Supporting Information

Can DNA-Protein Crosslinking Be Induced by One-Electron Oxidation of 8-Oxoguanosine? A Model Study of 9-Methyl-8-oxoguanine Radical Cation with Methylamine

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Table of Contents

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Table S1 Energetics for direct and HA_NH_2–mediated formation of X-$NHCH_3$[9MOG + H]$^{\bullet+}$

add site	stepwise or concerted paths	TS (eV) [a]	products and ΔH(298 K, eV) [a]	TS (eV) [a]	HA-NH_2-mediated paths [b]
N1	PT in N1-$^{+}NH_2CH_3$[9MOG]$^{\bullet}$	3.52/3.38 →	N1-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (3.28/3.21)	← 3.36/3.35	*async* HA_NH_2 + add
		3.38/3.32 →	N1-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (2.61/2.58)	← 2.55/2.56	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
	async add + PT	3.99/4.00 →	N1-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (2.59/2.54)	← 2.78/2.70	[9MOG + H_{N3}]$^{+}$···$^{\bullet}NHCH_3$
	sync add + PT	3.97/3.90 →	N1-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$ (2.61/2.63)	← 2.79/2.82	[9MOG + H_{C5}]$^{+}$···$^{\bullet}NHCH_3$
	N/A		N1-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (1.92/1.94)	← 3.38/3.39	*async* HA_NH_2 + add
			N1-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (2.52/2.51)	← 3.33/3.34	[9MOG + H_{C4}]$^{+}$···$^{\bullet}NHCH_3$
			N1-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$ (3.49/3.45)	← 3.65/3.64	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
			N1-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (3.29/3.27)	← 3.34/3.39	*async* HA_NH_2 + add
			N1-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (2.75/2.71)	← 2.76/2.75	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$
			N1-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (3.45/3.46)	← 3.55/3.62	*async* HA_NH_2 + add
C2	PT in C2-$^{+}NH_2CH_3$[9MOG]$^{\bullet}$	1.45/1.38 →	C2-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (0.69/0.69)	← 2.40/2.37	[9MOG + H_{N1}]$^{+}$···$^{\bullet}NHCH_3$
		1.11/1.00 →	C2-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (0.24/0.22)	← 1.90/1.88	*async* HA_NH_2 + add
		1.26/1.14 →	C2-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (0.08/0.00)	← 1.64/1.47	[9MOG + H_{N3}]$^{+}$ ···$^{\bullet}NHCH_3$
		2.75/2.68 →	C2-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (2.36/2.39)	← 3.01/3.04	[9MOG + H_{C4}]$^{+}$···$^{\bullet}NHCH_3$
		1.76/1.61 →	C2-$^{+}\dot{N}CH_3$[9MOG + H_{C5}] (1.23/1.08)	← 1.33/1.23	[9MOG + H_{C5}]$^{+}$ ···$^{\bullet}NHCH_3$
		2.14/2.16 →	C2-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (0.64/0.69)	← 1.57/1.47	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
	sync add + PT	3.04/3.14 →	C2-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (1.95/1.97)	← 2.31/2.23	*async* HA_NH_2 + add
		3.09/3.12 →	C2-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (1.72/1.82)	← 2.55/2.52	*async* HA_NH_2 + add
	N/A		C2-$^{+}\dot{N}HCH_3$[9MOG + H_{C6}] (2.48/2.35)	← 2.68/2.61	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
			C2-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (1.02/1.04)	← 1.76/1.68	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$
N2	N/A		N2-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (3.41/3.33)	← 3.68 /3.63	[9MOG + H_{N1}]$^{+}$···$^{\bullet}NHCH_3$
			N2-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (1.53/1.47)	← 3.38/3.31	*async* HA_NH_2 + add
			N2-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (2.72/2.59)	← 2.94/2.84	[9MOG + H_{N3}]$^{+}$ ···$^{\bullet}NHCH_3$
			N2-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (2.57/2.57)	← 3.75/3.67	[9MOG + H_{C4}]$^{+}$···$^{\bullet}NHCH_3$
			N2-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$ (2.09/2.01)	← 2.33/2.30	[9MOG + H_{C5}]$^{+}$ ···$^{\bullet}NHCH_3$
			N2-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$ (3.30/3.23)	← 3.48/3.44	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
			N2-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (2.47/2.43)	← 2.61/2.60	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
			N2-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (3.26/3.20)	← 3.31/3.27	*async* HA_NH_2 + add
			N2-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (2.78/2.72)	← 2.88/2.83	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$
			N2-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (3.51/3.47)	← 3.62/3.61	*async* HA_NH_2 + add
N3	PT in N3-$^{+}NH_2CH_3$[9MOG]$^{\bullet}$	3.58/3.38 →	N3-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (1.48/1.35)	← 3.04/3.12	*async* HA_NH_2 + add
		3.73/3.52 →	N3-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$ (1.75/1.56)	← 2.31/2.28	[9MOG + H_{C5}]$^{+}$···$^{\bullet}NHCH_3$
	async add + PT	3.18/3.15 →	N3-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (2.83/2.70)	← 3.44/3.44	[9MOG + H_{N1}]$^{+}$···$^{\bullet}NHCH_3$
		2.63/2.47 →	N3-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (2.56/2.42)		
		3.86/3.60 →	N3-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (1.27/1.10)		
		3.80/3.77 →	N3-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (2.05/1.92)	← 2.13/2.14	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
		4.61/4.57 →	N3-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (2.93/2.80)	← 3.10/3.08	*async* HA_NH_2 + add
		3.53/3.39 →	N3-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (2.89)/2.80	← 3.09 /3.10	*async* HA_NH_2 + add
	N/A		N3-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$ (2.82/2.65)	← 3.40/3.32	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
			N3-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (2.29/2.16)	← 2.32/2.32	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$

Table S1 *continued*.

add site	stepwise or concerted paths	TS (eV) [a]	products and ΔH(298 K, eV) [a]	TS (eV) [a]	HA-NH_2-mediated paths [b]
C4	PT in C4-$^{+}NH_2CH_3$[9MOG]$^{\bullet}$	1.28/1.27 →	C4-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (1.32/1.32)		
		3.14/3.08 →	C4-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (2.59/2.59)	← 3.19/3.30	*async* HA_NH_2 + add
		1.26/1.11 →	C4-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (0.23/0.09)	← 1.30/1.24	[9MOG + H_{N3}]$^{+}$···$^{\bullet}NHCH_3$
		1.91/1.72 →	C4-$^{+}$ṄHCH_3[9MOG + H_{C5}] (0.85/0.62)	← 1.12/1.04	[9MOG + H_{C5}]$^{+}$···$^{\bullet}NHCH_3$
		2.41/2.36 →	C4-$^{+}$ṄHCH_3[9MOG + H_{O6}] (1.40/1.36)	← 1.53/1.45	[9MOG + H_{O6}]$^{+}$ ···$^{\bullet}NHCH_3$
		1.86/1.82 →	C4-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (1.47/1.48)	← 2.13/2.07	*async* HA_NH_2 + add
		1.40/1.29 →	C4-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (0.78/0.75)	← 1.89/1.92	*async* HA_NH_2 + add
	async add + PT	2.71/2.69 →	C4-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (1.52/1.53)	← 2.58/2.64	*async* HA_NH_2 + add
		2.65/2.61 →	C4-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (0.71/0.69)	← 1.46/1.47	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$
C5	*async* add + PT	1.66/1.63 →	C5-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (1.56/1.56)		
		1.47/1.37 →	C5-$^{+}$ṄHCH_3[9MOG + H_{C2}] (1.60/1.42)	← 2.81/2.72	*async* HA_NH_2 + add
		1.20/1.15 →	C5-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (1.14/1.10)		
		1.65/1.61 →	C5-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (0.53/0.41)	← 1.55/1.52	[9MOG + H_{N3}]$^{+}$···$^{\bullet}NHCH_3$
		1.80/1.64 →	C5-$^{+}$ṄHCH_3[9MOG + H_{C4}] (1.12/0.98)		
		2.17/1.93 →	C5-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$ (1.24/1.16)	← 3.12/3.05	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
		1.28/1.14 →	C5-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (0.44/0.35)	← 1.41/1.40	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
		1.53/1.40 →	C5-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (0.83/0.76)		
		2.08/2.11 →	C5-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (0.63/0.57)	← 1.43/1.45	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$
		1.66/1.64 →	C5-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (1.03/1.00)	← 2.10/2.14	*async* HA_NH_2 + add
C6	*async* add + PT	0.84/0.82 →	C6-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (-0.69/-0.72)	← 1.96/1.94	[9MOG + H_{N1}]$^{+}$···$^{\bullet}NHCH_3$
		2.49/2.23 →	C6-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$ (1.15/1.04)	← 1.31/1.24	[9MOG + H_{C5}]$^{+}$···$^{\bullet}NHCH_3$
		2.63/2.40 →	C6-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (2.25/2.08)	← 2.36/2.29	*async* HA_NH_2 + add
	sync. add + PT	3.59/3.32 →	C6-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (2.57/2.45)	← 2.70/2.67	[9MOG + H_{C4}]$^{+}$···$^{\bullet}NHCH_3$
		1.16/1.02 →	C6-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (-0.28/-0.35)	← 0.99/0.95	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
	N/A		C6-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (3.09/3.01)	← 3.39/3.48	*async* HA_NH_2 + add
			C6-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (0.57/0.57)	← 2.22/2.16	*async* HA_NH_2 + add
			C6-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (1.33/1.16)	← 1.71/1.59	[9MOG + H_{N3}]$^{+}$···$^{\bullet}NHCH_3$
			C6-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (1.75/1.54)	← 1.67/1.60	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$
			C6-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (2.45/2.26)	← 2.47/2.45	*async* HA_NH_2 + add
O6	PT in O6-$^{+}NH_2CH_3$[9MOG]$^{\bullet}$	3.23/3.05 →	O6-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$ (1.43/1.32)	← 2.96/2.94	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
	async add + PT	3.37/3.27 →	O6-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (3.30/3.26)	← 3.36/3.37	[9MOG + H_{N1}]$^{+}$···$^{\bullet}NHCH_3$
		4.74/4.42 →	O6-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (2.05/2.02)	← 4.53/4.56	*async* HA_NH_2 + add
		4.16/4.10 →	O6-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (2.93/2.87)	← 3.47/3.49	*async* HA_NH_2 + add
		4.00/3.93 →	O6-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (2.55/2.43)	← 2.50/2.43	[9MOG + H_{N3}]$^{+}$···$^{\bullet}NHCH_3$
		3.18/3.02 →	O6-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$ (2.13/1.97)	← 2.20/2.14	[9MOG + H_{C5}]$^{+}$···$^{\bullet}NHCH_3$
		3.11/3.01 →	O6-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (3.13/3.09)	← 3.07/3.03	*async* HA_NH_2 + add
	N/A		O6-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (2.22/2.14)	← 3.15/3.06	[9MOG + H_{C4}]$^{+}$···$^{\bullet}NHCH_3$
			O6-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (2.42/2.38)	← 2.48/2.46	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$
			O6-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (2.88/2.87)	← 3.15/3.19	*async* HA_NH_2 + add

Table S1 *continued*.

add site	stepwise or concerted paths	TS (eV) [a]	products and ΔH(298 K, eV) [a]	TS (eV) [a]	HA-NH_2-mediated paths [b]
N7	*async* add + PT	$\xrightarrow{5.06/5.07}$	N7-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (3.14/3.12)	$\xleftarrow{3.52/3.59}$	*async* HA_NH_2 + add
		$\xrightarrow{4.13/4.11}$	N7-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (2.52/2.54)	$\xleftarrow{2.95/3.00}$	[9MOG + H_{C4}]$^{+}$···$^{\bullet}NHCH_3$
		$\xrightarrow{3.78/3.69}$	N7-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$ (1.77/1.72)	$\xleftarrow{2.85/2.60}$	[9MOG + H_{C5}]$^{+}$···$^{\bullet}NHCH_3$
	N/A		N7-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (3.22/3.21)	$\xleftarrow{3.78/3.84}$	[9MOG + H_{N1}]$^{+}$···$^{\bullet}NHCH_3$
			N7-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (2.94/3.03)	$\xleftarrow{3.43/3.56}$	*async* HA_NH_2 + add
			N7-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (2.79/2.73)	$\xleftarrow{3.02/2.99}$	[9MOG + H_{N3}]$^{+}$···$^{\bullet}NHCH_3$
			N7-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$ (3.41/3.35)	$\xleftarrow{4.20/3.93}$	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
			N7-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (2.53/2.55)	$\xleftarrow{3.03/2.98}$	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
			N7-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (2.34/2.28)	$\xleftarrow{2.45/2.39}$	[9MOG + H_{C8}]$^{+}$···$^{\bullet}NHCH_3$
			N7-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (2.91/2.95)	$\xleftarrow{3.33/3.38}$	*async* HA_NH_2 + add
C8	PT in C8-$^{+}NH_2CH_3$[9MOG]$^{\bullet}$	$\xrightarrow{1.97/1.95}$	C8-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (1.70/1.65)	$\xleftarrow{1.93/1.82}$	[9MOG + H_{N3}]$^{+}$···$^{\bullet}NHCH_3$
	async add + PT	$\xrightarrow{3.07/3.00}$	C8-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (1.23/1.12)	$\xleftarrow{1.41/1.36}$	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
		$\xrightarrow{1.07/0.95}$	C8-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (-0.15/-0.20)	$\xleftarrow{1.40/1.33}$	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$
	N/A		C8-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (1.84/1.86)	$\xleftarrow{2.99/2.93}$	[9MOG + H_{N1}]$^{+}$···$^{\bullet}NHCH_3$
			C8-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (3.10/2.98)	$\xleftarrow{3.15/3.22}$	*async* HA_NH_2 + add
			C8-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (1.59/1.66)	$\xleftarrow{3.27/3.18}$	*async* HA_NH_2 + add
			C8-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (2.80/2.65)	$\xleftarrow{2.83/2.81}$	[9MOG + H_{C4}]$^{+}$···$^{\bullet}NHCH_3$
			C8-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$ (1.38/1.20)	$\xleftarrow{1.40/1.34}$	[9MOG + H_{C5}]$^{+}$···$^{\bullet}NHCH_3$
			C8-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$ (2.54/2.29)	$\xleftarrow{2.60/2.52}$	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
			C8-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (1.57/1.52)	$\xleftarrow{1.79/1.64}$	*async* HA_NH_2 + add
			C8-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (-0.42/-0.55)	$\xleftarrow{1.96/1.86}$	*async* HA_NH_2 + add
O8	*async* add + PT	$\xrightarrow{4.86/4.81}$	O8-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (3.16/3.09)	$\xleftarrow{3.36/3.21}$	[9MOG + H_{N3}]$^{+}$···$^{\bullet}NHCH_3$
		$\xrightarrow{3.91/3.69}$	O8-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$ (2.09/1.96)	$\xleftarrow{2.50/2.42}$	[9MOG + H_{C5}]$^{+}$···$^{\bullet}NHCH_3$
		$\xrightarrow{3.11/2.95}$	O8-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (2.94/2.82)	$\xleftarrow{2.95/2.88}$	*async* HA_NH_2 + add
		$\xrightarrow{3.29/3.18}$	O8-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$ (3.15/3.10)	$\xleftarrow{3.16/3.15}$	*async* HA_NH_2 + add
	N/A		O8-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (3.58/3.49)	$\xleftarrow{3.96/3.92}$	[9MOG + H_{N1}]$^{+}$···$^{\bullet}NHCH_3$
			O8-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (2.63/2.60)	$\xleftarrow{3.46/3.41}$	*async* HA_NH_2 + add
			O8-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (3.42/3.33)	$\xleftarrow{3.95/3.87}$	*async* HA_NH_2 + add
			O8-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (2.48/2.40)	$\xleftarrow{3.34/3.26}$	[9MOG + H_{C4}]$^{+}$···$^{\bullet}NHCH_3$
			O8-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$ (3.33/3.22)	$\xleftarrow{3.59/3.51}$	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
			O8-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (2.49/2.49)	$\xleftarrow{2.49/2.49}$	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
N9	*async* add + PT	$\xrightarrow{5.35/5.38}$	N9-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$ (3.32/3.36)	$\xleftarrow{3.67/3.79}$	*async* HA_NH_2 + add
		$\xrightarrow{4.05/3.97}$	N9-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$ (1.93/1.96)	$\xleftarrow{3.53/3.35}$	[9MOG + H_{C4}]$^{+}$···$^{\bullet}NHCH_3$
	N/A		N9-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$ (3.27/3.31)	$\xleftarrow{3.61/3.73}$	[9MOG + H_{N1}]$^{+}$···$^{\bullet}NHCH_3$
			N9-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$ (2.54/2.63)	$\xleftarrow{3.59/4.02}$	*async* HA_NH_2 + add
			N9-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$ (2.66/2.63)	$\xleftarrow{2.77/2.76}$	[9MOG + H_{N3}]$^{+}$···$^{\bullet}NHCH_3$
			N9-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$ (1.96/1.96)	$\xleftarrow{2.09/2.15}$	[9MOG + H_{C5}]$^{+}$···$^{\bullet}NHCH_3$
			N9-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$ (3.15/3.16)	$\xleftarrow{3.41/3.47}$	[9MOG + H_{C6}]$^{+}$···$^{\bullet}NHCH_3$
			N9-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$ (2.30/2.36)	$\xleftarrow{2.44/2.56}$	[9MOG + H_{O6}]$^{+}$···$^{\bullet}NHCH_3$
			N9-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$ (2.89/2.94)	$\xleftarrow{3.27/3.34}$	*async* HA_NH_2 + add
			N9-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$ (2.46/2.48)	$\xleftarrow{2.75/2.75}$	[9MOG + H_{O8}]$^{+}$···$^{\bullet}NHCH_3$

[a] Energies are relative to 9MOG$^{\bullet+}$ + CH_3NH_2. Values in black were obtained at DLPNO-CCSD(T)/aug-cc-pVQZ//ωB97XD/6-31+G(d,p), and those in blue were obtained at ωB97XD/6-31+G(d,p).

[b] The label "*async* HA_NH_2 + add" indicates asynchronous concerted amine-H abstraction and addition of $^{\bullet}NHCH_3$.

Table S2 Energetics for HA_CH_3, H⊖A_CH_3, and subsequent crosslinking

paths	products	ΔH(298K, eV) [a]	TS (eV) [a]
HA_CH_3 by N1	[9MOG + H_{N1}]$^+$···$^\bullet CH_2NH_2$	1.60/1.52	1.59/1.47
	→ [9MOG + H_{N1}]$^+$ + $^\bullet CH_2NH_2$	2.37/2.46	
add -$^\bullet CH_2NH_2$	→ C2-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	0.46/0.48	1.88/1.78
	→ N2-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	2.38/2.27	2.78/2.52
	→ N3-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	1.75/1.69	2.54/2.40
	→ C4-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	1.50/1.50	2.09/2.03
	→ C5-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	1.65/1.65	2.18/2.12
	→ C6-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	-0.25/-0.41	2.03/1.94
	→ O6-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	1.44/1.41	2.38/2.39
	→ N7-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	1.99/1.94	2.18/2.12
	→ C8-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	2.04/2.10	2.66/2.60
	→ O8-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	1.74/1.68	2.01/2.23
	→ N9-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$	2.06/2.09	2.32/2.26
H⊖A_CH_3 by C2	[9MOG + H_{C2}]$^\bullet$ ···$CH_2NH_2^+$	0.48/0.45	1.60/1.47
	→ [9MOG + H_{C2}]$^\bullet$ + $^+CH_2NH_2$	1.76/1.83	
add -$NH_2CH_2^+$	→ C5-$^+NH_2\dot{C}H_2$[9MOG + H_{C2}]	1.87/1.92	2.32/2.30
add -$^+CH_2NH_2$	→ N1-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$	0.81/0.83	1.02/1.02
	→ N2-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$	0.33/0.26	0.80/0.75
	→ N3-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$	0.22/0.17	1.16/1.19
	→ C4-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$	2.28/2.31	2.38/2.31
	→ C5-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$	1.37/1.22	1.28/1.21
	→ O6-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$	0.55/0.53	0.84/0.85
	→ O8-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$	0.91/0.88	0.93/0.94
	→ N9-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$	1.30/1.33	1.30/1.31
HA_CH_3 by N2	[9MOG + H_{N2}]$^+$···$^\bullet CH_2NH_2$	1.15/1.09	1.18/1.03
	→ [9MOG + H_{N2}]$^+$ + $^\bullet CH_2NH_2$	2.05/2.17	
add -$^\bullet CH_2NH_2$	→ N1-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	2.11/2.02	2.49/2.41
	→ C2-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	0.19/0.18	1.72/1.69
	→ N3-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	1.38/1.26	1.91/1.88
	→ C4-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	1.13/1.16	2.11/2.10
	→ C5-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	1.09/1.04	2.02/1.94
	→ C6-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	1.13/1.12	2.63/2.43
	→ O6-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	1.40/1.37	1.91/1.87
	→ N7-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	1.77/1.75	1.89/1.84
	→ C8-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	2.07/2.19	2.91/2.82
	→ O8-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	1.60/1.53	2.13/2.09
	→ N9-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$	2.08/2.12	2.30/2.26
HA_CH_3 by N3	[9MOG + H_{N3}]$^+$···$^\bullet CH_2NH_2$	0.53/0.42	0.83/0.59
	→ [9MOG + H_{N3}]$^+$ + $^\bullet CH_2NH_2$	1.09/1.11	
add -$^\bullet CH_2NH_2$	→ N1-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	1.45/1.33	1.54/1.39
	→ C2-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	-0.16/-0.24	1.04/0.86
	→ N2-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	1.48/1.33	1.76/1.47
	→ C4-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	-0.14/-0.24	1.02/0.89
	→ C5-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	0.23/0.15	1.23/1.10
	→ C6-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	1.02/0.98	1.42/1.30
	→ O6-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	0.77/0.68	1.33/1.19
	→ N7-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	1.47/1.40	1.89/1.61
	→ C8-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	0.75/0.76	1.83/1.65
	→ O8-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	1.59/1.51	1.80/1.79
	→ N9-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$	1.79/1.81	1.84/1.81

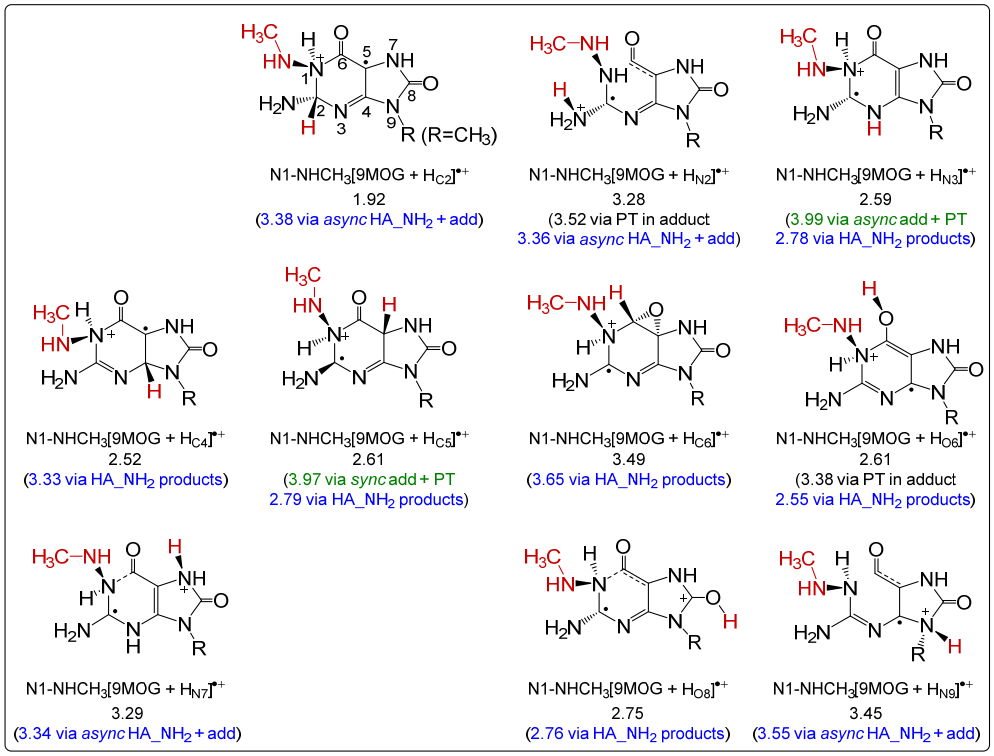
Table S2 *continued.*

paths	products	ΔH(298K, eV) [a]	TS (eV) [a]
H⊖A_CH_3 by C4	[9MOG + H_{C4}]• ···$CH_2NH_2^+$	0.61/0.60	1.47/1.26
	→ [9MOG + H_{C4}]• + $^+CH_2NH_2$	1.75/1.78	
add -$NH_2CH_2^+$	→ C5-$^+NH_2\dot{C}H_2$[9MOG + H_{C4}]•+	1.24/1.29	1.79/1.71
add -$^+CH_2NH_2$	→ N1-CH_2NH_2[9MOG + H_{C4}]•+	1.27/1.25	1.30/1.25
	→ C2-CH_2NH_2[9MOG + H_{C4}]•+	2.26/2.28	2.51/2.51
	→ N2-CH_2NH_2[9MOG + H_{C4}]•+	1.16/1.12	1.35/1.29
	→ C3-CH_2NH_2[9MOG + H_{C4}]•+	0.30/0.18	0.85/0.81
	→ C5-$CH_2\dot{N}H_2^+$[9MOG + H_{C4}]	0.99/0.75	1.02/0.96
	→ C6-CH_2NH_2[9MOG + H_{C4}]•+	2.34/2.31	2.34/2.30
	→ O6-CH_2NH_2[9MOG + H_{C4}]•+	0.76/0.70	1.00/0.99
	→ N7-CH_2NH_2[9MOG + H_{C4}]•+	1.08/1.08	1.12/1.07
	→ C8-CH_2NH_2[9MOG + H_{C4}]•+	2.72/2.58	2.69/2.67
	→ O8-CH_2NH_2[9MOG + H_{C4}]•+	0.81/0.73	0.83/0.77
	→ N9-CH_2NH_2[9MOG + H_{C4}]•+	0.74/0.75	1.20/1.18
HA_CH_3 by C5	[9MOG + H_{C5}]+···•CH_2NH_2	0.49/0.38	0.56/0.33
	→ [9MOG + H_{C5}]+ + •CH_2NH_2	0.88/0.93	
add -•CH_2NH_2	→ N1-CH_2NH_2[9MOG + H_{C5}]•+	1.52/1.50	1.51/1.47
	→ C2-CH_2NH_2[9MOG + H_{C5}]•+	1.40/1.27	1.50/1.26
	→ N2-CH_2NH_2[9MOG + H_{C5}]•+	0.89/0.78	1.20/0.96
	→ N3-CH_2NH_2[9MOG + H_{C5}]•+	0.35/0.25	1.22/1.04
	→ C4-$CH_2\dot{N}H_2^+$[9MOG + H_{C5}]	0.56/0.39	0.56/0.45
	→ C4-$^+NH_2\dot{C}H_2$[9MOG + H_{C5}]	0.55/0.53	0.58/0.60
	→ C6-CH_2NH_2[9MOG + H_{C5}]•+	0.88/0.67	0.85/0.69
	→ O6-CH_2NH_2[9MOG + H_{C5}]•+	0.66/0.53	0.95/0.84
	→ N7-CH_2NH_2[9MOG + H_{C5}]•+	0.51/0.46	0.86/0.81
	→ C8-CH_2NH_2[9MOG + H_{C5}]•+	1.49/1.37	1.47/1.35
	→ O8-CH_2NH_2[9MOG + H_{C5}]•+	0.53/0.43	0.81/0.76
	→ N9-CH_2NH_2[9MOG + H_{C5}]•+	0.70/0.68	0.96/0.78
HA_CH_3 by C6	[9MOG + H_{C6}]+···•CH_2NH_2	1.48/1.43	1.87/1.68
	→ [9MOG + H_{C6}]+ + •CH_2NH_2	2.00/2.02	
add -•CH_2NH_2	→ N1-CH_2NH_2[9MOG + H_{C6}]•+	2.28/2.22	2.53/2.38
	→ N2-CH_2NH_2[9MOG + H_{C6}]•+	2.04/1.97	2.42/2.20
	→ N3-CH_2NH_2[9MOG + H_{C6}]•+	1.59/1.48	2.37/2.22
	→ C5-CH_2NH_2[9MOG + H_{C6}]•+	0.94/0.86	2.19/2.04
	→ O6-CH_2NH_2[9MOG + H_{C6}]•+	0.06/-0.01	2.33/2.09
	→ N7-CH_2NH_2[9MOG + H_{C6}]•+	2.19/2.15	2.30/2.22
	→ C8-CH_2NH_2[9MOG + H_{C6}]•+	2.36/2.35	3.46/3.26
	→ O8-CH_2NH_2[9MOG + H_{C6}]•+	1.71/1.63	2.11/2.08
	→ N9-CH_2NH_2[9MOG + H_{C6}]•+	1.90/1.88	2.12/1.98
HA_CH_3 by O6	[9MOG + H_{O6}]+···•CH_2NH_2	0.09/0.01	0.28/0.19
	→ [9MOG + H_{O6}]+ + •CH_2NH_2	0.64/0.80	
add -•CH_2NH_2	→ N1-CH_2NH_2[9MOG + H_{O6}]•+	1.31/1.29	1.50/1.41
	→ C2-CH_2NH_2[9MOG + H_{O6}]•+	0.59/0.63	0.88/0.83
	→ N2-CH_2NH_2[9MOG + H_{O6}]•+	1.20/1.15	1.54/1.40
	→ N3-CH_2NH_2[9MOG + H_{O6}]•+	0.75/0.67	1.36/1.22
	→ C4-CH_2NH_2[9MOG + H_{O6}]•+	0.68/0.64	0.75/0.68
	→ C5-CH_2NH_2[9MOG + H_{O6}]•+	0.20/0.15	0.90/0.81
	→ C6-CH_2NH_2[9MOG + H_{O6}]•+	-0.44/-0.48	0.66/0.57
	→ N7-CH_2NH_2[9MOG + H_{O6}]•+	1.29/1.30	1.36/1.34
	→ C8-CH_2NH_2[9MOG + H_{O6}]•+	1.65/1.50	1.64/1.53

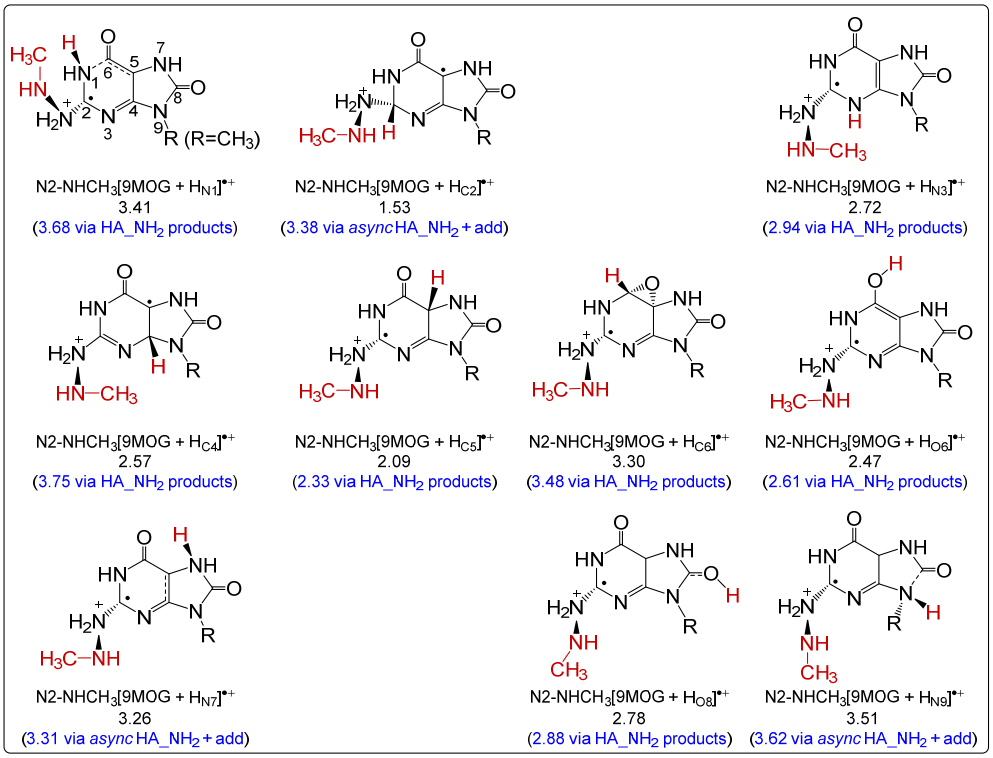
Table S2 *continued.*

paths	products	ΔH(298K, eV) [a]	TS (eV) [a]
	→ O8-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$	0.88/0.84	1.31/1.10
	→ N9-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$	1.09/1.14	1.29/1.23
HA_CH_3 by N7	[9MOG + H_{N7}]$^+$ + $^{\bullet}CH_2NH_2$	1.51/1.56	
	N1-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	2.07/2.04	2.21/2.12
	C2-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	1.61/1.65	1.78/1.66
	N2-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	2.04/1.99	2.23/2.10
	N3-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	1.95/1.91	2.48/2.41
	N4-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	1.32/1.36	1.68/1.57
async HA_CH_3 + add	C5-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	0.73/0.70	1.56/1.51
	C6-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	2.11/1.98	2.20/2.19
	O6-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	1.81/1.82	2.14/2.03
	C8-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	1.38/1.18	1.30/1.16
	O8-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	1.60/1.51	1.87/1.69
	N9-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$	1.85/1.89	2.09/2.03
HA_CH_3 by O8	[9MOG + H_{O8}]$^+$···$^{\bullet}CH_2NH_2$	0.16/0.04	0.20/0.17
	→ [9MOG + H_{O8}]$^+$ + $^{\bullet}CH_2NH_2$	0.85/0.90	
	→ N1-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	1.64/1.62	1.78/1.68
	→ C2-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	0.83/0.85	1.16/1.09
	→ N2-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	1.58/1.50	1.89/1.76
	→ N3-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	1.52/1.47	1.80/1.76
add -$^{\bullet}CH_2NH_2$	→ C4-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	0.64/0.63	1.15/1.07
	→ C5-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	0.44/0.38	1.00/0.96
	→ C6-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	1.50/1.34	1.69/1.42
	→ O6-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	0.98/0.96	1.42/1.32
	→ N7-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	1.07/0.99	1.21/1.13
	→ C8-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	-0.28/-0.32	0.73/0.60
	→ N9-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$	1.38/1.39	1.69/1.59
HA_CH_3 by N9	[9MOG + H_{N9}]$^+$···$^{\bullet}CH_2NH_2$	1.11/1.12	1.02/0.87
	→ [9MOG + H_{N9}]$^+$ + $^{\bullet}CH_2NH_2$	1.75/1.83	
	→ N1-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	2.12/2.10	2.32/2.26
	→ C2-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	1.36/1.45	1.89/1.85
	→ N2-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	2.37/2.32	2.54/2.40
	→ N3-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	1.78/1.74	2.56/2.44
	→ C4-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	0.64/0.67	1.62/1.56
add -$^{\bullet}CH_2NH_2$	→ C5-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	0.82/0.80	1.65/1.61
	→ C6-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	2.24/2.10	2.40/2.21
	→ O6-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	1.51/1.52	2.11/1.99
	→ 7N-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	1.81/1.82	2.36/2.18
	→ C8-$\dot{C}H_2NH_2$···[9MOG + H_{N9}]$^+$	1.57/1.48	1.53/1.45
	→ O8-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$	1.74/1.74	2.13/1.99

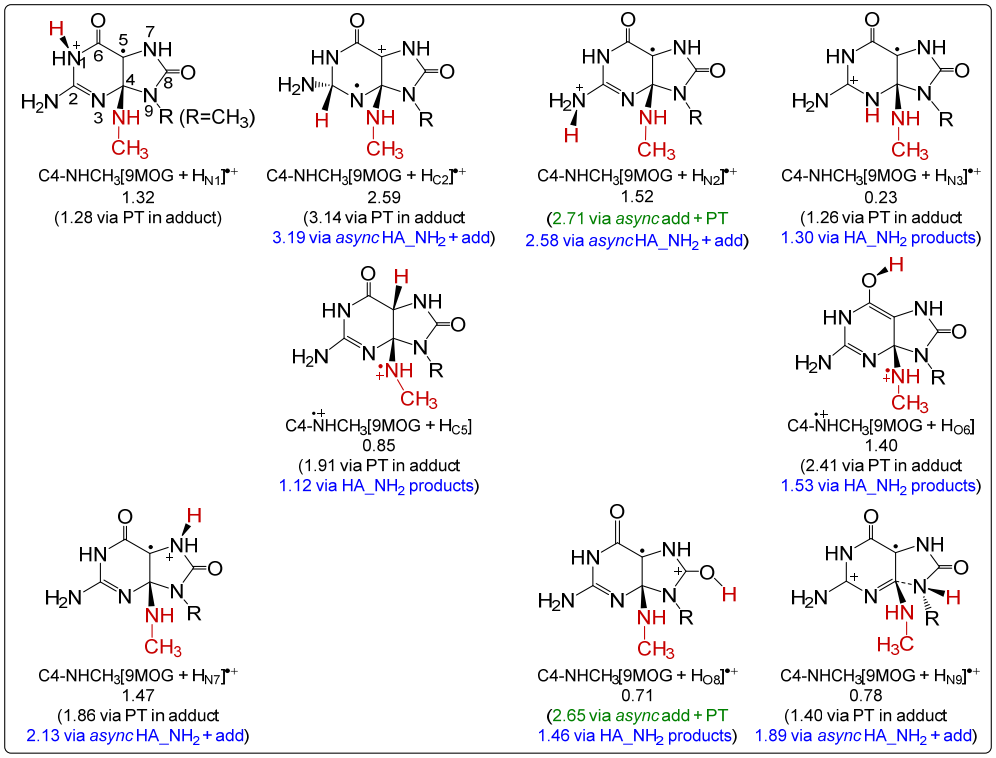
[a] Energies are relative to 9MOG$^{\bullet+}$ + CH_3NH_2. Values in black were obtained at DLPNO-CCSD(T)/aug-cc-pVQZ//ωB97XD/6-31+G(d,p), and those in blue were obtained at ωB97XD/6-31+G(d,p).



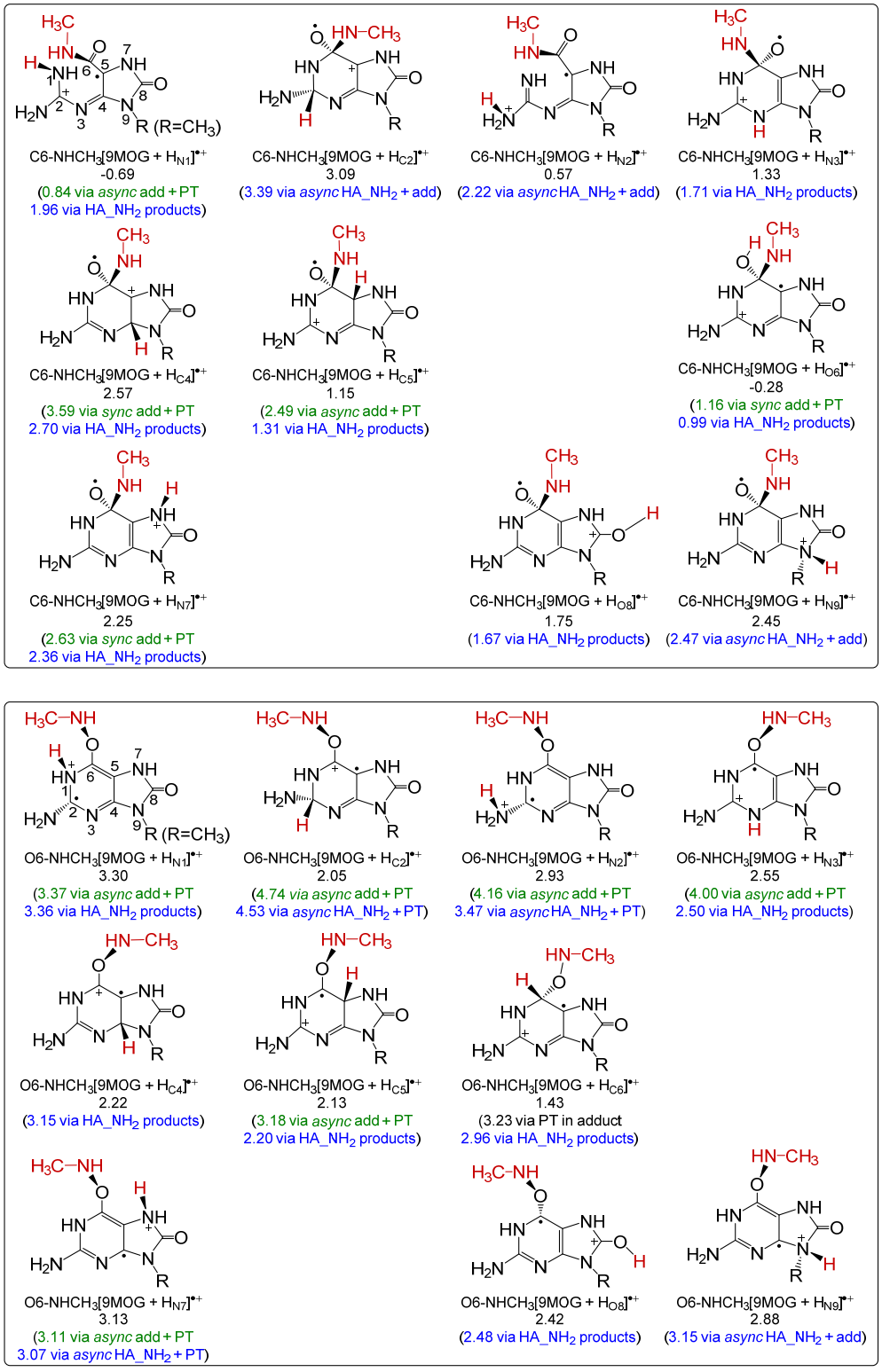
Scheme S1. Formation of N1-NHCH$_3$[9MOG + H]$^{\bullet+}$ (top) and C2-NHCH$_3$[9MOG + H]$^{\bullet+}$ (bottom). Product ΔH(298 K, eV) and activation barriers (in parentheses) were calculated relative to 9MOG$^{\bullet+}$ + CH$_3$NH$_2$ using DLPNO-CCSD(T)/aug-cc-pVQZ//ωB97XD/6-31+G(d,p). Activation barriers for concerted and stepwise pathways are distinguished in different colors.



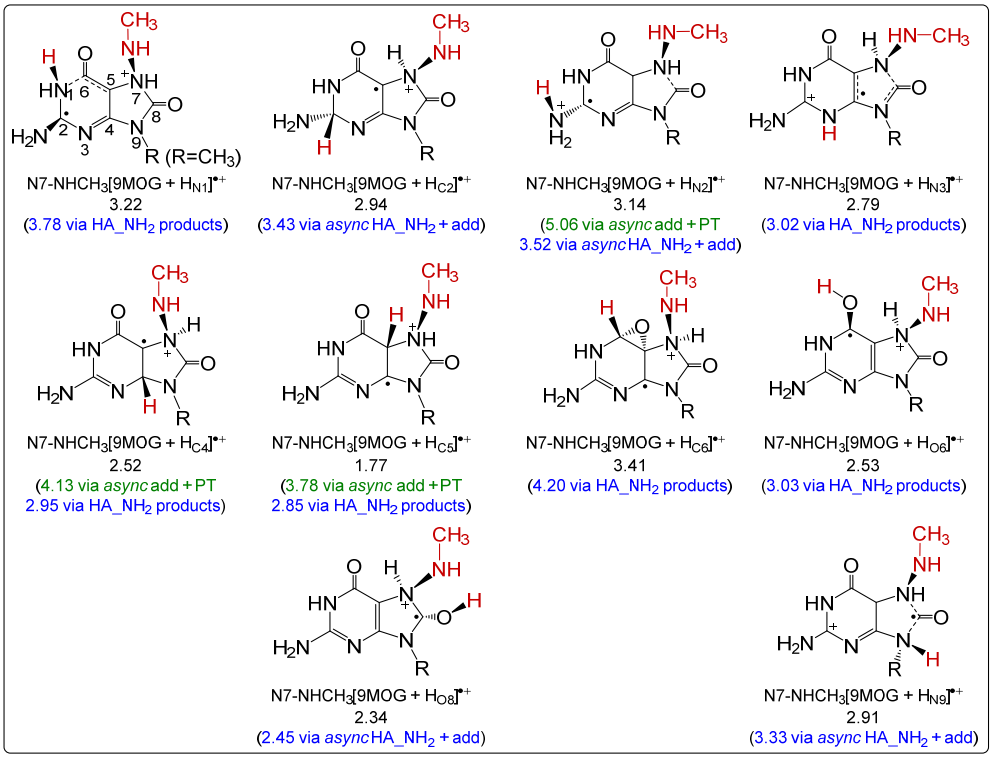
Scheme S1. (continued) Formation of N2-NHCH$_3$[9MOG + H]$^{\bullet+}$ (top) and N3-NHCH$_3$[9MOG + H]$^{\bullet+}$ (bottom).

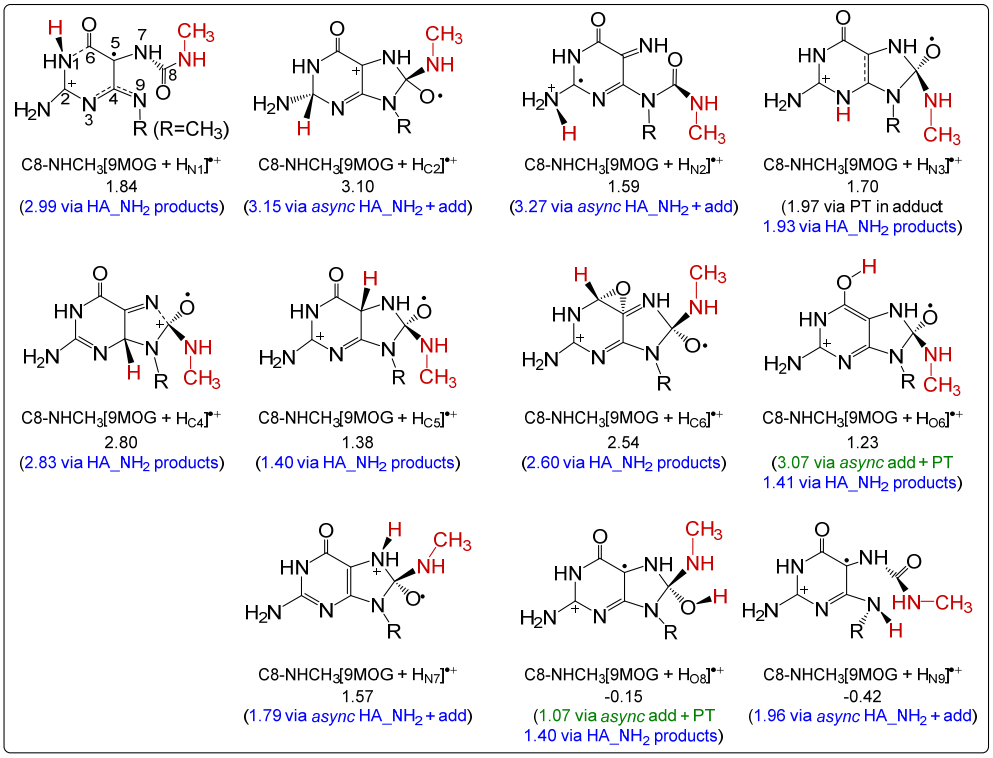


Scheme S1. (continued) Formation of C4-NHCH$_3$[9MOG + H]$^{\bullet+}$ (top) and C5-NHCH$_3$[9MOG + H]$^{\bullet+}$ (bottom).

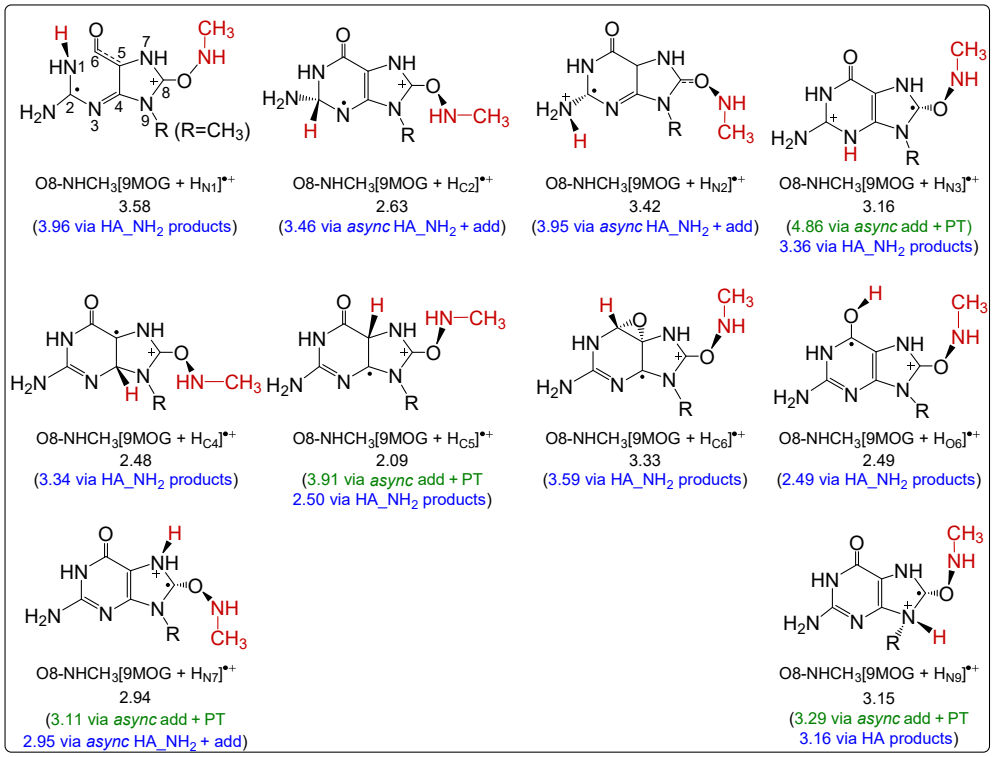


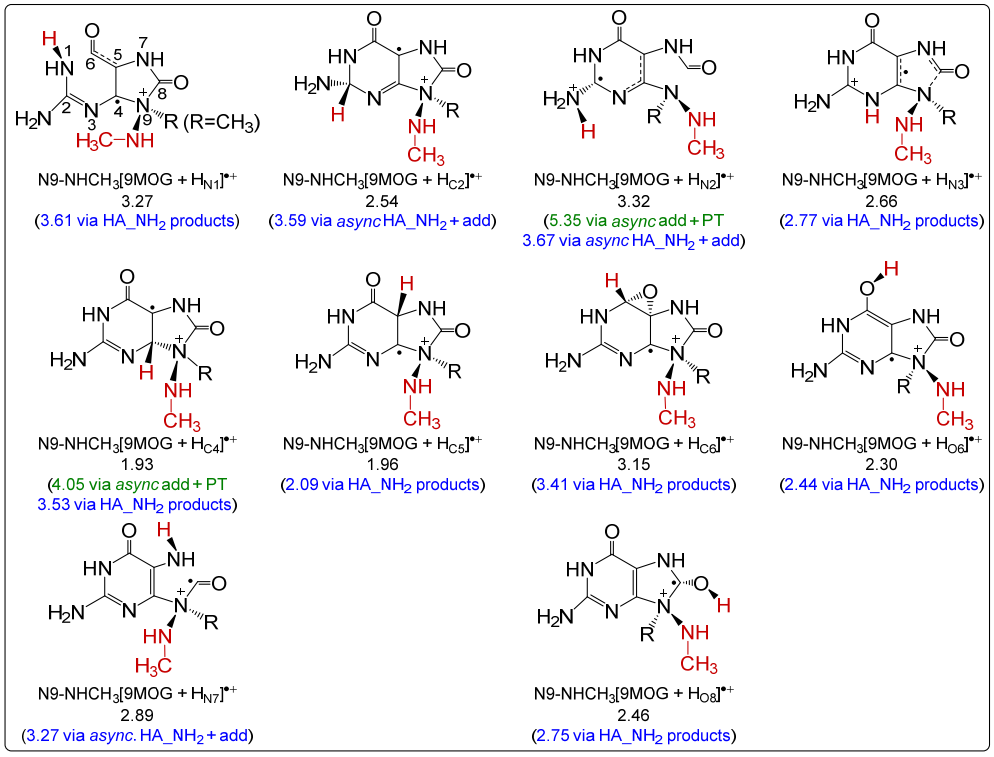
Scheme S1. (continued) Formation of C6-NHCH$_3$[9MOG + H]$^{\bullet+}$ (top) and O6-NHCH$_3$[9MOG + H]$^{\bullet+}$ (bottom).



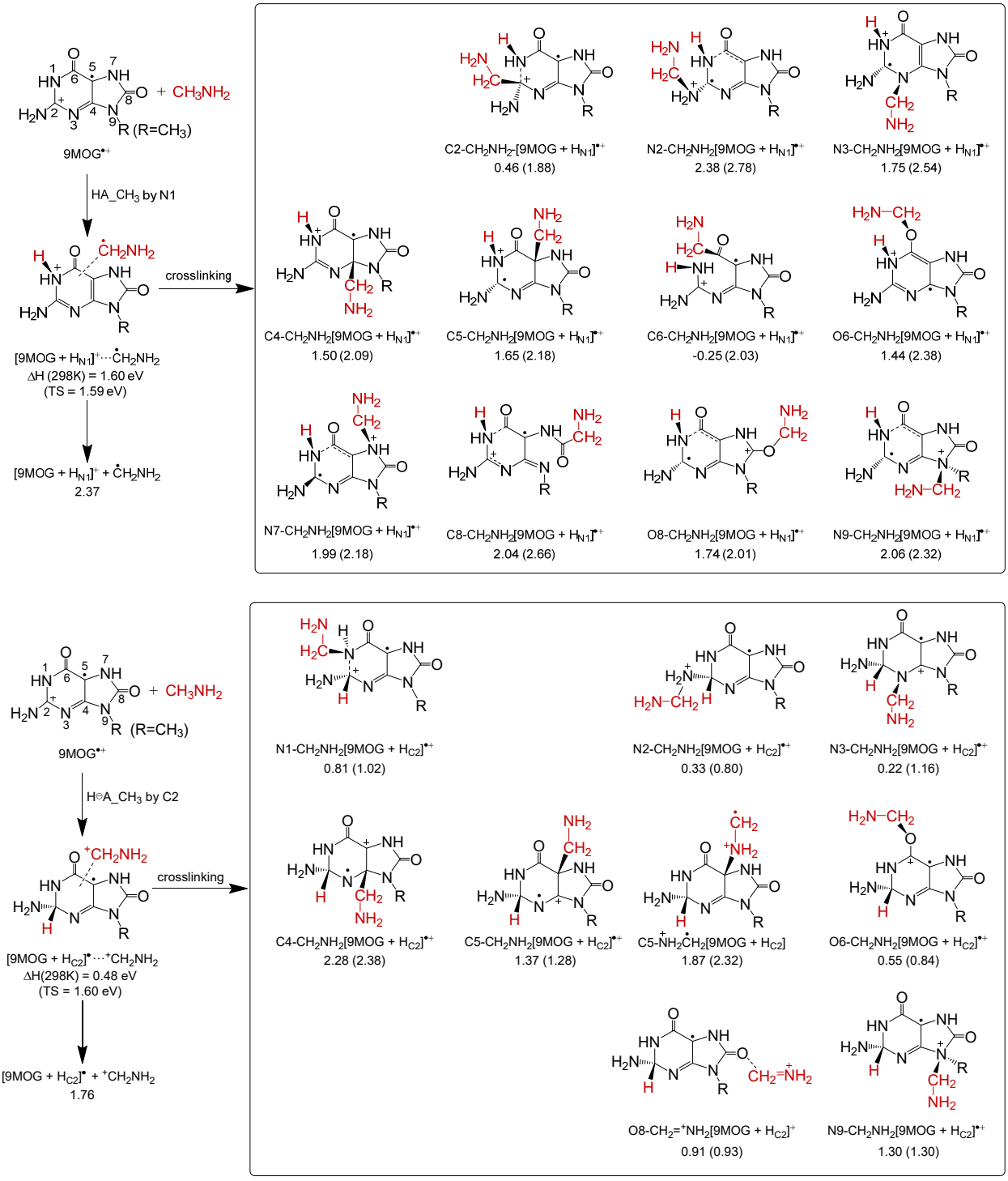


Scheme S1. (continued) Formation of N7-$NHCH_3$[9MOG + H]$^{\bullet+}$ (top) and C8-$NHCH_3$[9MOG + H]$^{\bullet+}$ (bottom).

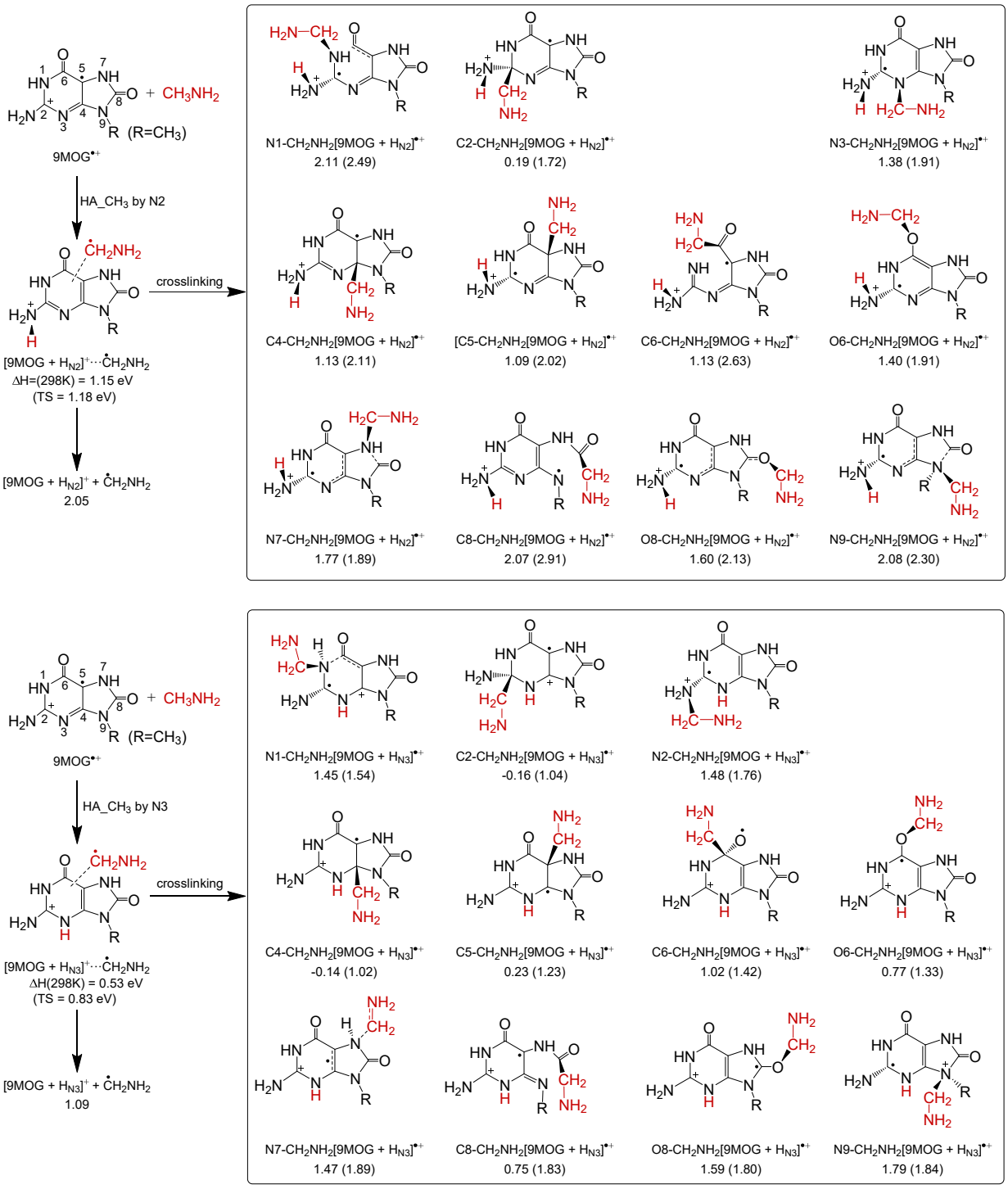




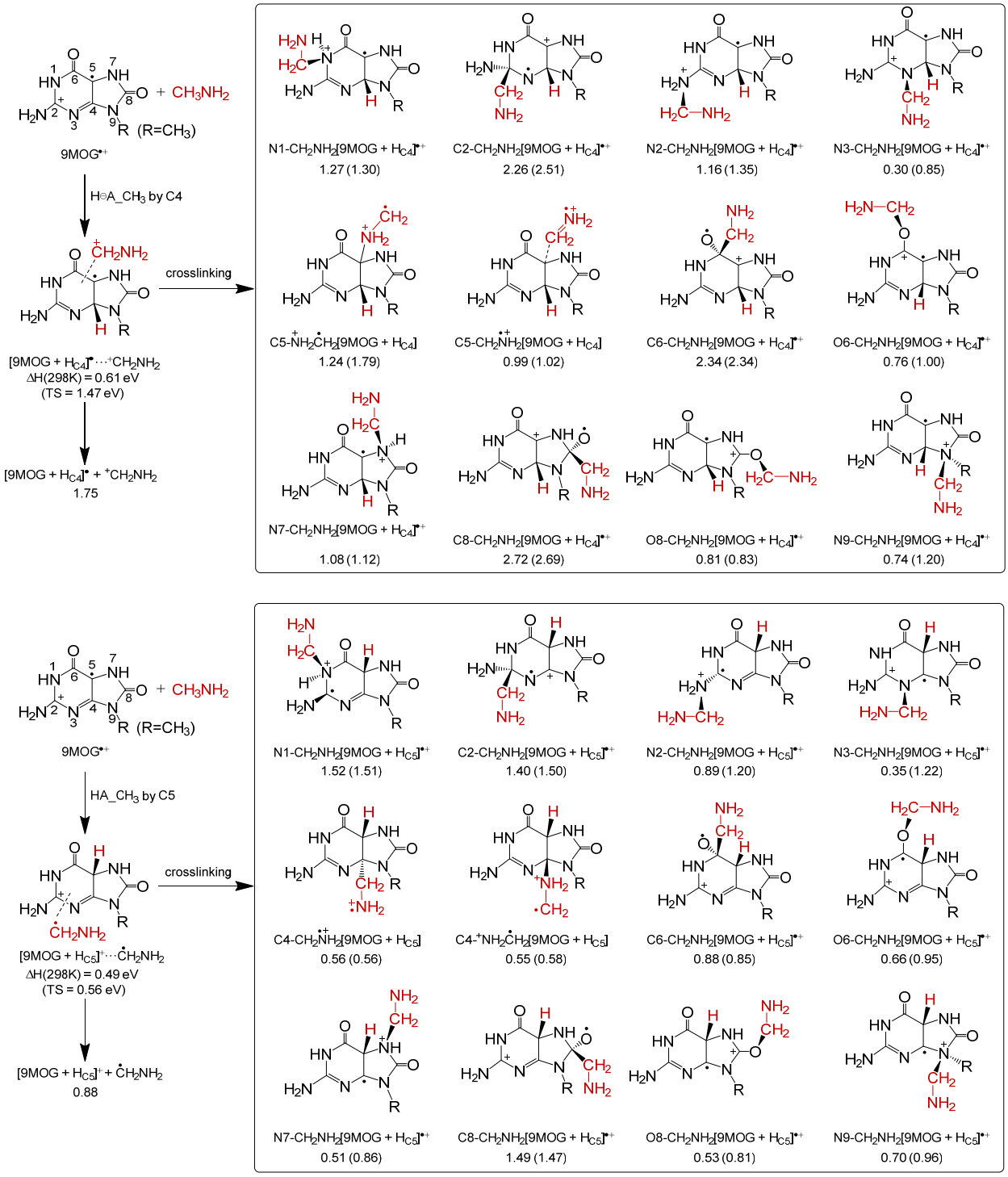
Scheme S1. (continued) Formation of O8-NHCH$_3$[9MOG + H]$^{\bullet+}$ (top) and N9-NHCH$_3$[9MOG + H]$^{\bullet+}$ (bottom).



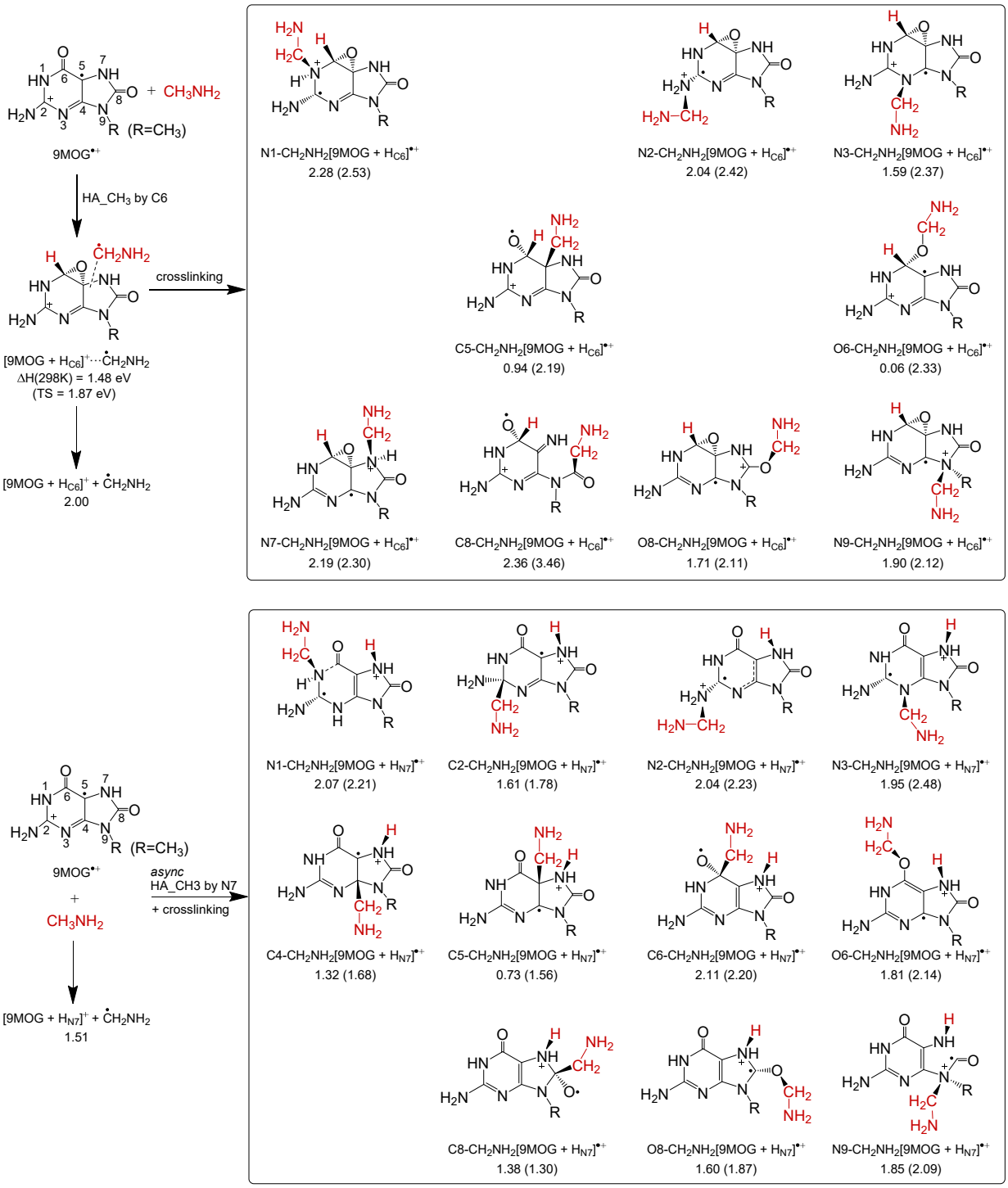
Scheme S2. Crosslinking following HA_CH_3 by N1 and H⊖A_CH_3 by C2 of $9MOG^{\bullet+}$. Reaction ΔH(298 K, eV) and activation barriers (in parentheses) were calculated relative to $9MOG^{\bullet+}$ + CH_3NH_2 using DLPNO-CCSD(T)/aug-cc-pVQZ//ωB97XD/6-31+G(d,p).



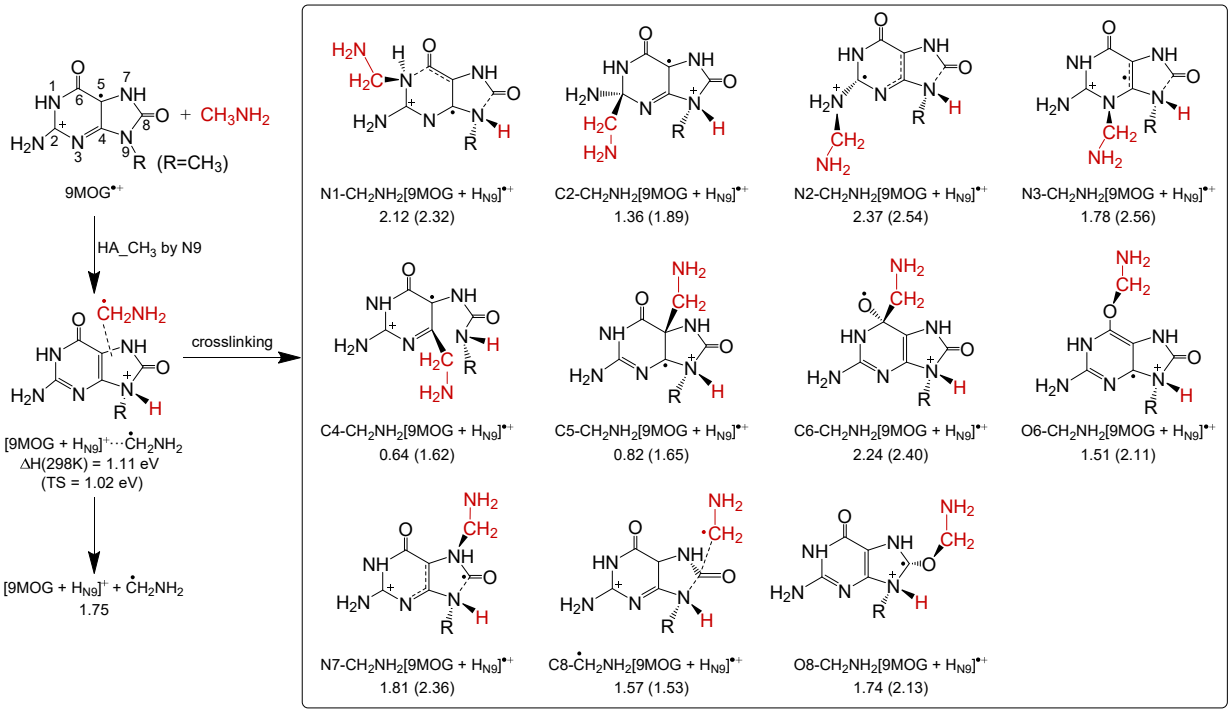
Scheme S2. (continued) Crosslinking following HA_CH_3 by N2 and N3 of 9MOG$^{\bullet+}$.



Scheme S2. (continued) Crosslinking following H⊖A_CH_3 by C4 and HA_CH_3 by C5 of 9MOG$^{\bullet+}$.



Scheme S2. (continued) Crosslinking following HA_CH_3 by C6, and asynchronous concerted HA_CH_3 by N7 and crosslinking.



Scheme S2. (continued) Crosslinking following HA_CH_3 by N9 of 9MOG$^{\bullet+}$.

Cartesian coordinates for reactants, CT, and PT products

1 9MOG^{++}

N1	1.540864	-0.777966	-0.002023
C2	0.057722	0.899800	0.000912
C3	-1.262756	1.482645	0.000727
O4	-1.541742	2.658507	0.001037
N5	-2.249671	0.468398	-0.000064
H6	-3.203177	0.815473	-0.000372
C7	-1.997672	-0.874469	-0.000350
N8	-3.021552	-1.718923	-0.001827
H9	-3.986613	-1.425407	-0.003151
H10	-2.817206	-2.708711	-0.001470
N11	-0.761474	-1.400361	0.001089
C12	0.217841	-0.520794	0.000662
C13	2.176393	-2.092013	0.002958
H14	1.988807	-2.589500	0.955429
H15	1.777062	-2.689366	-0.816998
H16	3.246322	-1.938309	-0.131786
C17	2.263325	0.435928	-0.000758
O18	3.449798	0.584010	-0.002681
N19	1.277471	1.452809	0.000861
H20	1.501771	2.441405	0.000327

Zero-point correction= 0.151699
Thermal correction to Energy= 0.162715
Thermal correction to Enthalpy= 0.163659
Thermal correction to Gibbs Free Energy= 0.114359
Sum of electronic and zero-point Energies= -656.531321
Sum of electronic and thermal Energies= -656.520305
Sum of electronic and thermal Enthalpies= -656.519361
Sum of electronic and thermal Free Energies= -656.568660

2 CH_3NH_2

N1	0.746992	0.000020	-0.117560
C2	-0.705875	0.000029	0.017459
H3	-1.078835	-0.000100	1.053415
H4	-1.113571	0.880155	-0.487496
H5	-1.113680	-0.880149	-0.487353
H6	1.156244	0.817244	0.319994
H7	1.156151	-0.817466	0.319604

Zero-point correction= 0.064793
Thermal correction to Energy= 0.068212
Thermal correction to Enthalpy= 0.069156
Thermal correction to Gibbs Free Energy= 0.041879
Sum of electronic and zero-point Energies= -95.772913
Sum of electronic and thermal Energies= -95.769494
Sum of electronic and thermal Enthalpies= -95.768550
Sum of electronic and thermal Free Energies= -95.795827

3 9MOG

N1	1.533332	-0.771865	-0.001474
C2	0.058677	0.886614	-0.007897
C3	-1.222321	1.488907	0.000415
O4	-1.536686	2.671654	0.008100
N5	-2.225511	0.479251	0.006566
H6	-3.168422	0.839195	0.078065
C7	-1.998684	-0.867399	0.001124
N8	-3.097149	-1.683680	0.055861
H9	-3.961309	-1.360421	-0.350254
H10	-2.889667	-2.659103	-0.097712
N11	-0.801405	-1.399129	-0.008766
C12	0.194266	-0.482226	-0.001044
C13	2.134804	-2.087223	0.012155
H14	1.916896	-2.600285	0.951949
H15	1.755655	-2.683263	-0.820512
H16	3.211587	-1.948084	-0.089371
C17	2.278235	0.420729	-0.004175
O18	3.492914	0.513714	-0.004313
N19	1.339133	1.427858	-0.008788
H20	1.576776	2.405576	-0.009720

Zero-point correction= 0.151257
Thermal correction to Energy= 0.162552
Thermal correction to Enthalpy= 0.163496
Thermal correction to Gibbs Free Energy= 0.114123
Sum of electronic and zero-point Energies= -656.800017
Sum of electronic and thermal Energies= -656.788722
Sum of electronic and thermal Enthalpies= -656.787778
Sum of electronic and thermal Free Energies= -656.837150

4 $CH_3NH_2^+$

N1	-0.708839	-0.000006	0.008294
C2	0.704534	-0.000092	0.014541
H3	1.091497	-0.915453	0.467741
H4	1.040130	0.002105	-1.047751
H5	1.091410	0.913823	0.470887
H6	-1.244285	-0.869799	-0.018150
H7	-1.244080	0.869918	-0.018029

Zero-point correction= 0.062230
Thermal correction to Energy= 0.066088
Thermal correction to Enthalpy= 0.067032
Thermal correction to Gibbs Free Energy= 0.037846
Sum of electronic and zero-point Energies= -95.447909
Sum of electronic and thermal Energies= -95.444051
Sum of electronic and thermal Enthalpies= -95.443107
Sum of electronic and thermal Free Energies= -95.472293

5 $CH_3NH_3^+$

N1	0.707743	-0.000010	-0.000030
C2	-0.796847	-0.000018	0.000147
H3	-1.139862	0.021932	-1.032781
H4	-1.140466	-0.905545	0.497007
H5	-1.140307	0.883758	0.534860
H6	1.082512	-0.815044	-0.493460
H7	1.082442	0.835056	-0.458812
H8	1.082563	-0.019980	0.952516

Zero-point correction= 0.080349
Thermal correction to Energy= 0.083789
Thermal correction to Enthalpy= 0.084733
Thermal correction to Gibbs Free Energy= 0.057179
Sum of electronic and zero-point Energies= -96.117881
Sum of electronic and thermal Energies= -96.114442
Sum of electronic and thermal Enthalpies= -96.113497
Sum of electronic and thermal Free Energies= -96.141051

6 [9MOG - H_{N1}]$^{\bullet}$

C1	-0.005573	0.872329	0.000717
C2	-0.177617	-0.536524	0.000730
C3	2.043434	-0.781775	-0.000346
C4	1.338312	1.440692	0.001019
C5	-2.225257	0.432298	-0.001150
N6	0.793526	-1.401407	0.001288
O7	1.507426	2.657677	0.001886
N8	-1.529428	-0.778624	-0.002292
N9	3.062636	-1.663318	-0.002435

H10	4.006787	-1.314896	-0.003817
H11	2.871336	-2.650380	-0.002343
C12	-2.165702	-2.080353	0.003588
H13	-1.782031	-2.680983	-0.823109
H14	-1.967465	-2.594088	0.946775
H15	-3.237961	-1.924415	-0.114195
O16	-3.422563	0.597148	-0.002645
N17	-1.235697	1.430079	-0.000045
H18	-1.439635	2.419328	-0.000468
N19	2.341032	0.502818	0.000038

Zero-point correction= 0.138108
Thermal correction to Energy= 0.149229
Thermal correction to Enthalpy= 0.150173
Thermal correction to Gibbs Free Energy= 0.100385
Sum of electronic and zero-point Energies= -656.164668
Sum of electronic and thermal Energies= -656.153547
Sum of electronic and thermal Enthalpies= -656.152603
Sum of electronic and thermal Free Energies= -656.202391

7 [9MOG - H_{N2a}]$^{\bullet}$

C1	0.024329	0.857276	0.000359
C2	-0.180696	-0.543318	-0.000131
C3	2.048051	-0.994295	-0.000629
C4	1.361049	1.410695	0.001233
C5	-2.207386	0.484393	-0.001497
N6	0.740246	-1.463643	0.000449
O7	1.635535	2.601085	0.002293
N8	-1.544704	-0.740828	-0.003471
N9	3.078104	-1.756485	-0.002616
H10	2.768646	-2.726569	-0.003085
H11	3.268311	0.661248	0.000585
C12	-2.215017	-2.025569	0.004809
H13	-1.847811	-2.638171	-0.820499
H14	-2.030077	-2.542834	0.948728
H15	-3.282702	-1.840867	-0.112966
O16	-3.399430	0.685736	-0.002154
N17	-1.190866	1.454889	-0.000518
H18	-1.371139	2.448122	-0.000231
N19	2.292071	0.393127	0.000654

Zero-point correction= 0.138482
Thermal correction to Energy= 0.149252
Thermal correction to Enthalpy= 0.150196
Thermal correction to Gibbs Free Energy= 0.100986
Sum of electronic and zero-point Energies= -656.163081
Sum of electronic and thermal Energies= -656.152311
Sum of electronic and thermal Enthalpies= -656.151367
Sum of electronic and thermal Free Energies= -656.200577

8 [9MOG - H_{N2b}]$^{\bullet}$

C1	-0.016007	0.860294	0.000272
C2	0.184776	-0.541880	-0.000138
C3	-2.041395	-1.017484	-0.000630
C4	-1.350681	1.405924	0.001368
C5	2.215016	0.480138	-0.001625
N6	-0.728860	-1.464572	0.000664
O7	-1.643190	2.592130	0.002568
N8	1.550165	-0.741309	-0.003785
N9	-2.983497	-1.886938	-0.003005
H10	-3.904071	-1.448931	-0.004374
H11	-3.246865	0.692914	0.001305
C12	2.213609	-2.030190	0.005121
H13	2.034619	-2.540735	0.953709
H14	1.830926	-2.645165	-0.811092
H15	3.280934	-1.852818	-0.125791
O16	3.406988	0.682491	-0.002284
N17	1.200264	1.455463	-0.000713
H18	1.385940	2.447522	-0.000498
N19	-2.284326	0.381561	0.000876

Zero-point correction= 0.138137
Thermal correction to Energy= 0.148946
Thermal correction to Enthalpy= 0.149890
Thermal correction to Gibbs Free Energy= 0.100662
Sum of electronic and zero-point Energies= -656.154160
Sum of electronic and thermal Energies= -656.143352
Sum of electronic and thermal Enthalpies= -656.142408
Sum of electronic and thermal Free Energies= -656.191635

9 [9MOG - H_{N7}]$^{\bullet}$

C1	-0.109715	0.931903	-0.002694
C2	-0.239503	-0.492154	0.001299
C3	1.952546	-0.886139	-0.000418
C4	1.224549	1.493350	0.001303
C5	-2.232383	0.527580	-0.004071
N6	0.739046	-1.407669	-0.002090
O7	1.587960	2.649906	0.006835
N8	-1.556422	-0.740556	-0.000907
N9	3.013639	-1.724759	0.026370
H10	3.948345	-1.407761	-0.167524
H11	2.813559	-2.707401	-0.071028
C12	-2.213740	-2.028353	0.010044
H13	-1.853950	-2.642106	-0.818490
H14	-2.024772	-2.546877	0.953109
H15	-3.282783	-1.843901	-0.099540
O16	-3.443501	0.622689	-0.007225
N17	-1.286517	1.546384	-0.005097
N18	2.204181	0.454208	0.001614
H19	3.155921	0.796905	0.034589

Zero-point correction= 0.137660
Thermal correction to Energy= 0.148829
Thermal correction to Enthalpy= 0.149773
Thermal correction to Gibbs Free Energy= 0.099921
Sum of electronic and zero-point Energies= -656.162233
Sum of electronic and thermal Energies= -656.151064
Sum of electronic and thermal Enthalpies= -656.150120
Sum of electronic and thermal Free Energies= -656.199972

Cartesian coordinates for products and TSs in Scheme 2

1 N1-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	2.286353	0.590208	0.157869
C2	0.588915	-0.872987	0.022399
C3	-0.687204	-1.305729	-0.131121
O4	-1.359743	-2.272891	-0.467309
N5	-1.671852	-0.050626	0.369725
H6	-1.769249	-0.184974	1.380318
C7	-1.178471	1.404223	0.113723
N8	-2.075429	2.092293	-0.720463
H9	-2.608381	2.816562	-0.247502
H10	-1.605713	2.503061	-1.524061
N11	0.133827	1.564901	0.056003
C12	0.933128	0.517617	0.136865
C13	3.076963	1.807774	0.192778
H14	2.942065	2.372239	-0.732456
H15	2.775034	2.420239	1.043397
H16	4.120764	1.512135	0.296592
C17	2.861209	-0.697183	0.003415
O18	4.038608	-0.949680	-0.009802
N19	1.792495	-1.561552	-0.129238
H20	1.911935	-2.562185	-0.132571
H21	-3.040260	0.482970	-0.910872
H22	-2.760469	-1.256558	-0.703544
H23	-3.919622	-1.211998	1.399374
H24	-4.196416	0.558755	1.209568
N25	-2.940112	-0.321913	-0.243101
C26	-4.090540	-0.396721	0.695340
H27	-4.981589	-0.604817	0.102676

Zero-point correction= 0.219443
Thermal correction to Energy= 0.234000
Thermal correction to Enthalpy= 0.234944
Thermal correction to Gibbs Free Energy= 0.177708
Sum of electronic and zero-point Energies= -752.180605
Sum of electronic and thermal Energies= -752.166048
Sum of electronic and thermal Enthalpies= -752.165104
Sum of electronic and thermal Free Energies= -752.222340

2 TS_N1-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	2.297802	0.580756	0.027449
C2	0.585369	-0.864626	0.129344
C3	-0.690262	-1.327128	0.078378
O4	-1.355017	-2.323754	-0.119533
N5	-1.711531	0.003544	0.385205
H6	-2.077314	-0.173395	1.326535
C7	-1.148887	1.403768	0.286332
N8	-2.111358	2.295769	-0.229341
H9	-2.606163	2.830894	0.480329
H10	-1.679703	2.948811	-0.878403
N11	0.146889	1.571023	0.093054
C12	0.945454	0.520305	0.117049
C13	3.099809	1.788548	-0.045421
H14	2.938730	2.293950	-1.000150
H15	2.833295	2.458299	0.773325
H16	4.144074	1.488529	0.040094
C17	2.854388	-0.720373	-0.041890
O18	4.027125	-0.987479	-0.111746
N19	1.774301	-1.580125	-0.014402
H20	1.883636	-2.580351	0.038813
H21	-2.977781	0.769096	-0.925353
H22	-2.563443	-0.907996	-1.197560
H23	-3.908631	-1.613761	0.631135
H24	-4.412526	0.103278	0.884254
N25	-2.866914	-0.193358	-0.520499
C26	-4.108670	-0.651905	0.158384
H27	-4.878574	-0.762290	-0.606094

Zero-point correction= 0.218941
Thermal correction to Energy= 0.233033
Thermal correction to Enthalpy= 0.233977
Thermal correction to Gibbs Free Energy= 0.178166
Sum of electronic and zero-point Energies= -752.179683
Sum of electronic and thermal Energies= -752.165592
Sum of electronic and thermal Enthalpies= -752.164648
Sum of electronic and thermal Free Energies= -752.220459

3 C2-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	-1.730717	-1.057349	0.102323
C2	-0.847369	0.995654	-0.089077
C3	0.192010	1.996073	-0.071177
O4	0.035336	3.193815	-0.180610
N5	1.452056	1.411921	0.107507
H6	2.189655	2.076663	0.314560
C7	1.727851	0.018593	0.331352
N8	2.605755	-0.127427	1.448483
H9	2.362571	0.524680	2.186064
H10	2.557220	-1.068172	1.827534
N11	0.636278	-0.897017	0.314478
C12	-0.542215	-0.385969	0.127702
C13	-1.915747	-2.487796	0.284793
H14	-2.988127	-2.678434	0.318167
H15	-1.471729	-3.034711	-0.549226
H16	-1.453432	-2.802580	1.221594
C17	-2.789660	-0.160671	-0.114254
O18	-3.960784	-0.409088	-0.189191
N19	-2.183003	1.108730	-0.229581
H20	-2.707249	1.961562	-0.377670
N21	2.611761	-0.419366	-0.916420
H22	2.030441	-0.291962	-1.747856
H23	3.382888	0.250046	-0.977291
C24	3.157486	-1.805510	-0.876270
H25	2.330278	-2.495554	-0.719994
H26	3.656196	-2.011176	-1.823193
H27	3.875808	-1.866874	-0.060235

Zero-point correction= 0.221826
Thermal correction to Energy= 0.236239
Thermal correction to Enthalpy= 0.237184
Thermal correction to Gibbs Free Energy= 0.179809
Sum of electronic and zero-point Energies= -752.303261
Sum of electronic and thermal Energies= -752.288848
Sum of electronic and thermal Enthalpies= -752.287904
Sum of electronic and thermal Free Energies= -752.345278

4 TS_C2-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	1.736183	-0.979761	-0.199986
C2	0.747381	1.013876	0.085795
C3	-0.323648	1.980117	-0.001856
O4	-0.239005	3.169864	0.218137
N5	-1.507489	1.365691	-0.427874
H6	-2.285913	1.999565	-0.563750
C7	-1.701797	-0.021157	-0.559275
N8	-2.742996	-0.389066	-1.371202
H9	-3.277141	0.321285	-1.847158
H10	-2.601011	-1.245717	-1.886339
N11	-0.609919	-0.884965	-0.614748
C12	0.528339	-0.354259	-0.274173
C13	2.004352	-2.376969	-0.506481
H14	3.060959	-2.558306	-0.311649
H15	1.393941	-3.019683	0.129728
H16	1.782245	-2.576813	-1.555983

C17	2.730153	-0.065796	0.187676
O18	3.900118	-0.272347	0.346972
N19	2.055788	1.165133	0.360758
H20	2.529238	2.024609	0.610049
N21	-2.364235	-0.453843	1.167839
H22	-1.663395	-0.196397	1.861948
H23	-3.173000	0.147838	1.319259
C24	-2.739752	-1.871594	1.296793
H25	-1.854085	-2.484037	1.127637
H26	-3.154572	-2.080706	2.284838
H27	-3.487664	-2.099410	0.536171

Zero-point correction= 0.219276
Thermal correction to Energy= 0.233690
Thermal correction to Enthalpy= 0.234634
Thermal correction to Gibbs Free Energy= 0.177674
Sum of electronic and zero-point Energies= -752.302032
Sum of electronic and thermal Energies= -752.287618
Sum of electronic and thermal Enthalpies= -752.286674
Sum of electronic and thermal Free Energies= -752.343634

5 N3-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	-1.564329	-0.697984	-0.273089
C2	-0.423462	1.160871	0.158296
C3	0.701966	2.079259	0.139020
O4	0.658428	3.273877	0.329165
N5	1.887371	1.412620	-0.204912
H6	2.715730	1.995640	-0.216313
C7	2.072127	0.034636	-0.209559
N8	3.234696	-0.579765	-0.694033
H9	4.067757	-0.375443	-0.155257
H10	2.120521	-2.225797	-0.075849
N11	0.903380	-0.764762	-0.491011
C12	-0.312685	-0.148978	-0.164811
C13	-1.955508	-2.013628	-0.736105
H14	-1.452060	-2.258372	-1.676309
H15	-1.776101	-2.784671	0.022881
H16	-3.031806	-1.976953	-0.915631
C17	-2.524142	0.316521	-0.009927
O18	-3.722822	0.171778	-0.025165
N19	-1.771296	1.444503	0.252267
H20	-2.173508	2.354065	0.425978
H21	3.415697	-0.455083	-1.690797
H22	0.555059	-2.750185	-0.323026
H23	-0.150294	-1.939511	1.851408
H24	1.511898	-1.317732	2.095338
N25	1.124584	-2.056533	0.167836
C26	0.906721	-2.104018	1.644253
H27	1.221312	-3.085718	1.999160

Zero-point correction= 0.221383
Thermal correction to Energy= 0.235573
Thermal correction to Enthalpy= 0.236517
Thermal correction to Gibbs Free Energy= 0.180397
Sum of electronic and zero-point Energies= -752.215344
Sum of electronic and thermal Energies= -752.201154
Sum of electronic and thermal Enthalpies= -752.200210
Sum of electronic and thermal Free Energies= -752.256329

6 TS_N3-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	-1.573507	-0.696056	-0.291094
C2	-0.416961	1.153343	0.137810
C3	0.721160	2.056828	0.147085
O4	0.694014	3.247400	0.368463
N5	1.897084	1.378865	-0.194923
H6	2.731585	1.952634	-0.215417
C7	2.057344	0.003679	-0.302297
N8	3.211526	-0.609367	-0.797432
H9	4.062130	-0.366626	-0.304230
H10	2.087256	-2.273271	0.013422
N11	0.889577	-0.796631	-0.501074
C12	-0.316092	-0.156853	-0.187617
C13	-1.971930	-2.015109	-0.737721
H14	-1.445708	-2.285317	-1.657794
H15	-1.821653	-2.772470	0.041415
H16	-3.042726	-1.969176	-0.945200
C17	-2.523418	0.323930	-0.026825
O18	-3.723592	0.192437	-0.039929
N19	-1.760078	1.447937	0.234068
H20	-2.155085	2.361502	0.403967
H21	3.350871	-0.543718	-1.805918
H22	0.507000	-2.772315	-0.147870
H23	-0.121799	-1.786252	1.966758
H24	1.548945	-1.154176	2.112692
N25	1.108246	-2.059087	0.272029
C26	0.929205	-1.974042	1.748401
H27	1.250042	-2.919804	2.185867

Zero-point correction= 0.220324
Thermal correction to Energy= 0.234061
Thermal correction to Enthalpy= 0.235005
Thermal correction to Gibbs Free Energy= 0.180205
Sum of electronic and zero-point Energies= -752.216265
Sum of electronic and thermal Energies= -752.202528
Sum of electronic and thermal Enthalpies= -752.201584
Sum of electronic and thermal Free Energies= -752.256384

7 C4-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	1.544406	-0.278347	-0.406552
C2	-0.117942	1.085118	0.329538
C3	-1.476824	1.538177	0.322998
O4	-1.866384	2.666794	0.551664
N5	-2.363871	0.485081	0.003766
H6	-3.339077	0.757528	-0.028767
C7	-1.948218	-0.686324	-0.606680
N8	-2.909121	-1.439287	-1.171820
H9	-3.819897	-1.068540	-1.391265
H10	-2.615110	-2.273900	-1.656216
N11	-0.709546	-1.108163	-0.624281
C12	0.214463	-0.342788	0.084448
C13	2.226858	-1.315272	-1.173813
H14	3.025273	-1.780633	-0.591380
H15	1.488765	-2.059268	-1.473169
H16	2.665873	-0.865171	-2.065061
C17	2.057717	1.007864	-0.316307
O18	3.144711	1.391777	-0.649512
N19	1.021644	1.807094	0.235530
H20	1.074954	2.818293	0.242712
N21	0.312422	-1.044642	1.596245
H22	0.951308	-0.482093	2.162752
H23	-0.614056	-0.960411	2.020280
C24	0.738242	-2.468787	1.589358
H25	1.784776	-2.520829	1.295176
H26	0.615642	-2.888890	2.587959
H27	0.117611	-3.004746	0.872300

Zero-point correction= 0.220782
Thermal correction to Energy= 0.235506
Thermal correction to Enthalpy= 0.236450
Thermal correction to Gibbs Free Energy= 0.178935
Sum of electronic and zero-point Energies= -752.300512
Sum of electronic and thermal Energies= -752.285788
Sum of electronic and thermal Enthalpies= -752.284844

Sum of electronic and thermal Free Energies= -752.342360

8 TS_C4-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	1.531344	-0.288327	-0.459167
C2	-0.101800	1.100530	0.263477
C3	-1.456135	1.562870	0.304922
O4	-1.835838	2.687346	0.566493
N5	-2.356435	0.517709	-0.008722
H6	-3.330810	0.795432	-0.012718
C7	-1.967022	-0.664976	-0.608817
N8	-2.942590	-1.424908	-1.133097
H9	-3.867956	-1.068135	-1.310416
H10	-2.665489	-2.271503	-1.606738
N11	-0.726693	-1.091388	-0.660865
C12	0.204678	-0.316368	-0.003712
C13	2.230150	-1.356571	-1.164116
H14	3.003869	-1.803509	-0.535972
H15	1.495465	-2.106229	-1.457013
H16	2.700959	-0.943051	-2.056687
C17	2.088593	0.976416	-0.308759
O18	3.204547	1.325731	-0.577069
N19	1.053995	1.796687	0.213722
H20	1.140863	2.803978	0.268520
N21	0.296727	-1.034782	1.629935
H22	0.961381	-0.487933	2.179120
H23	-0.621941	-0.906548	2.056068
C24	0.664403	-2.468250	1.623569
H25	1.709445	-2.565104	1.333605
H26	0.522593	-2.899244	2.615826
H27	0.030309	-2.979613	0.898987

Zero-point correction= 0.220035
Thermal correction to Energy= 0.234265
Thermal correction to Enthalpy= 0.235209
Thermal correction to Gibbs Free Energy= 0.178943
Sum of electronic and zero-point Energies= -752.301080
Sum of electronic and thermal Energies= -752.286851
Sum of electronic and thermal Enthalpies= -752.285907
Sum of electronic and thermal Free Energies= -752.342172

9 O6-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	2.232665	-0.547531	0.008404
C2	0.011896	-0.350747	-0.195874
C3	-1.209866	0.338986	-0.312948
O4	-2.243496	-0.169939	0.584491
N5	-1.022049	1.747493	-0.187969
H6	-1.728931	2.345315	-0.591947
C7	0.201730	2.340838	-0.005949
N8	0.228901	3.692430	0.019580
H9	-0.578786	4.224405	0.301252
H10	1.132261	4.112628	0.179571
N11	1.338844	1.681204	0.084259
C12	1.212336	0.351440	-0.050716
C13	3.642941	-0.248767	0.190573
H14	4.180872	-1.195769	0.153441
H15	3.989126	0.409272	-0.607593
H16	3.803398	0.232027	1.157291
C17	1.719481	-1.851341	-0.063978
O18	2.336579	-2.889114	-0.022843
N19	0.340298	-1.688368	-0.190806
H20	-0.274133	-2.482944	-0.244898
H21	-4.116663	0.236618	0.073732
H22	-4.845968	-1.986777	-0.352564
H23	-4.044310	-1.892702	1.251020
N24	-3.409455	-0.471133	-0.150242
C25	-3.902471	-1.831537	0.173180
H26	-3.154739	-2.550124	-0.156575
H27	-3.127510	-0.371423	-1.144232

Zero-point correction= 0.220064
Thermal correction to Energy= 0.234932
Thermal correction to Enthalpy= 0.235876
Thermal correction to Gibbs Free Energy= 0.177302
Sum of electronic and zero-point Energies= -752.198505
Sum of electronic and thermal Energies= -752.183637
Sum of electronic and thermal Enthalpies= -752.182693
Sum of electronic and thermal Free Energies= -752.241267

10 TS_O6-$^{+}$NH$_2$CH$_3$[9MOG]$^{\bullet}$

N1	2.189815	-0.442789	-0.081820
C2	-0.035077	-0.341311	0.109219
C3	-1.281460	0.304607	0.052711
O4	-2.353047	-0.201529	0.767937
N5	-1.167859	1.730506	0.094088
H6	-1.988009	2.273112	-0.134444
C7	0.039000	2.371967	-0.027720
N8	0.002429	3.724489	-0.118767
H9	-0.757538	4.245403	0.289746
H10	0.903906	4.178843	-0.120832
N11	1.198812	1.758993	-0.100762
C12	1.122863	0.412167	-0.038006
C13	3.589777	-0.074267	-0.200682
H14	4.171866	-0.993638	-0.139601
H15	3.768341	0.415889	-1.159183
H16	3.870042	0.598402	0.611676
C17	1.746692	-1.757427	0.079111
O18	2.414364	-2.761855	0.158928
N19	0.347145	-1.670843	0.135926
H20	-0.170213	-2.434154	0.542627
H21	-4.266400	-0.618392	0.384959
H22	-3.932776	-2.458959	-1.184222
H23	-3.085902	-2.719610	0.375668
N24	-3.393583	-0.717496	-0.142872
C25	-3.125559	-2.119465	-0.532561
H26	-2.175247	-2.136750	-1.068347
H27	-3.403343	-0.100712	-0.965943

Zero-point correction= 0.218505
Thermal correction to Energy= 0.233181
Thermal correction to Enthalpy= 0.234125
Thermal correction to Gibbs Free Energy= 0.175793
Sum of electronic and zero-point Energies= -752.197610
Sum of electronic and thermal Energies= -752.182935
Sum of electronic and thermal Enthalpies= -752.181990
Sum of electronic and thermal Free Energies= -752.240323

11 C8-NH$_2$CH$_3$[9MOG]$^{\bullet+}$

N1	-0.337110	2.010991	-0.409779
C2	-0.118618	-0.302729	-0.220864
C3	-0.697379	-1.628124	-0.206082
O4	-0.044442	-2.648452	-0.400612
N5	-2.059962	-1.632042	0.018279
H6	-2.510089	-2.538921	-0.001276
C7	-2.787430	-0.467531	0.205622
N8	-4.107760	-0.622299	0.444434
H9	-4.632112	0.215612	0.642917
N10	-2.270309	0.720877	0.127014
C11	-0.929479	0.849169	-0.161065
C12	-1.115885	3.218703	-0.350399
H13	-0.968969	3.763296	-1.289405
H14	-2.180390	3.065940	-0.160535
H15	-0.684660	3.849345	0.437523
C16	2.157809	0.433083	0.208679

O17	2.065832	1.236783	1.083372
N18	1.262187	-0.308498	-0.464527
H19	1.561705	-1.180830	-0.898510
H20	-4.503078	-1.502456	0.730960
H21	3.606901	0.049778	-1.322994
H22	5.257705	-1.121459	0.024280
H23	3.671905	-1.944003	0.091082
C24	4.224678	-1.044547	0.361317
N25	3.586574	0.142772	-0.303096
H26	4.184351	-0.885420	1.438250
H27	4.108079	0.991724	-0.063892

Zero-point correction= 0.217933
Thermal correction to Energy= 0.233682
Thermal correction to Enthalpy= 0.234626
Thermal correction to Gibbs Free Energy= 0.173101
Sum of electronic and zero-point Energies= -752.268592
Sum of electronic and thermal Energies= -752.252843
Sum of electronic and thermal Enthalpies= -752.251899
Sum of electronic and thermal Free Energies= -752.313424

12 TS_C8-NH_2CH_3[9MOG]$^{\bullet+}$

N1	0.244566	1.750808	-0.337444
C2	-0.144402	-0.526458	-0.011902
C3	-1.029668	-1.670362	-0.055872
O4	-0.637484	-2.825833	-0.125443
N5	-2.368967	-1.317247	-0.039521
H6	-3.028249	-2.083958	-0.091081
C7	-2.798281	0.000770	0.003323
N8	-4.131544	0.188523	0.063552
H9	-4.456547	1.139707	0.139985
N10	-1.998660	1.026109	-0.041648
C11	-0.644027	0.802671	-0.131334
C12	-0.254824	3.103247	-0.454612
H13	-0.997047	3.183923	-1.258081
H14	-0.758923	3.412950	0.469217
H15	0.575171	3.780128	-0.657933
C16	2.078161	-0.031342	0.689477
O17	1.959680	0.497501	1.747637
N18	1.217974	-0.788563	-0.049338
H19	1.482864	-1.710504	-0.386161
H20	-4.777612	-0.553749	0.273832
H21	3.104497	1.044226	-0.690473
H22	4.949927	-0.443378	-1.281179
H23	3.351674	-1.124018	-1.666213
C24	4.021049	-0.826654	-0.860456
N25	3.373999	0.266772	-0.072098
H26	4.230997	-1.663591	-0.194645
H27	4.016047	0.648887	0.628900

Zero-point correction= 0.217604
Thermal correction to Energy= 0.232486
Thermal correction to Enthalpy= 0.233430
Thermal correction to Gibbs Free Energy= 0.174903
Sum of electronic and zero-point Energies= -752.266381
Sum of electronic and thermal Energies= -752.251500
Sum of electronic and thermal Enthalpies= -752.250556
Sum of electronic and thermal Free Energies= -752.309083

13 O8-NH_2CH_3[9MOG]$^{\bullet+}$

N1	0.722728	-0.785806	0.147272
C2	-0.743382	0.872059	0.041935
C3	-2.032038	1.481064	0.012456
O4	-2.316400	2.664154	0.043400
N5	-3.032803	0.478310	-0.059185
H6	-3.978384	0.840873	-0.071160
C7	-2.806050	-0.873112	-0.072384
N8	-3.878671	-1.684586	-0.129170
H9	-4.818898	-1.344232	-0.237210
H10	-3.715045	-2.677791	-0.165499
N11	-1.600529	-1.409505	-0.021545
C12	-0.610351	-0.503413	0.040434
C13	1.291911	-2.113823	0.236983
H14	2.010968	-2.272207	-0.571422
H15	1.775373	-2.254034	1.208358
H16	0.482996	-2.837005	0.134493
C17	1.451547	0.405552	0.318125
O18	2.585511	0.492462	-0.632775
N19	0.516821	1.418869	0.128157
H20	0.686504	2.398427	0.297747
H21	4.198821	1.514150	-0.165348
H22	5.633794	-0.304029	0.384667
H23	4.867507	-0.586770	-1.214582
C24	4.700089	-0.509956	-0.141444
N25	3.773017	0.621001	0.100983
H26	4.233111	-1.415411	0.241779
H27	3.456069	0.666889	1.090975

Zero-point correction= 0.219907
Thermal correction to Energy= 0.234684
Thermal correction to Enthalpy= 0.235628
Thermal correction to Gibbs Free Energy= 0.177774
Sum of electronic and zero-point Energies= -752.198272
Sum of electronic and thermal Energies= -752.183496
Sum of electronic and thermal Enthalpies= -752.182552
Sum of electronic and thermal Free Energies= -752.240405

14 TS_O8-NH_2CH_3[9MOG]$^{\bullet+}$

N1	-0.709862	-0.801167	0.021992
C2	0.752584	0.871448	0.031080
C3	2.037049	1.482597	-0.018582
O4	2.316998	2.667550	-0.057725
N5	3.044937	0.482864	-0.027875
H6	3.987669	0.849571	-0.076030
C7	2.823998	-0.868183	-0.008395
N8	3.900902	-1.677519	-0.032654
H9	4.842962	-1.334597	0.048335
H10	3.741625	-2.670293	0.026954
N11	1.619366	-1.407588	0.015238
C12	0.623795	-0.503909	0.027278
C13	-1.284515	-2.125710	-0.051727
H14	-2.015391	-2.265589	0.749039
H15	-1.757918	-2.286611	-1.026774
H16	-0.479900	-2.850094	0.072817
C17	-1.442342	0.400964	-0.081175
O18	-2.603762	0.476346	0.618247
N19	-0.509932	1.433717	0.067059
H20	-0.679932	2.398222	-0.176496
H21	-4.174420	1.531573	-0.168610
H22	-5.661490	-0.318724	-0.652568
H23	-5.037064	-0.397748	1.024766
C24	-4.776910	-0.468756	-0.030777
N25	-3.799527	0.592390	-0.328298
H26	-4.312456	-1.429415	-0.248695
H27	-3.382702	0.532950	-1.271360

Zero-point correction= 0.217602
Thermal correction to Energy= 0.232449
Thermal correction to Enthalpy= 0.233393
Thermal correction to Gibbs Free Energy= 0.174797
Sum of electronic and zero-point Energies= -752.193168
Sum of electronic and thermal Energies= -752.178321
Sum of electronic and thermal Enthalpies= -752.177377
Sum of electronic and thermal Free Energies= -752.235973

Cartesian coordinates for HA_NH_2 products and TSs

1 [9MOG + H_{N1}]$^+$···˙$NHCH_3$

N1	1.735561	-0.794524	0.026057
C2	0.538108	1.029542	-0.446127
C3	-0.478852	1.904102	-0.483079
O4	-1.259724	2.734256	-0.650827
N5	-1.872394	-0.293316	-1.919959
H6	-1.077558	-0.045813	-2.489687
C7	-1.686940	-1.086363	-0.844169
N8	-2.725925	-1.758222	-0.350475
H9	-2.583285	-2.303011	0.485762
N10	-0.500429	-1.289889	-0.276061
C11	0.475855	-0.409571	-0.267842
C12	2.160076	-2.165752	0.261701
H13	1.652266	-2.565835	1.140721
H14	1.926324	-2.782316	-0.607315
H15	3.236845	-2.141800	0.427314
C16	2.645956	0.295528	0.037674
O17	3.834548	0.219222	0.201412
N18	1.876956	1.413068	-0.190030
H19	2.306175	2.265466	-0.518161
H20	-2.775910	-0.220767	-2.363033
H21	-3.633289	-1.769384	-0.787678
H22	-2.749717	1.474862	1.758515
C23	-1.622391	0.115668	2.709253
H24	-2.482351	-0.363165	3.202672
H25	-0.864815	-0.640769	2.489711
H26	-1.214998	0.824851	3.447085
N27	-2.017933	0.800159	1.511176

Zero-point correction= 0.212623
Thermal correction to Energy= 0.230164
Thermal correction to Enthalpy= 0.231108
Thermal correction to Gibbs Free Energy= 0.166202
Sum of electronic and zero-point Energies= -752.234624
Sum of electronic and thermal Energies= -752.217083
Sum of electronic and thermal Enthalpies= -752.216139
Sum of electronic and thermal Free Energies= -752.281045

2 TS_[9MOG + H_{N1}]$^+$···˙$NHCH_3$

N1	-1.773359	0.777329	-0.165091
C2	-0.494416	-1.030040	-0.366158
C3	0.568831	-1.867243	-0.437039
O4	1.145606	-2.873591	-0.430007
N5	1.927771	-0.401932	-1.312684
H6	1.741259	-0.544426	-2.304094
C7	1.657391	0.919740	-0.898011
N8	2.661209	1.782665	-0.804915
H9	2.472847	2.707675	-0.444347
N10	0.439550	1.315853	-0.631057
C11	-0.516685	0.394611	-0.442738
C12	-2.264606	2.147274	-0.122059
H13	-1.747451	2.703269	0.661428
H14	-2.102129	2.630643	-1.085634
H15	-3.330886	2.093574	0.095918
C16	-2.609664	-0.339657	0.130350
O17	-3.785931	-0.291360	0.375671
N18	-1.775181	-1.429312	0.069425
H19	-2.150073	-2.363754	0.002250
H20	2.853143	-0.735260	-1.058143
H21	3.606963	1.544989	-1.058714
H22	2.657908	-1.101863	2.192015
C23	1.551637	0.507082	2.627344
H24	2.285854	0.914988	3.338891
H25	1.040805	1.333815	2.126436
H26	0.821925	-0.047441	3.238423
N27	2.179655	-0.359917	1.670054

Zero-point correction= 0.212717
Thermal correction to Energy= 0.229268
Thermal correction to Enthalpy= 0.230213
Thermal correction to Gibbs Free Energy= 0.166587
Sum of electronic and zero-point Energies= -752.226914
Sum of electronic and thermal Energies= -752.210363
Sum of electronic and thermal Enthalpies= -752.209418
Sum of electronic and thermal Free Energies= -752.273044

3 [9MOG + H_{N1}]$^+$

N1	1.508662	-0.792513	-0.001418
C2	0.129398	0.945290	-0.000539
C3	-1.051923	1.654278	0.001333
O4	-1.473867	2.762941	0.003347
N5	-2.310931	0.484689	-0.003037
H6	-2.861105	0.738401	-0.830136
C7	-1.995369	-0.956360	-0.000603
N8	-3.054795	-1.767624	0.000743
H9	-2.888704	-2.765683	0.002928
N10	-0.785191	-1.379715	0.000120
C11	0.215388	-0.452779	-0.000341
C12	2.072659	-2.135887	0.002734
H13	1.863623	-2.627728	0.953802
H14	1.652853	-2.715710	-0.819407
H15	3.148987	-2.024795	-0.126695
C16	2.331038	0.383381	-0.000410
O17	3.532715	0.395596	-0.002107
N18	1.436574	1.427843	0.000967
H19	1.725157	2.394275	-0.001821
H20	-2.869335	0.740458	0.817857
H21	-4.009642	-1.443809	-0.001113

Zero-point correction= 0.162167
Thermal correction to Energy= 0.174412
Thermal correction to Enthalpy= 0.175356
Thermal correction to Gibbs Free Energy= 0.123089
Sum of electronic and zero-point Energies= -657.086907
Sum of electronic and thermal Energies= -657.074662
Sum of electronic and thermal Enthalpies= -657.073718
Sum of electronic and thermal Free Energies= -657.125985

4 ˙$NHCH_3$

H1	1.210701	0.788362	-0.000175
H2	-0.965617	0.586074	0.878574
H3	-1.125349	-0.959079	0.002699
H4	-0.965072	0.580358	-0.882384
C5	-0.627347	0.012814	0.000114
N6	0.801346	-0.153229	0.000086

Zero-point correction= 0.049366
Thermal correction to Energy= 0.052835
Thermal correction to Enthalpy= 0.053779
Thermal correction to Gibbs Free Energy= 0.025917
Sum of electronic and zero-point Energies= -95.117913
Sum of electronic and thermal Energies= -95.114444
Sum of electronic and thermal Enthalpies= -95.113500
Sum of electronic and thermal Free Energies= -95.141362

5 TS_([9MOG + H_{C2}]$^+$ + ˙$NHCH_3$)

N1	1.748689	-0.605083	0.543586
C2	0.292075	1.038165	0.011717
C3	-0.993811	1.767867	-0.010345

O4	-1.105686	2.907212	-0.407643
N5	-1.958679	0.977000	0.549412
H6	-2.903914	1.348341	0.571795
C7	-1.858734	-0.451777	0.720049
N8	-2.983499	-0.930563	1.427780
H9	-2.908969	-0.782605	2.429390
H10	-3.163571	-1.909815	1.246095
N11	-0.581493	-0.972898	1.020696
C12	0.410235	-0.275448	0.586598
C13	2.341795	-1.841642	1.039188
H14	3.409949	-1.803397	0.828066
H15	2.179557	-1.924769	2.114657
H16	1.892184	-2.696150	0.531441
C17	2.472417	0.417433	-0.041049
O18	3.640147	0.513465	-0.267921
N19	1.477323	1.434791	-0.356766
H20	1.709692	2.333441	-0.772704
H21	-1.860676	-0.808594	-0.450956
H22	-2.045588	-0.361258	-2.517297
H23	-0.182115	-2.444538	-1.602869
H24	-0.262584	-1.818466	-3.272710
C25	-0.836939	-1.989576	-2.349607
N26	-1.339458	-0.731525	-1.874472
H27	-1.642058	-2.689793	-2.611352

Zero-point correction= 0.210702
Thermal correction to Energy= 0.225941
Thermal correction to Enthalpy= 0.226885
Thermal correction to Gibbs Free Energy= 0.167263
Sum of electronic and zero-point Energies= -752.204171
Sum of electronic and thermal Energies= -752.188933
Sum of electronic and thermal Enthalpies= -752.187988
Sum of electronic and thermal Free Energies= -752.247610

6 [9MOG + H_{C2}]$^+$

N1	1.639846	-0.670221	0.111932
C2	-0.056829	0.841988	0.002901
C3	-1.455886	1.354741	0.121638
O4	-1.699052	2.537186	0.035127
N5	-2.283646	0.329803	0.428683
H6	-3.252944	0.586702	0.584569
C7	-1.991714	-1.111611	0.299931
N8	-2.465775	-1.571857	-0.987299
H9	-3.474587	-1.484525	-1.065687
H10	-2.220284	-2.547577	-1.128705
N11	-0.593925	-1.489090	0.359667
C12	0.264710	-0.574002	0.191524
C13	2.408575	-1.909978	0.217478
H14	3.459972	-1.662780	0.076395
H15	2.257821	-2.348444	1.204411
H16	2.081432	-2.605917	-0.555821
C17	2.198717	0.559525	-0.142051
O18	3.322124	0.911578	-0.294773
N19	1.032957	1.486889	-0.199007
H20	1.119672	2.492243	-0.355259
H21	-2.467298	-1.582455	1.170912

Zero-point correction= 0.163523
Thermal correction to Energy= 0.174912
Thermal correction to Enthalpy= 0.175856
Thermal correction to Gibbs Free Energy= 0.125790
Sum of electronic and zero-point Energies= -657.063477
Sum of electronic and thermal Energies= -657.052089
Sum of electronic and thermal Enthalpies= -657.051144
Sum of electronic and thermal Free Energies= -657.101210

7 TS_([9MOG + H_{N2}]$^+$ + $^{\bullet}NHCH_3$)

N1	2.175932	-1.045349	0.048404
C2	1.162719	0.933863	-0.002175
C3	0.095951	1.860251	-0.187874
O4	0.062598	3.064808	-0.052186
N5	-1.086939	1.147252	-0.595568
H6	-1.888259	1.745942	-0.761686
C7	-1.135122	-0.192678	-0.769730
N8	-2.427800	-0.750352	-1.129447
H9	-2.800284	-0.339528	-1.989348
H10	-2.277316	-1.748851	-1.299021
N11	-0.168220	-1.021929	-0.591908
C12	0.993796	-0.418767	-0.203443
C13	2.465643	-2.463966	-0.048691
H14	1.848841	-3.029254	0.652711
H15	2.290084	-2.818897	-1.066040
H16	3.518107	-2.591402	0.205593
C17	3.142328	-0.086046	0.423254
O18	4.294960	-0.299381	0.713541
N19	2.468939	1.128399	0.380507
H20	2.909616	2.011069	0.591002
H21	-3.194813	-0.620079	-0.235696
H22	-3.664600	-0.270846	1.833728
H23	-5.922269	0.330911	1.349331
H24	-5.763887	-1.397579	1.596105
C25	-5.468778	-0.577006	0.923484
N26	-4.045884	-0.453823	0.902042
H27	-5.867107	-0.758194	-0.074668

Zero-point correction= 0.213212
Thermal correction to Energy= 0.228282
Thermal correction to Enthalpy= 0.229226
Thermal correction to Gibbs Free Energy= 0.169005
Sum of electronic and zero-point Energies= -752.263774
Sum of electronic and thermal Energies= -752.248704
Sum of electronic and thermal Enthalpies= -752.247760
Sum of electronic and thermal Free Energies= -752.307981

8 [9MOG + H_{N2}]$^+$

N1	1.548495	-0.812913	-0.001284
C2	0.126583	0.900641	0.001422
C3	-1.136159	1.568797	0.000730
O4	-1.403499	2.747167	0.000475
N5	-2.198024	0.585029	0.000191
H6	-3.128432	0.990838	-0.000451
C7	-1.961489	-0.741631	-0.000100
N8	-3.139082	-1.638980	-0.001534
H9	-3.726629	-1.525373	-0.836562
H10	-2.763368	-2.596867	-0.000291
N11	-0.827965	-1.337794	0.000561
C12	0.231340	-0.474852	0.001210
C13	2.128086	-2.144979	0.002360
H14	1.894654	-2.661514	0.935477
H15	1.758319	-2.720027	-0.848350
H16	3.207692	-2.019786	-0.083098
C17	2.329466	0.365002	-0.000836
O18	3.532471	0.433947	-0.002192
N19	1.400165	1.403551	0.000206
H20	1.663651	2.378088	0.000161
H21	-3.729741	-1.524393	0.831147

Zero-point correction= 0.164670
Thermal correction to Energy= 0.176258
Thermal correction to Enthalpy= 0.177203
Thermal correction to Gibbs Free Energy= 0.126956
Sum of electronic and zero-point Energies= -657.096782
Sum of electronic and thermal Energies= -657.085194

Sum of electronic and thermal Enthalpies= -657.084250
Sum of electronic and thermal Free Energies= -657.134496

9 [9MOG + H_{N3}]$^+$···$^{\cdot}$NHCH$_3$

N1	-0.419973	-1.575256	-0.105115
C2	-1.585631	0.310700	0.050713
C3	-1.797030	1.716433	0.109436
O4	-2.816106	2.353361	0.219625
N5	-0.529513	2.417675	0.014926
H6	-0.629615	3.426279	0.054264
C7	0.688589	1.872357	-0.110847
N8	1.786746	2.632119	-0.185900
H9	1.737606	3.638389	-0.163088
H10	2.694821	2.202421	-0.281551
N11	0.808541	0.536918	-0.159773
C12	-0.336150	-0.223606	-0.078089
C13	0.645945	-2.548726	-0.239166
H14	0.176092	-3.532887	-0.210857
H15	1.162931	-2.426395	-1.194549
H16	1.351923	-2.466306	0.591463
C17	-1.791904	-1.948949	0.009356
O18	-2.211122	-3.079887	0.016933
N19	-2.471460	-0.752390	0.103764
H20	-3.474235	-0.691569	0.194422
H21	1.769253	0.119739	-0.266072
H22	3.955200	-0.538287	-1.257152
H23	4.351072	-2.030433	0.534902
H24	5.175212	-0.503765	0.781186
C25	4.174566	-0.957206	0.706647
H26	3.645341	-0.820605	1.650827
N27	3.441647	-0.386265	-0.384266

Zero-point correction= 0.215509
Thermal correction to Energy= 0.231562
Thermal correction to Enthalpy= 0.232506
Thermal correction to Gibbs Free Energy= 0.170952
Sum of electronic and zero-point Energies= -752.290016
Sum of electronic and thermal Energies= -752.273963
Sum of electronic and thermal Enthalpies= -752.273019
Sum of electronic and thermal Free Energies= -752.334572

10 TS_[9MOG + H_{N3}]$^+$···$^{\cdot}$NHCH$_3$

N1	-0.818864	-1.359383	-0.364421
C2	-1.256574	0.750027	0.158917
C3	-0.994095	2.139492	0.320920
O4	-1.722796	3.035758	0.684981
N5	0.365816	2.421614	-0.048203
H6	0.596265	3.407737	-0.002718
C7	1.291099	1.521377	-0.448887
N8	2.552978	1.953658	-0.705244
H9	2.748571	2.942915	-0.724771
H10	3.113342	1.395046	-1.329999
N11	1.019226	0.225468	-0.554666
C12	-0.280748	-0.106735	-0.275454
C13	-0.205679	-2.560775	-0.879242
H14	-0.994427	-3.308070	-0.982189
H15	0.249532	-2.375195	-1.855246
H16	0.544400	-2.953570	-0.180512
C17	-2.187355	-1.310077	0.012582
O18	-2.948504	-2.249444	0.026449
N19	-2.413039	0.010595	0.337003
H20	-3.311895	0.364712	0.626495
H21	2.064194	-0.848623	-0.273703
H22	3.318340	-2.207656	-0.513481
H23	2.790274	-2.888949	1.768416
H24	3.968405	-1.589391	1.795955
C25	2.928758	-1.827831	1.515833
H26	2.236143	-1.199104	2.073441
N27	2.761713	-1.632412	0.118226

Zero-point correction= 0.211382
Thermal correction to Energy= 0.226727
Thermal correction to Enthalpy= 0.227671
Thermal correction to Gibbs Free Energy= 0.167589
Sum of electronic and zero-point Energies= -752.283725
Sum of electronic and thermal Energies= -752.268379
Sum of electronic and thermal Enthalpies= -752.267435
Sum of electronic and thermal Free Energies= -752.327518

11 [9MOG + H_{N3}]$^+$

N1	1.549759	-0.779025	-0.000034
C2	0.096633	0.905617	-0.000041
C3	-1.183239	1.528130	-0.000018
O4	-1.493491	2.691300	-0.000063
N5	-2.234638	0.517154	0.000076
H6	-3.166303	0.920112	0.000093
C7	-2.090779	-0.811580	0.000132
N8	-3.147312	-1.627072	0.000215
H9	-4.088114	-1.262166	0.000240
H10	-3.048361	-2.630827	0.000254
N11	-0.840007	-1.317681	0.000103
C12	0.238740	-0.450766	0.000015
C13	2.163462	-2.095288	0.000001
H14	3.242711	-1.934914	-0.000153
H15	1.892089	-2.651536	0.901302
H16	1.891857	-2.651686	-0.901138
C17	2.316317	0.428515	-0.000125
O18	3.518307	0.492233	-0.000185
N19	1.373396	1.437375	-0.000127
H20	1.613280	2.417637	-0.000182
H21	-0.690881	-2.317904	0.000150

Zero-point correction= 0.163097
Thermal correction to Energy= 0.175053
Thermal correction to Enthalpy= 0.175997
Thermal correction to Gibbs Free Energy= 0.125420
Sum of electronic and zero-point Energies= -657.136074
Sum of electronic and thermal Energies= -657.124118
Sum of electronic and thermal Enthalpies= -657.123174
Sum of electronic and thermal Free Energies= -657.173752

12 [9MOG + H_{C4}]$^+$···$^{\cdot}$NHCH$_3$

N1	0.955271	1.139496	0.378877
C2	-0.348351	-0.713688	0.374110
C3	-1.599993	-1.511965	0.170367
O4	-1.665457	-2.700464	0.361574
N5	-2.609669	-0.687376	-0.253741
H6	-3.494315	-1.137236	-0.462327
C7	-2.497260	0.727619	-0.319542
N8	-3.678875	1.361530	-0.485162
H9	-4.540629	0.955852	-0.154392
H10	-3.640176	2.369572	-0.527855
N11	-1.384974	1.370720	-0.267388
C12	-0.183900	0.587059	-0.317582
C13	1.597982	2.377268	-0.036075
H14	2.078664	2.250172	-1.010625
H15	0.842283	3.161358	-0.090450
H16	2.347112	2.640226	0.710225
C17	1.554099	0.237577	1.184525
O18	2.567207	0.239971	1.817019
N19	0.600147	-0.917064	1.200152
H20	0.722326	-1.728496	1.804479
H21	0.112223	0.364036	-1.361306

H22	2.071598	-1.860370	-2.207024
H23	3.700979	0.109608	-0.786046
H24	4.217172	-1.502192	-1.342827
N25	2.158170	-1.107508	-1.516321
C26	3.526298	-0.667084	-1.533613
H27	3.795025	-0.277889	-2.528649

Zero-point correction= 0.214649
Thermal correction to Energy= 0.230791
Thermal correction to Enthalpy= 0.231735
Thermal correction to Gibbs Free Energy= 0.169166
Sum of electronic and zero-point Energies= -752.225818
Sum of electronic and thermal Energies= -752.209676
Sum of electronic and thermal Enthalpies= -752.208731
Sum of electronic and thermal Free Energies= -752.271300

13 TS_[9MOG + H_{C4}]$^{+}$···$^{\cdot}$NHCH$_3$

N1	1.239149	0.085524	1.045467
C2	-0.322331	-1.007043	-0.147424
C3	-1.675194	-1.263254	-0.698453
O4	-1.980489	-2.243419	-1.333806
N5	-2.523004	-0.228866	-0.355960
H6	-3.467393	-0.313396	-0.716137
C7	-2.199497	0.849607	0.494482
N8	-3.248380	1.648630	0.812426
H9	-4.181014	1.268444	0.869021
H10	-3.040414	2.400403	1.453801
N11	-1.005745	1.105462	0.909536
C12	0.004617	0.296943	0.345279
C13	1.990990	1.135808	1.712047
H14	2.371860	1.859995	0.986279
H15	1.339051	1.640604	2.425348
H16	2.827334	0.669964	2.232850
C17	1.752416	-1.146764	0.766114
O18	2.813339	-1.646705	1.017244
N19	0.687233	-1.813222	0.011769
H20	0.766032	-2.766815	-0.331417
H21	0.344998	0.802354	-0.700165
H22	0.723749	2.262316	-2.551412
H23	3.027832	0.780920	-1.460067
H24	2.763111	1.184954	-3.182624
N25	1.154980	1.588371	-1.913013
C26	2.564126	1.493331	-2.144961
H27	3.041652	2.478190	-2.027065

Zero-point correction= 0.211833
Thermal correction to Energy= 0.227139
Thermal correction to Enthalpy= 0.228083
Thermal correction to Gibbs Free Energy= 0.167899
Sum of electronic and zero-point Energies= -752.225290
Sum of electronic and thermal Energies= -752.209984
Sum of electronic and thermal Enthalpies= -752.209040
Sum of electronic and thermal Free Energies= -752.269224

14 [9MOG + H_{C4}]$^{+}$

N1	1.655265	-0.657630	0.210727
C2	-0.007736	0.889320	0.205750
C3	-1.421786	1.395687	0.203264
O4	-1.700441	2.564429	0.283845
N5	-2.289526	0.338884	0.105022
H6	-3.277602	0.565715	0.139833
C7	-1.864309	-0.989071	-0.162143
N8	-2.850979	-1.817376	-0.551506
H9	-3.704111	-1.475734	-0.965442
H10	-2.594900	-2.775498	-0.740428
N11	-0.650197	-1.402176	-0.027644
C12	0.275764	-0.511193	0.617554
C13	2.417096	-1.884849	0.410140
H14	2.571716	-2.066474	1.476377
H15	1.873337	-2.716488	-0.039804
H16	3.382472	-1.765710	-0.081044
C17	2.193757	0.479893	-0.275751
O18	3.274773	0.786338	-0.670815
N19	1.035681	1.447751	-0.269732
H20	1.098089	2.383692	-0.671372
H21	0.197922	-0.600533	1.716687

Zero-point correction= 0.163105
Thermal correction to Energy= 0.174445
Thermal correction to Enthalpy= 0.175389
Thermal correction to Gibbs Free Energy= 0.125963
Sum of electronic and zero-point Energies= -657.085122
Sum of electronic and thermal Energies= -657.073782
Sum of electronic and thermal Enthalpies= -657.072838
Sum of electronic and thermal Free Energies= -657.122264

15 [9MOG + H_{C5}]$^{+}$···$^{\cdot}$NHCH$_3$

N1	-0.829908	-1.472947	-0.041186
C2	0.031188	0.569572	0.517847
C3	1.316336	1.021778	1.161061
O4	1.427167	1.678377	2.156147
N5	2.431007	0.673861	0.364173
H6	3.315757	1.064292	0.670415
C7	2.395184	-0.275708	-0.622753
N8	3.494798	-0.495091	-1.329390
H9	4.344420	0.035904	-1.213394
H10	3.473175	-1.231945	-2.020703
N11	1.325622	-1.039686	-0.875207
C12	0.239072	-0.716962	-0.206626
C13	-1.060176	-2.800229	-0.596791
H14	-0.890905	-2.774812	-1.673326
H15	-0.385249	-3.520685	-0.131371
H16	-2.094745	-3.064478	-0.379683
C17	-1.736808	-0.857741	0.910630
O18	-2.800039	-1.317344	1.215523
N19	-1.101871	0.275184	1.344760
H20	-1.621910	0.988354	1.834948
H21	-0.242168	1.338839	-0.251362
H22	-1.346239	3.226946	-1.890451
H23	-3.087289	1.862871	-2.742255
H24	-3.148276	1.031241	-1.164239
C25	-2.897310	1.969895	-1.662993
H26	-3.584630	2.755111	-1.312855
N27	-1.530201	2.335316	-1.420484

Zero-point correction= 0.215207
Thermal correction to Energy= 0.231325
Thermal correction to Enthalpy= 0.232270
Thermal correction to Gibbs Free Energy= 0.168340
Sum of electronic and zero-point Energies= -752.280864
Sum of electronic and thermal Energies= -752.264745
Sum of electronic and thermal Enthalpies= -752.263801
Sum of electronic and thermal Free Energies= -752.327730

16 TS_[9MOG + H_{C5}]$^{+}$···$^{\cdot}$NHCH$_3$

N1	1.261928	-1.233034	0.009724
C2	0.009588	0.592696	-0.480702
C3	-1.266509	0.920649	-1.150550
O4	-1.442737	1.725936	-2.026757
N5	-2.344218	0.249807	-0.525600
H6	-3.263232	0.518718	-0.859779
C7	-2.197867	-0.811039	0.328012

N8	-3.288500	-1.345448	0.865573
H9	-4.216474	-0.981614	0.714852
H10	-3.174285	-2.155153	1.458611
N11	-1.018088	-1.369653	0.615146
C12	0.026586	-0.749052	0.097257
C13	1.729149	-2.529383	0.481774
H14	1.523288	-2.627409	1.548065
H15	1.226991	-3.328991	-0.065498
H16	2.802459	-2.571061	0.297984
C17	2.088757	-0.346449	-0.773366
O18	3.245673	-0.538175	-1.027845
N19	1.268578	0.695447	-1.123692
H20	1.597853	1.487346	-1.654390
H21	-0.049665	1.357742	0.580390
H22	0.014586	3.199041	1.321726
H23	1.553370	2.699484	3.074243
H24	1.658948	1.031292	2.446295
C25	1.481268	2.073124	2.174925
H26	2.275310	2.418057	1.493846
N27	0.177661	2.223905	1.589760

Zero-point correction= 0.210623
Thermal correction to Energy= 0.226134
Thermal correction to Enthalpy= 0.227078
Thermal correction to Gibbs Free Energy= 0.166108
Sum of electronic and zero-point Energies= -752.275108
Sum of electronic and thermal Energies= -752.259597
Sum of electronic and thermal Enthalpies= -752.258653
Sum of electronic and thermal Free Energies= -752.319623

17 [9MOG + H_{C5}]$^+$

N1	1.452322	-0.840561	0.023328
C2	0.071599	0.899975	0.595743
C3	-1.145492	1.486875	-0.100398
O4	-1.260942	2.612107	-0.487674
N5	-2.202769	0.555494	-0.142522
H6	-3.089591	0.924446	-0.470071
C7	-2.033938	-0.795743	0.031934
N8	-3.106065	-1.570925	0.026248
H9	-4.047931	-1.215060	-0.041338
H10	-2.970174	-2.569968	0.103234
N11	-0.834071	-1.379720	0.142907
C12	0.185924	-0.557418	0.246482
C13	2.009155	-2.137532	-0.344291
H14	1.782088	-2.864388	0.435869
H15	1.584099	-2.465624	-1.294246
H16	3.086712	-2.007369	-0.439429
C17	2.252253	0.377207	0.025627
O18	3.430872	0.402417	-0.164977
N19	1.363771	1.396599	0.247157
H20	1.684892	2.334103	0.440387
H21	-0.138853	0.981275	1.676381

Zero-point correction= 0.164150
Thermal correction to Energy= 0.175267
Thermal correction to Enthalpy= 0.176211
Thermal correction to Gibbs Free Energy= 0.127180
Sum of electronic and zero-point Energies= -657.141823
Sum of electronic and thermal Energies= -657.130707
Sum of electronic and thermal Enthalpies= -657.129762
Sum of electronic and thermal Free Energies= -657.178793

18 [9MOG + H_{C6}]$^+$···$^{\cdot}$$NHCH_3$

N1	2.378427	0.660295	-0.135583
C2	0.830121	-0.977108	0.230143
C3	-0.587274	-1.341790	0.109109
O4	0.120936	-1.446301	1.349868
N5	-1.501083	-0.265503	0.025227
H6	-2.522633	-0.446568	0.022845
C7	-1.104197	0.999065	0.283097
N8	-2.034343	1.923543	0.489188
H9	-3.015463	1.683522	0.511553
H10	-1.742046	2.879780	0.624030
N11	0.184821	1.417698	0.271048
C12	1.090253	0.489436	0.144642
C13	3.061614	1.930321	-0.341737
H14	4.106838	1.706024	-0.551617
H15	2.612799	2.457894	-1.185061
H16	2.981433	2.537503	0.560537
C17	3.021185	-0.612479	-0.333351
O18	4.179052	-0.760124	-0.593654
N19	2.027773	-1.564836	-0.204533
H20	2.256943	-2.543363	-0.109986
H21	-0.927310	-2.272714	-0.329719
H22	-4.928414	-0.715017	0.874617
H23	-5.652084	-1.330623	-1.296965
H24	-4.683924	0.019996	-1.955225
C25	-5.231059	-0.335900	-1.081082
N26	-4.380198	-0.392915	0.071534
H27	-6.097688	0.317714	-0.897808

Zero-point correction= 0.215461
Thermal correction to Energy= 0.231137
Thermal correction to Enthalpy= 0.232081
Thermal correction to Gibbs Free Energy= 0.169412
Sum of electronic and zero-point Energies= -752.250208
Sum of electronic and thermal Energies= -752.234533
Sum of electronic and thermal Enthalpies= -752.233588
Sum of electronic and thermal Free Energies= -752.296257

19 TS_[9MOG + H_{C6}]$^+$···$^{\cdot}$$NHCH_3$

N1	-2.229978	-0.642768	-0.133231
C2	-0.023838	-0.384310	0.141543
C3	1.224710	0.381279	0.435267
O4	1.517789	0.277823	1.744276
N5	0.962708	1.757566	-0.025026
H6	1.763632	2.373845	-0.000697
C7	-0.268488	2.308162	-0.126619
N8	-0.386257	3.630311	-0.244703
H9	0.394723	4.264404	-0.190216
H10	-1.312989	4.010136	-0.370848
N11	-1.414406	1.600228	-0.166244
C12	-1.251863	0.295193	-0.059625
C13	-3.649125	-0.397203	-0.353106
H14	-4.158653	-1.358841	-0.304829
H15	-4.029446	0.267714	0.423268
H16	-3.798292	0.056053	-1.334140
C17	-1.677178	-1.921060	0.036308
O18	-2.239402	-2.981411	0.028292
N19	-0.291334	-1.699118	0.210693
H20	0.357400	-2.454305	0.386455
H21	2.109045	-0.032563	-0.135443
H22	3.783643	-1.051286	-2.012167
H23	4.482783	-1.176442	0.836976
H24	5.606657	-0.824750	-0.506750
C25	4.676640	-1.342236	-0.224933
N26	3.576995	-0.884904	-1.022829
H27	4.865154	-2.413425	-0.395776

Zero-point correction= 0.211551
Thermal correction to Energy= 0.227412
Thermal correction to Enthalpy= 0.228356
Thermal correction to Gibbs Free Energy= 0.165828

Sum of electronic and zero-point Energies= -752.178178
Sum of electronic and thermal Energies= -752.162317
Sum of electronic and thermal Enthalpies= -752.161373
Sum of electronic and thermal Free Energies= -752.223901

20 [9MOG + H_{C6}]$^+$

N1	1.390948	0.838262	0.050235
C2	0.112932	-1.051831	0.060595
C3	-1.183479	-1.626099	-0.321405
O4	-0.683724	-1.718379	1.010035
N5	-2.242576	-0.694261	-0.500364
H6	-3.157321	-1.057792	-0.731879
C7	-2.119707	0.594595	-0.089735
N8	-3.205660	1.347824	0.025810
H9	-4.142398	0.995711	-0.097516
H10	-3.082115	2.319963	0.271842
N11	-0.935288	1.196171	0.140861
C12	0.128662	0.439376	0.104727
C13	1.873984	2.214035	0.037759
H14	2.957931	2.174657	-0.063910
H15	1.434250	2.748109	-0.805765
H16	1.602370	2.704487	0.973115
C17	2.269204	-0.297980	-0.105115
O18	3.459269	-0.232909	-0.176620
N19	1.444815	-1.404203	-0.192978
H20	1.819840	-2.339575	-0.128396
H21	-1.292175	-2.554384	-0.870714

Zero-point correction= 0.163943
Thermal correction to Energy= 0.174847
Thermal correction to Enthalpy= 0.175791
Thermal correction to Gibbs Free Energy= 0.127425
Sum of electronic and zero-point Energies= -657.101418
Sum of electronic and thermal Energies= -657.090514
Sum of electronic and thermal Enthalpies= -657.089570
Sum of electronic and thermal Free Energies= -657.137936

21 [9MOG + H_{O6}]$^+$···$^{\cdot}$$NHCH_3$

N1	-1.062722	-1.809164	-0.036273
C2	0.128877	0.065797	0.183477
C3	0.264941	1.425198	0.198374
O4	1.330611	2.162886	0.321463
N5	-0.912241	2.139145	0.074673
H6	-0.816073	3.147506	0.098212
C7	-2.136362	1.549713	-0.090091
N8	-3.213442	2.339570	-0.200006
H9	-3.174953	3.344542	-0.161417
H10	-4.110192	1.893612	-0.318856
N11	-2.287804	0.235729	-0.145716
C12	-1.165162	-0.464671	-0.009326
C13	-2.148166	-2.763080	-0.207102
H14	-2.610563	-2.630978	-1.186425
H15	-1.713189	-3.759289	-0.131229
H16	-2.894420	-2.621516	0.575984
C17	0.289105	-2.197642	0.153721
O18	0.707118	-3.324300	0.219588
N19	1.003859	-1.010835	0.238681
H20	1.957860	-0.994297	0.562530
H21	2.212721	1.631904	0.345814
H22	4.307689	1.065177	1.077989
H23	4.829532	-0.553816	-0.562584
H24	3.544248	0.137518	-1.608424
C25	4.271179	0.356431	-0.825429
H26	5.020485	1.063494	-1.217276
N27	3.632142	0.925123	0.322290

Zero-point correction= 0.215168
Thermal correction to Energy= 0.231092
Thermal correction to Enthalpy= 0.232036
Thermal correction to Gibbs Free Energy= 0.170710
Sum of electronic and zero-point Energies= -752.305152
Sum of electronic and thermal Energies= -752.289229
Sum of electronic and thermal Enthalpies= -752.288284
Sum of electronic and thermal Free Energies= -752.349610

22 TS_[9MOG + H_{O6}]$^+$···$^{\cdot}$$NHCH_3$

N1	-2.175294	-0.999179	0.091578
C2	-0.092253	-0.247285	-0.191146
C3	0.896469	0.734721	-0.262383
O4	2.129346	0.597352	-0.414758
N5	0.364450	2.031007	-0.153078
H6	1.049352	2.773876	-0.220597
C7	-0.958303	2.314638	0.036626
N8	-1.329447	3.600413	0.127477
H9	-0.688617	4.370939	0.037415
H10	-2.310393	3.796379	0.254867
N11	-1.887958	1.373949	0.139372
C12	-1.430605	0.129977	0.022034
C13	-3.614263	-1.080144	0.288245
H14	-4.132649	-0.613924	-0.551233
H15	-3.874005	-2.136895	0.344094
H16	-3.888872	-0.577523	1.216598
C17	-1.349829	-2.130576	-0.090398
O18	-1.696582	-3.284118	-0.117254
N19	-0.058142	-1.624283	-0.224967
H20	0.702450	-2.207994	-0.535072
H21	3.197497	-0.520471	0.007684
H22	3.941489	-1.771220	1.027853
H23	6.055066	-1.226807	-0.115004
H24	5.294790	0.324656	-0.599684
C25	5.341617	-0.443520	0.170149
H26	5.716426	-0.001922	1.106892
N27	4.046156	-1.007883	0.368692

Zero-point correction= 0.212998
Thermal correction to Energy= 0.228899
Thermal correction to Enthalpy= 0.229844
Thermal correction to Gibbs Free Energy= 0.167222
Sum of electronic and zero-point Energies= -752.302238
Sum of electronic and thermal Energies= -752.286336
Sum of electronic and thermal Enthalpies= -752.285392
Sum of electronic and thermal Free Energies= -752.348014

23 [9MOG + H_{O6}]$^+$

N1	1.556921	-0.766705	0.004139
C2	0.056045	0.894677	-0.008626
C3	-1.224565	1.345283	0.002801
O4	-1.713528	2.578321	0.010335
N5	-2.220414	0.391296	-0.001847
H6	-3.171344	0.742391	0.002760
C7	-1.962231	-0.951429	-0.003508
N8	-2.992277	-1.803085	-0.009695
H9	-3.957295	-1.515245	-0.015156
H10	-2.782879	-2.790326	-0.009667
N11	-0.725040	-1.429694	0.002057
C12	0.237453	-0.518570	-0.000278
C13	2.198382	-2.074705	0.016254
H14	2.010080	-2.573937	0.967883
H15	1.812277	-2.679696	-0.804674
H16	3.267820	-1.909324	-0.110514
C17	2.286201	0.454001	-0.003267
O18	3.479829	0.571810	-0.014587
N19	1.322260	1.456894	0.004088

H20	1.588616	2.426582	-0.059479
H21	-1.035544	3.262020	0.051418

Zero-point correction= 0.163088
Thermal correction to Energy= 0.175193
Thermal correction to Enthalpy= 0.176137
Thermal correction to Gibbs Free Energy= 0.124542
Sum of electronic and zero-point Energies= -657.147788
Sum of electronic and thermal Energies= -657.135683
Sum of electronic and thermal Enthalpies= -657.134738
Sum of electronic and thermal Free Energies= -657.186333

24 TS_([9MOG + H_{N7}]$^+$ +˙$NHCH_3$)

N1	0.057978	-1.937455	0.062072
C2	0.026012	0.225040	-0.549878
C3	-0.476534	1.544804	-0.599928
O4	0.106355	2.581060	-0.879688
N5	-1.852580	1.547203	-0.242586
H6	-2.294196	2.457976	-0.292270
C7	-2.554314	0.455112	0.184130
N8	-3.848929	0.609680	0.491102
N9	-2.009003	-0.749643	0.322658
C10	-0.730457	-0.802313	-0.044879
C11	-0.388967	-3.240321	0.539357
H12	-0.828009	-3.133698	1.531819
H13	-1.130355	-3.650472	-0.147941
H14	0.480362	-3.895540	0.581037
C15	1.335791	-1.673741	-0.360008
O16	2.294366	-2.390512	-0.423338
N17	1.372254	-0.240098	-0.744835
H18	1.699296	-0.171661	-1.713053
H19	-4.342047	1.480318	0.382321
H20	2.202866	0.390627	-0.062472
H21	-4.360922	-0.204357	0.794302
H22	4.039572	0.850659	0.674017
H23	1.700916	2.506956	1.341731
H24	2.953509	3.146080	0.296080
N25	3.056474	1.119092	0.601770
C26	2.762212	2.418856	1.106848
H27	3.397427	2.692670	1.953525

Zero-point correction= 0.211626
Thermal correction to Energy= 0.226342
Thermal correction to Enthalpy= 0.227286
Thermal correction to Gibbs Free Energy= 0.168596
Sum of electronic and zero-point Energies= -752.284067
Sum of electronic and thermal Energies= -752.269351 Sum of electronic and thermal Enthalpies= -752.268407
Sum of electronic and thermal Free Energies= -752.327098

25 [9MOG + H_{N7}]$^+$

N1	1.535059	-0.800332	-0.003453
C2	0.013134	0.881065	0.002751
C3	-1.271204	1.485637	0.000549
O4	-1.562395	2.662733	-0.001265
N5	-2.264862	0.464502	0.000462
H6	-3.216849	0.814542	-0.000417
C7	-2.016339	-0.876697	0.000187
N8	-3.048028	-1.722299	-0.000159
H9	-2.849074	-2.711547	0.000618
N10	-0.781584	-1.391405	0.000290
C11	0.176461	-0.478740	0.000806
C12	2.076844	-2.160226	0.000357
H13	1.858256	-2.639441	0.955216
H14	1.620579	-2.724391	-0.812805
H15	3.153767	-2.091706	-0.146736
C16	2.314046	0.307574	0.000177
O17	3.487205	0.488165	0.001330
N18	1.314481	1.510334	-0.000291
H19	1.499335	2.093702	-0.826129
H20	-4.009734	-1.422468	0.000208
H21	1.502110	2.096859	0.822631

Zero-point correction= 0.164787
Thermal correction to Energy= 0.176196
Thermal correction to Enthalpy= 0.177140
Thermal correction to Gibbs Free Energy= 0.127359
Sum of electronic and zero-point Energies= -657.118991
Sum of electronic and thermal Energies= -657.107582
Sum of electronic and thermal Enthalpies= -657.106638
Sum of electronic and thermal Free Energies= -657.156420

26 [9MOG + H_{O8}]$^+$⋯˙$NHCH_3$

N1	-0.194924	1.441543	-0.059766
C2	0.529013	-0.656168	-0.095203
C3	1.468155	-1.729560	-0.071536
O4	1.262993	-2.925503	-0.134806
N5	2.776898	-1.198406	0.044607
C6	3.100688	0.133419	0.122975
N7	4.401354	0.454978	0.231121
H8	5.138608	-0.228951	0.253377
H9	4.643079	1.431603	0.285327
N10	2.200004	1.099602	0.097777
C11	0.944036	0.646032	-0.011763
C12	-0.244202	2.898928	-0.001283
H13	-0.842475	3.214308	0.854077
H14	0.779947	3.251627	0.111215
H15	-0.675121	3.293516	-0.921975
C16	-1.271902	0.631909	-0.170146
O17	-2.469882	1.090916	-0.236242
N18	-0.861755	-0.645611	-0.193795
H19	-1.451957	-1.460657	-0.271313
H20	-3.237915	0.365640	-0.317910
H21	3.503917	-1.903748	0.068303
H22	-4.827009	-0.472003	1.652099
H23	-6.240871	-0.392823	0.561375
H24	-4.781072	-0.952603	-1.254581
N25	-4.398865	-0.573600	-0.384961
C26	-5.254547	-0.855088	0.725493
H27	-5.440450	-1.935586	0.812290

Zero-point correction= 0.214622
Thermal correction to Energy= 0.230674
Thermal correction to Enthalpy= 0.231618
Thermal correction to Gibbs Free Energy= 0.168975
Sum of electronic and zero-point Energies= -752.304738
Sum of electronic and thermal Energies= -752.288686
Sum of electronic and thermal Enthalpies= -752.287742
Sum of electronic and thermal Free Energies= -752.350385

27 TS_[9MOG + H_{O8}]$^+$⋯˙$NHCH_3$

N1	0.288504	-1.270107	-0.038887
C2	-0.673743	0.727850	-0.010099
C3	-1.730560	1.682506	0.012133
O4	-1.665431	2.896978	0.011596
N5	-2.973345	1.000721	0.037497
C6	-3.141695	-0.361130	0.037611
N7	-4.400298	-0.836192	0.063267
H8	-5.213255	-0.244441	0.078720
H9	-4.526277	-1.835645	0.063365
N10	-2.134802	-1.214992	0.014554
C11	-0.934854	-0.616130	-0.008225
C12	0.503295	-2.711257	-0.044246

H13	0.972848	-3.023848	0.889499
H14	-0.472585	-3.184436	-0.143812
H15	1.138390	-2.985449	-0.887028
C16	1.279309	-0.339068	-0.056378
O17	2.512449	-0.645772	-0.080677
N18	0.711262	0.883378	-0.041819
H19	1.196601	1.766896	-0.023745
H20	3.393454	0.138083	-0.185131
H21	-3.777791	1.616182	0.055242
H22	5.491259	-0.645450	0.855371
H23	6.467298	0.155750	-0.422806
H24	4.627983	1.656713	-0.789998
N25	4.495447	0.791014	-0.265003
C26	5.687134	0.294057	0.340575
H27	6.085242	1.038285	1.047471

Zero-point correction= 0.211134
Thermal correction to Energy= 0.227003
Thermal correction to Enthalpy= 0.227947
Thermal correction to Gibbs Free Energy= 0.165805
Sum of electronic and zero-point Energies= -752.307404
Sum of electronic and thermal Energies= -752.291535
Sum of electronic and thermal Enthalpies= -752.290591
Sum of electronic and thermal Free Energies= -752.352733

28 [9MOG + H_{O8}]$^+$

N1	1.505189	-0.776171	-0.000043
C2	0.019484	0.875782	-0.000023
C3	-1.270771	1.498059	0.000008
O4	-1.545105	2.677511	0.000032
N5	-2.267436	0.490086	0.000013
H6	-3.213844	0.853503	0.000041
C7	-2.048121	-0.865210	-0.000007
N8	-3.118519	-1.672989	0.000000
H9	-4.065992	-1.333562	0.000016
H10	-2.961700	-2.668641	-0.000007
N11	-0.837216	-1.401505	-0.000029
C12	0.137859	-0.487411	-0.000031
C13	2.098141	-2.111048	0.000057
H14	2.695297	-2.261626	0.901998
H15	1.275407	-2.825390	-0.000462
H16	2.696212	-2.261359	-0.901321
C17	2.165457	0.398399	-0.000017
O18	3.460818	0.590191	0.000007
N19	1.304658	1.409133	-0.000015
H20	1.553199	2.390574	-0.000008
H21	3.976691	-0.226416	0.000026

Zero-point correction= 0.163679
Thermal correction to Energy= 0.175441
Thermal correction to Enthalpy= 0.176385
Thermal correction to Gibbs Free Energy= 0.126213
Sum of electronic and zero-point Energies= -657.143675
Sum of electronic and thermal Energies= -657.131914
Sum of electronic and thermal Enthalpies= -657.130970
Sum of electronic and thermal Free Energies= -657.181142

29 TS_([9MOG + H_{N9}]$^+$ + $^{\bullet}NHCH_3$)

N1	-1.092537	-0.241322	-0.645885
C2	0.672227	1.000717	0.042534
C3	2.022492	1.271455	0.444394
O4	2.510585	2.324284	0.794108
N5	2.783831	0.076380	0.379882
H6	3.753560	0.196754	0.650290
C7	2.320279	-1.153744	-0.003474
N8	3.181966	-2.184734	-0.003871
H9	4.162316	-2.081586	0.198749
H10	2.847717	-3.079236	-0.325656
N11	1.061335	-1.362421	-0.358242
C12	0.314952	-0.254090	-0.313395
C13	-1.463600	-0.845081	-1.959131
H14	-0.911111	-0.351318	-2.759275
H15	-1.210164	-1.903782	-1.924603
H16	-2.535043	-0.704302	-2.098182
C17	-1.520163	1.198704	-0.504017
O18	-2.646374	1.550306	-0.724166
N19	-0.427934	1.863496	-0.064855
H20	-0.418453	2.856633	0.121416
H21	-1.718394	-0.809667	0.167754
H22	-2.275159	-2.205466	1.739077
H23	-4.093102	-0.042943	0.874787
H24	-3.816181	-0.543043	2.574318
C25	-3.825361	-0.876091	1.524147
N26	-2.540445	-1.396125	1.173953
H27	-4.588138	-1.666911	1.468580

Zero-point correction= 0.211779
Thermal correction to Energy= 0.226534
Thermal correction to Enthalpy= 0.227478
Thermal correction to Gibbs Free Energy= 0.167284
Sum of electronic and zero-point Energies= -752.271016
Sum of electronic and thermal Energies= -752.256261
Sum of electronic and thermal Enthalpies= -752.255317
Sum of electronic and thermal Free Energies= -752.315510

30 [9MOG + H_{N9}]$^+$

N1	1.507433	-0.937661	-0.283705
C2	0.098932	0.827886	-0.020177
C3	-1.161818	1.508190	0.123272
O4	-1.357907	2.692649	0.269250
N5	-2.219106	0.565334	0.070719
H6	-3.139213	0.981629	0.166246
C7	-2.087691	-0.788551	-0.092475
N8	-3.196047	-1.538797	-0.125334
H9	-4.123995	-1.155592	-0.048632
H10	-3.094317	-2.533838	-0.253165
N11	-0.902725	-1.375461	-0.216948
C12	0.108513	-0.511717	-0.171567
C13	1.954229	-1.926778	0.756063
H14	1.769026	-1.491166	1.737529
H15	1.372546	-2.837782	0.624275
H16	3.018823	-2.104204	0.607703
C17	2.332554	0.399519	-0.195856
O18	3.518640	0.384121	-0.263047
N19	1.399839	1.355122	-0.034384
H20	1.632717	2.335567	0.060306
H21	1.684472	-1.339814	-1.211884

Zero-point correction= 0.164586
Thermal correction to Energy= 0.175775
Thermal correction to Enthalpy= 0.176719
Thermal correction to Gibbs Free Energy= 0.127959
Sum of electronic and zero-point Energies= -657.108815
Sum of electronic and thermal Energies= -657.097627
Sum of electronic and thermal Enthalpies= -657.096683
Sum of electronic and thermal Free Energies= -657.145442

Cartesian coordinates for products and TSs in Scheme S1 and Table S1

1 N1-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	-2.114658	0.384519	0.366807
C2	-0.280001	-0.684381	-0.400760
C3	1.090901	-0.891181	-0.686622
O4	1.648362	-1.809561	-1.236841
N5	1.916655	0.234843	-0.088615
H6	2.753453	0.310615	-0.677280
C7	1.230878	1.681710	-0.147188
N8	1.340167	2.121521	-1.482613
H9	1.985815	2.885939	-1.629508
H10	0.453607	2.300178	-1.934919
N11	-0.112536	1.655333	0.329266
C12	-0.778498	0.573357	0.134530
C13	-3.036353	1.397663	0.864520
H14	-4.000441	0.916214	1.024133
H15	-2.658995	1.801521	1.804517
H16	-3.139234	2.201645	0.133464
C17	-2.514878	-0.885481	-0.052553
O18	-3.606383	-1.374728	-0.023018
N19	-1.331430	-1.511627	-0.536579
H20	-1.322400	-2.461560	-0.887048
H21	1.872471	2.226285	0.549132
H22	1.536039	-0.060571	1.844178
H23	3.505752	-1.256662	2.435592
H24	4.093233	-1.107753	0.776937
C25	3.196534	-1.220420	1.390189
N26	2.364735	-0.020774	1.254622
H27	2.692847	-2.155852	1.126764

Zero-point correction= 0.220562
Thermal correction to Energy= 0.235015
Thermal correction to Enthalpy= 0.235959
Thermal correction to Gibbs Free Energy= 0.178797
Sum of electronic and zero-point Energies= -752.231823
Sum of electronic and thermal Energies= -752.217371
Sum of electronic and thermal Enthalpies= -752.216427
Sum of electronic and thermal Free Energies= -752.273588

2 TS$^{\text{via async HA_NH2 + add}}$_N1-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	-2.268394	0.398875	0.340266
C2	-0.411582	-0.718282	-0.329211
C3	0.973396	-0.921992	-0.682514
O4	1.444939	-1.964587	-1.109984
N5	1.706090	0.224957	-0.402271
H6	2.587389	0.285545	-0.910300
C7	1.162593	1.598905	-0.115838
N8	1.521873	2.426166	-1.222916
H9	1.699750	3.382536	-0.941982
H10	0.836771	2.414647	-1.970831
N11	-0.239847	1.646464	0.227208
C12	-0.920276	0.576458	0.114101
C13	-3.192640	1.435310	0.788273
H14	-4.163295	0.966937	0.946599
H15	-2.828250	1.866106	1.721457
H16	-3.273972	2.213266	0.027664
C17	-2.648004	-0.894454	0.033306
O18	-3.715445	-1.423513	0.087600
N19	-1.421484	-1.551058	-0.392948
H20	-1.385862	-2.524750	-0.682233
H21	1.718530	1.923237	0.767788
H22	2.108970	-0.776615	1.833243
H23	4.428564	-1.308685	1.953706
H24	4.645885	-0.462058	0.414819
C25	3.925725	-1.021788	1.015222
N26	2.818958	-0.180965	1.389121
H27	3.633915	-1.951380	0.509877

Zero-point correction= 0.215029
Thermal correction to Energy= 0.229902
Thermal correction to Enthalpy= 0.230847
Thermal correction to Gibbs Free Energy= 0.171579
Sum of electronic and zero-point Energies= -752.179184
Sum of electronic and thermal Energies= -752.164311
Sum of electronic and thermal Enthalpies= -752.163366
Sum of electronic and thermal Free Energies= -752.222633

3 N1-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	-2.176153	0.590261	0.149008
C2	-0.500676	-0.826388	-0.260096
C3	0.780972	-1.264824	-0.541994
O4	1.321681	-2.316497	-0.777649
N5	1.805258	-0.017241	-0.396920
H6	2.514059	-0.235083	-1.104840
C7	1.196251	1.304253	-0.652236
N8	2.167259	2.372769	-0.307920
H9	2.785775	2.626915	-1.081451
H10	1.617486	3.197946	-0.046863
N11	-0.030303	1.579529	-0.213200
C12	-0.847098	0.528293	-0.105058
C13	-2.971472	1.787890	0.352563
H14	-2.631704	2.319888	1.243059
H15	-2.899262	2.440520	-0.519380
H16	-4.003871	1.465721	0.489103
C17	-2.736528	-0.714367	0.140848
O18	-3.894142	-0.990640	0.331110
N19	-1.674199	-1.557022	-0.124126
H20	-1.773200	-2.558600	-0.181365
H21	2.732552	2.058290	0.503224
H22	1.776139	-0.182141	1.588924
H23	3.155255	-2.071123	0.869938
H24	4.317367	-0.866592	0.243791
N25	2.507660	-0.015659	0.897321
C26	3.544284	-1.058097	0.992659
H27	3.998043	-0.947649	1.978914

Zero-point correction= 0.221160
Thermal correction to Energy= 0.235616
Thermal correction to Enthalpy= 0.236561
Thermal correction to Gibbs Free Energy= 0.179330
Sum of electronic and zero-point Energies= -752.185352
Sum of electronic and thermal Energies= -752.170896
Sum of electronic and thermal Enthalpies= -752.169952
Sum of electronic and thermal Free Energies= -752.227183

4 TS$^{\text{via PT in adduct}}$_N1-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	2.282811	0.603732	0.139813
C2	0.596375	-0.868106	0.045731
C3	-0.680184	-1.320792	-0.127852
O4	-1.312657	-2.298897	-0.462061
N5	-1.681033	-0.077481	0.381098
H6	-1.791904	-0.248274	1.384921
C7	-1.181521	1.358971	0.180455
N8	-2.122346	2.013585	-0.691168
H9	-2.587441	2.810631	-0.259729
H10	-1.689637	2.324197	-1.563187
N11	0.121092	1.564367	0.060944
C12	0.932739	0.518379	0.138384
C13	3.067361	1.825875	0.163048
H14	2.940711	2.374275	-0.772849
H15	2.753754	2.450281	1.000461
H16	4.111289	1.536409	0.282144

C17	2.867149	-0.683251	-0.000121
O18	4.046980	-0.925168	-0.018436
N19	1.802656	-1.553432	-0.109263
H20	1.926023	-2.553697	-0.094769
H21	-2.885035	0.924807	-0.781561
H22	-2.833508	-1.056682	-0.877112
H23	-3.948457	-1.352477	1.227096
H24	-4.165166	0.430738	1.322905
N25	-2.949161	-0.228342	-0.269896
C26	-4.084345	-0.430821	0.657331
H27	-4.988799	-0.506222	0.053104

Zero-point correction= 0.216337
Thermal correction to Energy= 0.230340
Thermal correction to Enthalpy= 0.231284
Thermal correction to Gibbs Free Energy= 0.175007
Sum of electronic and zero-point Energies= -752.178651
Sum of electronic and thermal Energies= -752.164647
Sum of electronic and thermal Enthalpies= -752.163703
Sum of electronic and thermal Free Energies= -752.219980

5 $TS^{via\ async\ HA_NH2\ +\ add}$_N1-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$

N1	-2.218608	0.575256	0.154049
C2	-0.506387	-0.801202	-0.243465
C3	0.797662	-1.190348	-0.562664
O4	1.321699	-2.255423	-0.811590
N5	1.738576	0.018467	-0.471576
H6	2.500513	-0.171126	-1.128591
C7	1.158130	1.299075	-0.582828
N8	2.157516	2.349915	-0.331114
H9	2.719832	2.603627	-1.148118
H10	1.657163	3.185053	-0.009030
N11	-0.066551	1.594672	-0.200443
C12	-0.882868	0.537119	-0.090848
C13	-3.039814	1.753832	0.366406
H14	-2.715213	2.285032	1.263170
H15	-2.981677	2.416203	-0.499304
H16	-4.065271	1.407832	0.497291
C17	-2.743840	-0.738566	0.144856
O18	-3.892513	-1.052792	0.329791
N19	-1.653273	-1.557525	-0.115474
H20	-1.724809	-2.562072	-0.170483
H21	2.774247	1.984848	0.428060
H22	1.902581	-0.246711	1.645953
H23	3.209795	-2.070727	0.803504
H24	4.380930	-0.870906	0.178314
N25	2.646527	-0.002226	0.987789
C26	3.638035	-1.076364	0.953776
H27	4.153605	-1.046528	1.919614

Zero-point correction= 0.218820
Thermal correction to Energy= 0.233049
Thermal correction to Enthalpy= 0.233993
Thermal correction to Gibbs Free Energy= 0.177279
Sum of electronic and zero-point Energies= -752.179997
Sum of electronic and thermal Energies= -752.165768
Sum of electronic and thermal Enthalpies= -752.164824
Sum of electronic and thermal Free Energies= -752.221537

6 N1-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$

N1	-2.282779	0.557084	-0.137857
C2	-0.549106	-0.823330	0.099918
C3	0.771826	-1.236938	0.182906
O4	1.348094	-2.266925	0.393556
N5	1.749967	0.030289	-0.166356
H6	1.775359	0.087934	-1.198440
C7	1.233212	1.294859	0.389059
N8	2.132957	2.334825	0.347671
H9	3.066630	2.028983	0.607335
H10	1.853760	3.165552	0.856242
N11	-0.077051	1.542190	-0.057502
C12	-0.945741	0.502478	-0.049782
C13	-3.128517	1.731064	-0.270165
H14	-4.159879	1.375853	-0.266590
H15	-2.982569	2.408583	0.575169
H16	-2.932154	2.242328	-1.215676
C17	-2.822700	-0.771823	-0.017268
O18	-3.994288	-1.041959	-0.056858
N19	-1.727215	-1.578489	0.147874
H20	-1.792978	-2.581112	0.229207
H21	-0.401714	2.493742	-0.162456
H22	3.005370	-0.932213	0.998367
H23	3.549403	-1.621918	-1.272304
H24	4.076889	0.076314	-1.554826
N25	3.090465	-0.209590	0.282765
C26	3.939809	-0.709818	-0.807541
H27	4.914342	-0.926090	-0.368542

Zero-point correction= 0.220119
Thermal correction to Energy= 0.234860
Thermal correction to Enthalpy= 0.235805
Thermal correction to Gibbs Free Energy= 0.178249
Sum of electronic and zero-point Energies= -752.210127
Sum of electronic and thermal Energies= -752.195386
Sum of electronic and thermal Enthalpies= -752.194442
Sum of electronic and thermal Free Energies= -752.251997

7 $TS^{via\ async\ add\ +\ PT}$_N1-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$

N1	1.902602	0.693693	0.190036
C2	0.401882	-0.787515	-0.515062
C3	-0.855337	-1.345260	-0.669663
O4	-1.349640	-2.408834	-0.918733
N5	-1.948126	-0.160810	-0.339793
C6	-1.424726	1.188451	-0.809617
N7	-2.433442	2.129879	-0.909145
H8	-3.042506	2.049967	-1.716175
H9	-2.082406	3.075884	-0.800458
N10	-0.371899	1.488712	0.053585
C11	0.604393	0.541265	-0.098169
C12	2.584793	1.907119	0.614689
H13	3.386174	2.130913	-0.090490
H14	1.857319	2.717329	0.633166
H15	3.014538	1.758671	1.606257
C16	2.613275	-0.521910	-0.072982
O17	3.801402	-0.667800	0.051330
N18	1.650284	-1.415684	-0.481716
H19	1.877584	-2.327803	-0.846485
H20	-1.140976	0.860447	1.086683
H21	-1.065060	-1.629717	1.888484
H22	-2.165677	-0.788210	3.002269
N23	-2.080766	0.049386	1.112311
C24	-2.036819	-1.148536	1.980611
H25	-2.834514	-1.846286	1.722872
H26	-2.940890	0.586062	1.251051
H27	-2.833019	-0.472108	-0.753738

Zero-point correction= 0.215733
Thermal correction to Energy= 0.229714
Thermal correction to Enthalpy= 0.230658
Thermal correction to Gibbs Free Energy= 0.175235
Sum of electronic and zero-point Energies= -752.156018
Sum of electronic and thermal Energies= -752.142037
Sum of electronic and thermal Enthalpies= -752.141093

Sum of electronic and thermal Free Energies= -752.196516

8 $TS^{via\ HA_NH2\ products}$_N1-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$

N1	2.218859	0.535045	-0.192517
C2	0.471143	-0.778399	0.243943
C3	-0.850962	-1.119001	0.563082
O4	-1.375345	-2.156878	0.885937
N5	-1.775975	0.086806	0.386221
H6	-2.550160	-0.029505	1.046135
C7	-1.263397	1.378325	0.471117
N8	-2.161246	2.385730	0.614038
H9	-2.987020	2.363083	0.024573
H10	-1.850129	3.296546	0.916127
N11	0.036216	1.579185	0.062598
C12	0.887776	0.518082	0.018320
C13	3.078114	1.674080	-0.463236
H14	4.091648	1.283332	-0.563631
H15	2.792876	2.160466	-1.399657
H16	3.052381	2.385248	0.366546
C17	2.722580	-0.802337	-0.081458
O18	3.874303	-1.122593	-0.221764
N19	1.616579	-1.568847	0.206463
H20	1.657033	-2.569633	0.324060
H21	0.345806	2.514144	-0.164992
H22	-1.928762	-0.322100	-1.712487
H23	-3.219201	-2.114817	-0.782990
H24	-4.382463	-0.889099	-0.189172
N25	-2.677525	-0.042004	-1.073150
C26	-3.650126	-1.126753	-0.965216
H27	-4.182796	-1.137279	-1.922780

Zero-point correction= 0.216539
Thermal correction to Energy= 0.231535
Thermal correction to Enthalpy= 0.232479
Thermal correction to Gibbs Free Energy= 0.174340
Sum of electronic and zero-point Energies= -752.204499
Sum of electronic and thermal Energies= -752.189503
Sum of electronic and thermal Enthalpies= -752.188559
Sum of electronic and thermal Free Energies= -752.246698

9 N1-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.192108	0.524193	0.249175
C2	-0.387174	-0.841732	-0.018454
C3	0.910551	-1.150418	-0.432044
O4	1.403007	-2.150314	-0.919011
N5	1.846416	0.075227	-0.279036
H6	2.517603	-0.056126	-1.046637
C7	1.148455	1.401165	-0.484935
N8	1.948287	2.278814	-1.135369
H9	2.936948	2.282319	-0.919652
H10	1.543956	3.195203	-1.279594
N11	-0.044028	1.595312	-0.121545
C12	-0.774489	0.515859	0.503432
C13	-3.058498	1.602540	0.695398
H14	-3.049694	1.685956	1.787166
H15	-2.727336	2.540940	0.248931
H16	-4.071223	1.378339	0.361080
C17	-2.667473	-0.716473	-0.078938
O18	-3.792366	-1.098293	-0.240686
N19	-1.499513	-1.549027	-0.228605
H20	-1.552553	-2.473365	-0.640080
H21	-0.600196	0.590463	1.592058
H22	1.990766	0.291033	1.697777
H23	2.934145	-1.951209	1.244257
H24	4.203616	-1.104362	0.317953
C25	3.491351	-1.015705	1.141209
N26	2.649472	0.169592	0.930303
H27	4.052820	-0.820525	2.055852

Zero-point correction= 0.220329
Thermal correction to Energy= 0.234685
Thermal correction to Enthalpy= 0.235629
Thermal correction to Gibbs Free Energy= 0.178308
Sum of electronic and zero-point Energies= -752.210765
Sum of electronic and thermal Energies= -752.196409
Sum of electronic and thermal Enthalpies= -752.195465
Sum of electronic and thermal Free Energies= -752.252786

10 $TS^{via\ HA_NH2\ products}$_N1-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.239045	0.517715	0.290771
C2	-0.432185	-0.829340	-0.034900
C3	0.905853	-1.133003	-0.457666
O4	1.340602	-2.223889	-0.800968
N5	1.704507	0.040065	-0.496696
H6	2.444960	-0.078783	-1.187937
C7	1.084377	1.357470	-0.542319
N8	1.885511	2.278404	-1.124195
H9	2.884740	2.196093	-0.988844
H10	1.524147	3.222613	-1.129067
N11	-0.085989	1.603337	-0.098278
C12	-0.808876	0.517044	0.495894
C13	-3.099627	1.611722	0.715799
H14	-3.130999	1.683629	1.807047
H15	-2.723814	2.542599	0.290190
H16	-4.102955	1.415742	0.338420
C17	-2.713669	-0.713899	-0.035577
O18	-3.824934	-1.133127	-0.173892
N19	-1.510417	-1.532280	-0.241114
H20	-1.549635	-2.474753	-0.620167
H21	-0.602336	0.532443	1.584247
H22	2.390050	0.481773	1.677857
H23	2.968801	-1.789748	1.450888
H24	4.219956	-1.313363	0.256146
C25	3.657566	-0.997704	1.136652
N26	3.047149	0.293363	0.912347
H27	4.379102	-0.840087	1.952952

Zero-point correction= 0.215826
Thermal correction to Energy= 0.230347
Thermal correction to Enthalpy= 0.231291
Thermal correction to Gibbs Free Energy= 0.173411
Sum of electronic and zero-point Energies= -752.180623
Sum of electronic and thermal Energies= -752.166103
Sum of electronic and thermal Enthalpies= -752.165159
Sum of electronic and thermal Free Energies= -752.223039

11 N1-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$

N1	-2.152740	0.589905	0.158636
C2	-0.340007	-0.831512	0.395112
C3	0.772350	-1.048604	-0.596237
O4	0.925710	-1.835882	-1.466224
N5	1.841941	0.027436	-0.381549
H6	2.484971	-0.060253	-1.184517
C7	1.254365	1.441638	-0.383919
N8	2.221099	2.380928	-0.079331
H9	2.848536	2.642291	-0.833361
H10	1.834830	3.203311	0.370332
N11	-0.034368	1.611248	-0.100620
C12	-0.805430	0.598391	0.157249
C13	-3.008964	1.745093	-0.060302
H14	-2.813079	2.496981	0.705204
H15	-2.822943	2.169440	-1.049339
H16	-4.040041	1.399802	0.011031

C17	-2.650593	-0.741816	0.195545
O18	-3.808395	-1.051490	0.204168
N19	-1.541663	-1.573600	0.192365
H20	-1.654033	-2.532809	0.485698
H21	0.090275	-0.919475	1.404023
H22	2.912856	0.630024	1.155828
H23	3.127383	-2.241601	0.432020
H24	4.310121	-0.995912	-0.069693
N25	2.519278	-0.268939	0.872392
C26	3.567973	-1.276581	0.689778
H27	4.069611	-1.381334	1.652622

Zero-point correction= 0.219377
Thermal correction to Energy= 0.233775
Thermal correction to Enthalpy= 0.234719
Thermal correction to Gibbs Free Energy= 0.177716
Sum of electronic and zero-point Energies= -752.206643
Sum of electronic and thermal Energies= -752.192246
Sum of electronic and thermal Enthalpies= -752.191301
Sum of electronic and thermal Free Energies= -752.248304

12 $TS^{via\ sync\ add\ +\ PT}$_N1-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	-2.037828	0.608611	0.146762
C2	-0.287228	-0.824098	-0.075513
C3	0.819438	-1.074824	-0.939715
O4	1.270643	-1.884734	-1.676408
N5	1.873795	0.060479	-0.345818
H6	2.791533	-0.074303	-0.782622
C7	1.354615	1.424965	-0.517132
N8	2.304469	2.392407	-0.204923
H9	3.037476	2.534539	-0.892207
H10	1.866577	3.276213	0.032340
N11	0.062684	1.639348	-0.205209
C12	-0.704037	0.591519	-0.045484
C13	-2.870477	1.797092	0.239313
H14	-2.524694	2.429093	1.058580
H15	-2.829554	2.355372	-0.697870
H16	-3.889618	1.461400	0.429750
C17	-2.570020	-0.710588	0.149135
O18	-3.722423	-0.999651	0.329887
N19	-1.498250	-1.549441	-0.086408
H20	-1.584178	-2.540332	0.078781
H21	0.742117	-0.714607	1.039107
H22	2.145483	0.551663	1.630163
H23	2.637710	-2.284420	0.860250
H24	3.928001	-1.076423	1.169480
N25	1.942319	-0.315204	1.121966
C26	2.910775	-1.387459	1.418478
H27	2.844657	-1.596159	2.487340

Zero-point correction= 0.213607
Thermal correction to Energy= 0.228163
Thermal correction to Enthalpy= 0.229107
Thermal correction to Gibbs Free Energy= 0.171854
Sum of electronic and zero-point Energies= -752.160339
Sum of electronic and thermal Energies= -752.145784
Sum of electronic and thermal Enthalpies= -752.144839
Sum of electronic and thermal Free Energies= -752.202093

13 $TS^{via\ HA_NH2\ products}$_N1-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	2.188466	0.560518	-0.206793
C2	0.362242	-0.842634	-0.310967
C3	-0.815218	-1.020327	0.610880
O4	-1.097010	-1.887984	1.367038
N5	-1.784413	0.110785	0.392716
H6	-2.531332	0.028844	1.091544
C7	-1.206817	1.407376	0.352082
N8	-2.101409	2.443993	0.281173
H9	-2.877824	2.462524	0.931485
H10	-1.659108	3.347937	0.170140
N11	0.089719	1.613691	0.056186
C12	0.847090	0.584975	-0.168986
C13	3.065416	1.715664	-0.088010
H14	2.829074	2.434308	-0.873305
H15	2.938853	2.183848	0.890636
H16	4.088148	1.357483	-0.201856
C17	2.668438	-0.782178	-0.141428
O18	3.821960	-1.104838	-0.145574
N19	1.548045	-1.592110	-0.047026
H20	1.638924	-2.572755	-0.269681
H21	-0.045915	-0.983625	-1.326168
H22	-2.741544	0.519097	-1.447492
H23	-3.546357	-2.019395	-0.184489
H24	-4.476672	-0.483281	-0.128725
N25	-2.526102	-0.399537	-1.051859
C26	-3.766704	-1.087106	-0.709333
H27	-4.242682	-1.348397	-1.660008

Zero-point correction= 0.217088
Thermal correction to Energy= 0.231458
Thermal correction to Enthalpy= 0.232403
Thermal correction to Gibbs Free Energy= 0.175535
Sum of electronic and zero-point Energies= -752.199445
Sum of electronic and thermal Energies= -752.185075
Sum of electronic and thermal Enthalpies= -752.184131
Sum of electronic and thermal Free Energies= -752.240998

14 N1-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	2.085193	0.642625	-0.195413
C2	0.489562	-0.872101	0.430009
C3	-0.903589	-1.280090	0.477147
O4	-0.197029	-1.157908	1.671229
N5	-1.907809	-0.191262	0.268817
H6	-2.665668	-0.332869	0.955041
C7	-1.360034	1.213012	0.530507
N8	-2.365707	2.149657	0.349251
H9	-3.033599	2.241335	1.108216
H10	-1.990825	3.056114	0.091917
N11	-0.095831	1.507187	0.219595
C12	0.781090	0.555369	0.147078
C13	2.803509	1.858106	-0.542714
H14	3.831626	1.576256	-0.767694
H15	2.344812	2.324236	-1.417069
H16	2.782550	2.551636	0.299383
C17	2.663667	-0.649367	-0.254972
O18	3.800912	-0.903017	-0.532136
N19	1.639441	-1.551041	0.041720
H20	1.840816	-2.523900	0.218249
H21	-1.288319	-2.251994	0.183811
H22	-2.694686	0.633981	-1.336784
H23	-3.320282	-2.228882	-0.938140
H24	-4.398481	-0.885755	-0.442529
N25	-2.425987	-0.318198	-1.088191
C26	-3.600557	-1.191888	-1.134375
H27	-3.985998	-1.143788	-2.153676

Zero-point correction= 0.219497
Thermal correction to Energy= 0.233621
Thermal correction to Enthalpy= 0.234565
Thermal correction to Gibbs Free Energy= 0.178122
Sum of electronic and zero-point Energies= -752.175983
Sum of electronic and thermal Energies= -752.161859
Sum of electronic and thermal Enthalpies= -752.160915

Sum of electronic and thermal Free Energies= -752.217358

15 $TS^{via\ HA_NH2\ products}$_N1-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	-1.968652	0.772557	0.197568
C2	-0.587383	-0.935661	-0.437480
C3	0.768100	-1.473718	-0.501226
O4	0.020982	-1.321194	-1.673971
N5	1.832257	-0.461376	-0.314563
H6	2.701221	-0.760269	-0.762186
C7	1.484761	0.863911	-0.661042
N8	2.519662	1.731037	-0.888826
H9	3.260214	1.453092	-1.520162
H10	2.221421	2.689755	-1.016234
N11	0.266558	1.371089	-0.357088
C12	-0.705421	0.528984	-0.197746
C13	-2.538853	2.072385	0.516242
H14	-3.590736	1.915882	0.753121
H15	-2.024024	2.506767	1.375424
H16	-2.444445	2.735967	-0.344560
C17	-2.691615	-0.447003	0.320999
O18	-3.836963	-0.551355	0.652868
N19	-1.793008	-1.466467	0.015901
H20	-2.108137	-2.416251	-0.114972
H21	1.081127	-2.462623	-0.184675
H22	1.602005	-0.156936	1.791042
H23	4.325179	-0.889163	0.960437
H24	3.757752	0.775307	1.335584
N25	2.261343	-0.781509	1.319615
C26	3.617555	-0.291011	1.541739
H27	3.836284	-0.475776	2.598839

Zero-point correction= 0.217165
Thermal correction to Energy= 0.231295
Thermal correction to Enthalpy= 0.232239
Thermal correction to Gibbs Free Energy= 0.175630
Sum of electronic and zero-point Energies= -752.169203
Sum of electronic and thermal Energies= -752.155073
Sum of electronic and thermal Enthalpies= -752.154129
Sum of electronic and thermal Free Energies= -752.210739

16 N1-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-2.307849	0.560792	0.134180
C2	-0.507444	-0.779885	-0.117036
C3	0.810881	-1.071453	-0.221306
O4	1.375634	-2.255902	-0.547527
N5	1.757069	0.055913	-0.249573
H6	2.295572	0.009405	-1.129957
C7	1.121723	1.428107	-0.212691
N8	2.043137	2.387229	-0.489713
H9	2.924867	2.322787	0.005611
H10	1.660726	3.321711	-0.551651
N11	-0.144121	1.627916	-0.054048
C12	-0.951216	0.569098	0.002588
C13	-3.180229	1.717665	0.245868
H14	-2.892645	2.317721	1.110721
H15	-3.120785	2.322898	-0.660961
H16	-4.196155	1.344694	0.374125
C17	-2.778555	-0.760346	0.066490
O18	-3.920664	-1.132094	0.116712
N19	-1.632605	-1.561095	-0.069048
H20	-1.698421	-2.554003	-0.232042
H21	1.455708	-2.847089	0.211045
H22	2.345710	-0.298420	1.634760
H23	3.786071	-1.808665	0.247139
H24	4.456655	-0.308825	-0.451673
C25	3.984718	-0.749742	0.430739
N26	2.806691	0.044783	0.794216
H27	4.687432	-0.647691	1.259392

Zero-point correction= 0.218565
Thermal correction to Energy= 0.233528
Thermal correction to Enthalpy= 0.234472
Thermal correction to Gibbs Free Energy= 0.176289
Sum of electronic and zero-point Energies= -752.209062
Sum of electronic and thermal Energies= -752.194100
Sum of electronic and thermal Enthalpies= -752.193156
Sum of electronic and thermal Free Energies= -752.251339

17 $TS^{via\ PT\ in\ adduct}$_N1-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	2.292286	0.613018	0.046996
C2	0.604332	-0.867605	0.043472
C3	-0.680206	-1.276614	-0.008328
O4	-1.343806	-2.331880	-0.147604
N5	-1.665420	-0.057231	0.224263
H6	-1.883415	-0.023127	1.234233
C7	-1.183594	1.313409	-0.232955
N8	-2.160142	2.282363	0.023369
H9	-2.610051	2.646454	-0.810135
H10	-1.775272	3.065199	0.545359
N11	0.116589	1.549882	-0.088668
C12	0.943408	0.529842	0.026894
C13	3.081187	1.831601	-0.012089
H14	2.934694	2.328119	-0.973336
H15	2.785687	2.502059	0.796104
H16	4.126550	1.546018	0.102611
C17	2.871722	-0.685430	0.039446
O18	4.048013	-0.933455	0.053969
N19	1.803939	-1.564652	0.006362
H20	1.925115	-2.563940	0.055922
H21	-2.527193	-1.628587	-0.456376
H22	-2.915861	-0.112214	-1.341161
H23	-4.064611	-0.886838	1.294082
H24	-4.258495	0.749001	0.563079
C25	-4.129518	-0.315121	0.367051
N26	-2.882368	-0.533910	-0.407426
H27	-4.948978	-0.706243	-0.236519

Zero-point correction= 0.216524
Thermal correction to Energy= 0.230608
Thermal correction to Enthalpy= 0.231552
Thermal correction to Gibbs Free Energy= 0.175406
Sum of electronic and zero-point Energies= -752.180833
Sum of electronic and thermal Energies= -752.166750
Sum of electronic and thermal Enthalpies= -752.165806
Sum of electronic and thermal Free Energies= -752.221952

18 $TS^{via\ HA_NH2\ products}$_N1-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-2.234190	0.542781	0.171040
C2	-0.443119	-0.761071	-0.222261
C3	0.860669	-0.969811	-0.545953
O4	1.487546	-2.115664	-0.883451
N5	1.755436	0.125497	-0.368651
H6	2.510227	0.070343	-1.059856
C7	1.150442	1.449533	-0.374155
N8	2.046028	2.435391	-0.612159
H9	2.968186	2.330650	-0.204743
H10	1.665463	3.371987	-0.587220
N11	-0.118606	1.651547	-0.153166
C12	-0.893865	0.575009	-0.044610
C13	-3.109897	1.681849	0.396088
H14	-2.797185	2.221250	1.291695
H15	-3.083343	2.350235	-0.466236
H16	-4.117831	1.290728	0.532693

C17	-2.690753	-0.789475	0.129620
O18	-3.814260	-1.177691	0.306229
N19	-1.558937	-1.564414	-0.160156
H20	-1.588930	-2.570342	-0.094977
H21	1.042509	-2.561279	-1.615542
H22	1.989023	0.085542	1.732562
H23	2.972692	-2.017123	1.142966
H24	4.213700	-1.114014	0.223339
C25	3.534144	-1.080936	1.078673
N26	2.716842	0.127903	1.014473
H27	4.147463	-0.972663	1.979013

Zero-point correction= 0.217472
Thermal correction to Energy= 0.232045
Thermal correction to Enthalpy= 0.232990
Thermal correction to Gibbs Free Energy= 0.175729
Sum of electronic and zero-point Energies= -752.209482
Sum of electronic and thermal Energies= -752.194909
Sum of electronic and thermal Enthalpies= -752.193965
Sum of electronic and thermal Free Energies= -752.251225

19 N1-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	-2.175039	0.596530	0.173723
C2	-0.408002	-0.776769	-0.290965
C3	0.886409	-1.179049	-0.548426
O4	1.405388	-2.234036	-0.838835
N5	1.845931	0.035541	-0.328747
H6	2.598096	-0.106357	-1.020192
C7	1.233278	1.377554	-0.535594
N8	2.178055	2.388497	-0.464705
H9	1.754131	3.294654	-0.304488
N10	-0.040041	1.608145	-0.203638
C11	-0.798553	0.557158	-0.086114
C12	-2.926512	1.820852	0.439905
H13	-2.534802	2.293645	1.341225
H14	-2.820430	2.498751	-0.407737
H15	-3.972978	1.554106	0.580323
C16	-2.745008	-0.623276	0.138660
O17	-3.853859	-1.026155	0.298314
N18	-1.585295	-1.617647	-0.197686
H19	-1.828096	-2.112041	-1.064749
H20	2.854859	2.429819	-1.219379
H21	-1.541854	-2.325140	0.545341
H22	2.717444	0.862665	1.241192
H23	4.310713	-0.786059	0.350245
H24	3.944296	-0.936952	2.086017
C25	3.523486	-1.017961	1.082461
N26	2.396591	-0.082285	1.030982
H27	3.174382	-2.038077	0.927302

Zero-point correction= 0.220477
Thermal correction to Energy= 0.235036
Thermal correction to Enthalpy= 0.235980
Thermal correction to Gibbs Free Energy= 0.178309
Sum of electronic and zero-point Energies= -752.183060
Sum of electronic and thermal Energies= -752.168501
Sum of electronic and thermal Enthalpies= -752.167557
Sum of electronic and thermal Free Energies= -752.225227

20 TS$^{\text{via async HA_NH2 + add}}$_N1-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	-2.194808	0.582557	0.184346
C2	-0.423388	-0.763169	-0.315161
C3	0.890201	-1.128650	-0.585641
O4	1.410656	-2.185034	-0.878896
N5	1.785293	0.067572	-0.376875
H6	2.610005	-0.061120	-0.971726
C7	1.215113	1.362983	-0.486868
N8	2.119400	2.394363	-0.537404
H9	1.689520	3.310294	-0.541216
N10	-0.062235	1.612148	-0.181632
C11	-0.821550	0.550598	-0.087862
C12	-2.952003	1.798280	0.474789
H13	-2.552475	2.263684	1.376484
H14	-2.863276	2.486940	-0.366070
H15	-3.994339	1.521191	0.625672
C16	-2.753747	-0.644216	0.144760
O17	-3.856710	-1.058047	0.310877
N18	-1.584070	-1.621906	-0.209970
H19	-1.828289	-2.118450	-1.075386
H20	2.904242	2.319494	-1.171782
H21	-1.515810	-2.330736	0.530408
H22	2.629231	0.757186	1.445019
H23	4.434919	-0.427565	0.418659
H24	4.099443	-1.036782	2.049738
C25	3.684421	-0.936030	1.041198
N26	2.426366	-0.212156	1.187521
H27	3.491367	-1.936309	0.651151

Zero-point correction= 0.218086
Thermal correction to Energy= 0.232619
Thermal correction to Enthalpy= 0.233563
Thermal correction to Gibbs Free Energy= 0.176015
Sum of electronic and zero-point Energies= -752.178592
Sum of electronic and thermal Energies= -752.164059
Sum of electronic and thermal Enthalpies= -752.163115
Sum of electronic and thermal Free Energies= -752.220663

21 N1-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-2.191304	0.559539	0.171334
C2	-0.401240	-0.758627	-0.187017
C3	0.900348	-1.131906	-0.506817
O4	1.417956	-2.174701	-0.880332
N5	1.850389	0.075544	-0.281901
C6	1.242406	1.428499	-0.322296
N7	2.158191	2.390331	-0.650399
H8	3.023403	2.377713	-0.121074
H9	1.761690	3.314942	-0.750478
N10	-0.024812	1.644404	-0.091619
C11	-0.792628	0.566013	0.003961
C12	-3.021969	1.733764	0.410845
H13	-3.503256	1.670112	1.389576
H14	-2.361005	2.599999	0.397220
H15	-3.763051	1.848130	-0.383775
C16	-2.604249	-0.707746	0.058900
O17	-3.829572	-1.164693	0.167236
N18	-1.577916	-1.524789	-0.166935
H19	-1.650830	-2.526078	-0.284413
H20	-4.489380	-0.472064	0.298166
H21	2.534757	0.014854	-1.047890
H22	2.004086	-0.121705	1.697454
H23	3.180107	-2.100657	0.836505
H24	4.337205	-0.965887	0.092635
N25	2.678188	-0.000944	0.942722
C26	3.638492	-1.112659	0.920272
H27	4.203093	-1.036832	1.851330

Zero-point correction= 0.219140
Thermal correction to Energy= 0.233895
Thermal correction to Enthalpy= 0.234839
Thermal correction to Gibbs Free Energy= 0.177166
Sum of electronic and zero-point Energies= -752.203977
Sum of electronic and thermal Energies= -752.189221
Sum of electronic and thermal Enthalpies= -752.188277

Sum of electronic and thermal Free Energies= -752.245951

22 $TS^{via\ HA_NH2\ products}$_N1-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-2.204964	0.553037	0.169095
C2	-0.413663	-0.747601	-0.186044
C3	0.903757	-1.092160	-0.529225
O4	1.403277	-2.153173	-0.877977
N5	1.800361	0.090376	-0.353440
C6	1.220329	1.410832	-0.353082
N7	2.134802	2.389721	-0.601821
H8	3.028651	2.286382	-0.134134
H9	1.759790	3.327896	-0.579458
N10	-0.046682	1.648029	-0.099832
C11	-0.811731	0.566446	-0.011782
C12	-3.043917	1.724852	0.396172
H13	-3.525215	1.666830	1.375078
H14	-2.387767	2.594669	0.375243
H15	-3.784546	1.825722	-0.400514
C16	-2.608741	-0.721788	0.076822
O17	-3.828346	-1.188131	0.199770
N18	-1.574499	-1.528484	-0.147233
H19	-1.632918	-2.532774	-0.250718
H20	-4.493982	-0.501092	0.331549
H21	2.533362	0.019264	-1.067571
H22	2.076044	-0.182918	1.713402
H23	3.232439	-2.091546	0.805788
H24	4.371983	-0.953357	0.037329
N25	2.775122	0.013502	0.993935
C26	3.706063	-1.110062	0.890395
H27	4.321143	-1.075025	1.795191

Zero-point correction= 0.217370
Thermal correction to Energy= 0.231970
Thermal correction to Enthalpy= 0.232914
Thermal correction to Gibbs Free Energy= 0.175121
Sum of electronic and zero-point Energies= -752.202218
Sum of electronic and thermal Energies= -752.187618
Sum of electronic and thermal Enthalpies= -752.186674
Sum of electronic and thermal Free Energies= -752.244467

23 N1-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	-2.153530	0.640787	0.504708
C2	-0.427322	-0.722848	-0.193389
C3	0.828559	-1.075781	-0.668222
O4	1.290468	-2.058451	-1.217432
N5	1.847208	0.064866	-0.320919
H6	2.554989	-0.015044	-1.067813
C7	1.276374	1.432613	-0.290829
N8	2.252560	2.410520	-0.308784
H9	2.852443	2.442572	-1.126256
H10	1.887216	3.327731	-0.082532
N11	0.047295	1.641581	0.082037
C12	-0.722504	0.569494	0.203506
C13	-2.678766	-0.810444	0.237800
O14	-3.824556	-1.079671	0.421399
N15	-1.605227	-1.497191	-0.181278
H16	-1.657052	-2.482022	-0.404765
H17	2.958905	0.651861	1.209640
H18	2.858342	-2.272063	0.782973
H19	4.156585	-1.231198	0.141743
C20	3.396298	-1.336448	0.928460
N21	2.461120	-0.209908	0.986848
H22	3.892846	-1.367707	1.899568
C23	-2.931123	1.651235	-0.287230
H24	-2.319611	0.820179	1.501653
H25	-2.770759	1.445495	-1.345056
H26	-3.983615	1.543772	-0.026648
H27	-2.552661	2.639881	-0.033110

Zero-point correction= 0.220265
Thermal correction to Energy= 0.234517
Thermal correction to Enthalpy= 0.235461
Thermal correction to Gibbs Free Energy= 0.179019
Sum of electronic and zero-point Energies= -752.175744
Sum of electronic and thermal Energies= -752.161492
Sum of electronic and thermal Enthalpies= -752.160548
Sum of electronic and thermal Free Energies= -752.216990

24 $TS^{via\ async\ HA_NH2\ +\ add}$_N1-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	-2.179496	0.619745	0.503378
C2	-0.451185	-0.698213	-0.231351
C3	0.836247	-1.018710	-0.691089
O4	1.292095	-2.033281	-1.186973
N5	1.773363	0.105914	-0.392006
H6	2.556502	0.027938	-1.048439
C7	1.247460	1.426347	-0.287370
N8	2.192107	2.424521	-0.301298
H9	2.894166	2.406566	-1.030366
H10	1.806309	3.347747	-0.151402
N11	0.011100	1.653760	0.100523
C12	-0.755480	0.577011	0.160955
C13	-2.682586	-0.846455	0.252509
O14	-3.817640	-1.137828	0.460168
N15	-1.600932	-1.508391	-0.188227
H16	-1.626860	-2.494993	-0.409610
H17	2.916457	0.598712	1.337751
H18	3.203948	-2.203627	0.497183
H19	4.358956	-0.884990	0.130069
C20	3.605660	-1.250787	0.842289
N21	2.518086	-0.317488	1.112994
H22	4.104037	-1.415734	1.804109
C23	-2.995273	1.615692	-0.268220
H24	-2.312299	0.800087	1.505233
H25	-2.858302	1.412288	-1.329813
H26	-4.038520	1.488012	0.018829
H27	-2.628690	2.611131	-0.022989

Zero-point correction= 0.218010
Thermal correction to Energy= 0.232206
Thermal correction to Enthalpy= 0.233150
Thermal correction to Gibbs Free Energy= 0.176687
Sum of electronic and zero-point Energies= -752.170040
Sum of electronic and thermal Energies= -752.155843
Sum of electronic and thermal Enthalpies= -752.154899
Sum of electronic and thermal Free Energies= -752.211362

25 C2-NHCH$_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	1.818303	-0.858240	-0.110583
C2	0.522198	0.987279	-0.167826
C3	-0.647770	1.772041	-0.304464
O4	-0.801126	2.963608	-0.188448
N5	-1.810318	0.897012	-0.674409
H6	-1.933385	0.910809	-1.692628
C7	-1.821368	-0.732833	-0.300939
N8	-2.609562	-1.295260	-1.313096
H9	-2.183871	-2.088403	-1.772669
N10	-0.497229	-1.251269	-0.358432
C11	0.510881	-0.467361	-0.229087
C12	2.289595	-2.235997	-0.097712
H13	1.801162	-2.784946	0.709038
H14	2.070512	-2.712580	-1.054228
H15	3.366499	-2.212671	0.066047
C16	2.655537	0.245642	0.060125

O17	3.843059	0.268830	0.206557
N18	1.794238	1.375979	0.029218
H19	2.137724	2.325843	0.101282
H20	-2.661969	1.298093	-0.267551
H21	-3.586513	-1.424839	-1.084398
H22	-2.829641	-1.683925	1.137900
C23	-1.744376	-0.236628	2.132438
H24	-0.759241	-0.696953	2.278511
H25	-1.627327	0.849452	2.063388
H26	-2.351273	-0.430843	3.016643
N27	-2.462051	-0.754136	0.969958

Zero-point correction= 0.219609
Thermal correction to Energy= 0.234260
Thermal correction to Enthalpy= 0.235205
Thermal correction to Gibbs Free Energy= 0.177972
Sum of electronic and zero-point Energies= -752.277982
Sum of electronic and thermal Energies= -752.263330
Sum of electronic and thermal Enthalpies= -752.262386
Sum of electronic and thermal Free Energies= -752.319619

26 $TS^{via\ PT\ in\ adduct}$_C2-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$

N1	1.893229	-0.992348	0.020605
C2	0.808970	0.980023	0.013105
C3	-0.293343	1.880871	-0.031543
O4	-0.272472	3.088958	-0.043477
N5	-1.565667	1.159919	-0.036756
H6	-2.227236	1.697080	-0.602412
C7	-1.663317	-0.374313	-0.322784
N8	-2.252898	-0.605299	-1.573546
H9	-1.992911	-1.500596	-1.966729
N10	-0.459135	-1.113131	-0.200557
C11	0.641888	-0.454732	-0.067384
C12	2.216288	-2.410677	-0.030032
H13	1.740470	-2.928650	0.804191
H14	1.872254	-2.836175	-0.974050
H15	3.299035	-2.504422	0.047108
C16	2.857572	0.018361	0.129725
O17	4.046004	-0.097697	0.217339
N18	2.127293	1.231856	0.116426
H19	2.568537	2.140220	0.187966
H20	-2.103363	0.726425	0.997953
H21	-3.244023	-0.421554	-1.660736
H22	-2.011025	-1.297728	1.516271
H23	-4.328784	-1.043288	1.806224
H24	-4.437889	-0.077776	0.335577
C25	-3.912759	-0.912340	0.807240
N26	-2.483279	-0.598198	0.945137
H27	-4.071925	-1.826366	0.228627

Zero-point correction= 0.215805
Thermal correction to Energy= 0.229858
Thermal correction to Enthalpy= 0.230802
Thermal correction to Gibbs Free Energy= 0.174497
Sum of electronic and zero-point Energies= -752.252183
Sum of electronic and thermal Energies= -752.238131
Sum of electronic and thermal Enthalpies= -752.237186
Sum of electronic and thermal Free Energies= -752.293491

27 $TS^{via\ HA_NH2\ products}$_C2-$NHCH_3$[9MOG + H_{N1}]$^{+}$

N1	1.772451	-0.819335	-0.164195
C2	0.474261	0.980134	-0.291684
C3	-0.699501	1.723710	-0.378176
O4	-1.004911	2.876879	-0.261378
N5	-1.896904	0.747132	-0.767001
H6	-2.105207	0.927763	-1.756340
C7	-1.733734	-0.733485	-0.591960
N8	-2.763150	-1.425730	-1.150990
H9	-2.580751	-2.410807	-1.293980
N10	-0.538333	-1.264483	-0.531187
C11	0.499987	-0.416253	-0.356596
C12	2.274107	-2.185461	-0.165574
H13	1.786213	-2.766023	0.618761
H14	2.096362	-2.650243	-1.136329
H15	3.345437	-2.128392	0.026553
C16	2.617650	0.309167	0.038285
O17	3.805767	0.281453	0.225210
N18	1.766398	1.397674	-0.021043
H19	2.095635	2.350303	0.026836
H20	-2.697756	1.069017	-0.213734
H21	-3.707334	-1.205894	-0.861892
H22	-2.391972	-1.654418	1.582708
C23	-1.361704	-0.120164	2.401507
H24	-0.372319	-0.602599	2.388368
H25	-1.244400	0.958558	2.288083
H26	-1.787746	-0.324406	3.393243
N27	-2.236091	-0.660315	1.390453

Zero-point correction= 0.215909
Thermal correction to Energy= 0.230633
Thermal correction to Enthalpy= 0.231577
Thermal correction to Gibbs Free Energy= 0.174154
Sum of electronic and zero-point Energies= -752.216383
Sum of electronic and thermal Energies= -752.201659
Sum of electronic and thermal Enthalpies= -752.200715
Sum of electronic and thermal Free Energies= -752.258137

28 C2-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$

N1	1.861219	-0.879832	-0.020121
C2	0.618596	0.986162	-0.107592
C3	-0.590884	1.766593	-0.207771
O4	-0.671685	2.974563	-0.136873
N5	-1.711324	0.946134	-0.402734
H6	-2.592738	1.423721	-0.246846
C7	-1.735472	-0.484169	-0.302422
N8	-2.385606	-0.994936	-1.643884
H9	-1.903261	-0.575519	-2.441692
H10	-2.283495	-2.011736	-1.703027
N11	-0.489697	-1.177644	-0.269986
C12	0.574557	-0.444092	-0.142681
C13	2.303179	-2.264784	0.013784
H14	1.796728	-2.794765	0.822255
H15	2.089419	-2.751592	-0.939310
H16	3.378580	-2.261112	0.190180
C17	2.733202	0.214861	0.104329
O18	3.925259	0.194370	0.234654
N19	1.905561	1.356929	0.044121
H20	2.261735	2.302080	0.106182
H21	-3.379114	-0.748945	-1.667086
H22	-2.678792	-1.919566	0.730516
H23	-1.396507	-0.605591	2.384935
H24	-3.123576	-0.857738	2.723584
C25	-2.415429	-0.387239	2.041755
N26	-2.685640	-0.902685	0.690186
H27	-2.585645	0.689535	2.078571

Zero-point correction= 0.221579
Thermal correction to Energy= 0.236006
Thermal correction to Enthalpy= 0.236950
Thermal correction to Gibbs Free Energy= 0.179737
Sum of electronic and zero-point Energies= -752.295093
Sum of electronic and thermal Energies= -752.280665
Sum of electronic and thermal Enthalpies= -752.279721

Sum of electronic and thermal Free Energies= -752.336935

29 TS$^{via\ PT\ in\ adduct}$_C2-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	1.932425	-0.886546	0.030977
C2	0.688785	0.977008	-0.084551
C3	-0.516740	1.753712	-0.245059
O4	-0.601321	2.963442	-0.230172
N5	-1.626487	0.924202	-0.445529
H6	-2.502314	1.427550	-0.521646
C7	-1.640335	-0.501072	-0.377425
N8	-2.465924	-1.073269	-1.518022
H9	-2.685906	-0.411332	-2.261139
H10	-2.015636	-1.899216	-1.914407
N11	-0.410192	-1.189448	-0.271706
C12	0.649456	-0.452784	-0.121814
C13	2.378377	-2.270599	0.061510
H14	1.887702	-2.801082	0.879353
H15	2.149499	-2.758455	-0.887361
H16	3.456389	-2.263356	0.220889
C17	2.800124	0.210452	0.168577
O18	3.989336	0.192496	0.321766
N19	1.971392	1.350935	0.091750
H20	2.326035	2.297010	0.148524
H21	-3.214193	-1.298305	-0.511492
H22	-2.212083	-1.878985	1.048294
H23	-2.198541	0.284547	2.292181
H24	-3.645385	-0.741490	2.464633
C25	-3.056964	-0.144312	1.768118
N26	-2.626275	-1.025250	0.670463
H27	-3.690473	0.656811	1.387752

Zero-point correction= 0.216393
Thermal correction to Energy= 0.230465
Thermal correction to Enthalpy= 0.231409
Thermal correction to Gibbs Free Energy= 0.174565
Sum of electronic and zero-point Energies= -752.266224
Sum of electronic and thermal Energies= -752.252151
Sum of electronic and thermal Enthalpies= -752.251207
Sum of electronic and thermal Free Energies= -752.308052

30 TS$^{via\ async\ HA_NH2\ +\ add}$_C2-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	1.872245	-0.858884	-0.058315
C2	0.578554	0.950061	-0.229490
C3	-0.629111	1.697949	-0.437429
O4	-0.801617	2.895378	-0.390143
N5	-1.703695	0.808013	-0.735711
H6	-2.610243	1.263688	-0.755398
C7	-1.601346	-0.551399	-0.620410
N8	-2.723232	-1.309527	-1.216078
H9	-2.996048	-0.972520	-2.145110
H10	-2.417202	-2.285706	-1.295335
N11	-0.472839	-1.215505	-0.546369
C12	0.595833	-0.439494	-0.288754
C13	2.362495	-2.226436	-0.037192
H14	1.861881	-2.796588	0.747700
H15	2.199612	-2.702645	-1.005732
H16	3.431474	-2.179055	0.170962
C17	2.701525	0.260171	0.153849
O18	3.883314	0.258232	0.382971
N19	1.846982	1.363792	0.043293
H20	2.166465	2.318722	0.124940
H21	-3.496293	-1.266696	-0.528430
H22	-2.074359	-1.788340	1.600675
H23	-1.036373	0.256737	2.227394
H24	-2.442183	-0.129278	3.213863
C25	-2.132186	0.126969	2.191847
N26	-2.519580	-0.920897	1.283338
H27	-2.594068	1.076920	1.916222

Zero-point correction= 0.216833
Thermal correction to Energy= 0.231499
Thermal correction to Enthalpy= 0.232443
Thermal correction to Gibbs Free Energy= 0.175083
Sum of electronic and zero-point Energies= -752.234254
Sum of electronic and thermal Energies= -752.219588
Sum of electronic and thermal Enthalpies= -752.218643
Sum of electronic and thermal Free Energies= -752.276004

31 C2-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	1.775857	-0.907722	-0.244438
C2	0.621881	0.985221	0.089925
C3	-0.499616	1.919313	-0.080137
O4	-0.394523	3.117035	0.074699
N5	-1.615413	1.258163	-0.547970
H6	-2.428431	1.835178	-0.727385
C7	-1.858442	-0.169709	-0.319466
N8	-2.872248	-0.709569	-1.160447
H9	-2.815906	-0.409975	-2.127038
H10	-3.806475	-0.593282	-0.789681
N11	-0.604366	-0.901273	-0.692773
C12	0.545297	-0.375205	-0.308993
C13	2.174310	-2.275951	-0.550364
H14	3.237815	-2.362878	-0.328213
H15	1.616393	-2.975138	0.076370
H16	2.010183	-2.487492	-1.608906
C17	2.689171	0.085716	0.213933
O18	3.863324	-0.053077	0.395256
N19	1.906259	1.235045	0.401580
H20	2.286751	2.131157	0.683698
H21	-0.707473	-1.862946	-0.991390
H22	-2.682242	0.353120	1.459317
H23	-1.620972	-2.404872	1.333429
H24	-2.539549	-1.664369	2.638516
C25	-2.432283	-1.705686	1.554175
N26	-2.073668	-0.367444	1.087785
H27	-3.357356	-2.102769	1.121052

Zero-point correction= 0.220634
Thermal correction to Energy= 0.234742
Thermal correction to Enthalpy= 0.235686
Thermal correction to Gibbs Free Energy= 0.179992
Sum of electronic and zero-point Energies= -752.302707
Sum of electronic and thermal Energies= -752.288598
Sum of electronic and thermal Enthalpies= -752.287654
Sum of electronic and thermal Free Energies= -752.343349

32 TS$^{via\ PT\ in\ adduct}$_C2-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	-1.804001	-1.065589	0.014082
C2	-0.866426	0.971400	0.055788
C3	0.213061	1.940326	-0.106025
O4	0.041168	3.135501	-0.219763
N5	1.452595	1.320884	-0.180844
H6	2.227932	1.974938	-0.183541
C7	1.746291	-0.041201	0.252870
N8	2.397364	-0.182117	1.507542
H9	1.745628	-0.149719	2.282129
H10	3.151985	0.478685	1.657108
N11	0.586619	-0.947045	0.202992
C12	-0.617005	-0.428330	0.101429
C13	-2.033276	-2.504369	0.041382
H14	-3.105422	-2.663456	0.153000
H15	-1.692841	-2.959468	-0.890283
H16	-1.502536	-2.940387	0.889350

C17	-2.846320	-0.109974	-0.063264
O18	-4.021968	-0.324095	-0.136035
N19	-2.198970	1.140730	-0.031133
H20	-2.688006	2.023780	-0.117812
H21	1.371440	-1.551161	-0.569559
H22	2.392575	-0.310387	-1.705448
H23	3.918457	-1.834404	0.321003
H24	4.158769	-1.876992	-1.441839
C25	3.875540	-1.250410	-0.595893
N26	2.490525	-0.801300	-0.817643
H27	4.568300	-0.406263	-0.530427

Zero-point correction= 0.215721
Thermal correction to Energy= 0.229968
Thermal correction to Enthalpy= 0.230913
Thermal correction to Gibbs Free Energy= 0.174142
Sum of electronic and zero-point Energies= -752.261298
Sum of electronic and thermal Energies= -752.247050
Sum of electronic and thermal Enthalpies= -752.246106
Sum of electronic and thermal Free Energies= -752.302877

33 $TS^{via\ HA_NH2\ products}$_C2-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$

N1	1.744309	-0.719620	-0.379356
C2	0.407227	1.017304	0.027318
C3	-0.773121	1.830270	-0.110867
O4	-0.895526	3.009784	0.131270
N5	-1.848029	1.060743	-0.628397
H6	-2.728166	1.555895	-0.703717
C7	-1.842204	-0.315721	-0.600526
N8	-2.970360	-0.962088	-1.003875
H9	-3.000274	-1.967860	-0.924719
H10	-3.859391	-0.510132	-0.849098
N11	-0.633563	-0.914015	-0.928784
C12	0.472910	-0.270929	-0.454863
C13	2.274543	-2.010930	-0.778345
H14	3.342077	-1.996325	-0.554540
H15	1.804894	-2.816905	-0.207628
H16	2.139853	-2.169815	-1.851098
C17	2.560243	0.315473	0.170828
O18	3.743447	0.237762	0.379475
N19	1.687386	1.362836	0.401752
H20	1.980896	2.258553	0.763201
H21	-0.601333	-1.864153	-1.267497
H22	-2.239066	0.087622	1.926661
H23	-0.771709	-2.408831	1.349962
H24	-0.928332	-1.649348	2.953252
C25	-1.416403	-1.787187	1.979668
N26	-1.646013	-0.520075	1.354141
H27	-2.358090	-2.323220	2.171609

Zero-point correction= 0.215098
Thermal correction to Energy= 0.230196
Thermal correction to Enthalpy= 0.231140
Thermal correction to Gibbs Free Energy= 0.173317
Sum of electronic and zero-point Energies= -752.250068
Sum of electronic and thermal Energies= -752.234970
Sum of electronic and thermal Enthalpies= -752.234026
Sum of electronic and thermal Free Energies= -752.291850

34 C2-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.801548	-0.973893	-0.324947
C2	-0.689473	1.013480	-0.173265
C3	0.456482	1.977689	-0.323989
O4	0.289977	3.173096	-0.361615
N5	1.593053	1.252388	-0.500526
H6	2.471623	1.754041	-0.580727
C7	1.677679	-0.111403	0.056618
N8	1.311564	-0.034445	1.453931
H9	1.921445	0.602905	1.960876
H10	1.324555	-0.943754	1.905592
N11	0.633976	-1.017647	-0.474297
C12	-0.594173	-0.340328	-0.800597
C13	-2.205912	-2.324548	-0.696268
H14	-2.406296	-2.381523	-1.769112
H15	-1.415835	-3.025680	-0.425130
H16	-3.115064	-2.564620	-0.145441
C17	-2.597889	-0.122824	0.366088
O18	-3.671570	-0.236654	0.870776
N19	-1.812953	1.148834	0.417620
H20	-2.133229	1.972451	0.925927
H21	-0.619157	-0.213427	-1.900572
H22	3.128794	-0.626409	-1.242483
H23	2.705043	-2.633626	0.300310
H24	4.372483	-2.109998	-0.016834
N25	2.993427	-0.573483	-0.237270
C26	3.420082	-1.809898	0.419808
H27	3.594965	-1.627179	1.482357

Zero-point correction= 0.219133
Thermal correction to Energy= 0.233274
Thermal correction to Enthalpy= 0.234218
Thermal correction to Gibbs Free Energy= 0.177811
Sum of electronic and zero-point Energies= -752.215221
Sum of electronic and thermal Energies= -752.201080
Sum of electronic and thermal Enthalpies= -752.200136
Sum of electronic and thermal Free Energies= -752.256543

35 $TS^{via\ PT\ in\ adduct}$_C2-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	1.707189	-0.936589	-0.206485
C2	0.639696	1.026661	0.110145
C3	-0.498824	1.998628	0.077366
O4	-0.338458	3.182804	0.259100
N5	-1.667019	1.355257	-0.210763
H6	-2.513114	1.915022	-0.238808
C7	-1.838387	-0.099769	-0.345527
N8	-3.050313	-0.304877	-1.052332
H9	-3.282123	-1.288924	-1.130569
H10	-2.995000	0.079327	-1.991206
N11	-0.641076	-0.707827	-0.961142
C12	0.410499	-0.381494	-0.094020
C13	1.999816	-2.344841	-0.435704
H14	1.709834	-2.941794	0.432672
H15	1.467100	-2.684976	-1.324511
H16	3.073720	-2.440707	-0.594242
C17	2.669715	-0.000985	0.056300
O18	3.859201	-0.078700	0.136984
N19	1.908582	1.244971	0.249648
H20	2.348780	2.143570	0.437021
H21	-0.296520	-0.589003	0.956811
H22	-2.431463	-0.096998	1.633140
H23	-1.605326	-2.701076	0.497075
H24	-2.069486	-2.401610	2.185270
N25	-1.853430	-0.677729	1.029733
C26	-2.234692	-2.094254	1.152195
H27	-3.286826	-2.261787	0.903539

Zero-point correction= 0.215209
Thermal correction to Energy= 0.228758
Thermal correction to Enthalpy= 0.229702
Thermal correction to Gibbs Free Energy= 0.175197
Sum of electronic and zero-point Energies= -752.203850
Sum of electronic and thermal Energies= -752.190301
Sum of electronic and thermal Enthalpies= -752.189357

Sum of electronic and thermal Free Energies= -752.243862

36 $TS^{via\ HA_NH2\ products}$_C2-NHCH$_3$[9MOG + H$_{C4}$]$^{\bullet+}$

N1	-1.732820	-1.100512	-0.194078
C2	-0.830013	0.982321	-0.274273
C3	0.241712	2.031776	-0.303870
O4	0.001568	3.188424	-0.559877
N5	1.448117	1.456472	-0.058635
H6	2.256318	2.068035	-0.064612
C7	1.571546	0.140280	0.524919
N8	2.312572	0.127136	1.684690
H9	3.239893	0.527893	1.649926
H10	2.251722	-0.737638	2.204694
N11	0.569993	-0.735538	0.449809
C12	-0.480046	-0.446476	-0.495082
C13	-1.903823	-2.545770	-0.216567
H14	-1.767862	-2.927419	-1.231354
H15	-1.179901	-3.003995	0.459948
H16	-2.915483	-2.771083	0.120190
C17	-2.714753	-0.238811	0.151251
O18	-3.855852	-0.374626	0.469671
N19	-2.050905	1.102819	0.083560
H20	-2.513255	1.961658	0.380598
H21	-0.198994	-0.637464	-1.544615
H22	2.270148	-0.670242	-1.704992
H23	2.725515	-2.712326	-0.525235
H24	4.195840	-2.003498	-1.208475
N25	2.732127	-0.606057	-0.793849
C26	3.394233	-1.844966	-0.475221
H27	3.843594	-1.784654	0.518161

Zero-point correction= 0.215134
Thermal correction to Energy= 0.229798
Thermal correction to Enthalpy= 0.230743
Thermal correction to Gibbs Free Energy= 0.172786
Sum of electronic and zero-point Energies= -752.191981
Sum of electronic and thermal Energies= -752.177316
Sum of electronic and thermal Enthalpies= -752.176372
Sum of electronic and thermal Free Energies= -752.234328

37 C2-$^{+}$ṄCH$_3$[9MOG + H$_{C5}$]

N1	1.654337	-1.011721	-0.151906
C2	0.595265	0.868918	0.659361
C3	-0.260478	1.893544	-0.072188
O4	0.066588	3.027654	-0.301463
N5	-1.499123	1.366227	-0.420779
H6	-2.019488	1.935149	-1.079302
C7	-1.775243	-0.051482	-0.391917
N8	-2.717829	-0.383499	-1.410110
H9	-3.589227	0.125658	-1.491783
H10	-2.723866	-1.354111	-1.699679
N11	-0.669597	-0.938310	-0.501193
C12	0.439418	-0.463138	-0.040422
C13	1.962428	-2.268869	-0.813628
H14	1.439785	-3.087066	-0.316193
H15	1.662717	-2.223510	-1.863035
H16	3.039622	-2.416570	-0.739831
C17	2.672504	-0.073782	0.233949
O18	3.851176	-0.287719	0.177480
N19	2.009110	1.056639	0.634245
H20	2.494431	1.856149	1.010437
H21	0.196458	0.779114	1.683456
H22	-3.155885	0.413178	1.169533
H23	-1.973967	-2.327745	1.014292
H24	-2.436630	-1.523882	2.544559
C25	-2.670754	-1.632017	1.479111
N26	-2.541813	-0.337770	0.854704
H27	-3.700484	-1.995846	1.399100

Zero-point correction= 0.217269
Thermal correction to Energy= 0.232045
Thermal correction to Enthalpy= 0.232990
Thermal correction to Gibbs Free Energy= 0.175073
Sum of electronic and zero-point Energies= -752.264047
Sum of electronic and thermal Energies= -752.249270
Sum of electronic and thermal Enthalpies= -752.248326
Sum of electronic and thermal Free Energies= -752.306243

38 $TS^{via\ PT\ in\ adduct}$_C2-$^{+}$ṄCH$_3$[9MOG + H$_{C5}$]

N1	1.713851	-0.821660	-0.385552
C2	0.342777	0.813292	0.484432
C3	-0.554323	1.844881	-0.223621
O4	-0.252766	2.993501	-0.406194
N5	-1.701556	1.200635	-0.608623
H6	-2.265265	1.612508	-1.343510
C7	-1.808385	-0.241892	-0.398075
N8	-2.941865	-0.735504	-1.056031
H9	-3.847144	-0.461649	-0.700181
H10	-2.873552	-1.702456	-1.340651
N11	-0.636006	-0.998587	-0.806116
C12	0.415545	-0.442895	-0.332072
C13	2.236176	-1.996671	-1.072431
H14	1.766696	-2.896644	-0.672466
H15	2.034757	-1.917028	-2.141603
H16	3.311219	-2.028339	-0.898027
C17	2.523352	0.094409	0.311954
O18	3.711236	0.066078	0.441249
N19	1.643039	1.071101	0.833216
H20	1.993705	1.944260	1.208026
H21	-0.477677	0.420728	1.314856
H22	-2.577901	0.304453	1.504902
H23	-1.029903	-2.227610	1.441282
H24	-1.877612	-1.520370	2.850387
C25	-1.895523	-1.649809	1.767987
N26	-1.874315	-0.335941	1.134556
H27	-2.804822	-2.192680	1.487363

Zero-point correction= 0.214430
Thermal correction to Energy= 0.228152
Thermal correction to Enthalpy= 0.229097
Thermal correction to Gibbs Free Energy= 0.174416
Sum of electronic and zero-point Energies= -752.243571
Sum of electronic and thermal Energies= -752.229849
Sum of electronic and thermal Enthalpies= -752.228904
Sum of electronic and thermal Free Energies= -752.283585

39 $TS^{via\ HA_NH2\ products}$_C2-$^{+}$ṄCH$_3$[9MOG + H$_{C5}$]

N1	1.667678	-0.966050	-0.214509
C2	0.522483	0.848857	0.618537
C3	-0.332422	1.887103	-0.096173
O4	-0.061863	3.052715	-0.203682
N5	-1.508532	1.321644	-0.576629
H6	-2.099460	1.932706	-1.127495
C7	-1.723456	-0.070787	-0.609593
N8	-2.775782	-0.465697	-1.377158
H9	-3.585777	0.112246	-1.536262
H10	-2.774955	-1.414724	-1.720408
N11	-0.643212	-0.937875	-0.661616
C12	0.440468	-0.453326	-0.137921
C13	2.042498	-2.192694	-0.901379
H14	1.501263	-3.035794	-0.470633
H15	1.811911	-2.109785	-1.965421
H16	3.114870	-2.326126	-0.761320

C17	2.642680	-0.024680	0.275273
O18	3.825795	-0.214943	0.281131
N19	1.929421	1.072866	0.681716
H20	2.371551	1.857169	1.135719
H21	0.065093	0.701683	1.612535
H22	-3.177820	0.255832	1.367603
H23	-1.728069	-2.324140	1.232321
H24	-2.342257	-1.585991	2.746923
C25	-2.498600	-1.682660	1.662799
N26	-2.432329	-0.382189	1.072107
H27	-3.490420	-2.135027	1.530195

Zero-point correction= 0.214968
Thermal correction to Energy= 0.229876
Thermal correction to Enthalpy= 0.230820
Thermal correction to Gibbs Free Energy= 0.172754
Sum of electronic and zero-point Energies= -752.258737
Sum of electronic and thermal Energies= -752.243829
Sum of electronic and thermal Enthalpies= -752.242885
Sum of electronic and thermal Free Energies= -752.300951

40 C2-$^{+}$ṄHCH$_3$[9MOG + H$_{C6}$]

N1	-1.639844	1.013096	-0.135358
C2	-0.856264	-1.126807	0.088936
C3	0.232383	-1.972291	0.555352
O4	-0.281555	-2.076297	-0.791462
N5	1.499671	-1.356124	0.710527
H6	2.261137	-2.027467	0.685961
C7	1.761990	-0.170877	-0.083124
N8	2.393071	-0.461933	-1.335361
H9	2.356900	-1.421615	-1.655716
H10	2.232366	0.223024	-2.064412
N11	0.703284	0.772478	-0.193039
C12	-0.493603	0.310246	-0.114907
C13	-1.760216	2.453043	-0.283078
H14	-2.822079	2.696364	-0.257086
H15	-1.243406	2.957580	0.536262
H16	-1.331756	2.763855	-1.237341
C17	-2.753245	0.164349	0.138075
O18	-3.897661	0.516986	0.185279
N19	-2.230897	-1.097950	0.364817
H20	-2.830382	-1.908650	0.400741
H21	0.069255	-2.835916	1.191191
H22	3.554060	-0.070176	1.088162
H23	3.297307	2.361010	1.469948
H24	2.416982	2.423885	-0.082981
C25	3.209937	1.923050	0.468416
N26	2.881533	0.530730	0.615165
H27	4.179725	2.026251	-0.030537

Zero-point correction= 0.217477
Thermal correction to Energy= 0.231967
Thermal correction to Enthalpy= 0.232911
Thermal correction to Gibbs Free Energy= 0.175938
Sum of electronic and zero-point Energies= -752.217069
Sum of electronic and thermal Energies= -752.202578
Sum of electronic and thermal Enthalpies= -752.201634
Sum of electronic and thermal Free Energies= -752.258607

41 TS$^{via\ HA_NH2\ products}$_C2-$^{+}$ṄHCH$_3$[9MOG + H$_{C6}$]

N1	1.583174	0.948431	0.324668
C2	0.846958	-1.161295	-0.159848
C3	-0.265523	-2.028294	-0.519091
O4	0.506675	-2.243722	0.675890
N5	-1.574023	-1.506631	-0.336190
H6	-2.264964	-2.218861	-0.134473
C7	-1.767738	-0.296602	0.356226
N8	-2.713681	-0.317561	1.338166
H9	-3.547326	-0.877629	1.243875
H10	-2.781934	0.504098	1.920191
N11	-0.723528	0.585817	0.626966
C12	0.467329	0.205387	0.316542
C13	1.690489	2.340007	0.729993
H14	2.731052	2.636680	0.601438
H15	1.046384	2.962826	0.105538
H16	1.400909	2.442387	1.776749
C17	2.667799	0.223758	-0.261299
O18	3.782875	0.639945	-0.392426
N19	2.146006	-0.994463	-0.669985
H20	2.768030	-1.762124	-0.879123
H21	-0.187381	-2.806835	-1.270310
H22	-2.894756	0.229981	-1.850157
H23	-2.332584	2.608017	-1.799190
H24	-2.409154	2.513888	-0.014730
C25	-2.810338	2.107438	-0.944863
N26	-2.565257	0.705044	-1.004579
H27	-3.887369	2.310927	-1.026802

Zero-point correction= 0.214990
Thermal correction to Energy= 0.229616
Thermal correction to Enthalpy= 0.230560
Thermal correction to Gibbs Free Energy= 0.172691
Sum of electronic and zero-point Energies= -752.207739
Sum of electronic and thermal Energies= -752.193113
Sum of electronic and thermal Enthalpies= -752.192169
Sum of electronic and thermal Free Energies= -752.250038

42 C2-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	1.727153	-1.109765	-0.012834
C2	0.848866	0.974624	-0.001655
C3	-0.220257	1.890190	0.076551
O4	-0.136161	3.201955	0.202466
N5	-1.425677	1.370740	0.025979
H6	-2.222948	1.993373	0.123355
C7	-1.797855	-0.112477	-0.243351
N8	-2.381593	-0.264873	-1.515320
H9	-3.245899	0.241663	-1.652741
H10	-1.751198	-0.232916	-2.303019
N11	-0.633328	-0.969354	-0.171332
C12	0.524336	-0.440239	-0.071289
C13	1.881438	-2.557440	-0.064222
H14	1.409451	-3.011145	0.808442
H15	1.419438	-2.943836	-0.973777
H16	2.948950	-2.774878	-0.064806
C17	2.787042	-0.222752	0.065955
O18	3.964276	-0.437690	0.114502
N19	2.192207	1.080150	0.078633
H20	2.779868	1.901881	0.107457
H21	0.762345	3.537429	0.302481
H22	-2.369374	-0.192043	1.685488
H23	-2.712946	-2.502940	0.816899
H24	-4.127768	-1.717967	1.571952
N25	-2.779257	-0.357834	0.771682
C26	-3.427359	-1.676803	0.737075
H27	-3.988647	-1.786804	-0.189519

Zero-point correction= 0.218974
Thermal correction to Energy= 0.233893
Thermal correction to Enthalpy= 0.234837
Thermal correction to Gibbs Free Energy= 0.176823
Sum of electronic and zero-point Energies= -752.278432
Sum of electronic and thermal Energies= -752.263513
Sum of electronic and thermal Enthalpies= -752.262569

Sum of electronic and thermal Free Energies= -752.320583

43 $TS^{via\ PT\ in\ adduct}$_C2-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$

N1	-2.043350	0.789435	0.002513
C2	-0.686849	-0.969778	-0.446473
C3	0.629757	-1.460619	-0.565559
O4	1.172927	-2.299519	0.252487
N5	1.441675	-0.578546	-1.238272
H6	2.363488	-0.993897	-1.369468
C7	1.574288	0.653414	-0.330245
N8	2.454634	1.621797	-0.838663
H9	3.316150	1.272633	-1.238651
H10	1.988021	2.261087	-1.469419
N11	0.282327	1.261626	-0.127069
C12	-0.733968	0.488646	-0.259153
C13	-2.551704	2.113387	0.341745
H14	-2.079416	2.471769	1.258382
H15	-2.340305	2.803479	-0.475277
H16	-3.627817	2.024537	0.485813
C17	-2.798992	-0.376753	0.130059
O18	-3.958084	-0.495780	0.396560
N19	-1.885674	-1.453071	-0.101596
H20	-2.184493	-2.420216	-0.090041
H21	1.752272	-1.482970	0.781179
H22	1.537261	0.420917	1.724002
H23	3.799603	1.235995	1.264376
H24	3.718998	-0.281467	2.205678
N25	2.072998	0.016518	0.956884
C26	3.513442	0.183306	1.241043
H27	4.103377	-0.343392	0.485977

Zero-point correction= 0.216451
Thermal correction to Energy= 0.229648
Thermal correction to Enthalpy= 0.230592
Thermal correction to Gibbs Free Energy= 0.176942
Sum of electronic and zero-point Energies= -752.222681
Sum of electronic and thermal Energies= -752.209484
Sum of electronic and thermal Enthalpies= -752.208540
Sum of electronic and thermal Free Energies= -752.262190

44 $TS^{via\ HA_NH2\ products}$_C2-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.699708	-0.976184	0.258902
C2	-0.700593	0.985490	-0.150799
C3	0.341172	1.845644	0.035852
O4	0.377875	3.162316	-0.117610
N5	1.529582	1.316712	0.451689
H6	2.314138	1.952544	0.510420
C7	1.742505	-0.074917	0.526153
N8	2.850381	-0.469456	1.240110
H9	3.518357	0.221159	1.543167
H10	2.690155	-1.231756	1.881456
N11	0.643138	-0.899973	0.655714
C12	-0.498604	-0.357766	0.276602
C13	-1.967401	-2.358586	0.623015
H14	-1.347565	-3.026432	0.022797
H15	-1.757593	-2.514492	1.682330
H16	-3.021745	-2.546718	0.421696
C17	-2.705284	-0.086234	-0.196730
O18	-3.860741	-0.356382	-0.387762
N19	-2.069569	1.138266	-0.382724
H20	-2.510258	1.829117	-0.971241
H21	-0.500402	3.554304	-0.191440
H22	1.357561	-0.416232	-1.837754
H23	2.183089	-2.645186	-1.439709
H24	3.317484	-1.695420	-2.409525
N25	2.125719	-0.556060	-1.177035
C26	2.846346	-1.770893	-1.420606
H27	3.614062	-1.897929	-0.656731

Zero-point correction= 0.215482
Thermal correction to Energy= 0.230473
Thermal correction to Enthalpy= 0.231418
Thermal correction to Gibbs Free Energy= 0.173747
Sum of electronic and zero-point Energies= -752.249988
Sum of electronic and thermal Energies= -752.234996
Sum of electronic and thermal Enthalpies= -752.234052
Sum of electronic and thermal Free Energies= -752.291722

45 C2-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	1.697338	-0.930475	-0.273420
C2	0.377764	0.830010	0.414636
C3	-0.519101	1.840390	-0.181677
O4	-0.153339	2.996901	-0.322423
N5	-1.644009	1.236845	-0.634352
H6	-2.208376	1.674786	-1.351469
C7	-1.844012	-0.194906	-0.355776
N8	-2.933805	-0.650854	-1.150900
H9	-2.813118	-1.604706	-1.464021
N10	-0.659421	-1.010678	-0.700618
C11	0.380900	-0.462646	-0.210207
C12	2.078950	-2.209037	-0.874631
H13	1.503138	-3.005193	-0.402052
H14	1.865603	-2.183998	-1.944177
H15	3.143747	-2.361623	-0.704948
C16	2.598537	-0.043925	0.208882
O17	3.778081	-0.050409	0.329673
N18	1.752275	1.180776	0.698952
H19	2.013486	2.053179	0.207585
H20	-3.842711	-0.510885	-0.728187
H21	1.949861	1.333970	1.695591
H22	-2.677527	0.432623	1.409198
H23	-2.324352	-1.430557	2.784755
H24	-3.096332	-2.056569	1.309678
N25	-1.980976	-0.245213	1.110837
C26	-2.204505	-1.555872	1.708347
H27	-1.342371	-2.199842	1.519110

Zero-point correction= 0.219785
Thermal correction to Energy= 0.234068
Thermal correction to Enthalpy= 0.235012
Thermal correction to Gibbs Free Energy= 0.178412
Sum of electronic and zero-point Energies= -752.230498
Sum of electronic and thermal Energies= -752.216215
Sum of electronic and thermal Enthalpies= -752.215271
Sum of electronic and thermal Free Energies= -752.271871

46 $TS^{via\ sync\ add\ +\ PT}$_C2-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	1.848317	-0.166852	-0.774651
C2	0.113160	1.235557	-0.290655
C3	-1.296799	1.721989	-0.270326
O4	-1.606519	2.885243	-0.152278
N5	-2.119051	0.645772	-0.450444
H6	-3.077040	0.762079	-0.757262
C7	-1.580002	-0.685890	-0.255103
N8	-2.569149	-1.641178	-0.526268
H9	-2.206711	-2.539949	-0.811569
N10	-0.375825	-1.003778	-1.039140
C11	0.455177	-0.050149	-0.899750
C12	2.647564	-1.247804	-1.348925
H13	2.153321	-2.204563	-1.163778
H14	2.752194	-1.085644	-2.421362
H15	3.628674	-1.229857	-0.876203
C16	2.212351	0.487281	0.376361

O17	3.239049	0.535116	0.972924
N18	0.944011	1.169429	0.874499
H19	1.125504	2.021762	1.411606
H20	-3.331128	-1.706059	0.135430
H21	0.198440	0.367159	1.375578
H22	-1.788769	-0.322708	1.796325
H23	-0.282115	-1.859891	2.758921
H24	-1.363070	-2.718166	1.640462
N25	-1.017793	-0.648455	1.211088
C26	-0.573285	-1.965452	1.712758
H27	0.287892	-2.304800	1.134932

Zero-point correction= 0.215921
Thermal correction to Energy= 0.229317
Thermal correction to Enthalpy= 0.230261
Thermal correction to Gibbs Free Energy= 0.176444
Sum of electronic and zero-point Energies= -752.186962
Sum of electronic and thermal Energies= -752.173566
Sum of electronic and thermal Enthalpies= -752.172622
Sum of electronic and thermal Free Energies= -752.226439

47 $TS^{via\ async\ HA_NH2\ +\ add}$_C2-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	1.701025	-0.921225	-0.278100
C2	0.486040	0.901065	0.366894
C3	-0.467447	1.886932	-0.038581
O4	-0.309055	3.097392	-0.025523
N5	-1.620687	1.271909	-0.540496
H6	-2.274380	1.865063	-1.034217
C7	-1.767821	-0.128120	-0.564648
N8	-2.853419	-0.565020	-1.293582
H9	-2.850374	-1.534090	-1.573580
N10	-0.643463	-0.934470	-0.712758
C11	0.418104	-0.361084	-0.218490
C12	2.015771	-2.259623	-0.769126
H13	2.003647	-2.977725	0.053078
H14	1.264368	-2.528735	-1.510428
H15	3.005014	-2.241316	-1.225501
C16	2.648465	-0.065246	0.170116
O17	3.827368	-0.160585	0.307236
N18	1.892488	1.226526	0.550635
H19	2.199942	2.004619	-0.051047
H20	-3.743501	-0.095219	-1.238368
H21	2.153366	1.483036	1.508359
H22	-2.974354	0.191128	1.496600
H23	-1.850532	-1.643213	2.725899
H24	-3.245960	-2.200689	1.799620
N25	-2.298991	-0.466224	1.096170
C26	-2.247116	-1.756324	1.706742
H27	-1.588404	-2.403383	1.125359

Zero-point correction= 0.216262
Thermal correction to Energy= 0.231103
Thermal correction to Enthalpy= 0.232047
Thermal correction to Gibbs Free Energy= 0.174076
Sum of electronic and zero-point Energies= -752.221637
Sum of electronic and thermal Energies= -752.206797
Sum of electronic and thermal Enthalpies= -752.205853
Sum of electronic and thermal Free Energies= -752.263823

48 C2-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$

N1	1.723389	-1.048514	-0.044024
C2	0.771329	0.985924	0.002625
C3	-0.284952	1.995344	0.088686
O4	-0.058158	3.186279	0.210341
N5	-1.503403	1.390501	0.052290
C6	-1.856237	-0.038506	-0.234291
N7	-2.460317	-0.233315	-1.513487
H8	-3.356893	0.237962	-1.568071
H9	-1.864448	0.044731	-2.283337
N10	-0.683066	-0.939452	-0.201049
C11	0.472813	-0.373833	-0.095148
C12	1.903611	-2.496017	-0.131109
H13	2.354149	-2.880358	0.786429
H14	0.909616	-2.929180	-0.246473
H15	2.504338	-2.753495	-1.006257
C16	2.673001	-0.119088	0.071239
O17	3.963775	-0.282270	0.139754
N18	2.131969	1.112025	0.107279
H19	2.646828	1.980954	0.204051
H20	4.247818	-1.206558	0.116946
H21	-2.303069	2.009466	0.122094
H22	-2.453192	-0.123156	1.695091
H23	-2.619811	-2.517586	0.919745
H24	-4.115974	-1.789071	1.560486
C25	-3.370262	-1.733821	0.766155
N26	-2.806223	-0.383327	0.781392
H27	-3.866555	-1.911217	-0.187207

Zero-point correction= 0.219613
Thermal correction to Energy= 0.234045
Thermal correction to Enthalpy= 0.234989
Thermal correction to Gibbs Free Energy= 0.178057
Sum of electronic and zero-point Energies= -752.264905
Sum of electronic and thermal Energies= -752.250473
Sum of electronic and thermal Enthalpies= -752.249529
Sum of electronic and thermal Free Energies= -752.306460

49 $TS^{via\ HA_NH2\ products}$_C2-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$

N1	1.700893	-0.949378	-0.207871
C2	0.666964	0.997654	0.088627
C3	-0.393827	1.970670	0.002593
O4	-0.314041	3.158918	0.241011
N5	-1.559442	1.353317	-0.457733
C6	-1.760526	-0.037756	-0.560029
N7	-2.870638	-0.417590	-1.281894
H8	-3.461006	0.302647	-1.666454
H9	-2.731153	-1.218616	-1.878580
N10	-0.683395	-0.888394	-0.642335
C11	0.455139	-0.307559	-0.272429
C12	1.952701	-2.352173	-0.520260
H13	2.407050	-2.857890	0.334838
H14	0.985327	-2.808815	-0.728481
H15	2.581999	-2.440326	-1.408779
C16	2.611844	-0.028907	0.161985
O17	3.898783	-0.202249	0.345827
N18	2.025832	1.147044	0.348787
H19	2.496038	2.001711	0.619942
H20	4.204667	-1.093114	0.132961
H21	-2.374281	1.954306	-0.448741
H22	-1.403865	-0.486297	1.809615
H23	-2.371042	-2.639227	1.367896
H24	-3.455435	-1.656080	2.364766
C25	-2.978477	-1.725584	1.378033
N26	-2.202531	-0.534359	1.172805
H27	-3.754182	-1.784192	0.612893

Zero-point correction= 0.215792
Thermal correction to Energy= 0.230840
Thermal correction to Enthalpy= 0.231784
Thermal correction to Gibbs Free Energy= 0.173581
Sum of electronic and zero-point Energies= -752.242197
Sum of electronic and thermal Energies= -752.227149
Sum of electronic and thermal Enthalpies= -752.226205

Sum of electronic and thermal Free Energies= -752.284408

50 C2-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	1.939360	-0.982568	0.308735
C2	0.566038	0.851971	-0.003158
C3	-0.598319	1.585563	-0.519328
O4	-0.557939	2.771707	-0.785205
N5	-1.619640	0.718861	-0.767552
H6	-2.388425	1.076671	-1.319508
C7	-1.729425	-0.641868	-0.221001
N8	-2.509216	-1.402061	-1.159072
H9	-3.478310	-1.102082	-1.192940
H10	-2.479549	-2.389444	-0.930342
N11	-0.429525	-1.344983	-0.114187
C12	0.547257	-0.545283	0.043133
C13	2.744224	0.339283	0.437820
O14	3.907769	0.340392	0.664828
N15	1.832405	1.327738	0.224671
H16	2.087794	2.310376	0.202760
H17	-2.186212	-1.475158	1.563663
H18	-3.349734	1.193906	1.132983
H19	-3.670854	0.075276	2.454639
N20	-2.162154	-0.540164	1.166661
C21	-3.439813	0.136780	1.390731
H22	-4.283401	-0.299627	0.836067
C23	2.520591	-1.891357	-0.741994
H24	1.989798	-1.459223	1.217023
H25	3.558963	-2.088393	-0.477986
H26	1.926519	-2.804047	-0.751698
H27	2.452837	-1.383337	-1.703647

Zero-point correction= 0.219935
Thermal correction to Energy= 0.234275
Thermal correction to Enthalpy= 0.235220
Thermal correction to Gibbs Free Energy= 0.178021
Sum of electronic and zero-point Energies= -752.236163
Sum of electronic and thermal Energies= -752.221823
Sum of electronic and thermal Enthalpies= -752.220879
Sum of electronic and thermal Free Energies= -752.278077

51 TS$^{\text{via sync add + PT}}$_C2-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	1.558281	-0.717304	-0.224425
C2	0.290033	1.111923	-0.548286
C3	-1.069113	1.702039	-0.388753
O4	-1.314643	2.883308	-0.346664
N5	-1.968778	0.676821	-0.215961
H6	-2.951897	0.906893	-0.294797
C7	-1.612865	-0.730766	-0.276127
N8	-2.769350	-1.488212	-0.526687
H9	-3.445938	-1.530876	0.224761
H10	-2.578536	-2.392803	-0.936968
N11	-0.554358	-1.064430	-1.215982
C12	0.421424	-0.192272	-0.969120
C13	2.302675	0.465330	0.270074
O14	3.403026	0.438421	0.723407
N15	1.421712	1.518721	0.103371
H16	1.641536	2.469591	0.377075
H17	-0.960922	-2.140779	1.097448
H18	-0.957667	0.569718	2.253873
H19	-0.669053	-0.964477	3.094468
N20	-0.800925	-1.137538	1.011659
C21	-1.210566	-0.489999	2.274448
H22	-2.285136	-0.590990	2.455071
C23	2.366155	-1.864280	-0.697812
H24	0.711924	-1.031076	0.622856
H25	3.004508	-2.189801	0.121961
H26	1.676168	-2.653629	-0.993799
H27	2.975425	-1.553843	-1.546254

Zero-point correction= 0.214712
Thermal correction to Energy= 0.228225
Thermal correction to Enthalpy= 0.229169
Thermal correction to Gibbs Free Energy= 0.175212
Sum of electronic and zero-point Energies= -752.187706
Sum of electronic and thermal Energies= -752.174193
Sum of electronic and thermal Enthalpies= -752.173249
Sum of electronic and thermal Free Energies= -752.227206

52 TS$^{\text{via async HA_NH2 + add}}$_C2-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	1.896474	-0.961667	0.279613
C2	0.497462	0.813625	-0.083885
C3	-0.633465	1.503444	-0.678116
O4	-0.692145	2.690143	-0.926749
N5	-1.609510	0.573511	-1.021792
H6	-2.404954	0.918864	-1.542728
C7	-1.630018	-0.721389	-0.479038
N8	-2.693370	-1.487235	-0.889106
H9	-3.618824	-1.087231	-0.845623
H10	-2.639501	-2.465634	-0.646238
N11	-0.443484	-1.401010	-0.291951
C12	0.524717	-0.552507	-0.062353
C13	2.666892	0.386763	0.488991
O14	3.814868	0.388781	0.798951
N15	1.752303	1.341080	0.232594
H16	1.972775	2.329144	0.258712
H17	-1.595774	-1.045350	1.947090
H18	-3.527053	0.951260	0.986595
H19	-3.197523	0.596936	2.692446
N20	-1.873640	-0.260633	1.350527
C21	-3.205949	0.169294	1.681558
H22	-3.940546	-0.648367	1.690106
C23	2.565932	-1.819780	-0.756996
H24	1.915199	-1.459909	1.176008
H25	3.593029	-1.991215	-0.436744
H26	2.006159	-2.750870	-0.831841
H27	2.540392	-1.284043	-1.705560

Zero-point correction= 0.216343
Thermal correction to Energy= 0.230696
Thermal correction to Enthalpy= 0.231641
Thermal correction to Gibbs Free Energy= 0.175160
Sum of electronic and zero-point Energies= -752.210634
Sum of electronic and thermal Energies= -752.196280
Sum of electronic and thermal Enthalpies= -752.195336
Sum of electronic and thermal Free Energies= -752.251817

53 N2-NHCH$_3$[9MOG + H$_{N1}$]$^{+}$

N1	1.863995	-1.120522	0.060039
C2	1.091301	0.970724	-0.008684
C3	0.194518	2.023043	0.036190
O4	0.211284	3.212431	-0.115538
N5	-1.299596	1.424899	0.319357
H6	-1.794941	1.502985	-0.582961
C7	-1.382479	0.058288	0.876459
N8	-2.736172	-0.500352	0.691323
H9	-2.698162	-1.439974	1.114308
N10	-0.453693	-0.851961	0.565846
C11	0.746186	-0.372614	0.229358
C12	1.988686	-2.556002	0.236785
H13	1.719064	-2.834014	1.257366
H14	1.348345	-3.083215	-0.472902
H15	3.032001	-2.809548	0.048198
C16	2.963887	-0.290384	-0.279400

O17	4.092197	-0.657186	-0.492227
N18	2.446851	0.990328	-0.306255
H19	3.002817	1.798650	-0.538617
H20	-1.699869	2.125652	0.948139
H21	-3.439303	0.036754	1.207607
H22	-2.478561	-1.139554	-1.158352
H23	-4.671777	-2.015711	-0.409617
H24	-5.225015	-0.309164	-0.424552
N25	-3.150042	-0.520061	-0.704506
C26	-4.519248	-1.024326	-0.854407
H27	-4.718950	-1.083512	-1.924933

Zero-point correction= 0.221620
Thermal correction to Energy= 0.236046
Thermal correction to Enthalpy= 0.236990
Thermal correction to Gibbs Free Energy= 0.179460
Sum of electronic and zero-point Energies= -752.180805
Sum of electronic and thermal Energies= -752.166379
Sum of electronic and thermal Enthalpies= -752.165434
Sum of electronic and thermal Free Energies= -752.222965

54 $TS^{via\ HA_NH2\ products}$_N2-$NHCH_3$[9MOG + H_{N1}]$^+$

N1	-1.992583	-1.065968	-0.031160
C2	-1.077303	0.964987	0.007023
C3	-0.116782	1.955760	-0.088151
O4	-0.045832	3.145387	0.027509
N5	1.316154	1.254586	-0.463640
H6	1.938350	1.425048	0.345417
C7	1.348084	-0.180935	-0.771543
N8	2.632310	-0.695088	-0.736517
H9	2.621119	-1.695726	-0.949651
N10	0.334524	-0.985481	-0.533776
C11	-0.829799	-0.400752	-0.210464
C12	-2.213118	-2.495097	-0.171066
H13	-1.971664	-2.814437	-1.186357
H14	-1.600818	-3.044383	0.546174
H15	-3.268939	-2.674775	0.031335
C16	-3.031894	-0.156753	0.307730
O17	-4.180536	-0.444034	0.529594
N18	-2.425219	1.082960	0.319217
H19	-2.923322	1.933079	0.533692
H20	1.658500	1.839226	-1.232696
H21	3.327041	-0.215027	-1.307830
H22	2.852025	-1.146902	1.380561
H23	4.956787	-1.840352	0.470880
H24	5.305615	-0.116056	0.117822
N25	3.365564	-0.432186	0.859060
C26	4.772110	-0.804183	0.779666
H27	5.193206	-0.670436	1.782356

Zero-point correction= 0.217908
Thermal correction to Energy= 0.232583
Thermal correction to Enthalpy= 0.233527
Thermal correction to Gibbs Free Energy= 0.175108
Sum of electronic and zero-point Energies= -752.170175
Sum of electronic and thermal Energies= -752.155500
Sum of electronic and thermal Enthalpies= -752.154556
Sum of electronic and thermal Free Energies= -752.212975

55 N2-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$

N1	1.604612	-1.251050	0.115143
C2	1.129786	0.936913	-0.025541
C3	0.316588	2.125633	0.082783
O4	0.708675	3.269385	0.001850
N5	-1.025202	1.799666	0.338577
H6	-1.560222	2.575792	0.710644
C7	-1.545401	0.475629	0.509283
N8	-2.533904	0.230038	-0.698263
H9	-1.993556	0.372370	-1.558378
H10	-3.265056	0.948738	-0.704086
N11	-0.668198	-0.637001	0.474862
C12	0.575813	-0.362663	0.212060
C13	1.519691	-2.691025	0.298937
H14	2.535987	-3.084287	0.297664
H15	1.037432	-2.909634	1.252765
H16	0.953269	-3.143990	-0.517171
C17	2.804573	-0.575078	-0.166269
O18	3.897239	-1.047298	-0.310366
N19	2.451038	0.788924	-0.246257
H20	3.123052	1.525312	-0.420839
H21	-2.194468	0.431251	1.388743
H22	-2.419366	-1.725311	-0.706098
H23	-4.640270	-2.213625	0.055036
H24	-3.774750	-1.246906	1.266806
N25	-3.174012	-1.046111	-0.799522
C26	-4.179178	-1.244678	0.248189
H27	-4.960950	-0.486038	0.154606

Zero-point correction= 0.222198
Thermal correction to Energy= 0.236520
Thermal correction to Enthalpy= 0.237465
Thermal correction to Gibbs Free Energy= 0.179317
Sum of electronic and zero-point Energies= -752.249108
Sum of electronic and thermal Energies= -752.234786
Sum of electronic and thermal Enthalpies= -752.233842
Sum of electronic and thermal Free Energies= -752.291990

56 $TS^{via\ async\ HA_NH2\ +\ add}$_N2-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$

N1	2.223143	-0.970650	-0.028648
C2	0.994230	0.915923	-0.073821
C3	-0.222587	1.747454	-0.127151
O4	-0.200131	2.956091	-0.027555
N5	-1.327455	0.961408	-0.274844
H6	-2.243327	1.406897	-0.284135
C7	-1.373579	-0.483445	-0.418878
N8	-2.182201	-1.019559	0.676729
H9	-1.780421	-0.815072	1.590842
H10	-2.347494	-2.020595	0.580232
N11	-0.136398	-1.204476	-0.378211
C12	0.934710	-0.511770	-0.165770
C13	2.649243	-2.363251	-0.084821
H14	3.728578	-2.383662	0.062758
H15	2.157239	-2.930231	0.706625
H16	2.399386	-2.789050	-1.057636
C17	3.096243	0.097702	0.125341
O18	4.284264	0.106074	0.258654
N19	2.250501	1.267723	0.092811
H20	2.604290	2.215571	0.185828
H21	-1.891532	-0.732943	-1.351947
H22	-4.190995	0.232877	1.375353
H23	-4.641058	-1.040095	-1.220606
H24	-5.895034	-0.201766	-0.306853
C25	-4.948274	-0.757598	-0.211130
N26	-3.997871	0.157078	0.372113
H27	-5.160648	-1.650000	0.388466

Zero-point correction= 0.214941
Thermal correction to Energy= 0.229861
Thermal correction to Enthalpy= 0.230805
Thermal correction to Gibbs Free Energy= 0.171256
Sum of electronic and zero-point Energies= -752.182193
Sum of electronic and thermal Energies= -752.167273
Sum of electronic and thermal Enthalpies= -752.166329

Sum of electronic and thermal Free Energies= -752.225878

57 N2-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	-1.930799	-1.010384	0.121484
C2	-0.897453	0.948869	-0.085334
C3	0.117996	1.925198	0.146654
O4	0.086709	3.118866	-0.054300
N5	1.298236	1.320192	0.692141
H6	1.928745	2.016474	1.077467
C7	1.452182	0.004381	1.104985
N8	2.767545	-0.562088	0.599403
H9	3.525282	0.028150	0.974319
H10	2.904027	-1.492352	1.005786
N11	0.394178	-0.857435	0.851279
C12	-0.762200	-0.351843	0.318812
C13	-2.236733	-2.404936	0.377048
H14	-3.276828	-2.556719	0.085116
H15	-1.599657	-3.058631	-0.224732
H16	-2.134867	-2.636889	1.440922
C17	-2.877327	-0.104239	-0.440064
O18	-4.012102	-0.376351	-0.745369
N19	-2.195810	1.090269	-0.545446
H20	-2.613696	1.937961	-0.897954
H21	0.367541	-1.756932	1.312956
H22	2.527896	0.183300	-1.216178
H23	4.476789	-2.025631	-0.908740
H24	4.187282	-1.068681	-2.360149
N25	2.836220	-0.712806	-0.841025
C26	4.199397	-1.032237	-1.270104
H27	4.948473	-0.295539	-0.948299

Zero-point correction= 0.221000
Thermal correction to Energy= 0.235615
Thermal correction to Enthalpy= 0.236559
Thermal correction to Gibbs Free Energy= 0.178449
Sum of electronic and zero-point Energies= -752.208136
Sum of electronic and thermal Energies= -752.193520
Sum of electronic and thermal Enthalpies= -752.192576
Sum of electronic and thermal Free Energies= -752.250686

58 TS$^{via\ HA_NH2\ products}$_N2-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	1.903467	-1.110751	-0.095308
C2	1.074827	0.947289	0.080712
C3	0.112641	1.994980	-0.047698
O4	0.248231	3.183010	0.135525
N5	-1.160449	1.478299	-0.463366
H6	-1.790736	2.216809	-0.757009
C7	-1.437279	0.179679	-0.826595
N8	-2.754670	-0.275284	-0.693742
H9	-3.429270	0.453911	-0.940412
H10	-2.944460	-1.092713	-1.274532
N11	-0.448474	-0.763263	-0.660009
C12	0.790399	-0.351350	-0.239486
C13	2.067896	-2.532520	-0.332076
H14	3.114322	-2.764036	-0.127970
H15	1.439901	-3.118364	0.344830
H16	1.848569	-2.778487	-1.374614
C17	2.973435	-0.272181	0.336416
O18	4.101362	-0.635291	0.560438
N19	2.414869	0.986146	0.426593
H20	2.937012	1.805547	0.697632
H21	-0.666927	-1.748257	-0.715036
H22	-2.880780	-0.155920	1.436952
H23	-5.030950	-1.695754	0.138777
H24	-4.941545	-1.334994	1.858602
N25	-3.208618	-0.911605	0.830136
C26	-4.666242	-0.964951	0.865677
H27	-5.168819	0.000032	0.713249

Zero-point correction= 0.218204
Thermal correction to Energy= 0.233005
Thermal correction to Enthalpy= 0.233949
Thermal correction to Gibbs Free Energy= 0.175215
Sum of electronic and zero-point Energies= -752.199239
Sum of electronic and thermal Energies= -752.184439
Sum of electronic and thermal Enthalpies= -752.183495
Sum of electronic and thermal Free Energies= -752.242229

59 N2-NHCH$_3$[9MOG + H$_{C4}$]$^{\bullet+}$

N1	-1.996421	-1.127004	-0.040870
C2	-1.112616	0.961717	-0.285759
C3	-0.092471	1.934024	-0.154439
O4	-0.188154	3.135258	0.015239
N5	1.222382	1.314566	-0.178203
H6	1.970287	1.971650	0.009498
C7	1.315358	-0.013946	0.113745
N8	2.637116	-0.473279	0.610940
H9	2.906551	0.026160	1.475149
H10	2.469557	-1.458630	0.855515
N11	0.439922	-0.919213	0.044101
C12	-0.821786	-0.486309	-0.561813
C13	-2.281780	-2.533033	-0.265575
H14	-2.363456	-2.752701	-1.335798
H15	-1.493323	-3.143397	0.177641
H16	-3.230425	-2.762663	0.219483
C17	-2.999257	-0.214838	0.213946
O18	-4.140314	-0.418580	0.531803
N19	-2.413830	1.071600	0.042142
H20	-2.883823	1.919607	0.330959
H21	-0.713797	-0.687921	-1.643815
H22	3.748365	0.503994	-0.732604
H23	4.822789	-2.027556	0.354094
H24	5.663141	-0.868852	-0.674739
C25	4.926695	-0.964783	0.123645
N26	3.659711	-0.456727	-0.409759
H27	5.284869	-0.419700	1.007334

Zero-point correction= 0.221314
Thermal correction to Energy= 0.235601
Thermal correction to Enthalpy= 0.236546
Thermal correction to Gibbs Free Energy= 0.178826
Sum of electronic and zero-point Energies= -752.208539
Sum of electronic and thermal Energies= -752.194252
Sum of electronic and thermal Enthalpies= -752.193308
Sum of electronic and thermal Free Energies= -752.251027

60 TS$^{via\ HA_NH2\ products}$_N2-NHCH$_3$[9MOG + H$_{C4}$]$^{\bullet+}$

N1	-1.931611	-1.090639	-0.133079
C2	-0.949682	0.957958	-0.238912
C3	0.117053	1.942031	-0.130204
O4	-0.014161	3.146212	-0.215026
N5	1.337064	1.301745	0.118141
H6	2.128808	1.922771	0.241814
C7	1.361852	-0.006876	0.586399
N8	2.523650	-0.395360	1.229375
H9	3.129344	0.317979	1.620783
H10	2.377909	-1.171538	1.869990
N11	0.428946	-0.882496	0.430283
C12	-0.655299	-0.493774	-0.443671
C13	-2.196528	-2.513588	-0.263336
H14	-2.068947	-2.835250	-1.301262
H15	-1.520069	-3.071868	0.385698
H16	-3.226581	-2.693270	0.044131

C17	-2.913791	-0.165386	0.044920
O18	-4.088499	-0.279736	0.245246
N19	-2.226662	1.124424	-0.022379
H20	-2.687338	1.998981	0.213211
H21	-0.388424	-0.710539	-1.495049
H22	3.350373	-2.130656	-0.015716
H23	4.333168	0.439298	-1.015238
H24	4.518247	-1.120789	-1.821021
C25	3.877103	-0.546451	-1.136141
N26	3.888185	-1.265932	0.111623
H27	2.893544	-0.462609	-1.621184

Zero-point correction= 0.215688
Thermal correction to Energy= 0.230129
Thermal correction to Enthalpy= 0.231073
Thermal correction to Gibbs Free Energy= 0.172824
Sum of electronic and zero-point Energies= -752.168614
Sum of electronic and thermal Energies= -752.154173
Sum of electronic and thermal Enthalpies= -752.153229
Sum of electronic and thermal Free Energies= -752.211478

61 N2-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	2.003973	-1.032176	0.086503
C2	0.910993	0.938286	0.581155
C3	-0.129303	1.769294	-0.161326
O4	0.012650	2.918021	-0.492660
N5	-1.321560	1.067408	-0.325778
H6	-2.156129	1.604344	-0.538754
C7	-1.427550	-0.287617	-0.024665
N8	-2.593736	-0.929448	-0.662073
H9	-2.485285	-0.914000	-1.687431
H10	-2.561597	-1.918170	-0.366348
N11	-0.363984	-1.116045	0.001641
C12	0.775933	-0.514651	0.210573
C13	2.329754	-2.398671	-0.283114
H14	1.936197	-3.088133	0.465141
H15	1.905664	-2.633482	-1.262182
H16	3.416387	-2.473074	-0.322577
C17	2.989361	0.013305	0.128201
O18	4.169729	-0.160871	0.003080
N19	2.292420	1.183851	0.298842
H20	2.770880	2.042335	0.526136
H21	0.675161	1.053613	1.654377
H22	-4.521447	-0.578858	-1.008392
H23	-3.507812	-0.082730	1.724775
H24	-5.189677	-0.001992	1.181060
N25	-3.823702	-0.249197	-0.345662
C26	-4.237380	-0.512720	1.036547
H27	-4.366094	-1.581162	1.252292

Zero-point correction= 0.221951
Thermal correction to Energy= 0.235945
Thermal correction to Enthalpy= 0.236889
Thermal correction to Gibbs Free Energy= 0.180255
Sum of electronic and zero-point Energies= -752.228946
Sum of electronic and thermal Energies= -752.214952
Sum of electronic and thermal Enthalpies= -752.214008
Sum of electronic and thermal Free Energies= -752.270642

62 TS$^{via\ HA_NH2\ products}$_N2-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	1.810155	-1.060682	-0.074894
C2	0.750904	0.878325	0.579999
C3	-0.109426	1.885066	-0.170040
O4	0.144705	3.049840	-0.317224
N5	-1.310591	1.307331	-0.596221
H6	-1.991437	1.955607	-0.977015
C7	-1.482041	-0.059025	-0.713879
N8	-2.756239	-0.539857	-0.949852
H9	-3.329208	0.022602	-1.577059
H10	-2.686793	-1.507670	-1.270975
N11	-0.512421	-0.967435	-0.519334
C12	0.608436	-0.483296	-0.047984
C13	2.128698	-2.372618	-0.615503
H14	1.556153	-3.136158	-0.087550
H15	1.896304	-2.406031	-1.682168
H16	3.195585	-2.533338	-0.462480
C17	2.828086	-0.112960	0.304197
O18	4.000768	-0.356682	0.337542
N19	2.168706	1.062443	0.564141
H20	2.644180	1.838539	0.999510
H21	0.343873	0.836658	1.605999
H22	-4.508292	-1.228771	0.134253
H23	-2.340334	-0.228209	1.842673
H24	-3.826721	-0.980633	2.406627
N25	-3.851164	-0.497283	0.421953
C26	-3.107492	-0.960989	1.580626
H27	-2.659206	-1.956504	1.480589

Zero-point correction= 0.218546
Thermal correction to Energy= 0.232756
Thermal correction to Enthalpy= 0.233701
Thermal correction to Gibbs Free Energy= 0.176101
Sum of electronic and zero-point Energies= -752.218455
Sum of electronic and thermal Energies= -752.204244
Sum of electronic and thermal Enthalpies= -752.203300
Sum of electronic and thermal Free Energies= -752.260899

63 N2-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	-1.891573	-1.021183	0.130122
C2	-1.033023	1.099436	-0.057320
C3	0.119163	1.966556	-0.309683
O4	-0.582871	2.025676	0.930959
N5	1.406065	1.361684	-0.219317
H6	2.163748	1.745135	-0.768503
C7	1.483454	0.035848	0.167353
N8	2.735410	-0.333760	0.830126
H9	2.881928	0.258694	1.660149
H10	2.610900	-1.308913	1.146016
N11	0.471746	-0.800809	0.414066
C12	-0.729821	-0.336496	0.199722
C13	-2.069349	-2.448749	0.324116
H14	-3.120925	-2.673290	0.147042
H15	-1.446908	-3.002720	-0.382260
H16	-1.800862	-2.722207	1.346130
C17	-2.939001	-0.158390	-0.292565
O18	-4.085045	-0.478009	-0.447993
N19	-2.358731	1.085381	-0.514485
H20	-2.940389	1.905621	-0.601067
H21	0.077669	2.848752	-0.940542
H22	4.704773	-0.159526	0.558295
H23	3.067821	-1.090895	-1.720304
H24	4.832616	-0.978335	-1.660971
N25	3.879327	-0.135732	-0.036340
C26	3.939037	-1.174988	-1.068037
H27	3.994483	-2.192026	-0.658424

Zero-point correction= 0.220500
Thermal correction to Energy= 0.234610
Thermal correction to Enthalpy= 0.235554
Thermal correction to Gibbs Free Energy= 0.178431
Sum of electronic and zero-point Energies= -752.184276
Sum of electronic and thermal Energies= -752.170166
Sum of electronic and thermal Enthalpies= -752.169222

Sum of electronic and thermal Free Energies= -752.226345

64 $TS^{via\ HA_NH2\ products}$_N2-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	1.769563	-1.007936	-0.229997
C2	1.000821	1.127828	0.095048
C3	-0.139428	1.995629	0.397247
O4	0.643740	2.179014	-0.786772
N5	-1.419488	1.418442	0.190151
H6	-2.251591	1.948134	0.410017
C7	-1.518926	0.258659	-0.538964
N8	-2.787624	-0.133042	-0.928767
H9	-3.333313	0.591626	-1.394182
H10	-2.714449	-0.976328	-1.502231
N11	-0.535080	-0.650755	-0.681231
C12	0.655339	-0.263521	-0.324673
C13	1.898485	-2.421719	-0.540203
H14	2.933852	-2.702035	-0.348331
H15	1.230693	-3.008017	0.094518
H16	1.656496	-2.592351	-1.590366
C17	2.827221	-0.239585	0.343073
O18	3.938045	-0.638000	0.550270
N19	2.290893	1.007197	0.631101
H20	2.896858	1.786021	0.843700
H21	-0.109910	2.790090	1.134611
H22	-4.663971	-0.812791	-0.081163
H23	-2.323687	-1.050871	1.679478
H24	-3.947687	-1.612530	2.072065
N25	-3.862663	-0.410513	0.413483
C26	-3.250184	-1.434734	1.246799
H27	-3.056749	-2.388146	0.740756

Zero-point correction= 0.218257
Thermal correction to Energy= 0.232232
Thermal correction to Enthalpy= 0.233177
Thermal correction to Gibbs Free Energy= 0.176768
Sum of electronic and zero-point Energies= -752.176351
Sum of electronic and thermal Energies= -752.162376
Sum of electronic and thermal Enthalpies= -752.161431
Sum of electronic and thermal Free Energies= -752.217840

65 N2-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-1.914938	-1.081088	0.125114
C2	-0.956940	0.950633	-0.037055
C3	0.063718	1.815831	0.152064
O4	0.102347	3.137388	-0.029509
N5	1.286893	1.310531	0.572565
H6	1.821201	1.989173	1.107349
C7	1.382787	-0.047634	0.962755
N8	2.698328	-0.637224	0.603331
H9	3.453252	-0.210502	1.158700
H10	2.622236	-1.620641	0.885869
N11	0.379628	-0.935010	0.749373
C12	-0.744935	-0.426588	0.326205
C13	-2.159485	-2.494233	0.356719
H14	-1.519252	-3.097309	-0.289879
H15	-1.961485	-2.736526	1.402196
H16	-3.206566	-2.684866	0.122555
C17	-2.889486	-0.199929	-0.393901
O18	-4.009033	-0.486273	-0.725919
N19	-2.284845	1.054678	-0.438475
H20	-2.710249	1.791966	-0.978192
H21	-0.777438	3.525244	-0.098037
H22	2.833365	0.338927	-1.112135
H23	4.489406	-2.098440	-0.823690
H24	4.551439	-0.927156	-2.139733
C25	4.373513	-1.040229	-1.069665
N26	2.994899	-0.622892	-0.819198
H27	5.122799	-0.448861	-0.523285

Zero-point correction= 0.221349
Thermal correction to Energy= 0.235914
Thermal correction to Enthalpy= 0.236858
Thermal correction to Gibbs Free Energy= 0.179093
Sum of electronic and zero-point Energies= -752.213921
Sum of electronic and thermal Energies= -752.199356
Sum of electronic and thermal Enthalpies= -752.198412
Sum of electronic and thermal Free Energies= -752.256177

66 $TS^{via\ HA_NH2\ products}$_N2-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	1.941108	-1.128398	-0.089628
C2	1.067737	0.939317	0.056775
C3	0.063762	1.832440	-0.111520
O4	0.071751	3.159470	0.005513
N5	-1.189972	1.340642	-0.419607
H6	-1.835156	2.031034	-0.786749
C7	-1.366080	-0.017461	-0.708383
N8	-2.668997	-0.509346	-0.651724
H9	-3.360150	0.051805	-1.154806
H10	-2.663155	-1.465356	-1.010494
N11	-0.380821	-0.925534	-0.576479
C12	0.785329	-0.439287	-0.233844
C13	2.121474	-2.558087	-0.281460
H14	1.464641	-3.110783	0.392296
H15	1.899038	-2.824641	-1.316127
H16	3.163070	-2.785040	-0.055386
C17	2.982679	-0.262845	0.315840
O18	4.112568	-0.576198	0.578599
N19	2.425803	1.015496	0.345086
H20	2.909645	1.753357	0.832771
H21	0.963569	3.524810	0.026184
H22	-3.112772	0.101044	1.344833
H23	-5.041236	-1.775616	0.149820
H24	-5.234230	-0.975375	1.705235
C25	-4.791955	-0.870198	0.709612
N26	-3.348507	-0.784067	0.890893
H27	-5.255792	0.003779	0.227621

Zero-point correction= 0.218223
Thermal correction to Energy= 0.232923
Thermal correction to Enthalpy= 0.233867
Thermal correction to Gibbs Free Energy= 0.175509
Sum of electronic and zero-point Energies= -752.207861
Sum of electronic and thermal Energies= -752.193160
Sum of electronic and thermal Enthalpies= -752.192216
Sum of electronic and thermal Free Energies= -752.250574

67 N2-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	1.849093	-1.035917	-0.095985
C2	0.844274	1.004363	-0.278157
C3	-0.247365	1.901263	-0.089156
O4	-0.194691	3.057898	0.295108
N5	-1.463168	1.250976	-0.370483
H6	-2.301172	1.813485	-0.294759
C7	-1.498677	-0.064618	-0.848495
N8	-2.829049	-0.676645	-0.828960
N9	-0.498035	-0.959653	-0.615034
C10	0.640450	-0.370641	-0.362591
C11	2.069931	-2.476229	-0.173565
H12	2.515207	-2.830067	0.756947
H13	1.100260	-2.947203	-0.327038
H14	2.733075	-2.708293	-1.008679
C15	2.838200	-0.175538	0.224366
O16	3.988063	-0.327880	0.499107

N17	2.202307	1.237262	0.173756
H18	2.766376	1.822213	-0.453195
H19	-3.396469	-0.296927	-1.592468
H20	2.260496	1.672948	1.104373
H21	-2.647694	-1.672576	-1.028633
H22	-4.526349	-0.857846	0.214045
H23	-3.658559	-0.960553	2.385717
H24	-2.774686	-2.162726	1.406030
C25	-2.972977	-1.092698	1.547850
N26	-3.606676	-0.457781	0.391111
H27	-2.041788	-0.575707	1.781583

Zero-point correction= 0.221922
Thermal correction to Energy= 0.236516
Thermal correction to Enthalpy= 0.237460
Thermal correction to Gibbs Free Energy= 0.178740
Sum of electronic and zero-point Energies= -752.185788
Sum of electronic and thermal Energies= -752.171193
Sum of electronic and thermal Enthalpies= -752.170249
Sum of electronic and thermal Free Energies= -752.228970

68 $TS^{via\ async\ HA_NH2\ +\ add}$_N2-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	1.859926	-1.059505	-0.097412
C2	0.880548	0.995107	-0.160026
C3	-0.183500	1.932921	-0.061546
O4	-0.120741	3.102640	0.270327
N5	-1.407121	1.304674	-0.389946
H6	-2.243427	1.855257	-0.231626
C7	-1.493994	-0.039303	-0.722953
N8	-2.774135	-0.541224	-0.935714
N9	-0.490529	-0.934483	-0.581134
C10	0.657266	-0.366435	-0.306251
C11	2.051948	-2.501434	-0.225728
H12	2.526942	-2.888474	0.676256
H13	1.068699	-2.951594	-0.353192
H14	2.676567	-2.719265	-1.093607
C15	2.873489	-0.226705	0.221593
O16	4.026748	-0.403975	0.459766
N17	2.257394	1.200628	0.237104
H18	2.801007	1.796069	-0.398923
H19	-3.326107	0.008227	-1.595748
H20	2.366686	1.605091	1.176594
H21	-2.688741	-1.510837	-1.251531
H22	-4.614239	-0.956879	0.059256
H23	-3.863339	-1.139529	2.330952
H24	-2.964572	-2.246899	1.263754
C25	-3.171223	-1.192196	1.485593
N26	-3.792390	-0.449761	0.396703
H27	-2.246767	-0.694510	1.785768

Zero-point correction= 0.219339
Thermal correction to Energy= 0.233931
Thermal correction to Enthalpy= 0.234875
Thermal correction to Gibbs Free Energy= 0.175740
Sum of electronic and zero-point Energies= -752.183363
Sum of electronic and thermal Energies= -752.168771
Sum of electronic and thermal Enthalpies= -752.167826
Sum of electronic and thermal Free Energies= -752.226962

69 N2-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$

N1	-1.931803	-1.015096	0.086987
C2	-0.884853	0.952988	-0.014650
C3	0.159048	1.915985	0.148153
O4	0.099494	3.117946	-0.030031
N5	1.344897	1.278739	0.584783
C6	1.411572	-0.086397	0.976799
N7	2.729862	-0.682060	0.599891
H8	3.481426	-0.262264	1.163785
H9	2.653548	-1.669084	0.863746
N10	0.404505	-0.966613	0.725001
C11	-0.696516	-0.378252	0.305636
C12	-2.201146	-2.431450	0.295073
H13	-2.454520	-2.919377	-0.649025
H14	-1.283600	-2.872003	0.684735
H15	-2.995231	-2.567542	1.033391
C16	-2.802466	-0.081057	-0.341261
O17	-4.064446	-0.254361	-0.661046
N18	-2.214969	1.103245	-0.412826
H19	-2.663820	1.963743	-0.698127
H20	-4.364895	-1.165581	-0.554986
H21	1.967352	1.935428	1.044091
H22	2.793633	0.313805	-1.103280
H23	4.651782	-1.974788	-0.827663
H24	4.628233	-0.782291	-2.126932
N25	3.035641	-0.634613	-0.820360
C26	4.446493	-0.927141	-1.061261
H27	5.135968	-0.282005	-0.496387

Zero-point correction= 0.221595
Thermal correction to Energy= 0.236040
Thermal correction to Enthalpy= 0.236984
Thermal correction to Gibbs Free Energy= 0.179631
Sum of electronic and zero-point Energies= -752.203235
Sum of electronic and thermal Energies= -752.188790
Sum of electronic and thermal Enthalpies= -752.187846
Sum of electronic and thermal Free Energies= -752.245199

70 $TS^{via\ HA_NH2\ products}$_N2-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$

N1	1.968552	-1.047342	-0.057422
C2	0.982623	0.952343	0.010599
C3	-0.053765	1.932561	-0.110597
O4	0.034783	3.137264	0.026934
N5	-1.272849	1.299015	-0.430227
C6	-1.398465	-0.069589	-0.731189
N7	-2.698738	-0.591213	-0.650020
H8	-3.390530	-0.045320	-1.169800
H9	-2.677917	-1.549198	-1.000887
N10	-0.399582	-0.961851	-0.561169
C11	0.741500	-0.385164	-0.230967
C12	2.186693	-2.480535	-0.207956
H13	2.507593	-2.922688	0.738168
H14	1.229911	-2.917738	-0.492599
H15	2.913570	-2.677525	-0.999572
C16	2.888316	-0.120029	0.271577
O17	4.162253	-0.313248	0.521517
N18	2.336767	1.083481	0.320044
H19	2.823553	1.942512	0.540917
H20	4.431734	-1.237825	0.453359
H21	-1.991700	1.951508	-0.721371
H22	-3.019760	0.004519	1.345141
H23	-5.173139	-1.609567	0.148630
H24	-5.241853	-0.836166	1.728016
N25	-3.363495	-0.829271	0.865508
C26	-4.812589	-0.753360	0.725350
H27	-5.188202	0.178255	0.274502

Zero-point correction= 0.218421
Thermal correction to Energy= 0.233194
Thermal correction to Enthalpy= 0.234138
Thermal correction to Gibbs Free Energy= 0.175166
Sum of electronic and zero-point Energies= -752.199527
Sum of electronic and thermal Energies= -752.184754
Sum of electronic and thermal Enthalpies= -752.183809

Sum of electronic and thermal Free Energies= -752.242782

71 N2-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	1.904598	-1.184106	0.195236
C2	0.933162	0.885279	0.009724
C3	-0.083894	1.854067	-0.261214
O4	0.014149	3.064212	-0.209260
N5	-1.299880	1.218224	-0.630605
H6	-1.890513	1.844210	-1.168714
C7	-1.402261	-0.174569	-0.878577
N8	-2.753039	-0.693334	-0.558224
H9	-3.451468	-0.292784	-1.200069
H10	-2.703769	-1.700266	-0.743270
N11	-0.437760	-1.045781	-0.497185
C12	0.670839	-0.452920	-0.137504
C13	2.935114	-0.064227	0.587500
O14	4.043763	-0.356877	0.915594
N15	2.260916	1.082559	0.434619
H16	2.683530	1.985591	0.605550
H17	-2.907271	0.431347	1.062003
H18	-4.789500	-1.841173	0.813384
H19	-4.816615	-0.582692	2.047794
C20	-4.577652	-0.786029	1.003180
N21	-3.148193	-0.532027	0.833931
H22	-5.219150	-0.159318	0.366277
C23	2.441134	-2.054938	-0.900167
H24	1.764562	-1.761518	1.031238
H25	1.700918	-2.826064	-1.107670
H26	2.597495	-1.432394	-1.780730
H27	3.383333	-2.482345	-0.558526

Zero-point correction= 0.221994
Thermal correction to Energy= 0.236066
Thermal correction to Enthalpy= 0.237011
Thermal correction to Gibbs Free Energy= 0.180090
Sum of electronic and zero-point Energies= -752.175226
Sum of electronic and thermal Energies= -752.161154
Sum of electronic and thermal Enthalpies= -752.160210
Sum of electronic and thermal Free Energies= -752.217131

72 TS$^{\text{via async HA_NH2 + add}}$_N2-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	1.949938	-1.198685	0.233134
C2	1.023397	0.884950	0.020573
C3	0.011285	1.869012	-0.229444
O4	0.132422	3.077194	-0.226446
N5	-1.228711	1.240572	-0.494409
H6	-1.933333	1.880709	-0.842068
C7	-1.395218	-0.144290	-0.625713
N8	-2.703912	-0.625737	-0.592693
H9	-3.350253	-0.122638	-1.205342
H10	-2.694851	-1.617715	-0.830432
N11	-0.423516	-1.027009	-0.336422
C12	0.719739	-0.446422	-0.055630
C13	3.035352	-0.092063	0.502045
O14	4.155897	-0.400753	0.764972
N15	2.379613	1.066396	0.347014
H16	2.832776	1.964474	0.454938
H17	-3.179886	0.203644	1.306918
H18	-5.235329	-1.573569	0.172662
H19	-5.416024	-0.611309	1.636194
C20	-4.918390	-0.648955	0.662440
N21	-3.483612	-0.690559	0.915988
H22	-5.262989	0.217110	0.076922
C23	2.389477	-2.142874	-0.844981
H24	1.847861	-1.727534	1.106462
H25	1.620833	-2.906095	-0.956295
H26	2.498783	-1.575122	-1.768568
H27	3.343425	-2.574486	-0.543626

Zero-point correction= 0.218765
Thermal correction to Energy= 0.233116
Thermal correction to Enthalpy= 0.234060
Thermal correction to Gibbs Free Energy= 0.175895
Sum of electronic and zero-point Energies= -752.170363
Sum of electronic and thermal Energies= -752.156012
Sum of electronic and thermal Enthalpies= -752.155068
Sum of electronic and thermal Free Energies= -752.213234

73 N3-NH$_2$CH$_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	-1.538002	-0.698764	-0.178367
C2	-0.448992	1.231501	0.016279
C3	0.606637	2.129596	0.166850
O4	0.687627	3.310628	0.360033
N5	1.977891	1.357007	0.102848
H6	2.326968	1.261554	1.070064
C7	2.011262	0.045160	-0.620438
N8	3.240476	-0.563131	-0.573659
H9	3.180864	-1.577469	-0.587697
N10	0.894269	-0.766902	-0.342622
C11	-0.311489	-0.137462	-0.167554
C12	-1.948633	-2.051871	-0.526273
H13	-1.560886	-2.328184	-1.509646
H14	-1.639203	-2.770564	0.234710
H15	-3.038712	-2.037020	-0.567606
C16	-2.532125	0.332212	-0.016850
O17	-3.720777	0.142889	-0.013153
N18	-1.816690	1.491626	0.101496
H19	-2.247661	2.399246	0.189898
H20	2.615192	2.012208	-0.359800
H21	3.954212	-0.190284	-1.187719
H22	0.617245	-2.715057	-0.632025
H23	-0.039404	-2.158739	1.793416
H24	1.711607	-1.873633	1.988361
C25	0.957105	-2.411020	1.409225
N26	1.135403	-2.105283	-0.011674
H27	1.128968	-3.480767	1.539427

Zero-point correction= 0.220690
Thermal correction to Energy= 0.234986
Thermal correction to Enthalpy= 0.235930
Thermal correction to Gibbs Free Energy= 0.179637
Sum of electronic and zero-point Energies= -752.203999
Sum of electronic and thermal Energies= -752.189703
Sum of electronic and thermal Enthalpies= -752.188759
Sum of electronic and thermal Free Energies= -752.245052

74 TS$^{\text{via async add + PT}}$_N3-NH$_2CH_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	-1.630827	-0.604715	-0.354400
C2	-0.276343	1.110386	0.032548
C3	0.970635	1.785471	0.234537
O4	1.220395	2.925698	0.508000
N5	2.084121	0.784391	0.106532
H6	1.954902	-0.076174	0.990156
C7	1.813466	-0.222750	-0.929939
N8	2.912073	-0.876348	-1.440734
H9	2.673608	-1.679713	-2.011592
N10	0.802055	-1.075979	-0.348912
C11	-0.338852	-0.231456	-0.231603
C12	-2.180430	-1.917208	-0.651664
H13	-1.378729	-2.560039	-1.014721
H14	-2.635480	-2.346610	0.243501
H15	-2.948896	-1.809036	-1.417835
C16	-2.461279	0.538581	-0.179477

O17	-3.664721	0.549504	-0.239684
N18	-1.577035	1.576853	0.061547
H19	-1.875453	2.531601	0.196360
H20	2.982402	1.266651	0.071930
H21	3.616493	-0.296207	-1.882022
H22	2.019034	-2.101199	0.873384
H23	-0.208913	-2.649809	1.659311
H24	-0.335521	-0.956592	2.231435
C25	0.347431	-1.776203	2.008784
N26	1.345821	-1.349292	1.017921
H27	0.889944	-2.029773	2.920778

Zero-point correction= 0.217061
Thermal correction to Energy= 0.230582
Thermal correction to Enthalpy= 0.231526
Thermal correction to Gibbs Free Energy= 0.177175
Sum of electronic and zero-point Energies= -752.186716
Sum of electronic and thermal Energies= -752.173195
Sum of electronic and thermal Enthalpies= -752.172251
Sum of electronic and thermal Free Energies= -752.226602

75 $TS^{via\ HA_NH2\ products}$_N3-$NHCH_3$[9MOG + H_{N1}]$^+$

N1	-1.555415	-0.567064	-0.412775
C2	-0.296204	1.202208	0.030363
C3	0.857368	1.968396	0.199279
O4	1.099531	3.103742	0.488153
N5	2.136363	1.049007	-0.047929
H6	2.584597	0.927968	0.871680
C7	1.960504	-0.279686	-0.706705
N8	3.122700	-0.941751	-0.915354
H9	3.037443	-1.933829	-1.092656
N10	0.812101	-0.933876	-0.571982
C11	-0.285391	-0.136214	-0.331171
C12	-2.031154	-1.880154	-0.816184
H13	-1.365503	-2.285380	-1.578915
H14	-2.082268	-2.553490	0.043562
H15	-3.035174	-1.754162	-1.221872
C16	-2.452054	0.509287	-0.119314
O17	-3.652971	0.439216	-0.128912
N18	-1.627870	1.579876	0.148104
H19	-1.977508	2.504830	0.348690
H20	2.767958	1.646901	-0.591158
H21	3.908709	-0.485605	-1.357260
H22	0.465915	-2.936267	0.327367
H23	-0.766522	-1.613463	1.898157
H24	0.782739	-0.875017	2.399134
C25	0.315271	-1.774974	1.989773
N26	1.001902	-2.195177	0.782592
H27	0.468627	-2.576434	2.724512

Zero-point correction= 0.215859
Thermal correction to Energy= 0.230800
Thermal correction to Enthalpy= 0.231744
Thermal correction to Gibbs Free Energy= 0.173685
Sum of electronic and zero-point Energies= -752.177345
Sum of electronic and thermal Energies= -752.162405
Sum of electronic and thermal Enthalpies= -752.161460
Sum of electronic and thermal Free Energies= -752.219519

76 N3-NH_2CH_3[9MOG + H_{C2}]$^{\bullet+}$

N1	-1.514501	-0.723681	-0.061623
C2	-0.364527	1.202461	0.044394
C3	0.739095	2.128790	-0.250048
O4	0.581525	3.326582	-0.352597
N5	1.897864	1.436314	-0.511128
H6	2.699848	1.978235	-0.806041
C7	2.105672	0.096011	-0.013204
N8	2.251126	0.129192	1.421435
H9	2.875105	0.873504	1.714223
H10	2.582212	-0.748820	1.807757
N11	0.923810	-0.759425	-0.326575
C12	-0.265423	-0.207756	-0.108137
C13	-1.968497	-2.110294	-0.094234
H14	-3.040837	-2.091803	0.101482
H15	-1.801618	-2.553606	-1.076796
H16	-1.472087	-2.690883	0.683989
C17	-2.441949	0.335494	0.166467
O18	-3.627668	0.227102	0.289267
N19	-1.664662	1.496939	0.220272
H20	-2.053177	2.429002	0.308986
H21	2.923833	-0.361674	-0.577679
H22	0.486866	-2.259432	-1.551585
C23	1.411021	-3.076033	0.151785
H24	1.478604	-4.021611	-0.387699
H25	2.376459	-2.906411	0.634603
H26	0.633106	-3.150322	0.920947
N27	1.161858	-2.027581	-0.834906

Zero-point correction= 0.220897
Thermal correction to Energy= 0.235136
Thermal correction to Enthalpy= 0.236080
Thermal correction to Gibbs Free Energy= 0.179626
Sum of electronic and zero-point Energies= -752.253280
Sum of electronic and thermal Energies= -752.239040
Sum of electronic and thermal Enthalpies= -752.238096
Sum of electronic and thermal Free Energies= -752.294550

77 $TS^{via\ PT\ in\ adduct}$_N3-NH_2CH_3[9MOG + H_{C2}]$^{\bullet+}$

N1	-1.576781	-0.723263	0.244354
C2	-0.454744	1.152587	-0.154941
C3	0.683923	2.029544	-0.338610
O4	0.663553	3.196830	-0.647486
N5	1.913137	1.357034	-0.119965
H6	2.739477	1.934696	-0.219328
C7	2.026662	0.065562	0.420545
N8	2.613871	-0.057372	1.657507
H9	2.684884	-0.981452	2.062847
H10	3.295905	0.626460	1.959191
N11	0.901002	-0.836357	0.205591
C12	-0.334328	-0.175633	0.095447
C13	-1.941994	-2.091211	0.560034
H14	-1.186234	-2.529230	1.214423
H15	-2.903021	-2.065308	1.075012
H16	-2.054685	-2.688652	-0.348904
C17	-2.543039	0.299873	0.088907
O18	-3.740340	0.166292	0.168036
N19	-1.801021	1.446262	-0.156243
H20	-2.215835	2.358730	-0.275222
H21	2.577647	-0.673207	-0.525257
H22	1.006621	-1.040135	-1.847153
H23	0.294377	-3.280118	-0.981591
H24	1.864276	-3.315494	-0.135490
C25	1.332795	-2.935786	-1.008082
N26	1.389902	-1.476298	-1.003090
H27	1.814465	-3.290926	-1.919795

Zero-point correction= 0.213757
Thermal correction to Energy= 0.228161
Thermal correction to Enthalpy= 0.229105
Thermal correction to Gibbs Free Energy= 0.172117
Sum of electronic and zero-point Energies= -752.179123
Sum of electronic and thermal Energies= -752.164719
Sum of electronic and thermal Enthalpies= -752.163775

Sum of electronic and thermal Free Energies= -752.220764

78 $TS^{via\ async\ HA_NH2\ +\ add}$_N3-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$

N1	-1.394974	-1.091109	0.259643
C2	-0.733125	1.030002	-0.152565
C3	0.216386	2.141040	-0.454627
O4	-0.164214	3.182634	-0.942068
N5	1.484588	1.725429	-0.222060
H6	2.222418	2.367602	-0.486404
C7	1.842325	0.573470	0.608973
N8	1.772706	0.964914	2.005126
H9	2.400883	1.739567	2.196644
H10	2.027239	0.191215	2.612263
N11	0.944509	-0.577890	0.499059
C12	-0.280267	-0.277370	0.238341
C13	-1.424136	-2.493266	0.658713
H14	-2.468040	-2.796383	0.733208
H15	-0.918804	-3.106604	-0.089088
H16	-0.933350	-2.605307	1.626465
C17	-2.524862	-0.356427	-0.042424
O18	-3.672665	-0.674359	-0.102298
N19	-2.022360	0.994809	-0.296208
H20	-2.617917	1.771124	-0.579258
H21	2.819997	0.238747	0.254190
H22	1.106323	-1.906894	-1.820880
C23	2.770582	-2.515147	-0.874162
H24	3.278825	-2.944759	-1.752419
H25	3.537019	-2.111525	-0.208444
H26	2.244677	-3.339624	-0.376515
N27	1.900438	-1.470036	-1.338178

Zero-point correction= 0.214746
Thermal correction to Energy= 0.229939
Thermal correction to Enthalpy= 0.230883
Thermal correction to Gibbs Free Energy= 0.170927
Sum of electronic and zero-point Energies= -752.189413
Sum of electronic and thermal Energies= -752.174220
Sum of electronic and thermal Enthalpies= -752.173275
Sum of electronic and thermal Free Energies= -752.233232

79 N3-NH_2CH_3[9MOG + H_{N2}]$^{\bullet+}$

N1	-1.544468	-0.711030	-0.192557
C2	-0.464881	1.213616	0.084219
C3	0.636660	2.123471	0.179249
O4	0.608367	3.318171	0.368968
N5	1.882315	1.449856	-0.008764
H6	2.668116	2.028151	0.270716
C7	2.048330	0.076806	0.008518
N8	3.187663	-0.425009	-0.829723
H9	4.095183	-0.164897	-0.438459
H10	3.091040	-1.454494	-0.786691
N11	0.930776	-0.724269	-0.260575
C12	-0.314100	-0.128776	-0.109917
C13	-1.928166	-2.056865	-0.582882
H14	-1.512836	-2.310754	-1.562280
H15	-1.637046	-2.794521	0.168286
H16	-3.016996	-2.053276	-0.657006
C17	-2.536619	0.307290	-0.049605
O18	-3.729646	0.128177	-0.093389
N19	-1.824328	1.469899	0.126382
H20	-2.254783	2.374319	0.247143
H21	3.144494	-0.114777	-1.811312
H22	0.655552	-2.650594	-0.630772
H23	-0.088960	-2.262497	1.739382
H24	1.625856	-1.905881	2.062326
N25	1.190969	-2.085667	0.019625
C26	0.940276	-2.460783	1.419541
H27	1.151118	-3.526582	1.518578

Zero-point correction= 0.221846
Thermal correction to Energy= 0.235944
Thermal correction to Enthalpy= 0.236888
Thermal correction to Gibbs Free Energy= 0.181197
Sum of electronic and zero-point Energies= -752.213751
Sum of electronic and thermal Energies= -752.199653
Sum of electronic and thermal Enthalpies= -752.198709
Sum of electronic and thermal Free Energies= -752.254401

80 $TS^{via\ async\ add\ +\ PT}$_N3-$NH_2CH_3$[9MOG + H_{N2}]$^{\bullet+}$

N1	-1.592872	-0.716641	-0.282956
C2	-0.430923	1.149753	0.038552
C3	0.718290	2.021522	0.106107
O4	0.727850	3.201768	0.368093
N5	1.924106	1.323341	-0.172879
H6	2.692272	1.956603	-0.370954
C7	1.969863	0.055202	-0.755305
N8	3.167701	-0.722226	-0.502903
H9	3.808627	-0.284781	0.160301
H10	2.531720	-1.663766	-0.002692
N11	0.852779	-0.825199	-0.553703
C12	-0.343199	-0.168588	-0.269016
C13	-1.988090	-2.057413	-0.666895
H14	-1.510680	-2.337505	-1.609116
H15	-1.749379	-2.784468	0.116103
H16	-3.070818	-2.043970	-0.801194
C17	-2.536842	0.303386	0.007268
O18	-3.735294	0.165472	0.055932
N19	-1.771362	1.439306	0.202306
H20	-2.167949	2.351057	0.375560
H21	3.673817	-0.974581	-1.351308
H22	0.854824	-2.788286	-0.116573
H23	-0.169785	-1.731024	1.890258
H24	1.393027	-0.907247	2.118066
N25	1.232976	-1.935171	0.289366
C26	0.907245	-1.802262	1.724701
H27	1.302501	-2.683421	2.232262

Zero-point correction= 0.217761
Thermal correction to Energy= 0.231290
Thermal correction to Enthalpy= 0.232234
Thermal correction to Gibbs Free Energy= 0.177460
Sum of electronic and zero-point Energies= -752.211686
Sum of electronic and thermal Energies= -752.198157
Sum of electronic and thermal Enthalpies= -752.197213
Sum of electronic and thermal Free Energies= -752.251986

81 N3-NH_2CH_3[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.578539	-0.597793	-0.252603
C2	-0.361921	1.334962	-0.232110
C3	0.816907	2.091274	-0.032717
O4	0.927310	3.247913	0.322450
N5	1.998846	1.295709	-0.270831
H6	2.865353	1.817087	-0.203354
C7	2.023506	-0.047844	-0.146028
N8	3.184759	-0.673823	0.040472
H9	4.028724	-0.159798	0.242305
H10	3.224055	-1.679084	0.102584
N11	0.877669	-0.743648	-0.241057
C12	-0.346243	-0.069936	-0.754503
C13	-2.203379	-1.804055	-0.787747
H14	-2.078136	-1.846162	-1.874405
H15	-1.769742	-2.697173	-0.340044
H16	-3.266214	-1.757612	-0.548729

C17	-2.381849	0.414848	0.261922
O18	-3.517339	0.338140	0.641814
N19	-1.592956	1.589321	0.253101
H20	-1.884273	2.445028	0.707984
H21	-0.308543	-0.131012	-1.855136
H22	1.392346	-2.586875	-0.879940
H23	-0.103128	-2.357609	1.676872
H24	1.670710	-2.463177	1.793775
N25	0.843335	-2.123132	-0.167078
C26	0.800060	-2.704423	1.170425
H27	0.734792	-3.787426	1.054494

Zero-point correction= 0.219834
Thermal correction to Energy= 0.234358
Thermal correction to Enthalpy= 0.235303
Thermal correction to Gibbs Free Energy= 0.178351
Sum of electronic and zero-point Energies= -752.263032
Sum of electronic and thermal Energies= -752.248508
Sum of electronic and thermal Enthalpies= -752.247563
Sum of electronic and thermal Free Energies= -752.304515

82 $TS^{via\ async\ add\ +\ PT}$_N3-$NH_2CH_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	1.481727	-0.928044	-0.344884
C2	0.639341	1.010890	0.433179
C3	-0.325467	2.058421	0.390557
O4	-0.192483	3.240729	0.661176
N5	-1.583087	1.603113	-0.174174
H6	-2.183539	2.380417	-0.435762
C7	-1.802927	0.382645	-0.684252
N8	-2.660086	0.160945	-1.684843
H9	-3.082165	0.911277	-2.213699
H10	-2.772736	-0.781743	-2.026965
N11	-1.048977	-0.695853	-0.200694
C12	0.330658	-0.361411	0.234849
C13	1.706046	-2.356972	-0.465685
H14	1.670912	-2.844935	0.515274
H15	0.955526	-2.792216	-1.128086
H16	2.694188	-2.505750	-0.900985
C17	2.552884	-0.051007	-0.175947
O18	3.721598	-0.260443	-0.376439
N19	1.984009	1.143434	0.314005
H20	2.515562	1.993920	0.440392
H21	-0.354598	-1.026759	1.410129
H22	-2.156523	-0.481921	1.541902
H23	-1.504954	-3.212646	0.596359
H24	-3.123221	-2.465360	0.419756
N25	-1.566282	-1.183336	1.079842
C26	-2.213759	-2.503361	1.023012
H27	-2.463151	-2.793610	2.044742

Zero-point correction= 0.213717
Thermal correction to Energy= 0.227912
Thermal correction to Enthalpy= 0.228857
Thermal correction to Gibbs Free Energy= 0.172458
Sum of electronic and zero-point Energies= -752.170735
Sum of electronic and thermal Energies= -752.156539
Sum of electronic and thermal Enthalpies= -752.155595
Sum of electronic and thermal Free Energies= -752.211994

83 N3-NH_2CH_3[9MOG + HC5]$^{\bullet+}$

N1	-1.213267	-1.117983	-0.062777
C2	-0.841233	1.083366	-0.743017
C3	-0.208012	2.083765	0.231983
O4	-0.784855	2.960704	0.814526
N5	1.169356	1.860779	0.375429
H6	1.679130	2.559884	0.904549
C7	1.832058	0.744749	-0.064699
N8	3.162457	0.804688	-0.265929
H9	3.621222	1.699219	-0.347389
H10	3.684383	-0.006578	-0.554723
N11	1.110747	-0.377367	-0.311150
C12	-0.246446	-0.261342	-0.465603
C13	-1.102617	-2.494915	0.386852
H14	-0.585015	-3.096094	-0.360276
H15	-0.570841	-2.545418	1.340584
H16	-2.120114	-2.859816	0.528487
C17	-2.477765	-0.445106	-0.074855
O18	-3.518321	-0.948224	0.251018
N19	-2.230214	0.828717	-0.516949
H20	-2.930202	1.551786	-0.446791
H21	-0.631282	1.426697	-1.769083
H22	2.134004	-1.714123	-1.394746
H23	1.776134	-2.223713	1.517920
H24	3.330155	-1.580827	0.945924
C25	2.444060	-2.159369	0.656964
N26	1.698437	-1.634041	-0.482606
H27	2.754943	-3.171302	0.393314

Zero-point correction= 0.218679
Thermal correction to Energy= 0.233660
Thermal correction to Enthalpy= 0.234604
Thermal correction to Gibbs Free Energy= 0.176518
Sum of electronic and zero-point Energies= -752.246396
Sum of electronic and thermal Energies= -752.231416
Sum of electronic and thermal Enthalpies= -752.230471
Sum of electronic and thermal Free Energies= -752.288558

84 $TS^{via\ PT\ in\ adduct}$_N3-NH_2CH_3[9MOG + H_{C5}]$^{\bullet+}$

N1	1.503377	-0.518571	-0.563641
C2	0.117562	0.937570	0.542189
C3	-1.048530	1.770816	0.161875
O4	-1.236714	2.944294	0.331875
N5	-2.057202	0.914310	-0.386922
H6	-2.881719	1.382793	-0.746068
C7	-1.757891	-0.362341	-0.787722
N8	-2.463562	-0.976912	-1.741295
H9	-2.958028	-0.456363	-2.451767
H10	-2.298109	-1.959696	-1.903502
N11	-0.854744	-1.160705	-0.027083
C12	0.222912	-0.269996	-0.260123
C13	2.080233	-1.691047	-1.197062
H14	1.679519	-2.596985	-0.738616
H15	1.864703	-1.688270	-2.267938
H16	3.159156	-1.638971	-1.049228
C17	2.308831	0.601986	-0.117161
O18	3.495809	0.682380	-0.285972
N19	1.446055	1.438835	0.539464
H20	1.750292	2.313513	0.938686
H21	-0.447933	0.182616	1.463795
H22	-2.109591	-1.175238	1.601688
H23	0.711583	-1.944167	1.995311
H24	-0.626360	-3.109715	1.782968
C25	-0.357379	-2.114201	2.143192
N26	-1.107667	-1.058847	1.449078
H27	-0.574501	-2.026406	3.209101

Zero-point correction= 0.214078
Thermal correction to Energy= 0.228330
Thermal correction to Enthalpy= 0.229274
Thermal correction to Gibbs Free Energy= 0.172834
Sum of electronic and zero-point Energies= -752.173713

Sum of electronic and thermal Energies= -752.159462
Sum of electronic and thermal Enthalpies= -752.158518
Sum of electronic and thermal Free Energies= -752.214958

85 $TS^{via\ HA_NH2\ products}$_N3-$NH_2CH_3$[9MOG + H_{C5}]$^{\bullet+}$

N1	-1.440282	-0.858146	-0.265637
C2	-0.554524	1.244938	-0.576601
C3	0.453172	1.943908	0.358252
O4	0.166100	2.848297	1.096178
N5	1.714160	1.405112	0.200380
H6	2.468573	1.797794	0.754355
C7	1.893922	0.264832	-0.585720
N8	3.130013	0.005813	-1.082113
H9	3.763801	0.776705	-1.237142
H10	3.219223	-0.765855	-1.727954
N11	0.934347	-0.698688	-0.627896
C12	-0.311408	-0.236877	-0.507631
C13	-1.756749	-2.284706	-0.184727
H14	-1.175987	-2.823409	-0.929999
H15	-1.520498	-2.664832	0.807045
H16	-2.825255	-2.374443	-0.379305
C17	-2.515307	0.126685	-0.061205
O18	-3.641505	-0.179266	0.191820
N19	-1.928596	1.342752	-0.214165
H20	-2.433186	2.207093	-0.084591
H21	-0.352312	1.604273	-1.597830
H22	1.688217	-2.708807	-0.254220
H23	1.239788	-1.154821	2.200022
H24	2.813481	-1.307377	1.353962
C25	1.849855	-1.792724	1.555657
N26	1.091216	-2.170448	0.375213
H27	2.057625	-2.719688	2.103058

Zero-point correction= 0.216621
Thermal correction to Energy= 0.230989
Thermal correction to Enthalpy= 0.231933
Thermal correction to Gibbs Free Energy= 0.175441
Sum of electronic and zero-point Energies= -752.219439
Sum of electronic and thermal Energies= -752.205071
Sum of electronic and thermal Enthalpies= -752.204127
Sum of electronic and thermal Free Energies= -752.260619

86 N3-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$

N1	1.418462	0.884550	-0.199679
C2	0.694338	-1.250549	0.274868
C3	-0.278874	-2.273051	-0.084071
O4	0.095189	-2.075989	1.275818
N5	-1.578525	-1.805495	-0.456868
H6	-2.321267	-2.489389	-0.506599
C7	-1.931263	-0.503171	-0.430125
N8	-3.211052	-0.177578	-0.636987
H9	-3.912285	-0.884987	-0.789660
H10	-3.512940	0.782777	-0.627681
N11	-1.011048	0.465031	-0.235343
C12	0.306821	0.170560	0.187304
C13	1.589447	2.330327	-0.260570
H14	2.660682	2.514551	-0.345167
H15	1.080143	2.743402	-1.131175
H16	1.203283	2.796536	0.647798
C17	2.551461	0.037022	-0.173563
O18	3.694116	0.383414	-0.316496
N19	2.073969	-1.245893	0.033434
H20	2.697504	-2.016806	0.217013
H21	-0.017515	-3.224115	-0.536161
H22	-1.749591	2.159734	-1.027945
H23	-1.256914	2.080363	1.906987
H24	-2.918916	1.749049	1.365565
C25	-1.976591	2.246211	1.102062
N26	-1.384381	1.803059	-0.155918
H27	-2.150629	3.319685	1.016546

Zero-point correction= 0.219134
Thermal correction to Energy= 0.233628
Thermal correction to Enthalpy= 0.234572
Thermal correction to Gibbs Free Energy= 0.177927
Sum of electronic and zero-point Energies= -752.205931
Sum of electronic and thermal Energies= -752.191438
Sum of electronic and thermal Enthalpies= -752.190493
Sum of electronic and thermal Free Energies= -752.247138

87 $TS^{via\ HA_NH2\ products}$_N3-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$

N1	1.560609	0.800635	-0.338099
C2	0.572666	-1.193211	0.208300
C3	-0.524436	-2.116241	-0.099688
O4	-0.292113	-1.692238	1.234353
N5	-1.649960	-1.507292	-0.746477
H6	-2.352836	-2.111913	-1.149979
C7	-1.826104	-0.173057	-0.800067
N8	-2.996688	0.314670	-1.199871
H9	-3.808872	-0.264693	-1.348718
H10	-3.076445	1.303224	-1.386235
N11	-0.849502	0.724306	-0.476289
C12	0.364955	0.181675	-0.265408
C13	1.814926	2.184950	-0.698544
H14	2.878848	2.367574	-0.549587
H15	1.557836	2.356009	-1.746241
H16	1.226852	2.838077	-0.051455
C17	2.591646	-0.116788	-0.001808
O18	3.765398	0.129571	0.034134
N19	1.962701	-1.334007	0.238392
H20	2.466352	-2.113618	0.633451
H21	-0.414393	-3.173330	-0.315276
H22	-1.719037	2.569219	0.333480
H23	-1.677922	0.297155	2.205285
H24	-3.151948	0.965091	1.430061
C25	-2.146107	1.199785	1.804642
N26	-1.247962	1.824004	0.847995
H27	-2.254369	1.909649	2.633202

Zero-point correction= 0.216843
Thermal correction to Energy= 0.230906
Thermal correction to Enthalpy= 0.231850
Thermal correction to Gibbs Free Energy= 0.176176
Sum of electronic and zero-point Energies= -752.180877
Sum of electronic and thermal Energies= -752.166813
Sum of electronic and thermal Enthalpies= -752.165869
Sum of electronic and thermal Free Energies= -752.221544

88 N3-NH_2CH_3[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.523241	-0.889263	-0.188149
C2	-0.603675	1.130502	0.159892
C3	0.428123	2.059934	0.292587
O4	0.297150	3.396781	0.107198
N5	1.692582	1.535049	-0.150638
H6	2.405027	2.227810	-0.346394
C7	1.967828	0.248566	-0.348149
N8	3.217994	-0.152258	-0.605548
H9	3.997290	0.483321	-0.541493
H10	3.410389	-1.104662	-0.870215
N11	0.967813	-0.679278	-0.285751
C12	-0.342402	-0.198577	-0.090540
C13	-1.774508	-2.284907	-0.508235
H14	-1.323504	-2.544637	-1.467698

H15	-1.387515	-2.940984	0.271999
H16	-2.857456	-2.392931	-0.576542
C17	-2.582020	0.016983	0.018353
O18	-3.762890	-0.235512	-0.005628
N19	-1.972802	1.246394	0.247651
H20	-2.501508	2.100161	0.334227
H21	0.355583	3.872888	0.943934
H22	1.579628	-2.504739	-0.859702
H23	1.063740	-2.043804	2.031770
H24	2.750745	-1.915355	1.462848
N25	1.218069	-2.024053	-0.047508
C26	1.768995	-2.361700	1.260400
H27	1.856569	-3.448163	1.308477

Zero-point correction= 0.217837
Thermal correction to Energy= 0.233406
Thermal correction to Enthalpy= 0.234350
Thermal correction to Gibbs Free Energy= 0.174782
Sum of electronic and zero-point Energies= -752.234011
Sum of electronic and thermal Energies= -752.218442
Sum of electronic and thermal Enthalpies= -752.217498
Sum of electronic and thermal Free Energies= -752.277066

89 TS$^{\text{via async add + PT}}$_N3-NH$_2CH_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-1.710933	-0.790561	0.054711
C2	-0.532471	1.054396	-0.440838
C3	0.750716	1.784440	-0.318199
O4	1.114740	2.125254	0.880165
N5	1.781062	0.979733	-1.041201
H6	2.476608	1.445825	-1.612561
C7	1.699742	-0.328764	-0.954496
N8	2.361317	-1.207535	-1.686447
H9	2.917627	-0.936845	-2.485596
H10	2.224018	-2.191432	-1.501572
N11	0.800761	-0.869087	0.024123
C12	-0.467352	-0.298718	-0.321792
C13	-2.178889	-2.164428	-0.049478
H14	-2.326283	-2.449105	-1.095252
H15	-1.457087	-2.835464	0.418894
H16	-3.131420	-2.232016	0.475596
C17	-2.613032	0.283536	0.032626
O18	-3.811404	0.237859	0.166599
N19	-1.824024	1.421668	-0.221186
H20	-2.226732	2.342409	-0.319084
H21	1.229340	0.895329	1.343134
H22	0.435255	-0.626229	1.981472
H23	3.296176	-0.556727	1.253658
H24	2.414330	-2.016472	1.816097
N25	1.209900	-0.328551	1.384796
C26	2.469721	-0.927794	1.861674
H27	2.624287	-0.599863	2.890540

Zero-point correction= 0.215201
Thermal correction to Energy= 0.228917
Thermal correction to Enthalpy= 0.229861
Thermal correction to Gibbs Free Energy= 0.174714
Sum of electronic and zero-point Energies= -752.163992
Sum of electronic and thermal Energies= -752.150276
Sum of electronic and thermal Enthalpies= -752.149332
Sum of electronic and thermal Free Energies= -752.204478

90 TS$^{\text{via HA_NH2 products}}$_N3-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-1.637543	-0.745332	-0.285631
C2	-0.441871	1.123440	-0.025502
C3	0.740468	1.817053	0.066579
O4	0.964247	3.085947	0.402534
N5	1.867356	1.132494	-0.287881
H6	2.737036	1.654767	-0.275496
C7	1.838464	-0.164801	-0.721272
N8	2.973834	-0.731294	-1.199030
H9	3.718809	-0.155875	-1.563167
H10	2.863783	-1.629442	-1.647616
N11	0.756856	-0.970978	-0.494877
C12	-0.388026	-0.246954	-0.312163
C13	-2.047852	-2.125229	-0.499011
H14	-1.581739	-2.506350	-1.408679
H15	-1.749000	-2.733348	0.355871
H16	-3.132091	-2.125123	-0.607951
C17	-2.558186	0.296336	-0.007989
O18	-3.755791	0.202062	0.027581
N19	-1.778163	1.434054	0.196154
H20	-2.207573	2.344967	0.135270
H21	0.240813	3.469901	0.911516
H22	1.326559	-2.825860	0.415417
H23	1.227512	-0.549879	2.280588
H24	2.733070	-1.215893	1.565585
N25	0.860590	-2.028221	0.846870
C26	1.705856	-1.447978	1.878657
H27	1.761545	-2.178205	2.692722

Zero-point correction= 0.216094
Thermal correction to Energy= 0.231051
Thermal correction to Enthalpy= 0.231995
Thermal correction to Gibbs Free Energy= 0.174595
Sum of electronic and zero-point Energies= -752.225354
Sum of electronic and thermal Energies= -752.210397
Sum of electronic and thermal Enthalpies= -752.209453
Sum of electronic and thermal Free Energies= -752.266853

91 N3-NH$_2$CH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	1.456702	-0.930218	-0.131753
C2	0.574478	1.171138	-0.237138
C3	-0.388953	2.172835	0.140988
O4	-0.110185	3.304292	0.496520
N5	-1.677336	1.654128	0.103707
H6	-2.429773	2.320716	0.224447
C7	-1.992689	0.395724	-0.447734
N8	-3.299585	-0.058257	-0.486308
N9	-0.971821	-0.602624	-0.264261
C10	0.290501	-0.174120	-0.234036
C11	1.640715	-2.386165	-0.223747
H12	1.175565	-2.876080	0.629859
H13	1.198390	-2.755025	-1.146394
H14	2.715185	-2.566635	-0.217396
C15	2.542698	-0.113377	-0.006304
O16	3.706332	-0.339874	0.078829
N17	1.999080	1.323273	-0.020540
H18	2.486618	1.848932	-0.756204
H19	-3.856402	0.074479	0.353295
H20	2.221703	1.796820	0.867179
H21	-3.817907	0.199252	-1.316469
H22	-1.948120	-2.152461	-0.938357
H23	-0.995774	-2.233376	1.851276
H24	-2.680831	-1.862306	1.393585
N25	-1.256413	-1.973653	-0.215491
C26	-1.768888	-2.389310	1.094946
H27	-1.979401	-3.458549	1.033064

Zero-point correction= 0.220633
Thermal correction to Energy= 0.235220
Thermal correction to Enthalpy= 0.236164
Thermal correction to Gibbs Free Energy= 0.178802
Sum of electronic and zero-point Energies= -752.200316

Sum of electronic and thermal Energies= -752.185729
Sum of electronic and thermal Enthalpies= -752.184785
Sum of electronic and thermal Free Energies= -752.242147

92 TS$^{via\ async\ add\ +\ PT}$_N3-NH$_2CH_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	1.773916	-0.693525	-0.384896
C2	0.228565	0.938341	-0.793888
C3	-1.079440	1.441307	-0.750530
O4	-1.534340	2.540068	-0.495559
N5	-2.047335	0.330501	-0.975870
H6	-2.959878	0.583286	-1.343095
C7	-1.816096	-0.844493	-0.426814
N8	-2.697581	-1.822951	-0.337957
N9	-0.527479	-1.114695	0.124006
C10	0.440207	-0.475762	-0.790486
C11	2.540564	-1.906795	-0.628283
H12	2.009773	-2.767683	-0.216651
H13	2.693089	-2.048737	-1.700128
H14	3.506198	-1.802772	-0.133108
C15	2.332920	0.461683	0.090278
O16	3.453762	0.708655	0.436989
N17	1.196479	1.386387	0.200743
H18	1.465534	2.367013	0.265222
H19	-3.632991	-1.752665	-0.716019
H20	0.496515	0.734999	1.110394
H21	-2.378312	-2.719805	0.001998
H22	0.243106	-1.004529	1.975648
H23	-2.058563	0.817313	1.714619
H24	-2.148537	-0.846390	2.393300
N25	-0.307397	-0.338130	1.435972
C26	-1.508130	0.021169	2.217217
H27	-1.157081	0.404373	3.177422

Zero-point correction= 0.216100
Thermal correction to Energy= 0.229413
Thermal correction to Enthalpy= 0.230357
Thermal correction to Gibbs Free Energy= 0.176423
Sum of electronic and zero-point Energies= -752.134225
Sum of electronic and thermal Energies= -752.120911
Sum of electronic and thermal Enthalpies= -752.119967
Sum of electronic and thermal Free Energies= -752.173901

93 TS$^{via\ async\ HA_NH2\ +\ add}$_N3-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	1.624595	-0.762999	-0.294231
C2	0.370489	1.113802	-0.076555
C3	-0.807658	1.924889	0.100702
O4	-0.828125	3.082830	0.482758
N5	-1.934918	1.167691	-0.195791
H6	-2.826550	1.635793	-0.075519
C7	-1.875095	-0.117563	-0.719424
N8	-3.028398	-0.680023	-1.192229
N9	-0.797920	-0.946744	-0.492754
C10	0.342470	-0.217804	-0.307225
C11	1.968845	-2.169508	-0.511624
H12	1.680564	-2.749261	0.364876
H13	1.430676	-2.526792	-1.389641
H14	3.042947	-2.228538	-0.682849
C15	2.556570	0.187513	-0.041247
O16	3.740031	0.174303	0.053076
N17	1.747409	1.515469	0.113033
H18	2.089285	2.197157	-0.575721
H19	-3.704964	-0.070079	-1.630606
H20	1.925924	1.921656	1.040581
H21	-2.907102	-1.560376	-1.673771
H22	-1.290869	-2.791779	0.418815
H23	-1.187178	-0.522312	2.292348
H24	-2.688806	-1.185564	1.581036
N25	-0.828110	-1.982330	0.829476
C26	-1.660937	-1.420107	1.885699
H27	-1.705881	-2.161757	2.689289

Zero-point correction= 0.217586
Thermal correction to Energy= 0.232158
Thermal correction to Enthalpy= 0.233102
Thermal correction to Gibbs Free Energy= 0.176130
Sum of electronic and zero-point Energies= -752.190240
Sum of electronic and thermal Energies= -752.175668
Sum of electronic and thermal Enthalpies= -752.174724
Sum of electronic and thermal Free Energies= -752.231696

94 N3-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-1.506653	-0.794993	-0.188613
C2	-0.489662	1.158223	0.113025
C3	0.557172	2.162899	0.145172
O4	0.372914	3.355276	0.292499
N5	1.791854	1.576881	-0.063667
C6	2.101085	0.193415	-0.051726
N7	3.285429	-0.235920	-0.651827
H8	3.492199	0.159846	-1.565780
H9	4.099124	-0.230383	-0.052183
N10	0.981643	-0.678685	-0.301402
C11	-0.262617	-0.165548	-0.118210
C12	-1.836557	-2.200886	-0.451299
H13	-2.403267	-2.278628	-1.382290
H14	-0.895910	-2.738243	-0.555436
H15	-2.397424	-2.613128	0.390994
C16	-2.443884	0.166246	-0.008471
O17	-3.745008	0.009994	0.020307
N18	-1.864975	1.341462	0.163535
H19	-2.338304	2.224421	0.314744
H20	-4.034762	-0.889943	-0.177138
H21	2.580025	2.209763	-0.000094
H22	1.908181	-2.307532	-0.808653
H23	0.729776	-2.220164	1.895264
H24	2.456525	-1.937118	1.562220
C25	1.552097	-2.446006	1.211059
N26	1.169279	-2.063951	-0.154683
H27	1.718749	-3.524651	1.215202

Zero-point correction= 0.219668
Thermal correction to Energy= 0.234581
Thermal correction to Enthalpy= 0.235525
Thermal correction to Gibbs Free Energy= 0.177542
Sum of electronic and zero-point Energies= -752.224156
Sum of electronic and thermal Energies= -752.209243
Sum of electronic and thermal Enthalpies= -752.208299
Sum of electronic and thermal Free Energies= -752.266282

95 TS$^{via\ HA_NH2\ products}$_N3-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-1.611588	-0.718993	-0.298542
C2	-0.367971	1.099009	-0.020927
C3	0.819263	1.926599	0.101138
O4	0.852004	3.091188	0.451878
N5	1.937930	1.167976	-0.216745
C6	1.898509	-0.128035	-0.726339
N7	3.078927	-0.686876	-1.149455
H8	2.965960	-1.545021	-1.672219
H9	3.763276	-0.066534	-1.560632
N10	0.831883	-0.965655	-0.515360
C11	-0.308004	-0.226697	-0.302436
C12	-2.005982	-2.109042	-0.523297
H13	-2.195431	-2.282399	-1.583735
H14	-1.185596	-2.731861	-0.166973

H15	-2.889894	-2.341821	0.073908
C16	-2.423994	0.321155	-0.042096
O17	-3.730751	0.326806	0.055070
N18	-1.706210	1.429141	0.127559
H19	-2.079768	2.349030	0.328005
H20	-4.145711	-0.505324	-0.205200
H21	2.823942	1.654273	-0.136777
H22	1.480864	-2.753164	0.424118
H23	1.007113	-0.523179	2.281222
H24	2.612006	-1.041141	1.685269
C25	1.592908	-1.373696	1.920384
N26	0.896648	-2.012729	0.810259
H27	1.651710	-2.102615	2.734852

Zero-point correction= 0.216806
Thermal correction to Energy= 0.231632
Thermal correction to Enthalpy= 0.232576
Thermal correction to Gibbs Free Energy= 0.175346
Sum of electronic and zero-point Energies= -752.218281
Sum of electronic and thermal Energies= -752.203455
Sum of electronic and thermal Enthalpies= -752.202511
Sum of electronic and thermal Free Energies= -752.259741

96 N3-NH_2CH_3[9MOG + H_{N9}]$^{\bullet+}$

N1	1.316993	-1.203013	0.121887
C2	0.747810	0.955343	-0.430311
C3	0.016873	2.109210	-0.132810
O4	0.348821	3.280295	-0.075354
N5	-1.380288	1.769876	0.153271
H6	-1.951904	2.578236	0.369035
C7	-1.882495	0.538776	0.296102
N8	-3.176778	0.375610	0.595589
H9	-3.798732	1.167688	0.640873
H10	-3.588761	-0.539366	0.672507
N11	-1.075270	-0.538630	0.145899
C12	0.222070	-0.352413	-0.406182
C13	1.328561	-1.478886	1.600354
H14	1.252406	-0.525240	2.123583
H15	0.480865	-2.119775	1.836917
H16	2.267011	-1.977644	1.843194
C17	2.593421	-0.386469	-0.249701
O18	3.666424	-0.909104	-0.256370
N19	2.148139	0.859407	-0.464682
H20	2.773066	1.616940	-0.707164
H21	1.377009	-2.092987	-0.376967
H22	-2.059164	-2.143176	0.833364
H23	-1.558924	-1.900978	-2.087009
H24	-3.170728	-1.515835	-1.436604
N25	-1.579899	-1.839174	-0.005393
C26	-2.260026	-2.105430	-1.275443
H27	-2.511670	-3.166709	-1.295988

Zero-point correction= 0.220052
Thermal correction to Energy= 0.234603
Thermal correction to Enthalpy= 0.235547
Thermal correction to Gibbs Free Energy= 0.178835
Sum of electronic and zero-point Energies= -752.200402
Sum of electronic and thermal Energies= -752.185851
Sum of electronic and thermal Enthalpies= -752.184907
Sum of electronic and thermal Free Energies= -752.241619

97 $TS^{via\ async\ add\ +\ PT}$_N3-$NH_2CH_3$[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.566255	-0.677150	-0.299474
C2	-0.234621	1.175621	-0.304164
C3	0.996727	1.812920	-0.152600
O4	1.339977	2.920046	0.235390
N5	2.081805	0.859218	-0.548976
H6	2.978443	1.315330	-0.693995
C7	2.003860	-0.452901	-0.500319
N8	3.068708	-1.260749	-0.449491
H9	4.004633	-0.886284	-0.383516
H10	2.974867	-2.210578	-0.779581
N11	0.748464	-1.057319	-0.459250
C12	-0.330574	-0.136607	-0.807783
C13	-2.365367	-1.583508	-1.157478
H14	-2.630101	-1.077780	-2.087032
H15	-1.768881	-2.469296	-1.381724
H16	-3.265605	-1.863156	-0.611007
C17	-2.339515	0.477510	0.210901
O18	-3.494105	0.416737	0.526696
N19	-1.481041	1.541523	0.195683
H20	-1.774595	2.475240	0.445840
H21	-0.846423	-1.402207	0.587107
H22	0.566622	-2.702234	0.747594
H23	0.573409	-0.054032	2.095615
H24	1.944403	-1.206910	2.162808
N25	0.369629	-1.706111	0.811735
C26	0.861484	-1.106175	2.070390
H27	0.375109	-1.629405	2.895921

Zero-point correction= 0.215804
Thermal correction to Energy= 0.229483
Thermal correction to Enthalpy= 0.230427
Thermal correction to Gibbs Free Energy= 0.175767
Sum of electronic and zero-point Energies= -752.177795
Sum of electronic and thermal Energies= -752.164115
Sum of electronic and thermal Enthalpies= -752.163171
Sum of electronic and thermal Free Energies= -752.217831

98 $TS^{via\ async\ HA_NH2\ +\ add}$_N3-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$

N1	1.584966	-0.902784	0.103609
C2	0.418924	1.046498	0.084646
C3	-0.753531	1.912137	0.040322
O4	-0.753242	3.097636	-0.232761
N5	-1.895598	1.168568	0.315371
H6	-2.759852	1.699624	0.293686
C7	-1.914926	-0.165656	0.696045
N8	-3.109657	-0.732370	1.050791
H9	-3.804777	-0.138392	1.481881
H10	-3.030766	-1.637837	1.493523
N11	-0.857678	-1.009533	0.417529
C12	0.290218	-0.267804	0.293311
C13	2.083601	-1.747093	1.238692
H14	2.111320	-1.131503	2.137349
H15	1.389991	-2.577201	1.362977
H16	3.082024	-2.097343	0.979250
C17	2.547653	0.287991	-0.204318
O18	3.709423	0.112301	-0.377961
N19	1.752774	1.380774	-0.168949
H20	2.099481	2.320397	-0.316437
H21	1.492004	-1.499371	-0.735407
H22	-1.351060	-2.737225	-0.694905
H23	-1.131026	-0.269139	-2.291053
H24	-2.671045	-1.008955	-1.763866
N25	-0.866201	-1.890221	-0.984504
C26	-1.625818	-1.208827	-2.028828
H27	-1.612714	-1.847069	-2.917362

Zero-point correction= 0.217051
Thermal correction to Energy= 0.231523
Thermal correction to Enthalpy= 0.232468
Thermal correction to Gibbs Free Energy= 0.175871
Sum of electronic and zero-point Energies= -752.189384

Sum of electronic and thermal Energies= -752.174911
Sum of electronic and thermal Enthalpies= -752.173967
Sum of electronic and thermal Free Energies= -752.230563

99 C4-NHCH$_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	1.650772	-0.364641	-0.241667
C2	-0.005012	1.118502	0.277174
C3	-1.324450	1.566260	0.400620
O4	-1.867593	2.638413	0.512466
N5	-2.222391	0.278740	0.361831
H6	-3.202711	0.567809	0.387448
C7	-1.825074	-0.611249	-0.768315
N8	-2.839477	-1.047254	-1.535372
H9	-2.593548	-1.630011	-2.323857
N10	-0.602167	-0.932486	-0.879565
C11	0.262406	-0.372571	0.154133
C12	2.395605	-1.529135	-0.700882
H13	2.915507	-2.021410	0.124111
H14	1.702132	-2.223002	-1.178267
H15	3.132990	-1.197325	-1.432545
C16	2.192734	0.890679	-0.273554
O17	3.303336	1.241133	-0.561247
N18	1.133503	1.790275	0.102351
H19	1.247765	2.795753	0.066480
H20	-1.947778	-0.268323	1.212848
H21	-3.729257	-0.575401	-1.578923
H22	0.463719	-0.557446	2.172255
H23	-0.332047	-2.810147	2.453775
H24	-0.428679	-2.947032	0.692284
N25	-0.072666	-1.006161	1.433765
C26	0.103702	-2.466904	1.514632
H27	1.153483	-2.772645	1.482396

Zero-point correction= 0.220342
Thermal correction to Energy= 0.234489
Thermal correction to Enthalpy= 0.235433
Thermal correction to Gibbs Free Energy= 0.179901
Sum of electronic and zero-point Energies= -752.254386
Sum of electronic and thermal Energies= -752.240239
Sum of electronic and thermal Enthalpies= -752.239294
Sum of electronic and thermal Free Energies= -752.294826

100 TS$^{\text{via PT in adduct}}$_C4-NHCH$_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	1.660082	-0.407356	-0.180097
C2	0.027385	1.134638	0.240508
C3	-1.302424	1.563177	0.392490
O4	-1.843674	2.633258	0.539810
N5	-2.135588	0.265735	0.383863
H6	-3.120439	0.468345	0.556885
C7	-1.811845	-0.550300	-0.794798
N8	-2.839562	-0.937420	-1.566063
H9	-2.618083	-1.485880	-2.385501
N10	-0.587860	-0.890074	-0.944892
C11	0.261908	-0.358305	0.113094
C12	2.371660	-1.592790	-0.641872
H13	2.805759	-2.146413	0.193362
H14	1.680082	-2.225966	-1.200266
H15	3.176364	-1.270002	-1.303152
C16	2.229795	0.843898	-0.245609
O17	3.357017	1.149301	-0.515265
N18	1.186579	1.776007	0.069457
H19	1.331257	2.777070	0.030250
H20	-1.558014	-0.370071	1.179467
H21	-3.722126	-0.450079	-1.564520
H22	0.319392	-0.538558	2.167834
H23	-0.609173	-2.758242	2.406674
H24	-0.564752	-2.903157	0.638534
N25	-0.187032	-0.972977	1.398176
C26	-0.085905	-2.443553	1.503187
H27	0.953214	-2.775508	1.558957

Zero-point correction= 0.216954
Thermal correction to Energy= 0.230610
Thermal correction to Enthalpy= 0.231554
Thermal correction to Gibbs Free Energy= 0.176812
Sum of electronic and zero-point Energies= -752.255873
Sum of electronic and thermal Energies= -752.242217
Sum of electronic and thermal Enthalpies= -752.241273
Sum of electronic and thermal Free Energies= -752.296014

101 C4-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	1.673906	-0.267831	-0.199494
C2	-0.247794	0.768977	0.453579
C3	-1.734178	0.931168	0.626447
O4	-2.232905	1.641836	1.462991
N5	-2.342895	0.098020	-0.268864
H6	-3.354799	0.060516	-0.272086
C7	-1.590689	-0.364442	-1.432507
N8	-1.044128	0.803591	-2.106880
H9	-1.776191	1.463765	-2.356142
H10	-0.530083	0.552172	-2.946582
N11	-0.397809	-1.145267	-1.096045
C12	0.283795	-0.590010	0.051221
C13	2.656411	-1.242008	-0.658320
H14	3.597996	-0.718036	-0.820495
H15	2.804519	-2.023350	0.091842
H16	2.315850	-1.688670	-1.592895
C17	1.997599	0.989998	0.201258
O18	3.030275	1.586815	0.219186
N19	0.716230	1.586892	0.655537
H20	0.650664	2.540037	1.006191
H21	-2.253331	-0.997398	-2.028246
H22	0.931127	-1.520997	1.756402
H23	-0.839960	-2.973562	2.211192
H24	-1.795949	-2.306996	0.895618
N25	0.078914	-1.402778	1.224201
C26	-0.782569	-2.586087	1.193716
H27	-0.413791	-3.370646	0.526235

Zero-point correction= 0.219055
Thermal correction to Energy= 0.233575
Thermal correction to Enthalpy= 0.234519
Thermal correction to Gibbs Free Energy= 0.177681
Sum of electronic and zero-point Energies= -752.208044
Sum of electronic and thermal Energies= -752.193524
Sum of electronic and thermal Enthalpies= -752.192580
Sum of electronic and thermal Free Energies= -752.249418

102 TS$^{\text{via PT in adduct}}$_C4-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	1.747664	-0.226308	0.049294
C2	-0.255052	0.912765	0.051942
C3	-1.600659	1.243822	0.644946
O4	-1.849515	2.119634	1.429474
N5	-2.479521	0.329747	0.097239
H6	-3.392870	0.193342	0.511126
C7	-1.818879	-0.650049	-0.711003
N8	-2.493898	-1.025509	-1.857734
H9	-2.010610	-1.579318	-2.553393
H10	-3.468349	-0.799467	-2.009512
N11	-0.465769	-0.185705	-0.993793
C12	0.360496	-0.425033	0.220508
C13	2.649954	-1.217312	-0.535314
H14	3.517458	-0.675941	-0.914290

H15	2.992495	-1.933976	0.210979
H16	2.161870	-1.735606	-1.367291
C17	1.995178	1.136350	-0.234855
O18	3.048976	1.612268	-0.555066
N19	0.778758	1.810718	-0.102822
H20	0.683610	2.782023	-0.361200
H21	-1.606630	-1.579040	-0.013259
H22	-0.554540	-0.992976	1.976781
H23	-0.066931	-3.283799	1.990490
H24	0.788400	-3.134909	0.438777
N25	-0.162321	-1.396339	1.129962
C26	0.566737	-2.636837	1.383239
H27	1.499370	-2.444009	1.923730

Zero-point correction= 0.215625
Thermal correction to Energy= 0.229025
Thermal correction to Enthalpy= 0.229969
Thermal correction to Gibbs Free Energy= 0.176217
Sum of electronic and zero-point Energies= -752.189249
Sum of electronic and thermal Energies= -752.175849
Sum of electronic and thermal Enthalpies= -752.174905
Sum of electronic and thermal Free Energies= -752.228657

103 TS$^{\text{via async HA_NH2 + add}}$_C4-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	1.718448	0.520371	0.186426
C2	-0.077194	-0.876329	0.221111
C3	-1.520540	-1.271110	0.174369
O4	-1.856821	-2.430844	0.080897
N5	-2.288045	-0.155807	0.135763
H6	-3.287976	-0.312364	0.074465
C7	-1.833788	1.182931	0.561161
N8	-1.894057	1.243669	2.008687
H9	-2.845053	1.134611	2.349551
H10	-1.532659	2.131483	2.344965
N11	-0.461696	1.527793	0.229161
C12	0.329159	0.514073	-0.033423
C13	2.581034	1.692368	0.104696
H14	3.481727	1.492116	0.684385
H15	2.862426	1.896053	-0.931432
H16	2.048659	2.544136	0.528235
C17	2.188070	-0.740403	0.405811
O18	3.284743	-1.172810	0.574808
N19	0.963464	-1.586016	0.446434
H20	0.983826	-2.589222	0.627329
H21	-2.485834	1.892245	0.035516
H22	0.743930	1.262564	-2.142943
H23	-0.707763	0.434050	-3.746377
H24	-1.469567	-0.628264	-2.547992
N25	0.280498	0.369261	-1.945597
C26	-0.966319	0.329119	-2.684719
H27	-1.647916	1.153016	-2.441491

Zero-point correction= 0.215821
Thermal correction to Energy= 0.230554
Thermal correction to Enthalpy= 0.231499
Thermal correction to Gibbs Free Energy= 0.172823
Sum of electronic and zero-point Energies= -752.182370
Sum of electronic and thermal Energies= -752.167637
Sum of electronic and thermal Enthalpies= -752.166692
Sum of electronic and thermal Free Energies= -752.225368

104 C4-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	1.633280	-0.624497	-0.336966
C2	0.126524	1.002504	0.174222
C3	-1.139724	1.634613	0.067769
O4	-1.414552	2.818966	0.130252
N5	-2.178772	0.668163	-0.215035
H6	-3.107347	1.057731	-0.321609
C7	-1.818701	-0.568231	-0.647546
N8	-2.884869	-1.322760	-1.375800
H9	-3.202340	-0.836293	-2.222133
H10	-2.454087	-2.216134	-1.647342
N11	-0.718196	-1.177157	-0.572469
C12	0.315940	-0.502864	0.231360
C13	2.317566	-1.895291	-0.512912
H14	2.520458	-2.379364	0.445321
H15	1.702936	-2.553875	-1.128408
H16	3.258856	-1.692290	-1.023502
C17	2.292651	0.582870	-0.376575
O18	3.434040	0.810968	-0.679707
N19	1.336543	1.568045	0.003194
H20	1.515811	2.556886	-0.114950
H21	-3.699793	-1.520601	-0.784785
H22	1.153972	-0.882151	2.030765
H23	-0.676940	-1.373910	3.356243
H24	-1.741509	-1.420641	1.964521
C25	-0.873482	-0.908177	2.390099
N26	0.294591	-1.111595	1.543033
H27	-1.128605	0.147221	2.561324

Zero-point correction= 0.221131
Thermal correction to Energy= 0.235465
Thermal correction to Enthalpy= 0.236409
Thermal correction to Gibbs Free Energy= 0.180384
Sum of electronic and zero-point Energies= -752.246748
Sum of electronic and thermal Energies= -752.232414
Sum of electronic and thermal Enthalpies= -752.231470
Sum of electronic and thermal Free Energies= -752.287495

105 TS$^{\text{via async add + PT}}$_C4-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	1.575934	-0.609764	-0.304117
C2	0.051798	1.037282	0.064095
C3	-1.199041	1.689582	-0.107356
O4	-1.468601	2.869735	0.000544
N5	-2.216511	0.701680	-0.378390
H6	-3.176864	0.979834	-0.212850
C7	-1.867168	-0.511349	-0.868275
N8	-2.681407	-1.599499	-0.358967
H9	-3.660111	-1.432424	-0.115927
H10	-2.571496	-2.438452	-0.932575
N11	-0.696529	-0.932493	-1.184611
C12	0.175267	-0.451474	-0.129840
C13	2.221470	-1.844727	-0.712599
H14	2.220484	-2.586259	0.092748
H15	1.723653	-2.249142	-1.596335
H16	3.257970	-1.609517	-0.955428
C17	2.268427	0.575833	-0.139021
O18	3.450461	0.767631	-0.213513
N19	1.285855	1.566598	0.134437
H20	1.508851	2.553831	0.142861
H21	-1.858968	-1.656523	0.556842
H22	0.071561	-2.188780	0.961246
H23	-0.516875	-1.473941	3.121174
H24	-0.726615	0.180703	2.516563
C25	-0.166104	-0.746415	2.388032
N26	-0.400298	-1.286600	1.033573
H27	0.896330	-0.550116	2.561741

Zero-point correction= 0.216867
Thermal correction to Energy= 0.230097
Thermal correction to Enthalpy= 0.231041
Thermal correction to Gibbs Free Energy= 0.177310
Sum of electronic and zero-point Energies= -752.203231

Sum of electronic and thermal Energies= -752.190001
Sum of electronic and thermal Enthalpies= -752.189057
Sum of electronic and thermal Free Energies= -752.242788

106 TS$^{\text{via async HA_NH2 + add}}$_C4-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	1.619389	-0.682040	-0.463907
C2	0.213243	1.012755	-0.052163
C3	-1.030798	1.702437	-0.060473
O4	-1.275703	2.878960	0.099621
N5	-2.109941	0.774529	-0.331361
H6	-3.027520	1.204420	-0.366400
C7	-1.867359	-0.511422	-0.666817
N8	-3.030730	-1.307307	-1.132921
H9	-3.466451	-0.916293	-1.976749
H10	-2.656952	-2.238810	-1.359070
N11	-0.763497	-1.141714	-0.668697
C12	0.304220	-0.390249	-0.182551
C13	2.186086	-2.016921	-0.535758
H14	1.977427	-2.552275	0.393901
H15	1.763614	-2.556540	-1.384842
H16	3.261525	-1.905380	-0.672450
C17	2.402889	0.468072	-0.296017
O18	3.603118	0.552632	-0.351427
N19	1.488354	1.500607	-0.041446
H20	1.765586	2.463917	0.079677
H21	-3.752463	-1.415115	-0.410967
H22	0.838310	-0.264299	2.174506
H23	-0.936080	-1.231618	3.460586
H24	-1.766299	-1.583649	1.950591
C25	-1.060196	-0.891876	2.423193
N26	0.223133	-0.974134	1.763945
H27	-1.495500	0.116549	2.469895

Zero-point correction= 0.217282
Thermal correction to Energy= 0.231967
Thermal correction to Enthalpy= 0.232911
Thermal correction to Gibbs Free Energy= 0.175777
Sum of electronic and zero-point Energies= -752.206424
Sum of electronic and thermal Energies= -752.191739
Sum of electronic and thermal Enthalpies= -752.190795
Sum of electronic and thermal Free Energies= -752.247930

107 C4-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	1.582520	-0.351756	-0.434390
C2	-0.010603	1.095877	0.315430
C3	-1.338804	1.583569	0.400300
O4	-1.718392	2.710913	0.649342
N5	-2.303817	0.550669	0.097362
H6	-3.268126	0.800855	0.281383
C7	-2.017737	-0.532686	-0.642764
N8	-2.989413	-1.200226	-1.268264
H9	-3.912339	-0.806484	-1.373808
H10	-2.830303	-2.120481	-1.648818
N11	-0.743052	-0.918624	-0.758930
C12	0.268471	-0.379703	0.178844
C13	2.448149	-1.509257	-0.619378
H14	3.202992	-1.248360	-1.361219
H15	2.951465	-1.795386	0.308283
H16	1.866146	-2.354787	-0.991944
C17	2.148789	0.910453	-0.361916
O18	3.269458	1.235550	-0.645584
N19	1.132981	1.777153	0.115492
H20	1.233105	2.784122	0.111699
H21	-0.459257	-1.505478	-1.530952
H22	0.581291	-0.545777	2.177283
H23	-0.180915	-2.789715	2.518260
H24	-0.414639	-2.965046	0.785402
C25	0.209278	-2.487388	1.545414
N26	0.084331	-1.034928	1.441683
H27	1.231940	-2.866365	1.448107

Zero-point correction= 0.220169
Thermal correction to Energy= 0.234666
Thermal correction to Enthalpy= 0.235610
Thermal correction to Gibbs Free Energy= 0.179081
Sum of electronic and zero-point Energies= -752.300120
Sum of electronic and thermal Energies= -752.285623
Sum of electronic and thermal Enthalpies= -752.284679
Sum of electronic and thermal Free Energies= -752.341209

108 TS$^{\text{via PT in adduct}}$_C4-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	1.441141	-0.316035	-0.554100
C2	-0.124171	1.007219	0.424648
C3	-1.462885	1.508985	0.334985
O4	-1.817441	2.657521	0.498654
N5	-2.408844	0.508392	-0.035269
H6	-3.351537	0.862835	-0.150920
C7	-2.090639	-0.745451	-0.459485
N8	-3.077505	-1.552793	-0.853800
H9	-4.047110	-1.278174	-0.834770
H10	-2.843026	-2.452535	-1.245804
N11	-0.845897	-1.219750	-0.457264
C12	0.207094	-0.417850	0.148782
C13	2.016990	-1.351482	-1.398138
H14	3.058618	-1.088333	-1.583278
H15	1.976675	-2.321403	-0.898633
H16	1.482973	-1.418208	-2.348728
C17	1.966203	0.961548	-0.472644
O18	3.003394	1.371051	-0.915986
N19	1.006843	1.731894	0.242552
H20	1.044529	2.743879	0.241559
H21	-0.454340	-2.004056	0.484645
H22	-0.316445	-1.013301	2.079685
H23	1.494278	-2.215180	2.859819
H24	2.281657	-2.149250	1.274304
C25	1.645797	-1.604914	1.969274
N26	0.327602	-1.348236	1.361444
H27	2.132398	-0.667482	2.251298

Zero-point correction= 0.216167
Thermal correction to Energy= 0.230294
Thermal correction to Enthalpy= 0.231238
Thermal correction to Gibbs Free Energy= 0.175093
Sum of electronic and zero-point Energies= -752.262272
Sum of electronic and thermal Energies= -752.248145
Sum of electronic and thermal Enthalpies= -752.247201
Sum of electronic and thermal Free Energies= -752.303346

109 TS$^{\text{via HA_NH2 products}}$_C4-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	1.373874	-0.567835	-0.702424
C2	-0.087680	0.994426	-0.060396
C3	-1.382254	1.568080	0.052092
O4	-1.712273	2.722835	0.181597
N5	-2.411678	0.545767	-0.032688
H6	-3.352279	0.919015	0.038565
C7	-2.228862	-0.750000	-0.318791
N8	-3.266527	-1.583415	-0.410895
H9	-4.213647	-1.256237	-0.294198
H10	-3.146613	-2.545225	-0.690822
N11	-0.978807	-1.206633	-0.510037
C12	0.110029	-0.375903	-0.211789
C13	2.030007	-1.845485	-0.908089
H14	1.621737	-2.350883	-1.786960

H15	3.087684	-1.642275	-1.080201
H16	1.917212	-2.471971	-0.017919
C17	2.078060	0.656684	-0.654335
O18	3.246509	0.820268	-0.892453
N19	1.131688	1.597130	-0.255447
H20	1.334225	2.582314	-0.167830
H21	-0.818006	-2.205213	-0.459916
H22	-0.425969	-0.590715	2.265260
H23	1.633172	-0.856618	3.387535
H24	2.444456	-0.964377	1.816229
C25	1.580925	-0.543448	2.335704
N26	0.349220	-1.033977	1.760047
H27	1.658395	0.553958	2.330849

Zero-point correction= 0.216336
Thermal correction to Energy= 0.231124
Thermal correction to Enthalpy= 0.232068
Thermal correction to Gibbs Free Energy= 0.175142
Sum of electronic and zero-point Energies= -752.258122
Sum of electronic and thermal Energies= -752.243335
Sum of electronic and thermal Enthalpies= -752.242391
Sum of electronic and thermal Free Energies= -752.299317

110 C4-$^{+}$ṄCH$_3$[9MOG + H$_{C5}$]

N1	1.057037	-0.423066	-0.784858
C2	-0.015418	0.823755	0.861286
C3	-1.284345	1.500703	0.336939
O4	-1.387470	2.701264	0.302514
N5	-2.295405	0.649732	-0.056372
H6	-3.146285	1.100169	-0.372687
C7	-2.136471	-0.725168	-0.175864
N8	-3.234464	-1.406169	-0.540815
H9	-4.153850	-0.995213	-0.543827
H10	-3.160177	-2.408440	-0.622563
N11	-1.019677	-1.354165	0.024298
C12	0.141742	-0.616365	0.328405
C13	1.406805	-1.415750	-1.782834
H14	2.389208	-1.851666	-1.580643
H15	0.634775	-2.185302	-1.789557
H16	1.448961	-0.922841	-2.755705
C17	1.708946	0.834063	-0.711374
O18	2.563902	1.198569	-1.474350
N19	1.170282	1.491880	0.373297
H20	1.221078	2.503498	0.389137
H21	-0.076013	0.831157	1.955051
H22	0.780353	-2.455523	1.023624
H23	2.144878	-0.018306	2.123755
H24	1.940723	-1.551562	3.018161
N25	0.929116	-1.466073	1.217175
C26	2.066505	-1.099945	2.028318
H27	2.990085	-1.497369	1.591616

Zero-point correction= 0.218705
Thermal correction to Energy= 0.233170
Thermal correction to Enthalpy= 0.234114
Thermal correction to Gibbs Free Energy= 0.177279
Sum of electronic and zero-point Energies= -752.280497
Sum of electronic and thermal Energies= -752.266033
Sum of electronic and thermal Enthalpies= -752.265089
Sum of electronic and thermal Free Energies= -752.321924

111 TS$^{\text{via PT in adduct}}$_C4-$^{+}$ṄCH$_3$[9MOG + H$_{C5}$]

N1	1.406282	-0.482406	-0.546825
C2	-0.116689	0.973572	0.431205
C3	-1.525935	1.454453	0.204963
O4	-1.847802	2.612570	0.270701
N5	-2.400071	0.422808	-0.076310
H6	-3.363737	0.710146	-0.202885
C7	-2.017405	-0.891570	-0.376004
N8	-3.021473	-1.698522	-0.759978
H9	-3.940388	-1.359029	-0.992917
H10	-2.784161	-2.643205	-1.022345
N11	-0.810944	-1.356002	-0.284427
C12	0.194940	-0.508492	0.202568
C13	1.972324	-1.635879	-1.232400
H14	2.202015	-2.430365	-0.519769
H15	1.272525	-2.012589	-1.980295
H16	2.892677	-1.308300	-1.715678
C17	1.872324	0.800149	-0.736354
O18	2.849204	1.172341	-1.325704
N19	0.943672	1.664282	-0.081107
H20	1.021889	2.672883	-0.135523
H21	-0.013321	0.627456	1.692736
H22	-0.278419	-1.422423	2.072453
H23	2.382558	-0.081355	1.994059
H24	1.694674	-1.033705	3.329188
N25	0.422562	-0.781385	1.698870
C26	1.768137	-0.947865	2.245384
H27	2.236110	-1.846441	1.833254

Zero-point correction= 0.214218
Thermal correction to Energy= 0.228537
Thermal correction to Enthalpy= 0.229482
Thermal correction to Gibbs Free Energy= 0.172822
Sum of electronic and zero-point Energies= -752.239970
Sum of electronic and thermal Energies= -752.225650
Sum of electronic and thermal Enthalpies= -752.224706
Sum of electronic and thermal Free Energies= -752.281365

112 TS$^{\text{via HA_NH2 products}}$_C4-$^{+}$ṄCH$_3$[9MOG + H$_{C5}$]

N1	-1.145225	-0.112151	0.764910
C2	0.199883	0.818972	-0.859776
C3	1.542854	1.393387	-0.406030
O4	1.818738	2.561632	-0.449165
N5	2.457238	0.412846	-0.027870
H6	3.390797	0.748090	0.181245
C7	2.091485	-0.885764	0.289072
N8	3.081348	-1.722392	0.614536
H9	4.053180	-1.458132	0.602694
H10	2.837433	-2.655650	0.910063
N11	0.851282	-1.305361	0.333903
C12	-0.111808	-0.425015	-0.046624
C13	-1.649719	-0.930967	1.854741
H14	-2.033603	-1.880006	1.472451
H15	-0.855351	-1.125710	2.576327
H16	-2.458660	-0.373767	2.327256
C17	-1.696365	1.165880	0.437799
O18	-2.639432	1.664045	0.988816
N19	-0.938749	1.648803	-0.600481
H20	-0.966404	2.630661	-0.836249
H21	0.315071	0.578845	-1.921905
H22	-0.436328	-2.325795	-1.797461
H23	-2.936779	-0.968099	-0.971294
H24	-2.721087	-1.862761	-2.508518
N25	-0.994113	-1.562480	-1.403332
C26	-2.399889	-1.784427	-1.459518
H27	-2.663834	-2.740353	-0.981454

Zero-point correction= 0.215423
Thermal correction to Energy= 0.230286
Thermal correction to Enthalpy= 0.231230
Thermal correction to Gibbs Free Energy= 0.172886
Sum of electronic and zero-point Energies= -752.265521

Sum of electronic and thermal Energies= -752.250659
Sum of electronic and thermal Enthalpies= -752.249715
Sum of electronic and thermal Free Energies= -752.308058

113 C4-$^{+}$ṄHCH$_3$[9MOG + H$_{O6}$]

N1	1.530113	-0.268333	-0.454362
C2	-0.153286	1.065961	0.303202
C3	-1.447339	1.398813	0.272016
O4	-2.030368	2.603385	0.386640
N5	-2.367073	0.389640	0.009403
H6	-3.346894	0.608953	0.120521
C7	-1.952347	-0.805964	-0.529508
N8	-2.923121	-1.623462	-0.999938
H9	-3.792800	-1.244508	-1.340934
H10	-2.608735	-2.481289	-1.427596
N11	-0.704710	-1.180803	-0.569785
C12	0.207854	-0.373528	0.127667
C13	2.267487	-1.343739	-1.079792
H14	2.846208	-1.916098	-0.345497
H15	1.562656	-1.996802	-1.595459
H16	2.967571	-0.901238	-1.789671
C17	2.041844	1.043112	-0.323915
O18	3.130663	1.401680	-0.687887
N19	1.048167	1.802382	0.281602
H20	1.097107	2.802572	0.149961
H21	-1.506671	3.212396	0.917386
H22	0.916550	-0.344603	2.154693
H23	1.862505	-2.614700	1.669505
H24	0.360686	-2.689704	2.605051
C25	0.786071	-2.394207	1.640365
N26	0.564179	-0.986928	1.447102
H27	0.304874	-2.945653	0.833645

Zero-point correction= 0.217178
Thermal correction to Energy= 0.232255
Thermal correction to Enthalpy= 0.233199
Thermal correction to Gibbs Free Energy= 0.175667
Sum of electronic and zero-point Energies= -752.254019
Sum of electronic and thermal Energies= -752.238941
Sum of electronic and thermal Enthalpies= -752.237997
Sum of electronic and thermal Free Energies= -752.295529

114 TS$^{via\ PT\ in\ adduct}$_C4-$^{+}$ṄHCH$_3$[9MOG + H$_{O6}$]

N1	1.683763	0.348660	0.099695
C2	-0.001035	-0.674834	-1.061394
C3	-1.408829	-0.713923	-1.215747
O4	-1.962213	0.312717	-1.778294
N5	-1.989388	-1.344125	-0.125605
H6	-3.005642	-1.396043	-0.154358
C7	-1.488185	-0.641518	1.054488
N8	-2.194905	-0.912382	2.163979
H9	-2.777542	-1.733049	2.218028
H10	-1.891912	-0.492165	3.029499
N11	-0.510713	0.203530	1.059408
C12	0.268915	0.499268	-0.133965
C13	2.415835	1.169048	1.056969
H14	2.554671	2.176815	0.660402
H15	1.881729	1.205187	2.010066
H16	3.394390	0.711811	1.204200
C17	2.091188	-0.930523	-0.201785
O18	3.127939	-1.484236	0.028824
N19	0.983405	-1.546282	-0.893927
H20	1.021554	-2.508245	-1.208071
H21	-1.243295	1.143681	-1.577055
H22	0.584182	2.058612	-1.397357
H23	0.172222	3.132949	0.820188
H24	-0.839983	3.703325	-0.534115
C25	-0.601399	2.851457	0.102634
N26	-0.163332	1.745954	-0.778489
H27	-1.496936	2.547934	0.641707

Zero-point correction= 0.215144
Thermal correction to Energy= 0.228820
Thermal correction to Enthalpy= 0.229764
Thermal correction to Gibbs Free Energy= 0.175118
Sum of electronic and zero-point Energies= -752.215743
Sum of electronic and thermal Energies= -752.202067
Sum of electronic and thermal Enthalpies= -752.201123
Sum of electronic and thermal Free Energies= -752.255769

115 TS$^{via\ HA_NH2\ products}$_C4-$^{+}$ṄHCH$_3$[9MOG + H$_{O6}$]

N1	1.527667	-0.281093	-0.481797
C2	-0.129360	1.106706	0.183114
C3	-1.426388	1.437135	0.246454
O4	-2.016656	2.619619	0.464952
N5	-2.349720	0.429203	-0.007349
H6	-3.325612	0.661324	0.120185
C7	-1.965607	-0.768346	-0.552181
N8	-2.944399	-1.602846	-0.959853
H9	-3.860258	-1.260222	-1.203678
H10	-2.645933	-2.461413	-1.397366
N11	-0.710571	-1.131458	-0.663921
C12	0.195081	-0.300288	-0.061103
C13	2.249977	-1.378982	-1.096417
H14	2.774009	-1.981189	-0.347860
H15	1.541081	-1.998257	-1.646588
H16	2.989441	-0.957069	-1.777426
C17	2.094233	0.995682	-0.296743
O18	3.225969	1.310208	-0.554848
N19	1.085401	1.799740	0.234420
H20	1.189331	2.799748	0.143733
H21	-1.447219	3.231736	0.942931
H22	1.061169	-0.447692	2.191097
H23	1.733474	-2.712838	1.680352
H24	0.279145	-2.727811	2.680255
C25	0.671425	-2.428147	1.698488
N26	0.502506	-1.016758	1.549322
H27	0.124522	-2.944998	0.908098

Zero-point correction= 0.215563
Thermal correction to Energy= 0.230512
Thermal correction to Enthalpy= 0.231456
Thermal correction to Gibbs Free Energy= 0.174204
Sum of electronic and zero-point Energies= -752.250596
Sum of electronic and thermal Energies= -752.235647
Sum of electronic and thermal Enthalpies= -752.234703
Sum of electronic and thermal Free Energies= -752.291955

116 C4-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	1.238459	-0.202225	-0.648665
C2	-0.183435	0.883754	0.739301
C3	-1.446666	1.475080	0.332022
O4	-1.638109	2.678066	0.339694
N5	-2.364017	0.528810	-0.064513
H6	-3.263713	0.887647	-0.360826
C7	-2.010987	-0.807383	-0.325742
N8	-3.011249	-1.557745	-0.829629
N9	-0.840274	-1.318450	-0.137802
C10	0.205210	-0.521128	0.395925
C11	1.649513	-1.113665	-1.717378
H12	2.644598	-1.515805	-1.518409
H13	0.918362	-1.919800	-1.755519
H14	1.655793	-0.576959	-2.666981

C15	1.824099	0.982862	-0.498631
O16	2.710588	1.572117	-1.024648
N17	1.000770	1.682144	0.686758
H18	0.816955	2.673049	0.480589
H19	-3.973466	-1.261796	-0.814077
H20	1.561923	1.598212	1.543716
H21	-2.823777	-2.538343	-0.971874
H22	0.170338	-1.234716	2.267306
H23	2.543453	-2.115546	0.786080
H24	1.893208	-2.738460	2.295120
C25	1.617211	-2.327022	1.324025
N26	0.878146	-1.078171	1.554277
H27	1.033986	-3.074474	0.774414

Zero-point correction= 0.220285
Thermal correction to Energy= 0.234795
Thermal correction to Enthalpy= 0.235739
Thermal correction to Gibbs Free Energy= 0.178796
Sum of electronic and zero-point Energies= -752.249033
Sum of electronic and thermal Energies= -752.234523
Sum of electronic and thermal Enthalpies= -752.233579
Sum of electronic and thermal Free Energies= -752.290522

117 $TS^{via\ PT\ in\ adduct}$_C4-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	-1.123827	-0.215923	0.770163
C2	0.175418	0.903060	-0.681307
C3	1.421694	1.514776	-0.288855
O4	1.663405	2.703401	-0.300977
N5	2.338902	0.538067	0.100472
H6	3.248261	0.891170	0.372819
C7	2.051581	-0.824299	0.213724
N8	3.086025	-1.593954	0.591956
N9	0.889521	-1.370907	-0.006278
C10	-0.159062	-0.511988	-0.340559
C11	-1.424135	-1.089743	1.897354
H12	-2.393290	-1.577338	1.767456
H13	-0.636446	-1.841416	1.948361
H14	-1.434381	-0.504237	2.817546
C15	-1.777742	0.937441	0.529271
O16	-2.656562	1.523266	1.077079
N17	-1.132805	1.431166	-0.792451
H18	-1.282687	2.420165	-0.993315
H19	4.033459	-1.256930	0.638328
H20	-1.480432	0.500595	-1.504100
H21	2.928808	-2.587710	0.659279
H22	-0.383238	-1.087754	-2.293510
H23	-2.693106	-1.812601	-0.618154
H24	-2.344166	-2.321757	-2.272725
C25	-1.893542	-2.071822	-1.312369
N26	-1.007362	-0.909460	-1.506687
H27	-1.335964	-2.932989	-0.934574

Zero-point correction= 0.216557
Thermal correction to Energy= 0.230367
Thermal correction to Enthalpy= 0.231311
Thermal correction to Gibbs Free Energy= 0.176036
Sum of electronic and zero-point Energies= -752.235750
Sum of electronic and thermal Energies= -752.221940
Sum of electronic and thermal Enthalpies= -752.220995
Sum of electronic and thermal Free Energies= -752.276270

118 $TS^{via\ async\ HA_NH2\ +\ add}$_C4-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	1.554227	-0.627541	-0.491858
C2	0.120266	0.958739	0.312730
C3	-1.072920	1.707981	0.135315
O4	-1.211336	2.911526	0.259347
N5	-2.139264	0.864907	-0.252429
H6	-3.028320	1.337463	-0.366794
C7	-1.954353	-0.405469	-0.746083
N8	-3.025572	-1.029590	-1.260463
N9	-0.798509	-1.036783	-0.731381
C10	0.213479	-0.387195	-0.099464
C11	2.035548	-1.929187	-0.941755
H12	1.862441	-2.662597	-0.151820
H13	1.494209	-2.217012	-1.842946
H14	3.101012	-1.844127	-1.150798
C15	2.367876	0.416639	-0.260913
O16	3.540034	0.595361	-0.371171
N17	1.441463	1.552590	0.271329
H18	1.488010	2.360614	-0.364387
H19	-3.898804	-0.560618	-1.437881
H20	1.811602	1.880398	1.170563
H21	-2.884180	-1.944479	-1.660624
H22	0.726417	-0.663890	2.321363
H23	-1.550923	-2.281190	1.408574
H24	-0.867354	-2.259412	3.057023
C25	-1.043017	-1.664547	2.151866
N26	0.225403	-1.231850	1.630311
H27	-1.689210	-0.824153	2.443569

Zero-point correction= 0.216746
Thermal correction to Energy= 0.231548
Thermal correction to Enthalpy= 0.232492
Thermal correction to Gibbs Free Energy= 0.174462
Sum of electronic and zero-point Energies= -752.227672
Sum of electronic and thermal Energies= -752.212870
Sum of electronic and thermal Enthalpies= -752.211926
Sum of electronic and thermal Free Energies= -752.269956

119 C4-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$

N1	1.603850	-0.581207	-0.311277
C2	0.059327	0.960894	0.385682
C3	-1.201590	1.640249	0.222705
O4	-1.388739	2.828403	0.411054
N5	-2.190801	0.757574	-0.209030
C6	-1.873769	-0.458661	-0.819491
N7	-2.874679	-1.022658	-1.530551
H8	-3.638692	-0.476451	-1.894749
H9	-2.666721	-1.895258	-1.991473
N10	-0.732598	-1.062352	-0.711425
C11	0.193888	-0.532862	0.224594
C12	2.246249	-1.828096	-0.703826
H13	2.968016	-2.154052	0.048731
H14	1.457542	-2.575521	-0.783426
H15	2.718837	-1.717697	-1.683305
C16	2.157313	0.603994	-0.225625
O17	3.382019	0.947410	-0.513089
N18	1.296159	1.545213	0.223837
H19	1.489636	2.539559	0.237630
H20	3.928952	0.207625	-0.811899
H21	-3.119281	1.150016	-0.300969
H22	0.842101	-0.888612	2.121635
H23	-1.650161	-2.271483	1.392965
H24	-0.875007	-2.188283	2.973889
N25	0.216044	-1.312493	1.442971
C26	-1.074066	-1.628969	2.059009
H27	-1.671382	-0.744185	2.317277

Zero-point correction= 0.219771
Thermal correction to Energy= 0.234316
Thermal correction to Enthalpy= 0.235260
Thermal correction to Gibbs Free Energy= 0.178764
Sum of electronic and zero-point Energies= -752.278042

Sum of electronic and thermal Energies= -752.263498
Sum of electronic and thermal Enthalpies= -752.262554
Sum of electronic and thermal Free Energies= -752.319050

120 $TS^{via\ async\ add\ +\ PT}$_C4-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$

N1	1.284070	-0.036744	-1.046257
C2	-0.285027	1.118891	0.114598
C3	-1.687805	1.442654	0.156070
O4	-2.158449	2.556562	0.260721
N5	-2.468030	0.283291	0.077630
C6	-1.966306	-0.976828	-0.235279
N7	-2.890587	-1.931196	-0.442971
H8	-3.869360	-1.726217	-0.559134
H9	-2.561716	-2.845987	-0.710659
N10	-0.702519	-1.284364	-0.305505
C11	0.215609	-0.289783	-0.003012
C12	2.148333	-1.128395	-1.486227
H13	2.896675	-1.413337	-0.740570
H14	1.502379	-1.974394	-1.720731
H15	2.659916	-0.810306	-2.394657
C16	1.814494	1.063512	-0.458143
O17	2.921176	0.996448	0.180497
N18	0.807154	1.924992	-0.088036
H19	0.966690	2.831607	0.335940
H20	2.423421	0.189181	0.873619
H21	-3.467181	0.437813	0.131113
H22	0.694244	-0.087499	2.032921
H23	1.701671	-2.555201	0.784880
H24	1.886169	-2.057167	2.477685
N25	1.101059	-0.574583	1.235062
C26	1.240123	-2.001902	1.600311
H27	0.270722	-2.451251	1.820477

Zero-point correction= 0.215044
Thermal correction to Energy= 0.228616
Thermal correction to Enthalpy= 0.229560
Thermal correction to Gibbs Free Energy= 0.175395
Sum of electronic and zero-point Energies= -752.206719
Sum of electronic and thermal Energies= -752.193147
Sum of electronic and thermal Enthalpies= -752.192203
Sum of electronic and thermal Free Energies= -752.246368

121 $TS^{via\ HA_NH2\ products}$_C4-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$

N1	1.552116	-0.599381	-0.513472
C2	0.112227	1.008471	0.108954
C3	-1.136734	1.700722	0.076965
O4	-1.342344	2.880078	0.285476
N5	-2.170541	0.799966	-0.261035
C6	-1.976634	-0.486735	-0.724236
N7	-3.068459	-1.143424	-1.165010
H8	-3.920991	-0.664392	-1.405319
H9	-2.924669	-2.064324	-1.549615
N10	-0.814822	-1.093117	-0.725427
C11	0.191758	-0.373650	-0.149706
C12	2.093954	-1.928649	-0.752231
H13	2.347445	-2.402249	0.199381
H14	1.315388	-2.506912	-1.249200
H15	2.957089	-1.873308	-1.418807
C16	2.232488	0.514406	-0.238766
O17	3.524407	0.704513	-0.294589
N18	1.411066	1.503145	0.127166
H19	1.694760	2.454356	0.324366
H20	4.023773	-0.096373	-0.501283
H21	-3.092651	1.218525	-0.290090
H22	0.571465	-0.240512	2.240229
H23	-1.352009	-2.325761	1.520932
H24	-0.838957	-1.913988	3.169776
N25	0.285897	-1.043337	1.670440
C26	-0.991239	-1.517042	2.157682
H27	-1.758883	-0.733889	2.231941

Zero-point correction= 0.216609
Thermal correction to Energy= 0.231322
Thermal correction to Enthalpy= 0.232266
Thermal correction to Gibbs Free Energy= 0.175321
Sum of electronic and zero-point Energies= -752.249615
Sum of electronic and thermal Energies= -752.234903
Sum of electronic and thermal Enthalpies= -752.233959
Sum of electronic and thermal Free Energies= -752.290904

122 C4-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.434859	-1.033416	-0.162861
C2	-0.068232	0.866944	-0.118714
C3	1.164546	1.530761	-0.440105
O4	1.261596	2.669937	-0.857643
N5	2.263814	0.692436	-0.223232
H6	3.170042	1.109940	-0.394157
C7	2.128830	-0.686820	-0.112497
N8	3.258327	-1.400737	-0.270338
H9	4.095104	-1.011957	-0.673130
H10	3.198477	-2.401909	-0.168115
N11	1.010183	-1.298716	0.153017
C12	-0.082656	-0.489245	0.517216
C13	-1.269228	-1.956918	-1.325874
H14	-0.692340	-1.446918	-2.097440
H15	-0.727292	-2.834945	-0.982167
H16	-2.261638	-2.215408	-1.695554
C17	-2.209701	0.193065	-0.573378
O18	-3.366623	0.170802	-0.856767
N19	-1.308235	1.220664	-0.573376
H20	-1.542176	2.135336	-0.946014
H21	-1.946087	-1.509241	0.588025
H22	0.435988	-0.975940	2.401732
H23	-1.969225	0.760813	2.260224
H24	-0.382147	1.527466	2.513552
C25	-0.946695	0.592387	2.612854
N26	-0.335548	-0.537741	1.916908
H27	-1.015452	0.338381	3.670484

Zero-point correction= 0.219987
Thermal correction to Energy= 0.234545
Thermal correction to Enthalpy= 0.235489
Thermal correction to Gibbs Free Energy= 0.178480
Sum of electronic and zero-point Energies= -752.275710
Sum of electronic and thermal Energies= -752.261153
Sum of electronic and thermal Enthalpies= -752.260209
Sum of electronic and thermal Free Energies= -752.317217

123 $TS^{via\ PT\ in\ adduct}$_C4-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.609482	-0.755604	-0.098210
C2	-0.001266	0.945566	0.011414
C3	1.289300	1.511014	-0.276856
O4	1.514338	2.686798	-0.489276
N5	2.286026	0.524086	-0.302040
H6	3.221489	0.865213	-0.486576
C7	1.988883	-0.824648	-0.443362
N8	3.007981	-1.620060	-0.810641
H9	3.868898	-1.258225	-1.187279
H10	2.817628	-2.604129	-0.921342
N11	0.813954	-1.346327	-0.214143
C12	-0.155577	-0.498688	0.328552
C13	-1.935145	-1.923704	-0.942075
H14	-1.404182	-1.856766	-1.892518

H15	-1.633266	-2.828571	-0.416849
H16	-3.012436	-1.919760	-1.104006
C17	-2.182858	0.514178	-0.537832
O18	-3.286886	0.654067	-0.968780
N19	-1.206585	1.478124	-0.340411
H20	-1.338069	2.434832	-0.650097
H21	-1.657393	-0.912393	1.148597
H22	-0.031091	-1.709531	1.991818
H23	-0.610550	1.122390	2.638654
H24	0.992061	0.362104	2.838453
C25	-0.086689	0.183316	2.820041
N26	-0.453344	-0.802493	1.788184
H27	-0.402437	-0.208373	3.787127

Zero-point correction= 0.216103
Thermal correction to Energy= 0.230104
Thermal correction to Enthalpy= 0.231048
Thermal correction to Gibbs Free Energy= 0.175376
Sum of electronic and zero-point Energies= -752.255571
Sum of electronic and thermal Energies= -752.241570
Sum of electronic and thermal Enthalpies= -752.240626
Sum of electronic and thermal Free Energies= -752.296298

124 TS$^{\text{via async HA_NH2 + add}}$_C4-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	-1.472046	-1.039449	0.055348
C2	-0.084288	0.700707	-0.492487
C3	1.156573	1.322306	-0.848330
O4	1.318320	2.413422	-1.354342
N5	2.234643	0.464511	-0.534560
H6	3.145657	0.843074	-0.767252
C7	2.114751	-0.826151	-0.069656
N8	3.243963	-1.541465	0.068909
H9	4.132021	-1.235241	-0.293184
H10	3.161942	-2.493020	0.391849
N11	0.959305	-1.367801	0.255351
C12	-0.090362	-0.515434	0.169658
C13	-1.644529	-2.201482	-0.871312
H14	-1.271529	-1.921286	-1.856417
H15	-1.069815	-3.035683	-0.473282
H16	-2.708157	-2.433590	-0.914380
C17	-2.299577	0.183210	-0.407151
O18	-3.487452	0.150811	-0.449423
N19	-1.382895	1.129786	-0.725542
H20	-1.644429	2.037609	-1.089523
H21	-1.802727	-1.255000	1.004927
H22	0.232874	-0.560947	2.545339
H23	-0.804552	2.094544	1.867142
H24	0.868862	1.688564	2.357337
C25	-0.188052	1.411036	2.455117
N26	-0.470631	0.035657	2.099298
H27	-0.460571	1.543278	3.510898

Zero-point correction= 0.216721
Thermal correction to Energy= 0.231348
Thermal correction to Enthalpy= 0.232293
Thermal correction to Gibbs Free Energy= 0.175067
Sum of electronic and zero-point Energies= -752.232981
Sum of electronic and thermal Energies= -752.218354
Sum of electronic and thermal Enthalpies= -752.217409
Sum of electronic and thermal Free Energies= -752.274635

125 C5-NHCH$_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	-1.572237	-1.044388	0.184561
C2	-0.089937	0.765019	0.102386
C3	0.881263	0.842483	-1.064335
O4	0.781992	1.201798	-2.190498
N5	2.166988	0.162609	-0.595677
H6	2.519788	0.735559	0.188132
C7	1.951782	-1.243086	-0.031386
N8	3.098434	-1.795181	0.461998
H9	2.941554	-2.558847	1.107938
N10	0.738077	-1.605518	0.297143
C11	-0.254655	-0.747992	0.244435
C12	-2.146464	-2.379970	0.216313
H13	-1.727038	-2.986925	-0.588992
H14	-1.939657	-2.851431	1.178280
H15	-3.221863	-2.269868	0.079394
C16	-2.331533	0.113466	-0.120855
O17	-3.518467	0.146501	-0.294051
N18	-1.429185	1.158290	-0.188438
H19	-1.723328	2.074900	-0.488012
H20	2.833860	0.164260	-1.373393
H21	3.859771	-1.976600	-0.181956
H22	0.204652	0.934290	2.107033
H23	-0.468140	3.203949	1.404903
H24	1.130513	3.131019	2.173378
C25	0.547615	2.802411	1.312484
N26	0.586804	1.334821	1.254806
H27	1.011094	3.224879	0.414684

Zero-point correction= 0.218166
Thermal correction to Energy= 0.233145
Thermal correction to Enthalpy= 0.234089
Thermal correction to Gibbs Free Energy= 0.175771
Sum of electronic and zero-point Energies= -752.246350
Sum of electronic and thermal Energies= -752.231371
Sum of electronic and thermal Enthalpies= -752.230427
Sum of electronic and thermal Free Energies= -752.288745

126 TS$^{\text{via async add + PT}}$_C5-NHCH$_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	1.602584	-1.008645	-0.212319
C2	0.087169	0.759159	-0.063928
C3	-0.879284	0.745320	1.113602
O4	-0.781827	1.030261	2.264528
N5	-2.107504	0.171010	0.481435
H6	-1.935586	0.809516	-0.501884
C7	-1.922633	-1.223434	-0.006968
N8	-3.066128	-1.857056	-0.382880
H9	-2.916004	-2.733594	-0.865875
N10	-0.719232	-1.611220	-0.332247
C11	0.272827	-0.735601	-0.276674
C12	2.202541	-2.332253	-0.264802
H13	1.789403	-2.961331	0.526482
H14	2.011270	-2.790556	-1.236437
H15	3.274781	-2.205801	-0.117923
C16	2.333111	0.155309	0.093662
O17	3.513963	0.222617	0.292994
N18	1.412625	1.207244	0.128726
H19	1.655846	2.043782	0.639601
H20	-2.948030	0.320240	1.040461
H21	-3.847895	-1.876495	0.259894
H22	-0.438836	0.930727	-2.059716
H23	0.365553	3.167449	-1.428133
H24	-1.300386	3.153087	-2.059955
C25	-0.654816	2.819755	-1.247665
N26	-0.718872	1.347199	-1.172268
H27	-1.025006	3.250676	-0.313180

Zero-point correction= 0.215461
Thermal correction to Energy= 0.229372
Thermal correction to Enthalpy= 0.230316
Thermal correction to Gibbs Free Energy= 0.175063
Sum of electronic and zero-point Energies= -752.242900

Sum of electronic and thermal Energies= -752.228989
Sum of electronic and thermal Enthalpies= -752.228045
Sum of electronic and thermal Free Energies= -752.283298

127 C5-$^{+}$ṄHCH$_3$[9MOG + H$_{C2}$]

N1	-1.384140	-1.240885	0.237308
C2	-0.183369	0.727913	0.091779
C3	1.052115	1.056426	-0.899442
O4	0.876098	1.900124	-1.741391
N5	2.134575	0.345752	-0.583814
H6	2.961542	0.463384	-1.161906
C7	2.227486	-0.780467	0.389344
N8	3.259487	-1.628811	-0.101465
H9	2.910601	-2.290052	-0.788246
H10	3.724531	-2.136341	0.640676
N11	0.949485	-1.451190	0.565015
C12	-0.105635	-0.786727	0.356591
C13	-1.753382	-2.647426	0.338116
H14	-2.821840	-2.720674	0.139182
H15	-1.195557	-3.235573	-0.394125
H16	-1.532420	-3.008483	1.342759
C17	-2.202247	-0.287065	-0.401563
O18	-3.308055	-0.464846	-0.822579
N19	-1.468780	0.906166	-0.452993
H20	-1.680116	1.595867	-1.162371
H21	2.561755	-0.377716	1.354310
H22	0.875018	1.274364	1.811959
H23	-1.636413	2.693294	1.331362
H24	-0.195284	3.504287	0.680323
C25	-0.553927	2.797495	1.445489
N26	0.065772	1.512177	1.244693
H27	-0.297204	3.172063	2.434746

Zero-point correction= 0.218109
Thermal correction to Energy= 0.232798
Thermal correction to Enthalpy= 0.233742
Thermal correction to Gibbs Free Energy= 0.176391
Sum of electronic and zero-point Energies= -752.251229
Sum of electronic and thermal Energies= -752.236540
Sum of electronic and thermal Enthalpies= -752.235596
Sum of electronic and thermal Free Energies= -752.292947

128 TS$^{\text{via async add + PT}}$_C5-$^{+}$ṄHCH$_3$[9MOG + H$_{C2}$]

N1	1.515205	0.963890	-0.210367
C2	0.016856	-0.772592	0.166846
C3	-0.981239	-1.246654	-0.922088
O4	-0.801511	-2.208236	-1.624640
N5	-2.063415	-0.403034	-0.928929
H6	-2.759087	-0.482557	-1.661470
C7	-2.009333	0.750163	-0.064054
N8	-3.164514	1.488677	-0.044070
H9	-3.097291	2.435144	0.305275
H10	-4.054821	1.023783	0.062332
N11	-0.806453	1.517048	-0.116560
C12	0.207276	0.724568	-0.072194
C13	2.131551	2.244955	-0.529453
H14	3.120922	2.270376	-0.074287
H15	2.227357	2.364387	-1.610566
H16	1.500210	3.036255	-0.123945
C17	2.249743	-0.261849	-0.200693
O18	3.422712	-0.358328	-0.411014
N19	1.339430	-1.269249	0.100064
H20	1.549669	-2.220173	-0.174669
H21	-1.771696	0.135759	1.010119
H22	-1.146328	-1.818925	1.542679
H23	0.318391	0.516222	2.622565
H24	0.944793	-1.144037	2.781489
C25	0.041073	-0.538816	2.670257
N26	-0.695179	-0.910152	1.454953
H27	-0.612801	-0.692616	3.528346

Zero-point correction= 0.215398
Thermal correction to Energy= 0.229111
Thermal correction to Enthalpy= 0.230055
Thermal correction to Gibbs Free Energy= 0.175249
Sum of electronic and zero-point Energies= -752.252240
Sum of electronic and thermal Energies= -752.238527
Sum of electronic and thermal Enthalpies= -752.237583
Sum of electronic and thermal Free Energies= -752.292388

129 TS$^{\text{via async HA_NH2 + add}}$_ C5-$^{+}$ṄHCH$_3$[9MOG + H$_{C2}$]

N1	1.748689	-0.605083	0.543586
C2	0.292075	1.038165	0.011717
C3	-0.993811	1.767867	-0.010345
O4	-1.105686	2.907212	-0.407643
N5	-1.958679	0.977000	0.549412
H6	-2.903914	1.348341	0.571795
C7	-1.858734	-0.451777	0.720049
N8	-2.983499	-0.930563	1.427780
H9	-2.908969	-0.782605	2.429390
H10	-3.163571	-1.909815	1.246095
N11	-0.581493	-0.972898	1.020696
C12	0.410235	-0.275448	0.586598
C13	2.341795	-1.841642	1.039188
H14	3.409949	-1.803397	0.828066
H15	2.179557	-1.924769	2.114657
H16	1.892184	-2.696150	0.531441
C17	2.472417	0.417433	-0.041049
O18	3.640147	0.513465	-0.267921
N19	1.477323	1.434791	-0.356766
H20	1.709692	2.333441	-0.772704
H21	-1.860676	-0.808594	-0.450956
H22	-2.045588	-0.361258	-2.517297
H23	-0.182115	-2.444538	-1.602869
H24	-0.262584	-1.818466	-3.272710
C25	-0.836939	-1.989576	-2.349607
N26	-1.339458	-0.731525	-1.874472
H27	-1.642058	-2.689793	-2.611352

Zero-point correction= 0.210702
Thermal correction to Energy= 0.225941
Thermal correction to Enthalpy= 0.226885
Thermal correction to Gibbs Free Energy= 0.167263
Sum of electronic and zero-point Energies= -752.204171
Sum of electronic and thermal Energies= -752.188933
Sum of electronic and thermal Enthalpies= -752.187988
Sum of electronic and thermal Free Energies= -752.247610

130 C5-NHCH$_3$[9MOG + H$_{N2}$]$^{\cdot+}$

N1	1.549811	-0.870733	-0.314067
C2	-0.049346	0.730489	0.227302
C3	-1.051124	1.324385	-0.774631
O4	-0.981892	2.428812	-1.247900
N5	-2.069985	0.413839	-1.030687
H6	-2.732549	0.684096	-1.749880
C7	-1.934844	-0.933530	-0.673023
N8	-2.951059	-1.374947	0.331477
H9	-3.913706	-1.187115	0.042851
H10	-2.840028	-2.378399	0.502488
N11	-0.734112	-1.529613	-0.456823
C12	0.234449	-0.691076	-0.229807
C13	2.234288	-2.088362	-0.721477
H14	2.140052	-2.847204	0.057204
H15	1.800134	-2.459217	-1.651598

H16	3.284553	-1.838283	-0.869065
C17	2.232629	0.383223	-0.117941
O18	3.415162	0.533000	-0.237714
N19	1.262204	1.301676	0.201693
H20	1.453281	2.292570	0.162260
H21	-2.748500	-0.859373	1.205828
H22	-1.051724	1.616823	1.752846
H23	1.012611	0.622209	2.746646
H24	0.223607	-0.945238	2.447986
N25	-0.749518	0.674899	1.514263
C26	0.047199	0.120685	2.618687
H27	-0.524780	0.223916	3.541695

Zero-point correction= 0.221916
Thermal correction to Energy= 0.236051
Thermal correction to Enthalpy= 0.236995
Thermal correction to Gibbs Free Energy= 0.181046
Sum of electronic and zero-point Energies= -752.262552
Sum of electronic and thermal Energies= -752.248418
Sum of electronic and thermal Enthalpies= -752.247473
Sum of electronic and thermal Free Energies= -752.303422

131 TS$^{\text{via async add + PT}}$_C5-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	1.613879	-0.741733	-0.371597
C2	-0.141022	0.643539	0.248475
C3	-1.112772	1.308114	-0.749940
O4	-1.058561	2.469932	-1.064186
N5	-2.034664	0.377654	-1.176120
H6	-2.719343	0.664187	-1.866003
C7	-1.880818	-0.988490	-0.822236
N8	-2.627583	-1.300754	0.402935
H9	-3.618954	-1.070594	0.338319
H10	-2.523343	-2.283979	0.654963
N11	-0.603430	-1.529282	-0.783622
C12	0.275004	-0.683564	-0.366569
C13	2.421816	-1.828135	-0.908994
H14	2.410193	-2.678069	-0.224566
H15	2.021741	-2.129851	-1.878286
H16	3.439743	-1.455222	-1.019224
C17	2.164837	0.507182	0.047005
O18	3.326472	0.790763	0.025127
N19	1.095982	1.296820	0.463921
H20	1.188226	2.304149	0.419322
H21	-1.966910	-0.526249	1.130047
H22	-1.331125	1.228265	1.826735
H23	0.722180	0.311041	2.827650
H24	0.144237	-1.284438	2.276754
N25	-0.944663	0.344506	1.490966
C26	-0.161073	-0.281108	2.582376
H27	-0.802395	-0.360508	3.460677

Zero-point correction= 0.217746
Thermal correction to Energy= 0.230980
Thermal correction to Enthalpy= 0.231924
Thermal correction to Gibbs Free Energy= 0.177988
Sum of electronic and zero-point Energies= -752.259814
Sum of electronic and thermal Energies= -752.246580
Sum of electronic and thermal Enthalpies= -752.245636
Sum of electronic and thermal Free Energies= -752.299572

132 C5-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	1.334974	-1.134706	-0.016147
C2	0.127986	0.876527	0.104495
C3	-0.946480	1.084395	-0.976064
O4	-0.918754	1.926583	-1.829512
N5	-2.048420	0.202645	-0.878048
H6	-2.823146	0.416426	-1.496239
C7	-2.135906	-0.854795	-0.037350
N8	-3.318379	-1.436757	0.168179
H9	-4.172455	-1.023330	-0.174467
H10	-3.402808	-2.294744	0.692094
N11	-1.026137	-1.294198	0.561076
C12	0.183973	-0.582893	0.473410
C13	1.787252	-2.501292	0.151165
H14	2.732802	-2.596999	-0.383251
H15	1.949739	-2.729733	1.208602
H16	1.061181	-3.197192	-0.278381
C17	2.170243	-0.116099	-0.546525
O18	3.271688	-0.295028	-0.997111
N19	1.459719	1.054501	-0.432103
H20	1.749396	1.881349	-0.933801
H21	-1.106763	-2.042358	1.238697
H22	-0.405992	2.665200	0.894575
H23	1.615565	1.866732	2.191339
H24	0.183106	2.364957	3.125060
N25	-0.286664	1.706165	1.207206
C26	0.562187	1.644815	2.399334
H27	0.494729	0.649758	2.846834

Zero-point correction= 0.220034
Thermal correction to Energy= 0.234716
Thermal correction to Enthalpy= 0.235661
Thermal correction to Gibbs Free Energy= 0.178587
Sum of electronic and zero-point Energies= -752.288204
Sum of electronic and thermal Energies= -752.273521
Sum of electronic and thermal Enthalpies= -752.272577
Sum of electronic and thermal Free Energies= -752.329651

133 TS$^{\text{via async add + PT}}$_C5-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	1.430826	1.022801	0.253476
C2	0.067636	-0.815991	-0.063349
C3	-1.113069	-1.285422	0.787640
O4	-1.191325	-2.291981	1.430341
N5	-2.188337	-0.343197	0.755004
H6	-3.014673	-0.623868	1.273319
C7	-2.138756	0.842490	0.084832
N8	-3.244758	1.534021	-0.131441
H9	-4.168271	1.187457	0.083824
H10	-3.153100	2.453284	-0.542430
N11	-0.965351	1.277516	-0.451294
C12	0.114990	0.652454	0.228787
C13	1.949223	2.351771	0.539408
H14	3.026767	2.329144	0.379396
H15	1.487872	3.070342	-0.138706
H16	1.742878	2.629520	1.576498
C17	2.221179	-0.141253	0.438608
O18	3.395376	-0.163304	0.688355
N19	1.368295	-1.231582	0.268670
H20	1.678299	-2.177171	0.432827
H21	-0.909893	0.422332	-1.364202
H22	-0.943954	-1.677612	-1.716468
H23	1.450399	-1.652445	-2.389960
H24	0.316825	-0.830933	-3.496952
N25	-0.344277	-0.879383	-1.518152
C26	0.758386	-0.815857	-2.500241
H27	1.302120	0.121854	-2.374652

Zero-point correction= 0.216394
Thermal correction to Energy= 0.230112
Thermal correction to Enthalpy= 0.231056
Thermal correction to Gibbs Free Energy= 0.176066
Sum of electronic and zero-point Energies= -752.243461
Sum of electronic and thermal Energies= -752.229744

Sum of electronic and thermal Enthalpies= -752.228800
Sum of electronic and thermal Free Energies= -752.283789

134 TS$^{via\ HA_NH2\ products_C5}$_NHCH3[9MOG + H_{N3}]$^{\bullet+}$

N1	-1.522249	0.946001	-0.305105
C2	-0.056568	-0.768896	-0.207909
C3	1.202187	-1.293115	-0.724082
O4	1.431088	-2.387390	-1.167541
N5	2.246006	-0.324898	-0.606005
H6	3.169464	-0.683184	-0.822569
C7	2.113066	0.936706	-0.158090
N8	3.189959	1.685200	0.094346
H9	4.112534	1.277673	0.108001
H10	3.114658	2.650175	0.376649
N11	0.874096	1.447688	-0.025033
C12	-0.212311	0.618973	-0.200737
C13	-2.140690	2.256755	-0.246784
H14	-3.207389	2.110061	-0.421067
H15	-2.004281	2.708406	0.740117
H16	-1.739595	2.908355	-1.027707
C17	-2.266650	-0.252154	-0.501468
O18	-3.460087	-0.321770	-0.639427
N19	-1.321287	-1.264056	-0.497554
H20	-1.558232	-2.232910	-0.650069
H21	0.751448	2.397099	0.301969
H22	0.479264	-2.145217	1.695293
H23	-1.594855	-1.109118	2.235761
H24	-0.451106	-1.017178	3.578782
N25	0.499725	-1.120849	1.732708
C26	-0.624352	-0.693884	2.544537
H27	-0.691750	0.399205	2.554292

Zero-point correction= 0.215953
Thermal correction to Energy= 0.231156
Thermal correction to Enthalpy= 0.232100
Thermal correction to Gibbs Free Energy= 0.173871
Sum of electronic and zero-point Energies= -752.248280
Sum of electronic and thermal Energies= -752.233077
Sum of electronic and thermal Enthalpies= -752.232132
Sum of electronic and thermal Free Energies= -752.290361

135 C5-$^{+}$ṄHCH$_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	1.382926	-1.027102	0.297467
C2	0.042261	0.854907	0.011371
C3	-1.392094	1.325921	-0.263114
O4	-1.604227	2.500412	-0.490749
N5	-2.333736	0.353831	-0.242423
H6	-3.287605	0.654301	-0.407570
C7	-2.064486	-0.971682	0.167948
N8	-3.132760	-1.798223	0.072203
H9	-3.862561	-1.625761	-0.601653
H10	-2.968043	-2.762668	0.320399
N11	-0.942702	-1.367336	0.634662
C12	0.147696	-0.466419	0.830685
C13	1.879491	-2.318579	0.750775
H14	2.058819	-2.277123	1.826924
H15	1.160832	-3.111106	0.529632
H16	2.817282	-2.517650	0.232096
C17	1.645184	-0.572281	-0.969781
O18	2.455460	-0.954295	-1.773600
N19	0.758506	0.513211	-1.184968
H20	0.878664	1.136004	-1.974967
H21	0.269435	-0.251695	1.899891
H22	0.326882	2.891991	0.280759
H23	2.513692	1.021278	1.086810
H24	2.611479	2.819685	0.967841
C25	1.996894	1.967285	1.260511
N26	0.747742	1.995755	0.549806
H27	1.781747	2.047943	2.337033

Zero-point correction= 0.218484
Thermal correction to Energy= 0.233024
Thermal correction to Enthalpy= 0.233969
Thermal correction to Gibbs Free Energy= 0.176788
Sum of electronic and zero-point Energies= -752.267444
Sum of electronic and thermal Energies= -752.252904
Sum of electronic and thermal Enthalpies= -752.251959
Sum of electronic and thermal Free Energies= -752.309140

136 TS$^{via\ async\ add\ +\ PT}$_C5-$^{+}$ṄHCH$_3$[9MOG + H_{C4}]

N1	-1.705706	-0.787452	-0.199658
C2	-0.046372	0.851053	-0.063546
C3	1.127598	0.957796	0.897094
O4	1.347316	1.934798	1.567749
N5	1.936720	-0.164829	0.902887
H6	2.745605	-0.101930	1.511117
C7	1.653500	-1.360959	0.240929
N8	2.599334	-2.306031	0.313572
H9	3.447902	-2.204768	0.846747
H10	2.404743	-3.198116	-0.116939
N11	0.545812	-1.607089	-0.405755
C12	-0.370437	-0.584517	-0.497941
C13	-2.453080	-2.003309	-0.460652
H14	-2.570663	-2.154142	-1.536734
H15	-1.925571	-2.854887	-0.027290
H16	-3.433433	-1.888559	0.001354
C17	-2.281942	0.362449	0.384481
O18	-3.413095	0.460242	0.771052
N19	-1.282715	1.329687	0.431497
H20	-1.367952	2.132248	1.041047
H21	-0.265638	-0.017050	-1.704439
H22	-0.377716	2.163547	-1.654558
H23	2.182022	0.668987	-1.856484
H24	1.601839	1.963828	-2.911136
N25	0.248691	1.389547	-1.437660
C26	1.629917	1.610824	-1.880733
H27	2.135037	2.353661	-1.255067

Zero-point correction= 0.214391
Thermal correction to Energy= 0.228524
Thermal correction to Enthalpy= 0.229469
Thermal correction to Gibbs Free Energy= 0.173574
Sum of electronic and zero-point Energies= -752.242860
Sum of electronic and thermal Energies= -752.228727
Sum of electronic and thermal Enthalpies= -752.227782
Sum of electronic and thermal Free Energies= -752.283677

137 C5-NHCH$_3$[9MOG + H_{C6}]$^{\bullet+}$

N1	1.328458	1.060155	-0.019874
C2	0.093305	-0.914918	0.002953
C3	-1.085416	-1.227545	-0.978867
O4	-0.822164	-0.965986	-2.264029
N5	-2.259899	-0.516190	-0.440062
H6	-3.164332	-0.820742	-0.776243
C7	-2.152738	0.719369	0.101838
N8	-3.249693	1.386026	0.441910
H9	-4.181970	1.028449	0.302360
H10	-3.137752	2.313106	0.827029
N11	-0.974561	1.344128	0.305128
C12	0.093955	0.613154	0.117167
C13	1.765420	2.449775	0.022264
H14	2.848524	2.451796	-0.095641
H15	1.298110	3.008018	-0.790863

H16	1.487764	2.888930	0.980758
C17	2.206612	-0.022439	-0.410297
O18	3.379239	0.103355	-0.610211
N19	1.410719	-1.134481	-0.506013
H20	1.826894	-2.053425	-0.557731
H21	-1.272126	-2.316352	-0.916913
H22	-1.129921	-1.666657	1.461067
H23	1.727198	-1.408802	2.157218
H24	0.513331	-0.227444	2.717560
C25	0.668837	-1.262784	2.383389
N26	-0.144695	-1.638106	1.226115
H27	0.415539	-1.934220	3.204206

Zero-point correction= 0.219195
Thermal correction to Energy= 0.233398
Thermal correction to Enthalpy= 0.234342
Thermal correction to Gibbs Free Energy= 0.178167
Sum of electronic and zero-point Energies= -752.260428
Sum of electronic and thermal Energies= -752.246226
Sum of electronic and thermal Enthalpies= -752.245282
Sum of electronic and thermal Free Energies= -752.301456

138 $TS^{via\ async\ add\ +\ PT}$_C5-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$

N1	1.349637	1.225045	0.130277
C2	0.125297	-0.722790	0.006269
C3	-1.088249	-1.179355	-0.859974
O4	-0.995936	-1.747525	-1.967795
N5	-2.203408	-0.242563	-0.629565
H6	-3.076835	-0.525920	-1.057429
C7	-2.137241	0.889253	0.085203
N8	-3.248797	1.557449	0.394816
H9	-4.168784	1.246784	0.124059
H10	-3.151263	2.462573	0.831236
N11	-0.967299	1.458554	0.476343
C12	0.109080	0.759639	0.249988
C13	1.759289	2.620553	0.223650
H14	2.824504	2.661422	-0.001563
H15	1.199734	3.219222	-0.497450
H16	1.573236	2.988963	1.232860
C17	2.200994	0.204364	-0.424638
O18	3.328421	0.377646	-0.781183
N19	1.435189	-0.943715	-0.473803
H20	1.674273	-1.689524	-1.113748
H21	-1.200607	-1.998530	0.235560
H22	-0.656511	-0.939453	1.963937
H23	1.034686	-3.185903	1.057373
H24	1.667949	-1.901027	2.115692
C25	0.767573	-2.434575	1.800730
N26	-0.239161	-1.521674	1.238477
H27	0.316164	-2.933770	2.658112

Zero-point correction= 0.214275
Thermal correction to Energy= 0.228415
Thermal correction to Enthalpy= 0.229359
Thermal correction to Gibbs Free Energy= 0.172826
Sum of electronic and zero-point Energies= -752.232006
Sum of electronic and thermal Energies= -752.217865
Sum of electronic and thermal Enthalpies= -752.216921
Sum of electronic and thermal Free Energies= -752.273454

139 $TS^{via\ HA_NH2\ products}$_C5-$NHCH_3$[9MOG + H_{C6}]$^{\bullet+}$

N1	-1.326049	-1.026192	-0.046669
C2	-0.079700	0.827662	-0.454316
C3	1.199850	1.244783	-1.085970
N4	2.294674	0.635749	-0.276486
H5	3.221376	1.013665	-0.424589
C6	2.183736	-0.637651	0.148757
N7	3.258410	-1.318970	0.530546
H8	4.198270	-0.968093	0.430350
H9	3.125725	-2.264316	0.860689
N10	0.998053	-1.291474	0.268145
C11	-0.060030	-0.601898	-0.056018
C12	-1.793486	-2.369159	0.272913
H13	-2.880799	-2.333007	0.329773
H14	-1.483668	-3.064635	-0.508656
H15	-1.373672	-2.677907	1.230550
C16	-2.193478	0.011422	-0.504320
O17	-3.379657	-0.062235	-0.619238
N18	-1.369029	1.113300	-0.747676
H19	-1.733024	1.997959	-1.070821
H20	1.036345	1.522011	1.848013
O21	0.874557	0.545557	-2.170176
H22	1.396543	2.318517	-1.176172
N23	0.102906	1.712062	1.469297
C24	-0.882197	1.249738	2.407201
H25	-0.843660	1.912149	3.286175
H26	-1.885714	1.325094	1.981508
H27	-0.697847	0.231274	2.778908

Zero-point correction= 0.214042
Thermal correction to Energy= 0.229123
Thermal correction to Enthalpy= 0.230067
Thermal correction to Gibbs Free Energy= 0.171364
Sum of electronic and zero-point Energies= -752.192029
Sum of electronic and thermal Energies= -752.176948
Sum of electronic and thermal Enthalpies= -752.176004
Sum of electronic and thermal Free Energies= -752.234707

140 C5-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$

N1	1.347928	1.050320	-0.213008
C2	0.051923	-0.848333	0.206859
C3	-1.044468	-1.237854	-0.756136
O4	-0.833877	-1.774725	-1.959537
N5	-2.184501	-0.457581	-0.650124
H6	-3.034992	-0.779696	-1.096126
C7	-2.134040	0.768649	-0.058244
N8	-3.264995	1.382644	0.287224
H9	-4.171573	0.951848	0.200634
H10	-3.204989	2.317097	0.663432
N11	-0.965772	1.412458	0.108364
C12	0.098679	0.664762	0.050697
C13	1.792512	2.411175	-0.484425
H14	1.310149	2.786467	-1.388890
H15	1.539640	3.051974	0.360974
H16	2.872971	2.378590	-0.620342
C17	2.203980	-0.086411	-0.337752
O18	3.387328	-0.040130	-0.514798
N19	1.386287	-1.207744	-0.251660
H20	1.829256	-2.056197	0.078381
H21	0.036991	-2.196575	-1.989517
H22	-0.585785	-2.193046	1.589374
H23	1.566907	-1.095229	2.527998
H24	0.124552	-1.168599	3.560684
N25	-0.341825	-1.210560	1.535427
C26	0.522956	-0.769655	2.627805
H27	0.500179	0.321452	2.701693

Zero-point correction= 0.219449
Thermal correction to Energy= 0.234091
Thermal correction to Enthalpy= 0.235035
Thermal correction to Gibbs Free Energy= 0.178378
Sum of electronic and zero-point Energies= -752.290486
Sum of electronic and thermal Energies= -752.275843

Sum of electronic and thermal Enthalpies= -752.274899
Sum of electronic and thermal Free Energies= -752.331556

141 $TS^{via\ async\ add\ +\ PT}$_C5-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.315023	-1.213781	0.155390
C2	-0.078934	0.702296	-0.181090
C3	1.196449	1.125645	-0.863752
O4	1.394020	2.402936	-0.740482
N5	2.295475	0.257527	-0.559928
H6	3.201917	0.618616	-0.834696
C7	2.197559	-0.928634	0.048224
N8	3.279406	-1.675522	0.278363
H9	4.209411	-1.397568	0.007063
H10	3.144956	-2.589226	0.685364
N11	1.003295	-1.477942	0.416083
C12	-0.057642	-0.765086	0.189672
C13	-1.733281	-2.587504	0.404879
H14	-1.199685	-3.266210	-0.263874
H15	-1.520266	-2.848126	1.441678
H16	-2.804707	-2.641585	0.215387
C17	-2.128767	-0.294936	-0.601878
O18	-3.260454	-0.500348	-0.932670
N19	-1.320650	0.782847	-0.874373
H20	-1.623955	1.552881	-1.452094
H21	0.601205	2.466725	0.293979
H22	0.554792	1.347843	1.720337
H23	-1.936027	2.666491	0.846516
H24	-1.118725	2.799890	2.411557
N25	-0.073664	1.688866	0.992025
C26	-1.350917	2.124899	1.586967
H27	-1.926121	1.275521	1.962937

Zero-point correction= 0.216183
Thermal correction to Energy= 0.230108
Thermal correction to Enthalpy= 0.231052
Thermal correction to Gibbs Free Energy= 0.175483
Sum of electronic and zero-point Energies= -752.260852
Sum of electronic and thermal Energies= -752.246927
Sum of electronic and thermal Enthalpies= -752.245982
Sum of electronic and thermal Free Energies= -752.301551

142 $TS^{via\ HA_NH2\ products}$_C5-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$

N1	1.460685	0.923432	-0.413525
C2	0.003581	-0.786240	-0.126509
C3	-1.237247	-1.193694	-0.634284
O4	-1.604815	-2.384836	-1.089834
N5	-2.266521	-0.307905	-0.462863
H6	-3.204976	-0.644753	-0.644966
C7	-2.043347	0.994233	-0.110769
N8	-3.089850	1.775127	0.166683
H9	-4.027087	1.423522	0.278311
H10	-2.905562	2.739066	0.401629
N11	-0.818652	1.524283	-0.126001
C12	0.159934	0.654919	-0.223796
C13	2.064591	2.243841	-0.527551
H14	1.636762	2.773492	-1.379801
H15	1.885515	2.809101	0.388306
H16	3.134370	2.098591	-0.673897
C17	2.202311	-0.284109	-0.506401
O18	3.392574	-0.378194	-0.614440
N19	1.261122	-1.315826	-0.453825
H20	1.586524	-2.225496	-0.157388
H21	-0.853881	-2.893551	-1.421478
H22	-0.401002	-1.914639	1.937198
H23	1.776298	-0.968835	2.266854
H24	0.699779	-0.662073	3.631414
N25	-0.344829	-0.894080	1.854799
C26	0.846951	-0.459873	2.562604
H27	0.976861	0.620149	2.451369

Zero-point correction= 0.216461
Thermal correction to Energy= 0.231274
Thermal correction to Enthalpy= 0.232219
Thermal correction to Gibbs Free Energy= 0.174901
Sum of electronic and zero-point Energies= -752.252316
Sum of electronic and thermal Energies= -752.237502
Sum of electronic and thermal Enthalpies= -752.236558
Sum of electronic and thermal Free Energies= -752.293876

143 C5-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	1.444711	-1.006405	-0.201471
C2	0.025663	0.842965	0.235231
C3	-1.069888	1.285525	-0.725752
O4	-0.956607	2.240482	-1.469700
N5	-2.169434	0.458629	-0.657911
H6	-2.953489	0.733085	-1.239781
C7	-2.083669	-0.869837	-0.225469
N8	-3.240359	-1.563116	-0.156370
N9	-0.923664	-1.444361	0.008030
C10	0.124668	-0.635631	0.049222
C11	1.888924	-2.392896	-0.322554
H12	1.696726	-2.914231	0.615859
H13	1.340947	-2.878076	-1.131758
H14	2.956336	-2.388664	-0.538389
C15	2.265670	0.042197	-0.419227
O16	3.433377	0.132165	-0.654721
N17	1.378614	1.289618	-0.308936
H18	1.278353	1.756385	-1.222812
H19	-4.132948	-1.100459	-0.097180
H20	1.800122	1.963031	0.339566
H21	-3.189385	-2.524206	0.145007
H22	-0.938856	1.949146	1.669347
H23	1.107893	0.051089	2.671453
H24	-0.612034	-0.403551	2.733970
N25	-0.144002	1.333514	1.560836
C26	0.086389	0.440034	2.696917
H27	-0.015421	1.025975	3.610625

Zero-point correction= 0.219241
Thermal correction to Energy= 0.234243
Thermal correction to Enthalpy= 0.235188
Thermal correction to Gibbs Free Energy= 0.176482
Sum of electronic and zero-point Energies= -752.275886
Sum of electronic and thermal Energies= -752.260883
Sum of electronic and thermal Enthalpies= -752.259939
Sum of electronic and thermal Free Energies= -752.318644

144 $TS^{via\ async\ add\ +\ PT}$_C5-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	-1.471257	1.030105	-0.035683
C2	-0.050564	-0.812537	0.033731
C3	1.144021	-1.201873	-0.801580
O4	1.184165	-2.219884	-1.462291
N5	2.185676	-0.305856	-0.680683
H6	3.041533	-0.585775	-1.146913
C7	2.060283	0.983819	-0.164573
N8	3.193853	1.697779	0.005282
N9	0.890014	1.490323	0.150622
C10	-0.142189	0.655343	0.121088
C11	-1.936986	2.411500	-0.013569
H12	-1.721798	2.852211	0.960398
H13	-1.430919	2.984085	-0.793415
H14	-3.011345	2.404522	-0.192751
C15	-2.251226	-0.002352	-0.483204

O16	-3.396097	-0.016418	-0.832108
N17	-1.403458	-1.215418	-0.441819
H18	-1.472991	-1.798102	-1.280010
H19	4.078623	1.402989	-0.374732
H20	-1.346907	-1.795343	0.673883
H21	3.092394	2.670517	0.252864
H22	0.448011	-2.437683	1.285413
H23	-0.699593	-0.094440	2.686248
H24	1.038628	-0.491789	2.708907
N25	-0.150157	-1.611511	1.334579
C26	0.029846	-0.901557	2.613144
H27	-0.151996	-1.612798	3.418994

Zero-point correction= 0.215099
Thermal correction to Energy= 0.229471
Thermal correction to Enthalpy= 0.230416
Thermal correction to Gibbs Free Energy= 0.173709
Sum of electronic and zero-point Energies= -752.251657
Sum of electronic and thermal Energies= -752.237284
Sum of electronic and thermal Enthalpies= -752.236340
Sum of electronic and thermal Free Energies= -752.293046

145 C5-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	1.622049	0.956040	0.172996
C2	-0.013314	-0.728500	0.146839
C3	-1.190173	-0.860648	-0.821396
O4	-1.331833	-1.766837	-1.609606
N5	-2.135912	0.142036	-0.642129
C6	-1.873630	1.362129	-0.027451
N7	-2.902080	2.229017	0.075390
H8	-3.858868	1.942948	-0.052157
H9	-2.728522	3.109448	0.534526
N10	-0.671212	1.697010	0.383221
C11	0.244402	0.732751	0.358545
C12	2.298196	2.234000	0.362282
H13	2.740745	2.580417	-0.575184
H14	1.541410	2.954260	0.670785
H15	3.053684	2.155285	1.147622
C16	2.155266	-0.164019	-0.318287
O17	3.409577	-0.362861	-0.630192
N18	1.252334	-1.124428	-0.480567
H19	1.481011	-2.060556	-0.783649
H20	3.965974	0.419127	-0.518753
H21	-2.974988	0.038012	-1.201033
H22	-0.674953	-0.828466	2.075023
H23	-0.172662	-3.413064	0.711025
H24	-1.819638	-2.807999	0.959784
C25	-0.792127	-2.771649	1.343025
N26	-0.218423	-1.426636	1.396520
H27	-0.774159	-3.187485	2.351047

Zero-point correction= 0.218500
Thermal correction to Energy= 0.233697
Thermal correction to Enthalpy= 0.234641
Thermal correction to Gibbs Free Energy= 0.176514
Sum of electronic and zero-point Energies= -752.283128
Sum of electronic and thermal Energies= -752.267931
Sum of electronic and thermal Enthalpies= -752.266987
Sum of electronic and thermal Free Energies= -752.325115

146 TS$^{\text{via async add + PT}}$_C5-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	1.177667	1.497147	-0.236016
C2	0.223236	-0.566203	-0.239823
C3	-1.077749	-1.266491	-0.600665
O4	-1.138435	-2.364959	-1.084135
N5	-2.217105	-0.535636	-0.263028
C6	-2.213692	0.773103	0.187868
N7	-3.389841	1.307154	0.503075
H8	-4.263494	0.807394	0.446051
H9	-3.404827	2.275549	0.790702
N10	-1.127318	1.516314	0.306370
C11	0.025448	0.935575	-0.026746
C12	1.548145	2.886068	-0.037494
H13	2.470423	2.905125	0.546604
H14	1.724663	3.351975	-1.008691
H15	0.747010	3.403576	0.489074
C16	2.160434	0.441487	-0.641825
O17	2.914432	0.030139	0.321120
N18	1.235751	-0.540279	-1.232350
H19	1.676903	-1.427027	-1.450670
H20	1.890212	-0.663922	0.985086
H21	-3.094385	-0.997888	-0.477563
H22	0.351857	-0.714325	1.897944
H23	1.392220	-2.994490	0.318062
H24	-0.083822	-3.040486	1.311697
C25	0.903426	-2.591847	1.204557
N26	0.814307	-1.113851	1.079333
H27	1.515541	-2.813003	2.078901

Zero-point correction= 0.217220
Thermal correction to Energy= 0.230518
Thermal correction to Enthalpy= 0.231462
Thermal correction to Gibbs Free Energy= 0.177543
Sum of electronic and zero-point Energies= -752.224423
Sum of electronic and thermal Energies= -752.211125
Sum of electronic and thermal Enthalpies= -752.210181
Sum of electronic and thermal Free Energies= -752.264100

147 TS$^{\text{via HA_NH2 products}}$_C5-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	1.528293	-1.091472	-0.057766
C2	0.028982	0.558129	0.239049
C3	-1.248280	0.962355	0.812958
O4	-1.488682	1.980059	1.424383
N5	-2.243036	0.012274	0.511591
C6	-2.018021	-1.234276	-0.030912
N7	-3.084986	-2.015325	-0.266812
H8	-4.033400	-1.706173	-0.133884
H9	-2.925073	-2.935016	-0.646938
N10	-0.806239	-1.687583	-0.298346
C11	0.163489	-0.808699	-0.052604
C12	2.136612	-2.369074	-0.413301
H13	2.643790	-2.805759	0.450095
H14	1.329470	-3.033507	-0.719796
H15	2.824020	-2.239777	-1.252226
C16	2.164019	0.004555	0.388188
O17	3.450987	0.165897	0.554763
N18	1.295112	0.962722	0.698673
H19	1.555625	1.906975	0.949377
H20	3.975423	-0.607465	0.310127
H21	-3.168583	0.265142	0.838396
H22	-0.800985	1.035933	-1.973543
H23	0.695212	3.319054	-0.897500
H24	-1.078861	3.151072	-0.862869
C25	-0.164660	2.865464	-1.400135
N26	0.043596	1.433993	-1.551730
H27	-0.217094	3.308888	-2.403137

Zero-point correction= 0.216209
Thermal correction to Energy= 0.231328
Thermal correction to Enthalpy= 0.232272
Thermal correction to Gibbs Free Energy= 0.174075
Sum of electronic and zero-point Energies= -752.250737
Sum of electronic and thermal Energies= -752.235617

Sum of electronic and thermal Enthalpies= -752.234673
Sum of electronic and thermal Free Energies= -752.292871

148 C5-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	-1.383387	1.167374	0.354710
C2	-0.104531	-0.869728	-0.001756
C3	1.038660	-1.059182	-1.006221
O4	0.989727	-1.799654	-1.954441
N5	2.172223	-0.316529	-0.681479
H6	2.974154	-0.488055	-1.277839
C7	2.153068	0.808436	0.132030
N8	3.326090	1.411186	0.383718
H9	4.212609	1.007265	0.128914
H10	3.322457	2.238488	0.960351
N11	1.029646	1.310891	0.602145
C12	-0.056486	0.565793	0.445244
C13	-2.226382	0.119119	-0.428575
O14	-3.360254	0.356619	-0.706922
N15	-1.410255	-0.916488	-0.646966
H16	-1.753746	-1.764026	-1.082830
H17	0.939774	-2.242509	1.124520
H18	-1.762095	-1.535112	2.087211
H19	-0.563673	-2.518941	2.906989
N20	-0.003288	-1.895681	1.003562
C21	-0.687267	-1.646129	2.265365
H22	-0.314197	-0.761468	2.802173
C23	-1.449581	2.514205	-0.303410
H24	-1.827511	1.249258	1.278276
H25	-2.498619	2.800298	-0.369262
H26	-0.876441	3.212802	0.303062
H27	-1.010587	2.425923	-1.296553

Zero-point correction= 0.219785
Thermal correction to Energy= 0.234400
Thermal correction to Enthalpy= 0.235344
Thermal correction to Gibbs Free Energy= 0.178058
Sum of electronic and zero-point Energies= -752.266819
Sum of electronic and thermal Energies= -752.252204
Sum of electronic and thermal Enthalpies= -752.251260
Sum of electronic and thermal Free Energies= -752.308546

149 TS$^{\text{via async add + PT}}$_C5-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	1.383364	-1.066214	0.222950
C2	0.059331	0.658976	-0.114148
C3	-1.242419	1.264812	-0.583766
O4	-1.359026	2.384661	-1.016150
N5	-2.306646	0.389570	-0.410756
H6	-3.207998	0.766416	-0.682240
C7	-2.206828	-0.945672	-0.001846
N8	-3.360481	-1.604761	0.196686
H9	-4.264349	-1.163048	0.159513
H10	-3.311371	-2.583556	0.435446
N11	-1.053164	-1.557229	0.163898
C12	0.008833	-0.828961	-0.173214
C13	2.130976	-0.129232	-0.673959
O14	3.254226	-0.293480	-1.037666
N15	1.255707	0.908206	-0.869488
H16	1.512928	1.779332	-1.312090
H17	-0.397722	0.653813	1.933578
H18	0.227416	3.015472	1.460764
H19	1.105341	2.224784	2.798514
N20	0.402177	0.893331	1.347808
C21	0.929880	2.219817	1.722301
H22	1.881111	2.387699	1.217823
C23	1.927803	-2.420966	0.387695
H24	1.220774	-0.236681	1.196326
H25	2.980803	-2.333047	0.651381
H26	1.373196	-2.918774	1.181851
H27	1.826096	-2.974832	-0.546403

Zero-point correction= 0.215784
Thermal correction to Energy= 0.229939
Thermal correction to Enthalpy= 0.230883
Thermal correction to Gibbs Free Energy= 0.175013
Sum of electronic and zero-point Energies= -752.242739
Sum of electronic and thermal Energies= -752.228585
Sum of electronic and thermal Enthalpies= -752.227641
Sum of electronic and thermal Free Energies= -752.283511

150 TS$^{\text{via async HA_NH2 + add}}$_C5-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	-1.632135	-0.907199	-0.372185
C2	-0.134780	0.662814	0.334537
C3	1.117077	1.069674	0.960300
O4	1.330771	2.104019	1.550891
N5	2.114509	0.098813	0.751102
H6	3.020365	0.351114	1.131059
C7	1.921793	-1.141026	0.187185
N8	2.982249	-1.949886	0.053934
H9	3.915079	-1.686672	0.326392
H10	2.834284	-2.868615	-0.334549
N11	0.729685	-1.556967	-0.218187
C12	-0.233414	-0.664226	-0.036735
C13	-2.389971	0.306874	0.269332
O14	-3.577421	0.335437	0.295862
N15	-1.415698	1.126886	0.699803
H16	-1.613907	2.045946	1.072509
H17	-0.124576	2.521167	-1.226354
H18	1.334279	0.275592	-2.401700
H19	1.104485	1.826620	-3.206493
N20	-0.094684	1.545812	-1.541835
C21	1.169982	1.342638	-2.222216
H22	2.042439	1.771713	-1.711301
C23	-2.210701	-2.229130	0.014328
H24	-1.742914	-0.760501	-1.387396
H25	-3.271285	-2.212541	-0.233402
H26	-1.682467	-3.004684	-0.537641
H27	-2.069987	-2.362715	1.086044

Zero-point correction= 0.216817
Thermal correction to Energy= 0.231480
Thermal correction to Enthalpy= 0.232425
Thermal correction to Gibbs Free Energy= 0.174991
Sum of electronic and zero-point Energies= -752.224863
Sum of electronic and thermal Energies= -752.210199
Sum of electronic and thermal Enthalpies= -752.209255
Sum of electronic and thermal Free Energies= -752.266689

151 C6-NHCH$_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	0.476536	1.842895	0.018510
C2	0.679707	-0.391241	0.178447
C3	0.466735	-1.849742	0.379823
O4	-0.428046	-2.224476	1.140441
N5	-2.757501	-0.877798	0.849186
H6	-1.925315	-1.293850	1.277033
C7	-2.610260	0.010939	-0.128483
N8	-3.635122	0.266113	-0.953536
H9	-3.553205	1.035240	-1.599623
N10	-1.536145	0.789953	-0.306472
C11	-0.269836	0.689115	-0.011416
C12	-0.056896	3.184247	-0.157607
H13	-0.516525	3.273442	-1.143315
H14	-0.800401	3.391936	0.612954
H15	0.776250	3.880741	-0.069237

C16	1.825597	1.584941	0.233540
O17	2.736444	2.363935	0.329953
N18	1.900930	0.186972	0.315238
H19	2.766249	-0.280463	0.548765
H20	-3.634852	-1.360163	0.972775
H21	-4.503856	-0.242050	-0.912814
H22	1.169452	-3.666703	0.055987
H23	2.029652	-1.507497	-1.796622
H24	3.297409	-2.382456	-0.897454
N25	1.314414	-2.702333	-0.217931
C26	2.275376	-2.437869	-1.283264
H27	2.223631	-3.246798	-2.012788

Zero-point correction= 0.218943
Thermal correction to Energy= 0.234498
Thermal correction to Enthalpy= 0.235442
Thermal correction to Gibbs Free Energy= 0.175191
Sum of electronic and zero-point Energies= -752.330769
Sum of electronic and thermal Energies= -752.315214
Sum of electronic and thermal Enthalpies= -752.314270
Sum of electronic and thermal Free Energies= -752.374522

152 $TS^{via\ async\ add\ +\ PT}$_C6-$NHCH_3$[9MOG + H_{N1}]$^{\bullet+}$

N1	-1.936570	0.476157	0.231136
C2	-0.062383	-0.612726	-0.371434
C3	1.302819	-1.116298	-0.580679
O4	1.690863	-1.700881	-1.552021
N5	2.108687	0.991602	-0.260568
H6	3.008884	1.268406	-0.643259
C7	1.297653	1.994761	-0.047787
N8	1.625983	3.295706	-0.143707
H9	0.913575	3.990152	0.018194
N10	-0.028349	1.812930	0.308751
C11	-0.576309	0.655944	0.099469
C12	-2.875345	1.523788	0.604859
H13	-2.589812	1.942836	1.569796
H14	-2.875024	2.312478	-0.149799
H15	-3.863344	1.069505	0.669990
C16	-2.334904	-0.768289	-0.237042
O17	-3.442762	-1.228278	-0.320049
N18	-1.135760	-1.414721	-0.600514
H19	-1.129432	-2.331135	-1.028592
H20	2.552155	3.597365	-0.397956
N21	2.087454	-1.378221	0.718336
H22	2.167956	-0.464320	1.182681
H23	3.028742	-1.629848	0.401966
C24	1.515608	-2.456571	1.573628
H25	0.520832	-2.155727	1.901804
H26	1.464711	-3.377578	0.992921
H27	2.163004	-2.596695	2.438696

Zero-point correction= 0.218839
Thermal correction to Energy= 0.233453
Thermal correction to Enthalpy= 0.234397
Thermal correction to Gibbs Free Energy= 0.176200
Sum of electronic and zero-point Energies= -752.273217
Sum of electronic and thermal Energies= -752.258603
Sum of electronic and thermal Enthalpies= -752.257659
Sum of electronic and thermal Free Energies= -752.315856

153 $TS^{via\ HA_NH2\ products}$_C6-$NHCH_3$[9MOG + H_{N1}]$^{+}$

N1	1.739366	-0.796105	0.168720
C2	0.489753	0.948979	-0.441335
C3	-0.512805	1.851515	-0.530184
O4	-1.113779	2.789493	-0.842875
N5	-1.820321	-0.726591	-1.835747
H6	-1.013841	-0.421822	-2.357816
C7	-1.657686	-1.300880	-0.627573
N8	-2.701953	-1.932921	-0.076258
H9	-2.550822	-2.399944	0.804451
N10	-0.508025	-1.336456	0.033069
C11	0.461437	-0.451823	-0.097817
C12	2.194835	-2.130839	0.524592
H13	1.710854	-2.452580	1.447801
H14	1.958334	-2.834187	-0.275350
H15	3.273856	-2.071703	0.664675
C16	2.638656	0.289245	-0.014983
O17	3.835759	0.239922	0.097114
N18	1.844221	1.353883	-0.357491
H19	2.235515	2.201625	-0.738590
H20	-2.687884	-0.802479	-2.343471
H21	-3.542288	-2.145038	-0.589883
H22	-2.969036	1.495750	0.971972
C23	-1.727830	0.781955	2.403051
H24	-2.514007	0.201216	2.907471
H25	-0.776490	0.251363	2.481591
H26	-1.655233	1.734038	2.951707
N27	-2.062283	1.020982	1.031567

Zero-point correction= 0.211760
Thermal correction to Energy= 0.228727
Thermal correction to Enthalpy= 0.229671
Thermal correction to Gibbs Free Energy= 0.166618
Sum of electronic and zero-point Energies= -752.234584
Sum of electronic and thermal Energies= -752.217617
Sum of electronic and thermal Enthalpies= -752.216673
Sum of electronic and thermal Free Energies= -752.279726

154 C6-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$

N1	-2.036128	0.484625	0.219087
C2	-0.069491	-0.538687	-0.306009
C3	1.434875	-0.679150	-0.425218
O4	1.859207	-1.582921	-1.291639
N5	1.784786	0.677215	-0.708749
H6	2.692741	0.801857	-1.144048
C7	1.423162	1.732737	0.233096
N8	1.903516	2.954623	-0.312054
H9	1.918671	3.705944	0.366429
H10	1.385658	3.241397	-1.135857
N11	-0.025229	1.753468	0.510456
C12	-0.664885	0.705354	0.195038
C13	-3.034686	1.465899	0.634573
H14	-4.017760	1.015169	0.504336
H15	-2.876575	1.721064	1.682756
H16	-2.947826	2.361025	0.017112
C17	-2.341222	-0.739705	-0.314838
O18	-3.377692	-1.292507	-0.510169
N19	-1.023096	-1.344066	-0.623865
H20	-0.921364	-2.278055	-1.017179
H21	1.887726	1.579810	1.219755
H22	3.021673	-1.143470	0.791479
H23	1.997881	-2.523281	2.430561
H24	0.436792	-2.357652	1.626147
N25	2.006539	-1.218357	0.824006
C26	1.513117	-2.436402	1.456622
H27	1.732329	-3.333236	0.871215

Zero-point correction= 0.218553
Thermal correction to Energy= 0.232913
Thermal correction to Enthalpy= 0.233857
Thermal correction to Gibbs Free Energy= 0.177117
Sum of electronic and zero-point Energies= -752.192581
Sum of electronic and thermal Energies= -752.178221

Sum of electronic and thermal Enthalpies= -752.177277
Sum of electronic and thermal Free Energies= -752.234017

155 $TS^{via\ async\ HA_NH2\ +\ add}$_C6-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$

N1	1.968185	0.167776	-0.347588
C2	-0.143687	-0.224691	0.418059
C3	-1.640862	-0.195497	0.266379
O4	-2.412344	-0.828424	1.033400
N5	-1.993759	1.009441	-0.376287
H6	-2.960547	1.259388	-0.202165
C7	-1.058968	2.125436	-0.301861
N8	-0.835614	2.474231	1.098993
H9	-1.668312	2.882736	1.516240
H10	-0.074880	3.141404	1.203426
N11	0.283914	1.815174	-0.815436
C12	0.695602	0.708166	-0.358747
C13	3.149035	0.795776	-0.935037
H14	3.991462	0.120147	-0.792569
H15	2.974357	0.955652	-1.998765
H16	3.345214	1.750384	-0.443612
C17	2.025587	-0.897418	0.521289
O18	2.933395	-1.581593	0.873964
N19	0.633310	-1.086523	0.981435
H20	0.360135	-1.834940	1.613872
H21	-1.472327	2.927585	-0.917685
H22	-2.310735	-1.014763	-1.673894
H23	-1.391239	-3.225947	-1.841739
H24	-0.731236	-3.064430	-0.203431
N25	-1.565668	-1.339639	-1.052196
C26	-1.554460	-2.770327	-0.858205
H27	-2.496364	-3.148975	-0.452294

Zero-point correction= 0.216524
Thermal correction to Energy= 0.230809
Thermal correction to Enthalpy= 0.231753
Thermal correction to Gibbs Free Energy= 0.174950
Sum of electronic and zero-point Energies= -752.175397
Sum of electronic and thermal Energies= -752.161113
Sum of electronic and thermal Enthalpies= -752.160168
Sum of electronic and thermal Free Energies= -752.216972

156 C6-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$

N1	-1.810649	0.929183	0.006335
C2	-0.180532	-0.631952	-0.117990
C3	1.112918	-1.249762	-0.475041
O4	1.944439	-0.591998	-1.126452
N5	2.145945	1.283991	1.563980
H6	3.161424	1.272107	1.613620
C7	1.657122	1.641247	0.465719
N8	2.499783	1.983459	-0.748111
H9	2.452603	1.089044	-1.290197
H10	2.067572	2.742086	-1.280897
N11	0.343735	1.807173	0.147404
C12	-0.449644	0.786706	0.037505
C13	-2.522778	2.185740	0.180771
H14	-2.257201	2.631075	1.140907
H15	-2.264388	2.873418	-0.625740
H16	-3.589249	1.964821	0.151636
C17	-2.444077	-0.302392	-0.133054
O18	-3.620624	-0.539696	-0.190480
N19	-1.396950	-1.239999	-0.191194
H20	-1.583805	-2.208722	-0.407243
H21	3.468708	2.218632	-0.528247
H22	2.210026	-2.891183	-0.502195
H23	-0.083458	-4.040378	0.283821
H24	0.038263	-2.738460	1.506128
C25	0.596667	-3.359027	0.803930
N26	1.341889	-2.524672	-0.132172
H27	1.304663	-3.956194	1.379134

Zero-point correction= 0.219609
Thermal correction to Energy= 0.234743
Thermal correction to Enthalpy= 0.235687
Thermal correction to Gibbs Free Energy= 0.176825
Sum of electronic and zero-point Energies= -752.282938
Sum of electronic and thermal Energies= -752.267803
Sum of electronic and thermal Enthalpies= -752.266859
Sum of electronic and thermal Free Energies= -752.325722

157 $TS^{via\ async\ HA_NH2\ +\ add}$_C6-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$

N1	1.995351	0.602086	-0.112189
C2	0.137307	-0.650258	0.091637
C3	-1.285336	-0.922283	0.578001
O4	-1.287973	-0.838847	1.831769
N5	-2.012315	0.462374	-0.072941
H6	-3.021699	0.399718	0.007548
C7	-1.365183	1.585816	-0.105092
N8	-2.134905	2.875148	-0.130702
H9	-3.072768	2.787968	0.270522
H10	-1.599222	3.563455	0.411284
N11	-0.075803	1.803093	-0.132238
C12	0.645235	0.665538	-0.071001
C13	2.926615	1.708400	-0.273335
H14	2.772459	2.186159	-1.242137
H15	2.780555	2.434210	0.527906
H16	3.933384	1.295171	-0.220577
C17	2.403905	-0.735158	0.043301
O18	3.526517	-1.163934	0.050792
N19	1.205441	-1.460572	0.163501
H20	1.196906	-2.457456	0.333015
H21	-2.213997	3.231698	-1.088870
H22	-2.123127	-2.731539	0.598587
H23	-0.759530	-2.655464	-1.620707
H24	-1.958756	-1.424274	-2.064854
C25	-1.780701	-2.295485	-1.426345
N26	-2.042491	-1.949713	-0.038547
H27	-2.480554	-3.073724	-1.733393

Zero-point correction= 0.218391
Thermal correction to Energy= 0.232178
Thermal correction to Enthalpy= 0.233122
Thermal correction to Gibbs Free Energy= 0.177395
Sum of electronic and zero-point Energies= -752.223098
Sum of electronic and thermal Energies= -752.209311
Sum of electronic and thermal Enthalpies= -752.208367
Sum of electronic and thermal Free Energies= -752.264093

158 C6-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$

N1	-2.006477	0.545013	0.103072
C2	-0.106516	-0.634382	-0.068373
C3	1.316711	-0.795244	-0.536187
O4	1.144609	-0.660130	-1.810112
N5	2.004028	0.519745	0.103805
H6	3.014393	0.444442	0.147630
C7	1.450766	1.706066	0.122441
N8	2.137382	2.853578	0.198078
H9	3.143019	2.850886	0.123772
H10	1.696960	3.727902	0.438776
N11	0.079879	1.789385	0.085536
C12	-0.663526	0.636673	0.046546
C13	-2.987664	1.607543	0.253913
H14	-3.962935	1.129261	0.349346
H15	-2.782467	2.185264	1.158293
H16	-2.995814	2.252656	-0.628363

C17	-2.367960	-0.827432	-0.002387
O18	-3.484564	-1.270083	0.021395
N19	-1.154950	-1.502553	-0.095172
H20	-1.103809	-2.505464	-0.198555
H21	-0.362057	2.680952	-0.088736
H22	2.203826	-2.569133	-0.792354
H23	0.984208	-2.757860	1.504343
H24	2.152678	-1.513160	1.990277
C25	1.974243	-2.332011	1.287192
N26	2.127128	-1.855585	-0.079676
H27	2.726392	-3.098403	1.476950

Zero-point correction= 0.217698
Thermal correction to Energy= 0.233041
Thermal correction to Enthalpy= 0.233985
Thermal correction to Gibbs Free Energy= 0.175468
Sum of electronic and zero-point Energies= -752.261401
Sum of electronic and thermal Energies= -752.246058
Sum of electronic and thermal Enthalpies= -752.245114
Sum of electronic and thermal Free Energies= -752.303631

159 $TS^{via\ HA_NH2\ products_C6}$_NHCH$_3$[9MOG + H_{N3}]$^{\bullet+}$

N1	1.908221	0.722703	-0.151577
C2	0.142774	-0.488979	0.451374
C3	-1.271040	-0.819541	0.611043
O4	-1.727370	-1.723599	1.333690
N5	-2.019474	0.462463	0.602889
H6	-2.935069	0.399220	1.032668
C7	-1.624256	1.610526	0.058017
N8	-2.466883	2.640357	-0.094063
H9	-3.456870	2.526402	0.058570
H10	-2.129863	3.578708	-0.244923
N11	-0.339091	1.735412	-0.327307
C12	0.546893	0.702678	-0.032787
C13	2.770419	1.819862	-0.547385
H14	3.796641	1.468459	-0.429810
H15	2.610248	2.086719	-1.595661
H16	2.618831	2.687983	0.100069
C17	2.408779	-0.524627	0.292970
O18	3.572577	-0.843275	0.357840
N19	1.280474	-1.259907	0.624484
H20	1.333453	-2.140218	1.114309
H21	-0.046838	2.528517	-0.880493
H22	-2.724341	-1.942281	-0.811520
H23	-0.825455	-3.427724	-0.920350
H24	0.061245	-2.116066	-1.756562
C25	-0.923669	-2.545074	-1.565592
N26	-1.791589	-1.552672	-0.982042
H27	-1.364639	-2.882302	-2.511067

Zero-point correction= 0.215645
Thermal correction to Energy= 0.230790
Thermal correction to Enthalpy= 0.231734
Thermal correction to Gibbs Free Energy= 0.173283
Sum of electronic and zero-point Energies= -752.245708
Sum of electronic and thermal Energies= -752.230563
Sum of electronic and thermal Enthalpies= -752.229619
Sum of electronic and thermal Free Energies= -752.288070

160 6C-NHCH$_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.271644	0.080254	0.254633
C2	-0.096153	-0.584165	0.254507
C3	1.396860	-0.461815	0.459150
O4	1.733008	-0.714456	1.730800
N5	1.748948	0.843397	-0.043419
H6	2.625595	1.188303	0.333316
C7	0.768833	1.822186	-0.263493
N8	1.271213	2.994711	-0.715002
H9	2.120034	3.005288	-1.258762
H10	0.600874	3.726441	-0.898906
N11	-0.506392	1.693955	-0.076252
C12	-0.965799	0.545724	0.669435
C13	-3.478828	0.880915	0.402528
H14	-3.702036	1.027200	1.461511
H15	-3.332928	1.845733	-0.086899
H16	-4.301444	0.346262	-0.071712
C17	-2.234989	-1.105290	-0.382883
O18	-3.057959	-1.797815	-0.901607
N19	-0.782809	-1.476458	-0.353755
H20	-0.427644	-2.279627	-0.867346
H21	-0.941595	0.720814	1.754724
H22	1.991023	-2.422047	0.283734
H23	4.163442	-1.083826	0.201761
H24	3.852238	-2.247469	-1.100461
N25	2.122859	-1.541824	-0.211524
C26	3.501910	-1.324376	-0.637295
H27	3.525817	-0.526229	-1.378954

Zero-point correction= 0.219009
Thermal correction to Energy= 0.233286
Thermal correction to Enthalpy= 0.234230
Thermal correction to Gibbs Free Energy= 0.177668
Sum of electronic and zero-point Energies= -752.213000
Sum of electronic and thermal Energies= -752.198723
Sum of electronic and thermal Enthalpies= -752.197779
Sum of electronic and thermal Free Energies= -752.254341

161 $TS^{via\ sync\ add\ +\ PT}$_C6-NHCH$_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	1.973981	0.492033	0.385190
C2	0.245745	-0.723532	-0.465091
C3	-1.259293	-1.069666	-0.406706
O4	-1.740541	-2.050124	-1.016876
N5	-1.892982	0.264215	-0.723812
H6	-2.730461	0.164818	-1.286082
C7	-1.342635	1.475241	-0.483929
N8	-2.011186	2.583874	-0.827355
H9	-2.928824	2.562623	-1.242129
H10	-1.557734	3.475082	-0.693851
N11	-0.137885	1.642690	0.079107
C12	0.558192	0.479563	0.319200
C13	2.771628	1.565771	0.963019
H14	2.506495	2.511001	0.486720
H15	2.590794	1.627988	2.037565
H16	3.821581	1.337812	0.781984
C17	2.511552	-0.581738	-0.264510
O18	3.636822	-0.942103	-0.427649
N19	1.329666	-1.336101	-0.768937
H20	1.406168	-2.246813	-1.219724
H21	-0.960507	-2.101561	1.401184
H22	-3.384419	-1.339050	1.288945
H23	-2.522610	-1.239261	2.846565
N24	-1.295421	-1.168366	1.155065
C25	-2.557045	-0.859121	1.825598
H26	-2.715213	0.219650	1.850272
H27	-0.027585	-0.101990	1.284463

Zero-point correction= 0.212140
Thermal correction to Energy= 0.226468
Thermal correction to Enthalpy= 0.227412
Thermal correction to Gibbs Free Energy= 0.171114
Sum of electronic and zero-point Energies= -752.181269
Sum of electronic and thermal Energies= -752.166941
Sum of electronic and thermal Enthalpies= -752.165997

Sum of electronic and thermal Free Energies= -752.222295

162 $TS^{via\ HA_NH2\ products}$_C6-NHCH$_3$[9MOG + H$_{C4}$]$^{\bullet+}$

N1	-2.149894	0.518914	-0.065544
C2	-0.274816	-0.631828	0.510446
C3	1.210308	-0.808425	0.727878
O4	1.675265	-1.783332	1.353343
N5	1.776115	0.483350	0.840790
H6	2.710346	0.514102	1.227804
C7	1.252220	1.575542	0.135300
N8	2.133341	2.543942	-0.191503
H9	3.128869	2.398566	-0.188784
H10	1.771598	3.385317	-0.613597
N11	-0.000667	1.681860	-0.171449
C12	-0.841545	0.743546	0.508420
C13	-3.118736	1.584304	-0.283447
H14	-3.491309	1.968537	0.669964
H15	-2.636966	2.383736	-0.847174
H16	-3.949092	1.174030	-0.857446
C17	-2.453574	-0.792100	-0.165905
O18	-3.432787	-1.391825	-0.493090
N19	-1.182033	-1.485443	0.220551
H20	-1.086304	-2.497254	0.170461
H21	-0.956328	1.032071	1.574684
H22	1.466678	-2.394129	-0.933755
H23	3.707897	-1.440857	-0.811572
H24	3.023012	-1.498952	-2.438271
N25	1.603683	-1.378759	-0.945444
C26	2.909665	-1.039913	-1.449545
H27	3.006830	0.042287	-1.545022
O27	-0.905717	-0.454662	1.788554

Zero-point correction= 0.214853
Thermal correction to Energy= 0.229758
Thermal correction to Enthalpy= 0.230703
Thermal correction to Gibbs Free Energy= 0.172226
Sum of electronic and zero-point Energies= -752.205808
Sum of electronic and thermal Energies= -752.190902
Sum of electronic and thermal Enthalpies= -752.189958
Sum of electronic and thermal Free Energies= -752.248435

163 C6-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	1.999601	0.435916	-0.171472
C2	-0.009761	-0.645920	-0.471036
C3	-1.233165	-0.620757	0.462621
N4	-1.900952	0.687444	0.157830
H5	-2.854225	0.767631	0.492089
C6	-1.201362	1.821463	-0.119198
N7	-1.845474	2.978253	-0.213097
H8	-2.840180	3.072432	-0.078954
H9	-1.302521	3.805501	-0.417371
N10	0.130911	1.843850	-0.286966
C11	0.708475	0.666808	-0.316077
C12	3.042643	1.432056	0.034098
H13	2.985040	2.182517	-0.754275
H14	2.913469	1.906359	1.008650
H15	3.999051	0.911797	-0.004262
C16	2.250616	-0.986450	-0.054167
O17	3.334618	-1.467988	0.102744
N18	1.021319	-1.581555	-0.140629
H19	0.934335	-2.583473	-0.213855
H20	-0.353807	-0.738665	-1.511095
N21	-2.044907	-1.755983	0.331802
H22	-2.684136	-1.863726	1.108372
C23	-2.522571	-2.211927	-0.967698
H24	-1.704927	-2.626581	-1.564495
H25	-3.237429	-3.017631	-0.802441
H26	-3.018605	-1.422079	-1.546274

Zero-point correction= 0.219361
Thermal correction to Energy= 0.233837
Thermal correction to Enthalpy= 0.234781
Thermal correction to Gibbs Free Energy= 0.177702
Sum of electronic and zero-point Energies= -752.264954
Sum of electronic and thermal Energies= -752.250478
Sum of electronic and thermal Enthalpies= -752.249534
Sum of electronic and thermal Free Energies= -752.306613

164 $TS^{via\ async\ add\ +\ PT}$_C6-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	2.133041	0.414840	-0.247544
C2	0.160538	-0.727971	-0.150664
C3	-1.301856	-0.777319	0.547716
N4	-1.798256	0.637457	0.464396
H5	-2.649820	0.764813	0.999438
C6	-1.101125	1.736568	0.131413
N7	-1.695851	2.927563	0.181381
H8	-2.667278	3.050865	0.419772
H9	-1.133291	3.744031	-0.009147
N10	0.204154	1.750927	-0.225016
C11	0.805750	0.592573	-0.227062
C12	3.146326	1.461061	-0.298195
H13	2.932102	2.126863	-1.134053
H14	3.146227	2.026095	0.635884
H15	4.111622	0.976192	-0.438691
C16	2.440404	-0.951005	-0.000829
O17	3.533301	-1.431468	0.084980
N18	1.206851	-1.586685	0.118388
H19	1.146885	-2.584189	0.266515
H20	-0.680323	-1.114816	-1.112620
N21	-1.950647	-1.518091	-0.652027
H22	-1.869508	-2.515567	-0.439656
C23	-3.300553	-1.208905	-1.134027
H24	-3.335140	-0.178673	-1.487777
H25	-3.532225	-1.877037	-1.964539
H26	-4.043582	-1.361325	-0.344965
O27	-1.435504	-1.342200	1.655356

Zero-point correction= 0.213154
Thermal correction to Energy= 0.227547
Thermal correction to Enthalpy= 0.228491
Thermal correction to Gibbs Free Energy= 0.171557
Sum of electronic and zero-point Energies= -752.221368
Sum of electronic and thermal Energies= -752.206976
Sum of electronic and thermal Enthalpies= -752.206031
Sum of electronic and thermal Free Energies= -752.262965

165 $TS^{via\ HA_NH2\ products}$_C6-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	2.194639	0.288229	-0.144531
C2	0.113507	-0.645769	-0.466601
C3	-1.128146	-0.541357	0.440210
N4	-1.678544	0.802068	0.294305
H5	-2.512645	0.962507	0.847469
C6	-0.906433	1.879325	-0.004311
N7	-1.464558	3.085139	-0.018556
H8	-2.453785	3.236460	0.101114
H9	-0.864923	3.881734	-0.180342
N10	0.417123	1.817879	-0.230581
C11	0.920733	0.609616	-0.278896
C12	3.305605	1.205023	0.073260
H13	3.317536	1.953484	-0.719086
H14	3.198042	1.692827	1.043724
H15	4.220677	0.613924	0.051769
C16	2.345091	-1.150104	-0.064237

O17	3.392819	-1.710689	0.079131
N18	1.078127	-1.655959	-0.166282
H19	0.928659	-2.648985	-0.249616
H20	-0.240142	-0.679993	-1.505554
N21	-2.390379	-1.550392	-0.587001
H22	-2.204046	-2.532774	-0.361437
C23	-3.793651	-1.270279	-0.437892
H24	-4.008350	-0.242270	-0.736098
H25	-4.366701	-1.952248	-1.077962
H26	-4.131067	-1.447084	0.592874
O27	-1.282612	-1.147443	1.494930

Zero-point correction= 0.216208
Thermal correction to Energy= 0.230779
Thermal correction to Enthalpy= 0.231723
Thermal correction to Gibbs Free Energy= 0.174223
Sum of electronic and zero-point Energies= -752.258014
Sum of electronic and thermal Energies= -752.243444
Sum of electronic and thermal Enthalpies= -752.242499
Sum of electronic and thermal Free Energies= -752.299999

166 C6-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-2.018847	0.572734	0.067773
C2	-0.112864	-0.565938	-0.197854
C3	1.348078	-0.770881	-0.442750
O4	1.636840	-0.917268	-1.806868
N5	1.972472	0.513019	-0.063858
H6	2.974880	0.526235	-0.206245
C7	1.334190	1.702408	0.051945
N8	2.059338	2.815624	0.157761
H9	3.065296	2.831917	0.105330
H10	1.565285	3.687387	0.280741
N11	-0.001243	1.849055	0.113997
C12	-0.671287	0.717681	0.001448
C13	-2.995353	1.633760	0.276307
H14	-2.835713	2.097527	1.250768
H15	-2.896974	2.382612	-0.510505
H16	-3.984471	1.178951	0.237519
C17	-2.360035	-0.780375	-0.084942
O18	-3.452481	-1.277546	-0.069937
N19	-1.126801	-1.448934	-0.255742
H20	-1.062886	-2.453497	-0.354637
H21	1.468202	-1.831048	-2.071306
H22	2.774825	-2.134681	-0.031301
H23	0.645177	-1.880655	2.007112
H24	2.198437	-1.035955	2.195036
C25	1.701436	-1.894061	1.725507
N26	1.831175	-1.908959	0.268035
H27	2.135421	-2.813626	2.118214

Zero-point correction= 0.220702
Thermal correction to Energy= 0.235066
Thermal correction to Enthalpy= 0.236010
Thermal correction to Gibbs Free Energy= 0.179569
Sum of electronic and zero-point Energies= -752.315934
Sum of electronic and thermal Energies= -752.301571
Sum of electronic and thermal Enthalpies= -752.300627
Sum of electronic and thermal Free Energies= -752.357068

167 TS$^{\text{via sync add + PT}}$_C6-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-1.981872	0.579462	0.154955
C2	-0.082677	-0.498745	-0.325884
C3	1.383668	-0.697222	-0.449472
O4	1.838022	-1.456115	-1.442532
N5	1.967237	0.661567	-0.408619
H6	2.827721	0.730294	-0.940727
C7	1.333643	1.789883	-0.006005
N8	2.018046	2.932884	0.036799
H9	3.006901	2.990822	-0.148287
H10	1.514258	3.776834	0.267474
N11	0.034669	1.847716	0.340106
C12	-0.636256	0.734725	0.095939
C13	-2.960143	1.607479	0.486464
H14	-2.731152	2.028018	1.465884
H15	-2.940516	2.394863	-0.268691
H16	-3.940501	1.132818	0.502821
C17	-2.330077	-0.713488	-0.275210
O18	-3.427867	-1.185129	-0.386054
N19	-1.099526	-1.349575	-0.551126
H20	-1.041301	-2.263457	-0.982269
H21	2.399683	-2.006885	-0.373091
H22	2.679282	-0.978250	1.254480
H23	0.587892	-3.048590	0.948880
H24	0.512524	-1.763216	2.190081
C25	1.175462	-2.370512	1.568583
N26	2.021174	-1.530353	0.704471
H27	1.824150	-2.967922	2.209546

Zero-point correction= 0.215990
Thermal correction to Energy= 0.230046
Thermal correction to Enthalpy= 0.230991
Thermal correction to Gibbs Free Energy= 0.174842
Sum of electronic and zero-point Energies= -752.265320
Sum of electronic and thermal Energies= -752.251264
Sum of electronic and thermal Enthalpies= -752.250320
Sum of electronic and thermal Free Energies= -752.306469

168 TS$^{\text{via HA_NH2 products}}$_C6-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-1.854182	0.787068	0.111543
C2	-0.100614	-0.432093	-0.546288
C3	1.256074	-0.681334	-0.645067
O4	1.759324	-1.670823	-1.396995
N5	2.045798	0.469338	-0.500702
H6	3.033600	0.354690	-0.688890
C7	1.569170	1.647642	-0.010223
N8	2.427491	2.649938	0.209909
H9	3.413924	2.591207	0.016064
H10	2.047074	3.532959	0.516150
N11	0.278999	1.846730	0.254231
C12	-0.515308	0.824310	-0.031647
C13	-2.716024	1.872119	0.559955
H14	-2.339040	2.272048	1.501645
H15	-2.745535	2.661545	-0.192857
H16	-3.713735	1.456947	0.698864
C17	-2.350993	-0.473955	-0.313077
O18	-3.500656	-0.817042	-0.341841
N19	-1.221570	-1.210150	-0.674631
H20	-1.290591	-2.101626	-1.142694
H21	2.368252	-2.187803	-0.846538
H22	1.605099	-0.887631	1.880031
H23	0.626025	-3.407668	0.740543
H24	-0.312021	-2.280684	1.765660
C25	0.693605	-2.657013	1.531702
N26	1.631507	-1.620477	1.164379
H27	1.065839	-3.156260	2.437482

Zero-point correction= 0.215953
Thermal correction to Energy= 0.230835
Thermal correction to Enthalpy= 0.231779
Thermal correction to Gibbs Free Energy= 0.174263
Sum of electronic and zero-point Energies= -752.268716
Sum of electronic and thermal Energies= -752.253833
Sum of electronic and thermal Enthalpies= -752.252889

Sum of electronic and thermal Free Energies= -752.310405

169 C6-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	2.167945	0.245559	-0.036680
C2	0.051176	-0.540124	-0.329030
C3	-1.379918	-0.538837	0.066585
O4	-1.175895	-0.829754	1.355792
N5	-1.792434	0.909611	-0.146875
H6	-2.787059	1.085802	-0.085559
C7	-0.952312	1.952619	-0.058906
N8	-1.426442	3.199869	-0.027493
N9	0.398861	1.833400	-0.028213
C10	0.824499	0.599088	-0.134366
C11	3.274672	1.193749	0.079650
H12	3.402612	1.722762	-0.865716
H13	3.046870	1.903723	0.874441
H14	4.177072	0.633019	0.319334
C15	2.341303	-1.100434	-0.049093
O16	3.302509	-1.797470	-0.006145
N17	0.917621	-1.693579	-0.167899
H18	0.677946	-2.207152	0.693380
H19	-2.409669	3.415703	0.003957
H20	0.892541	-2.361849	-0.945892
H21	-0.760795	3.957326	0.005090
H22	-2.332585	-1.176463	-1.603154
H23	-3.264654	-2.186307	1.018428
H24	-4.191112	-0.980551	0.094414
C25	-3.474340	-1.810866	0.016031
N26	-2.212854	-1.453135	-0.634894
H27	-3.943440	-2.611470	-0.556743

Zero-point correction= 0.219982
Thermal correction to Energy= 0.234479
Thermal correction to Enthalpy= 0.235423
Thermal correction to Gibbs Free Energy= 0.178435
Sum of electronic and zero-point Energies= -752.226689
Sum of electronic and thermal Energies= -752.212191
Sum of electronic and thermal Enthalpies= -752.211247
Sum of electronic and thermal Free Energies= -752.268236

170 TS$^{\text{via async add + PT}}$_C6-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	2.051546	0.384800	0.023029
C2	0.030873	-0.334760	0.719793
C3	-1.366601	-0.476112	0.271806
O4	-1.927654	-0.913863	1.403256
N5	-1.837460	0.847237	-0.185870
H6	-2.843855	0.957131	-0.174630
C7	-1.078645	1.972705	-0.084601
N8	-1.670399	3.161824	-0.175526
N9	0.262923	1.962861	0.010750
C10	0.756215	0.772807	0.294732
C11	3.124700	1.267901	-0.424424
H12	2.842415	1.749409	-1.361828
H13	3.309306	2.024332	0.338578
H14	4.017094	0.660085	-0.568300
C15	2.168019	-0.990824	0.059243
O16	3.114823	-1.686724	-0.137223
N17	0.819594	-1.508136	0.438626
H18	0.911144	-2.192827	1.192725
H19	-2.666090	3.280580	-0.272884
H20	0.046501	-1.895419	-0.386036
H21	-1.083584	3.982777	-0.149358
H22	-1.325197	-1.027919	-1.720644
H23	-2.395715	-3.025869	0.172757
H24	-3.400757	-2.081187	-0.945924
C25	-2.410668	-2.519359	-0.791197
N26	-1.346534	-1.496879	-0.817102
H27	-2.209658	-3.242513	-1.582183

Zero-point correction= 0.216733
Thermal correction to Energy= 0.230337
Thermal correction to Enthalpy= 0.231281
Thermal correction to Gibbs Free Energy= 0.176245
Sum of electronic and zero-point Energies= -752.214271
Sum of electronic and thermal Energies= -752.200667
Sum of electronic and thermal Enthalpies= -752.199723
Sum of electronic and thermal Free Energies= -752.254759

171 TS$^{\text{via async HA_NH2 + add}}$_C6-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	2.039180	0.461331	-0.193716
C2	0.019824	-0.505191	0.171143
C3	-1.380466	-0.533347	0.569309
O4	-1.822705	-1.332148	1.439324
N5	-1.858178	0.830414	0.554539
H6	-2.764085	0.963901	0.985616
C7	-1.189500	1.890273	0.027832
N8	-1.828396	3.062944	-0.066908
N9	0.089728	1.845190	-0.349431
C10	0.648751	0.654379	-0.153690
C11	3.017897	1.493693	-0.529159
H12	2.751449	1.937562	-1.488089
H13	3.021255	2.262447	0.244465
H14	3.996905	1.020735	-0.593381
C15	2.378872	-0.784904	0.196139
O16	3.412463	-1.363013	0.313258
N17	1.024761	-1.492175	0.511867
H18	1.004513	-1.760048	1.505501
H19	-2.815437	3.166099	0.100681
H20	0.988651	-2.364208	-0.026577
H21	-1.305002	3.859905	-0.395007
H22	-3.254217	-1.486233	-0.434301
H23	-0.767777	-2.237615	-1.822110
H24	-1.696096	-3.320997	-0.718239
C25	-1.755287	-2.473268	-1.413660
N26	-2.312277	-1.300565	-0.791150
H27	-2.402498	-2.780055	-2.243100

Zero-point correction= 0.216954
Thermal correction to Energy= 0.231710
Thermal correction to Enthalpy= 0.232654
Thermal correction to Gibbs Free Energy= 0.174592
Sum of electronic and zero-point Energies= -752.219430
Sum of electronic and thermal Energies= -752.204674
Sum of electronic and thermal Enthalpies= -752.203730
Sum of electronic and thermal Free Energies= -752.261792

172 C6-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-2.136577	0.293741	-0.023360
C2	-0.072920	-0.548721	-0.136760
C3	1.389498	-0.572877	0.104216
O4	1.314147	-0.795264	1.420936
N5	1.817277	0.848307	-0.226604
C6	1.026856	1.933319	-0.082412
N7	1.576150	3.156207	-0.087769
H8	2.570312	3.310145	-0.059811
H9	0.960198	3.951703	-0.026341
N10	-0.312925	1.874451	0.009959
C11	-0.780122	0.637588	-0.045838
C12	-3.249137	1.233984	0.067651
H13	-3.781364	1.103357	1.012326
H14	-2.817794	2.234308	0.039877
H15	-3.921589	1.114821	-0.784959
C16	-2.214478	-1.049234	-0.074024

O17	-3.294417	-1.789329	-0.087654
N18	-0.996982	-1.580257	-0.142906
H19	-0.784138	-2.569139	-0.178774
H20	-4.114139	-1.281351	-0.032482
H21	2.818619	0.991205	-0.243252
H22	2.198639	-1.288145	-1.611644
H23	3.800405	-2.780127	-0.655389
H24	4.160267	-1.163667	-0.017207
N25	2.124844	-1.543892	-0.633413
C26	3.403240	-1.960444	-0.055645
H27	3.232614	-2.327958	0.956932

Zero-point correction= 0.218534
Thermal correction to Energy= 0.233543
Thermal correction to Enthalpy= 0.234487
Thermal correction to Gibbs Free Energy= 0.176593
Sum of electronic and zero-point Energies= -752.247398
Sum of electronic and thermal Energies= -752.232389
Sum of electronic and thermal Enthalpies= -752.231445
Sum of electronic and thermal Free Energies= -752.289339

173 $TS^{via\ HA_NH2\ products}$_C6-$NHCH_3$[9MOG + H_{O8}]$^{\bullet+}$

N1	-1.924822	0.646266	-0.152752
C2	-0.072631	-0.454382	0.372731
C3	1.358657	-0.679776	0.585544
O4	1.827912	-1.566264	1.345551
N5	1.981080	0.620056	0.563982
C6	1.439712	1.754647	0.023382
N7	2.240437	2.834413	-0.075367
H8	3.243676	2.759957	-0.050988
H9	1.837011	3.676791	-0.453878
N10	0.174739	1.859924	-0.341918
C11	-0.530186	0.746679	-0.066274
C12	-2.827697	1.710204	-0.578872
H13	-3.504511	1.986895	0.232803
H14	-2.206184	2.570382	-0.827401
H15	-3.384336	1.404867	-1.467583
C16	-2.266214	-0.588910	0.250015
O17	-3.470570	-1.110674	0.331053
N18	-1.175574	-1.279463	0.568597
H19	-1.172108	-2.213958	0.955704
H20	-4.175500	-0.476047	0.151180
H21	2.903047	0.647101	0.979999
H22	2.959077	-1.643496	-0.767320
H23	1.765658	-2.960153	-2.349353
H24	1.393006	-3.483344	-0.700780
N25	1.965182	-1.459949	-0.933340
C26	1.299984	-2.649687	-1.407077
H27	0.245396	-2.434853	-1.596318

Zero-point correction= 0.216133
Thermal correction to Energy= 0.231142
Thermal correction to Enthalpy= 0.232086
Thermal correction to Gibbs Free Energy= 0.174108
Sum of electronic and zero-point Energies= -752.245066
Sum of electronic and thermal Energies= -752.230056
Sum of electronic and thermal Enthalpies= -752.229112
Sum of electronic and thermal Free Energies= -752.287090

174 C6-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.999359	0.694872	-0.435269
C2	-0.126091	-0.554041	0.025820
C3	1.256640	-0.741918	0.574907
O4	0.825037	-0.624386	1.830500
N5	2.020605	0.449864	0.064607
H6	3.018987	0.370188	0.217542
C7	1.479277	1.651671	-0.188976
N8	2.258662	2.729879	-0.323264
H9	3.248233	2.713935	-0.136662
H10	1.824315	3.606892	-0.566053
N11	0.151567	1.835280	-0.371576
C12	-0.537765	0.717695	-0.281238
C13	-2.729712	1.574371	0.545361
H14	-2.419203	1.284332	1.549126
H15	-2.443867	2.604813	0.341082
H16	-3.797983	1.415422	0.403347
C17	-2.385219	-0.798543	-0.241954
O18	-3.513061	-1.162388	-0.337499
N19	-1.216340	-1.424210	0.014089
H20	-1.184241	-2.409874	0.236906
H21	-2.277047	0.963991	-1.385918
H22	1.867111	-2.608393	0.980359
H23	2.538992	-1.571466	-1.721591
H24	1.136442	-2.637941	-1.508681
C25	2.111638	-2.351337	-1.086077
N26	2.042702	-1.887028	0.292897
H27	2.774979	-3.215692	-1.130916

Zero-point correction= 0.219223
Thermal correction to Energy= 0.233739
Thermal correction to Enthalpy= 0.234683
Thermal correction to Gibbs Free Energy= 0.177787
Sum of electronic and zero-point Energies= -752.220235
Sum of electronic and thermal Energies= -752.205719
Sum of electronic and thermal Enthalpies= -752.204775
Sum of electronic and thermal Free Energies= -752.261671

175 $TS^{via\ async\ HA_NH2\ +\ add}$_C6-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.962186	0.661913	-0.480310
C2	-0.132134	-0.429180	0.298823
C3	1.281768	-0.635678	0.648391
O4	1.669984	-1.459999	1.511630
N5	1.919647	0.656057	0.581238
H6	2.804092	0.707487	1.071068
C7	1.442223	1.746994	-0.089041
N8	2.252407	2.814090	-0.211028
H9	3.247325	2.753578	-0.071810
H10	1.885320	3.629406	-0.676423
N11	0.207859	1.817182	-0.562463
C12	-0.510439	0.724678	-0.261113
C13	-2.745263	1.760584	0.177536
H14	-2.527406	1.736380	1.244887
H15	-2.419354	2.704750	-0.255895
H16	-3.802998	1.574864	-0.005014
C17	-2.379375	-0.744697	0.064626
O18	-3.516623	-1.096732	0.042544
N19	-1.226085	-1.295570	0.484383
H20	-1.195458	-2.172634	0.987061
H21	-2.173230	0.670698	-1.484791
H22	2.976205	-1.689921	-0.513835
H23	0.329985	-2.587236	-1.450178
H24	1.445928	-3.548430	-0.428319
C25	1.376199	-2.764206	-1.191299
N26	1.994754	-1.532455	-0.762298
H27	1.900049	-3.124583	-2.084332

Zero-point correction= 0.216754
Thermal correction to Energy= 0.231322
Thermal correction to Enthalpy= 0.232266
Thermal correction to Gibbs Free Energy= 0.175205
Sum of electronic and zero-point Energies= -752.213456
Sum of electronic and thermal Energies= -752.198888
Sum of electronic and thermal Enthalpies= -752.197944

Sum of electronic and thermal Free Energies= -752.255006

176 O6-NHCH$_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	2.101845	-0.640946	-0.056746
C2	-0.128068	-0.312483	0.156805
C3	-1.238141	0.435021	0.256876
O4	-2.550153	0.147267	0.371280
N5	-1.103957	1.890873	0.112171
H6	-1.619545	2.338540	0.882061
C7	0.321642	2.434692	0.079814
N8	0.309468	3.767683	-0.263810
H9	1.204644	4.079726	-0.622174
N10	1.346531	1.637525	-0.044868
C11	1.153901	0.335077	-0.006742
C12	3.532601	-0.444983	-0.208778
H13	3.746762	0.024508	-1.170908
H14	3.910384	0.183688	0.599642
H15	4.001180	-1.427792	-0.164506
C16	1.497092	-1.907503	0.066060
O17	2.051338	-2.974446	0.061364
N18	0.129692	-1.661493	0.192318
H19	-0.565751	-2.380910	0.313203
H20	-1.584142	2.209077	-0.748205
H21	-0.054803	4.419688	0.423749
H22	-3.320491	-1.414124	1.197154
H23	-3.822062	-2.653209	-0.752042
H24	-2.970230	-1.440374	-1.722444
C25	-3.570035	-1.592019	-0.823255
N26	-2.763443	-1.280239	0.355243
H27	-4.490327	-1.002015	-0.881511

Zero-point correction= 0.218822
Thermal correction to Energy= 0.233941
Thermal correction to Enthalpy= 0.234885
Thermal correction to Gibbs Free Energy= 0.175182
Sum of electronic and zero-point Energies= -752.184138
Sum of electronic and thermal Energies= -752.169019
Sum of electronic and thermal Enthalpies= -752.168075
Sum of electronic and thermal Free Energies= -752.227778

177 TS$^{\text{via async add + PT}}$_O6-NHCH$_3$[9MOG + H$_{N1}$]$^{\bullet+}$

N1	-2.403456	0.189981	0.090066
C2	-0.346889	-0.629701	-0.309155
C3	0.981721	-0.519908	-0.618244
O4	1.984411	-1.442459	-0.404067
N5	1.576659	0.816887	-0.544813
H6	2.027944	1.067313	-1.432017
C7	0.697413	1.914996	-0.113417
N8	1.361726	3.067450	0.125864
H9	0.803737	3.882414	0.336621
N10	-0.568766	1.779575	0.069045
C11	-1.096844	0.544354	-0.087384
C12	-3.517631	1.076402	0.376617
H13	-3.367140	1.573693	1.336954
H14	-3.613245	1.822818	-0.413536
H15	-4.417603	0.462901	0.416246
C16	-2.524681	-1.205167	0.019676
O17	-3.529535	-1.860700	0.133570
N18	-1.224128	-1.679382	-0.205214
H19	-1.035088	-2.655158	-0.372972
H20	2.415767	0.395017	0.249288
H21	2.297659	3.225080	-0.212030
H22	2.432954	-1.257519	1.524196
H23	4.783320	-0.952568	1.282218
H24	4.567413	-0.885529	-0.486519
C25	4.194405	-1.322063	0.440103
N26	2.812192	-0.888259	0.650530
H27	4.260724	-2.410420	0.388005

Zero-point correction= 0.214935
Thermal correction to Energy= 0.229305
Thermal correction to Enthalpy= 0.230250
Thermal correction to Gibbs Free Energy= 0.173144
Sum of electronic and zero-point Energies= -752.183191
Sum of electronic and thermal Energies= -752.168821
Sum of electronic and thermal Enthalpies= -752.167877
Sum of electronic and thermal Free Energies= -752.224982

178 TS$^{\text{via HA_NH2 products}}$_O6-NHCH$_3$[9MOG + H$_{N1}$]$^{+}$

N1	-2.394357	0.057194	0.141270
C2	-0.290403	-0.592957	-0.275622
C3	1.042305	-0.412897	-0.566223
O4	2.039878	-1.214139	-0.648674
N5	1.526865	1.003362	-0.368145
H6	2.069951	1.285018	-1.193779
C7	0.523165	2.058061	-0.054826
N8	1.048313	3.302653	-0.078557
H9	0.408407	4.056656	0.133287
N10	-0.716889	1.795115	0.122242
C11	-1.120938	0.506694	-0.005081
C12	-3.576875	0.846436	0.444673
H13	-3.462565	1.336314	1.413249
H14	-3.737556	1.595013	-0.332857
H15	-4.420986	0.157731	0.475774
C16	-2.423377	-1.342511	-0.027917
O17	-3.387098	-2.061063	0.038184
N18	-1.098901	-1.704489	-0.280063
H19	-0.829059	-2.655309	-0.478942
H20	2.222668	0.826411	0.405336
H21	2.018618	3.470304	0.143974
H22	2.520998	-1.726560	1.339032
H23	4.905646	-1.386500	1.335059
H24	4.727755	-0.672852	-0.279184
C25	4.300618	-1.393841	0.420074
N26	2.962011	-0.982783	0.796105
H27	4.337633	-2.395883	-0.017458

Zero-point correction= 0.215989
Thermal correction to Energy= 0.230659
Thermal correction to Enthalpy= 0.231604
Thermal correction to Gibbs Free Energy= 0.173907
Sum of electronic and zero-point Energies= -752.179843
Sum of electronic and thermal Energies= -752.165172
Sum of electronic and thermal Enthalpies= -752.164228
Sum of electronic and thermal Free Energies= -752.221925

179 O6-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	2.066111	-0.677228	0.052828
C2	-0.136834	-0.291362	-0.265435
C3	-1.265280	0.546813	-0.315465
O4	-2.536823	0.192776	-0.357559
N5	-1.033562	1.848753	-0.288342
H6	-1.821805	2.486513	-0.236733
C7	0.313609	2.509163	-0.294765
N8	0.221215	3.594253	0.625895
H9	0.836132	4.357533	0.371317
H10	0.424576	3.307483	1.577789
N11	1.409086	1.599943	-0.065588
C12	1.159929	0.344533	-0.092696
C13	3.500043	-0.507671	0.236752
H14	3.941851	-1.500581	0.313736
H15	3.922652	0.023366	-0.617557
H16	3.690883	0.055585	1.151322

C17	1.435916	-1.914436	-0.030743
O18	1.913594	-3.011365	0.043652
N19	0.057473	-1.622768	-0.226170
H20	-0.668178	-2.322381	-0.306523
H21	0.440097	2.926625	-1.302179
H22	-3.318759	-1.377465	-1.145118
H23	-3.796824	-2.587149	0.821975
H24	-4.446004	-0.927473	0.939762
C25	-3.533597	-1.527935	0.879706
N26	-2.740400	-1.239840	-0.317097
H27	-2.920957	-1.369768	1.768666

Zero-point correction= 0.219909
Thermal correction to Energy= 0.234545
Thermal correction to Enthalpy= 0.235489
Thermal correction to Gibbs Free Energy= 0.176872
Sum of electronic and zero-point Energies= -752.229136
Sum of electronic and thermal Energies= -752.214500
Sum of electronic and thermal Enthalpies= -752.213556
Sum of electronic and thermal Free Energies= -752.272173

180 $TS^{\text{via async add + PT}}$_O6-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$

N1	-2.037715	0.662472	0.036223
C2	-0.266512	-0.499334	-0.801666
C3	1.049746	-0.597019	-1.093627
O4	1.850651	-1.642713	-0.661283
N5	1.699467	0.646753	-1.182539
H6	2.611388	0.672507	-1.622772
C7	1.477233	1.404160	0.005274
N8	2.292427	2.497279	0.207496
H9	3.283355	2.353754	0.330867
H10	1.893322	3.236838	0.768039
N11	0.121033	1.629972	0.307752
C12	-0.703395	0.779348	-0.210484
C13	-2.854000	1.638004	0.744692
H14	-3.858894	1.225866	0.829885
H15	-2.437525	1.821027	1.737828
H16	-2.880876	2.570295	0.179968
C17	-2.452806	-0.662702	-0.189606
O18	-3.546153	-1.122827	-0.021732
N19	-1.302900	-1.364964	-0.610826
H20	-1.369435	-2.307676	-0.967190
H21	1.887653	0.185481	0.737655
H22	3.212508	-1.358940	0.739574
H23	1.836112	-1.693514	2.667883
H24	1.695945	-3.077015	1.536796
C25	1.489845	-2.015737	1.683155
N26	2.203214	-1.209248	0.685274
H27	0.421110	-1.820465	1.595485

Zero-point correction= 0.213535
Thermal correction to Energy= 0.227341
Thermal correction to Enthalpy= 0.228285
Thermal correction to Gibbs Free Energy= 0.173518
Sum of electronic and zero-point Energies= -752.129341
Sum of electronic and thermal Energies= -752.115535
Sum of electronic and thermal Enthalpies= -752.114591
Sum of electronic and thermal Free Energies= -752.169357

181 $TS^{\text{via async HA_NH2 + add}}$_O6-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$

N1	1.303900	-1.272262	-0.354449
C2	0.153829	0.630543	0.272193
C3	-1.152916	1.193765	0.734315
O4	-1.039479	2.415555	0.161342
N5	-2.231909	0.393565	0.673616
H6	-3.134158	0.782385	0.923044
C7	-2.339064	-0.747614	-0.288783
N8	-3.295006	-1.646176	0.258595
H9	-2.928020	-2.154219	1.056906
H10	-3.636947	-2.303001	-0.432607
N11	-1.051967	-1.362998	-0.586840
C12	0.027095	-0.759924	-0.319677
C13	1.617561	-2.634211	-0.768033
H14	2.685697	-2.787643	-0.619712
H15	1.050028	-3.349598	-0.167905
H16	1.364495	-2.760489	-1.820625
C17	2.109656	-0.564189	0.548831
O18	3.217688	-0.837015	0.911603
N19	1.349350	0.545813	0.968312
H20	1.678724	1.166392	1.692924
H21	-2.745376	-0.362602	-1.233873
H22	-0.307081	1.621183	-1.683224
H23	2.119451	2.174803	-1.384698
H24	1.586260	3.101694	0.048981
C25	1.294812	2.736196	-0.934339
N26	0.148797	1.848236	-0.795598
H27	1.013269	3.572129	-1.575272

Zero-point correction= 0.217781
Thermal correction to Energy= 0.231682
Thermal correction to Enthalpy= 0.232626
Thermal correction to Gibbs Free Energy= 0.176888
Sum of electronic and zero-point Energies= -752.135237
Sum of electronic and thermal Energies= -752.121335
Sum of electronic and thermal Enthalpies= -752.120391
Sum of electronic and thermal Free Energies= -752.176129

182 O6-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$

N1	2.000028	-0.793543	-0.094940
C2	-0.185198	-0.304141	0.105556
C3	-1.216859	0.571272	0.152518
O4	-2.523838	0.354977	0.328964
N5	-0.946888	1.925011	-0.001360
H6	-1.732375	2.443274	-0.380976
C7	0.352028	2.342658	-0.373149
N8	0.709837	3.666825	0.258257
H9	0.675633	3.640539	1.287893
H10	1.676947	3.860336	-0.019516
N11	1.417305	1.507263	-0.278736
C12	1.128207	0.239917	-0.116994
C13	3.437668	-0.713458	-0.277966
H14	3.663302	-0.218992	-1.224231
H15	3.893921	-0.160177	0.545513
H16	3.819945	-1.734118	-0.290010
C17	1.314113	-2.013147	0.147655
O18	1.818277	-3.103934	0.225246
N19	-0.018546	-1.669876	0.270429
H20	-0.760045	-2.328438	0.444854
H21	0.120619	4.435577	-0.066967
H22	-3.403949	-1.085815	1.246489
H23	-4.013960	-2.400014	-0.613449
H24	-3.048916	-1.343701	-1.660027
N25	-2.836113	-1.049645	0.402184
C26	-3.663557	-1.375004	-0.758455
H27	-4.524402	-0.707645	-0.869092

Zero-point correction= 0.220666
Thermal correction to Energy= 0.235507
Thermal correction to Enthalpy= 0.236451
Thermal correction to Gibbs Free Energy= 0.177641
Sum of electronic and zero-point Energies= -752.198135
Sum of electronic and thermal Energies= -752.183294
Sum of electronic and thermal Enthalpies= -752.182350

Sum of electronic and thermal Free Energies= -752.241160

183 TS$^{via\ async\ add\ +\ PT}$_O6-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	2.110185	0.579854	0.068404
C2	0.325234	-0.515441	-0.773273
C3	-1.006539	-0.583051	-1.147102
O4	-1.923727	-1.494516	-0.650089
N5	-1.537539	0.705540	-1.397078
H6	-2.430033	0.752734	-1.869407
C7	-1.250831	1.584527	-0.360317
N8	-2.362570	1.720023	0.572682
H9	-2.563809	0.448401	0.671587
H10	-2.063965	2.183709	1.432345
N11	-0.053441	1.665857	0.151588
C12	0.810225	0.742090	-0.318166
C13	2.978082	1.584547	0.658590
H14	3.162060	2.386258	-0.058451
H15	2.521134	1.993870	1.562134
H16	3.918831	1.093749	0.907507
C17	2.469919	-0.773668	-0.052607
O18	3.539699	-1.268057	0.196293
N19	1.313911	-1.430635	-0.496780
H20	1.351890	-2.384525	-0.823190
H21	-3.171909	2.214470	0.193873
H22	-3.425626	-1.354344	0.581142
H23	-2.246096	-1.150576	2.654026
H24	-0.729474	-1.036088	1.728321
N25	-2.491127	-0.944061	0.593915
C26	-1.731706	-1.466994	1.742537
H27	-1.673017	-2.555164	1.703389

Zero-point correction= 0.215261
Thermal correction to Energy= 0.228781
Thermal correction to Enthalpy= 0.229726
Thermal correction to Gibbs Free Energy= 0.174712
Sum of electronic and zero-point Energies= -752.151603
Sum of electronic and thermal Energies= -752.138083
Sum of electronic and thermal Enthalpies= -752.137139
Sum of electronic and thermal Free Energies= -752.192152

184 TS$^{via\ async\ HA_NH2\ +\ add}$_O6-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	-2.282657	0.069202	-0.161210
C2	-0.159178	-0.506604	0.328150
C3	1.173073	-0.263132	0.612336
O4	2.074810	-1.097021	0.973810
N5	1.610224	1.084438	0.378921
H6	2.562929	1.069129	0.005442
C7	0.680328	1.999509	-0.050175
N8	1.126302	3.406044	-0.057024
H9	1.875578	3.591100	-0.733187
H10	0.310804	3.973883	-0.316163
N11	-0.594712	1.826153	-0.188045
C12	-1.009323	0.561223	-0.027430
C13	-3.478737	0.812881	-0.506653
H14	-3.691250	1.568141	0.253309
H15	-3.358336	1.291117	-1.481043
H16	-4.300326	0.097694	-0.549194
C17	-2.280369	-1.304961	0.111051
O18	-3.221883	-2.057388	0.090750
N19	-0.947486	-1.621007	0.409540
H20	-0.659906	-2.550256	0.675335
H21	1.457749	3.707636	0.869572
H22	4.031695	-1.434588	0.376105
H23	3.674070	-2.166688	-1.950941
H24	1.969775	-1.811339	-1.663778
N25	3.309960	-1.072180	-0.246884
C26	2.902310	-2.107910	-1.173018
H27	2.783751	-3.095131	-0.714604

Zero-point correction= 0.216403
Thermal correction to Energy= 0.231144
Thermal correction to Enthalpy= 0.232088
Thermal correction to Gibbs Free Energy= 0.174028
Sum of electronic and zero-point Energies= -752.175322
Sum of electronic and thermal Energies= -752.160581
Sum of electronic and thermal Enthalpies= -752.159637
Sum of electronic and thermal Free Energies= -752.217698

185 O6-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	-2.090392	0.672750	0.027428
C2	0.122247	0.309780	-0.097946
C3	1.250195	-0.483895	-0.344284
O4	2.560702	-0.216118	-0.094785
N5	1.007671	-1.887050	-0.240126
H6	1.784720	-2.481924	-0.501357
C7	-0.174366	-2.450197	0.000395
N8	-0.297711	-3.781052	0.098891
H9	0.509595	-4.384707	0.098166
H10	-1.202536	-4.223681	0.055172
N11	-1.267121	-1.670706	0.141809
C12	-1.101979	-0.276600	0.094259
C13	-3.511362	0.511364	0.258379
H14	-3.969269	1.489913	0.107628
H15	-3.940867	-0.193923	-0.458193
H16	-3.711609	0.186543	1.284266
C17	-1.478384	1.933490	-0.124425
O18	-2.039196	3.003891	-0.158148
N19	-0.119271	1.664214	-0.211693
H20	0.592549	2.363462	-0.354870
H21	-2.081277	-2.060335	0.598449
H22	3.375758	1.145922	-1.213249
H23	3.945274	2.680825	0.485462
H24	4.547580	1.052000	0.901098
N25	2.821078	1.175487	-0.358755
C26	3.650612	1.659723	0.740698
H27	3.056478	1.686244	1.655561

Zero-point correction= 0.218346
Thermal correction to Energy= 0.233898
Thermal correction to Enthalpy= 0.234842
Thermal correction to Gibbs Free Energy= 0.174590
Sum of electronic and zero-point Energies= -752.214888
Sum of electronic and thermal Energies= -752.199336
Sum of electronic and thermal Enthalpies= -752.198392
Sum of electronic and thermal Free Energies= -752.258644

186 TS$^{via\ async\ add\ +\ PT}$_O6-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	1.844744	0.624474	0.368047
C2	0.453232	-0.419728	-1.028787
C3	-0.902608	-0.839387	-1.214452
O4	-1.399402	-1.789860	-0.341173
N5	-1.763037	0.318509	-1.297570
H6	-2.515198	0.331563	-1.975371
C7	-1.577585	1.315966	-0.421569
N8	-2.410021	2.340767	-0.318194
H9	-3.269355	2.410538	-0.842992
H10	-2.152286	3.098212	0.298335
N11	-0.533376	1.219748	0.465459
C12	0.588331	0.628823	-0.149301
C13	2.445450	1.584931	1.280978
H14	3.296744	1.100683	1.758989
H15	2.794406	2.464379	0.735247
H16	1.711237	1.881232	2.030174

C17	2.577897	-0.432137	-0.221295
O18	3.748411	-0.673398	-0.054926
N19	1.654558	-1.110892	-1.013202
H20	1.951642	-1.811981	-1.675574
H21	-0.937159	0.100775	0.980270
H22	-0.486482	-1.783444	1.420237
H23	-2.352782	-1.276289	2.799422
H24	-2.735544	-2.614111	1.674640
N25	-1.261976	-1.243895	1.030897
C26	-2.501387	-1.551134	1.752519
H27	-3.313515	-0.960467	1.328803

Zero-point correction= 0.215372
Thermal correction to Energy= 0.229125
Thermal correction to Enthalpy= 0.230070
Thermal correction to Gibbs Free Energy= 0.174477
Sum of electronic and zero-point Energies= -752.158211
Sum of electronic and thermal Energies= -752.144458
Sum of electronic and thermal Enthalpies= -752.143513
Sum of electronic and thermal Free Energies= -752.199106

187 $TS^{via\ HA_NH2\ products}$_O6-NHCH$_3$[9MOG + H_{N3}]$^{\bullet+}$

N1	2.212456	0.035546	-0.128212
C2	0.077753	-0.419500	0.382468
C3	-1.264153	-0.115107	0.663840
O4	-2.246542	-0.902684	0.904438
N5	-1.589990	1.258129	0.362250
H6	-2.584346	1.453266	0.357112
C7	-0.734199	2.208539	-0.000017
N8	-1.136178	3.469975	-0.199537
H9	-2.083339	3.752389	-0.000294
H10	-0.537647	4.150021	-0.641483
N11	0.568848	1.888835	-0.162482
C12	0.960136	0.560664	0.014406
C13	3.439434	0.705603	-0.512216
H14	4.213444	-0.061241	-0.564052
H15	3.335793	1.170244	-1.496681
H16	3.732802	1.447639	0.235882
C17	2.148411	-1.346043	0.162400
O18	3.069009	-2.126046	0.135265
N19	0.814373	-1.584558	0.468421
H20	0.475677	-2.490790	0.751176
H21	1.260529	2.618332	-0.261466
H22	-3.986156	-1.469953	-0.010245
H23	-3.156464	-2.736342	-1.888821
H24	-2.491110	-3.264183	-0.322681
N25	-3.123216	-1.222558	-0.496787
C26	-2.535181	-2.434152	-1.036929
H27	-1.536173	-2.217156	-1.425352

Zero-point correction= 0.215375
Thermal correction to Energy= 0.230937
Thermal correction to Enthalpy= 0.231882
Thermal correction to Gibbs Free Energy= 0.171929
Sum of electronic and zero-point Energies= -752.215291
Sum of electronic and thermal Energies= -752.199729
Sum of electronic and thermal Enthalpies= -752.198785
Sum of electronic and thermal Free Energies= -752.258737

188 O6-NHCH$_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.105181	-0.660432	0.029262
C2	0.122776	-0.288313	0.340221
C3	1.241813	0.540772	0.315766
O4	2.524422	0.220441	0.287883
N5	0.992670	1.873700	0.285960
H6	1.769632	2.512189	0.405967
C7	-0.275499	2.359900	-0.144643
N8	-0.264303	3.669748	-0.503811
H9	0.537416	4.055629	-0.980539
H10	-1.159093	4.035695	-0.797734
N11	-1.330582	1.639358	-0.148426
C12	-1.220197	0.370771	0.519631
C13	-3.551230	-0.522976	0.038649
H14	-3.927082	-0.433704	1.062686
H15	-3.831301	0.361001	-0.535755
H16	-3.976163	-1.413442	-0.424148
C17	-1.473243	-1.853158	-0.140352
O18	-1.897922	-2.940409	-0.422994
N19	-0.066666	-1.575781	0.070578
H20	0.664618	-2.262163	-0.065987
H21	-1.406820	0.525147	1.600200
H22	3.202651	-1.291721	1.287384
H23	3.987122	-2.584554	-0.519028
H24	4.626233	-0.920446	-0.622548
C25	3.722439	-1.535150	-0.670575
N26	2.752632	-1.207250	0.375891
H27	3.249655	-1.430366	-1.647977

Zero-point correction= 0.220244
Thermal correction to Energy= 0.234541
Thermal correction to Enthalpy= 0.235486
Thermal correction to Gibbs Free Energy= 0.178667
Sum of electronic and zero-point Energies= -752.224398
Sum of electronic and thermal Energies= -752.210101
Sum of electronic and thermal Enthalpies= -752.209157
Sum of electronic and thermal Free Energies= -752.265975

189 $TS^{via\ HA_NH2\ products}$_O6-NHCH$_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.361771	-0.196131	0.292913
C2	-0.147568	-0.508803	-0.130247
C3	1.195633	-0.079641	-0.396545
O4	2.120342	-0.847234	-0.755809
N5	1.366643	1.269381	-0.182470
H6	2.305290	1.633522	-0.285545
C7	0.264545	2.155595	-0.142447
N8	0.581483	3.456760	-0.347787
H9	1.345104	3.709180	-0.956473
H10	-0.194363	4.102706	-0.319267
N11	-0.940294	1.778740	0.103778
C12	-1.084753	0.426534	0.561494
C13	-3.623378	0.330475	0.790569
H14	-3.696188	0.205124	1.874615
H15	-3.689599	1.387480	0.530666
H16	-4.432926	-0.217727	0.309133
C17	-2.236053	-1.428197	-0.254559
O18	-3.031680	-2.276431	-0.535807
N19	-0.787230	-1.572874	-0.513141
H20	-0.412867	-2.353914	-1.043870
H21	-0.875059	0.376153	1.648651
H22	2.957979	-2.441605	0.508021
H23	5.058724	-1.618066	1.263325
H24	4.803564	-1.422644	-0.478990
N25	3.088217	-1.466601	0.795032
C26	4.447709	-1.100595	0.505470
H27	4.594885	-0.028020	0.641974

Zero-point correction= 0.214722
Thermal correction to Energy= 0.229652
Thermal correction to Enthalpy= 0.230596
Thermal correction to Gibbs Free Energy= 0.171202
Sum of electronic and zero-point Energies= -752.191534
Sum of electronic and thermal Energies= -752.176604
Sum of electronic and thermal Enthalpies= -752.175660

Sum of electronic and thermal Free Energies= -752.235054

190 O6-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	0.739319	-1.867287	0.056665
C2	-0.152253	0.024155	-0.940098
C3	-0.310074	1.371172	-0.286901
O4	-1.348706	1.774586	0.453140
N5	0.880580	2.015515	0.000944
H6	0.829233	2.992379	0.266409
C7	2.074310	1.361666	0.030574
N8	3.208860	2.064458	0.098914
H9	3.237271	3.071337	0.097186
H10	4.076636	1.555315	0.176685
N11	2.143329	0.021861	0.046853
C12	1.038866	-0.608965	-0.251377
C13	1.584647	-2.799599	0.789396
H14	2.535228	-2.915938	0.268346
H15	1.760688	-2.426884	1.800434
H16	1.057271	-3.752270	0.827716
C17	-0.639548	-2.143161	-0.244719
O18	-1.180350	-3.197248	-0.060023
N19	-1.164274	-0.964696	-0.712679
H20	-2.061037	-0.942354	-1.173424
H21	0.071054	0.156585	-2.010801
H22	-2.888542	2.418941	-0.539644
H23	-4.499044	0.921062	0.299484
H24	-3.602958	1.680111	1.644612
N25	-2.595296	1.491249	-0.234425
C26	-3.523389	1.007600	0.784175
H27	-3.206343	0.018098	1.117863

Zero-point correction= 0.219457
Thermal correction to Energy= 0.234032
Thermal correction to Enthalpy= 0.234977
Thermal correction to Gibbs Free Energy= 0.177581
Sum of electronic and zero-point Energies= -752.230815
Sum of electronic and thermal Energies= -752.216240
Sum of electronic and thermal Enthalpies= -752.215296
Sum of electronic and thermal Free Energies= -752.272692

191 TS$^{\text{via async add + PT}}$_O6-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	-2.076280	-0.067841	0.217367
C2	0.107272	-0.443881	-0.220155
C3	1.282112	0.109668	-0.873358
O4	2.436530	-0.639837	-0.603854
N5	1.456631	1.489065	-0.600942
H6	2.289523	1.917988	-0.984224
C7	0.505995	2.276608	-0.018410
N8	0.771780	3.576568	0.150362
H9	1.620361	4.016838	-0.165592
H10	0.043755	4.153995	0.543802
N11	-0.675687	1.821765	0.384831
C12	-0.878212	0.523878	0.172615
C13	-3.340443	0.551928	0.585134
H14	-3.246654	1.020180	1.565128
H15	-3.620134	1.302011	-0.156683
H16	-4.089584	-0.238792	0.614000
C17	-1.984353	-1.403869	-0.282214
O18	-2.894217	-2.189521	-0.344954
N19	-0.671320	-1.559387	-0.657203
H20	-0.318585	-2.478791	-0.870097
H21	1.069454	-0.895263	0.779293
H22	2.916357	-0.563738	1.330654
H23	2.673378	-2.887831	1.822206
H24	3.760270	-2.668599	0.415460
C25	2.739270	-2.557029	0.783502
N26	2.325459	-1.152102	0.740888
H27	2.059432	-3.143422	0.166712

Zero-point correction= 0.215184
Thermal correction to Energy= 0.229271
Thermal correction to Enthalpy= 0.230215
Thermal correction to Gibbs Free Energy= 0.174261
Sum of electronic and zero-point Energies= -752.192152
Sum of electronic and thermal Energies= -752.178064
Sum of electronic and thermal Enthalpies= -752.177120
Sum of electronic and thermal Free Energies= -752.233075

192 TS$^{\text{via HA_NH2 products}}$_O6-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	-2.144563	0.534073	-0.111033
C2	0.139308	0.389374	-0.367818
C3	1.151256	-0.356020	0.445996
O4	2.274964	0.123698	0.811069
N5	1.011158	-1.753050	0.312938
H6	1.791943	-2.311593	0.636850
C7	-0.160205	-2.346700	-0.026692
N8	-0.224121	-3.672347	-0.122098
H9	0.571581	-4.277969	0.003946
H10	-1.119755	-4.086367	-0.337209
N11	-1.297784	-1.652237	-0.214658
C12	-1.168549	-0.349950	-0.241104
C13	-3.562276	0.243259	0.057333
H14	-3.890459	-0.422985	-0.740425
H15	-3.732713	-0.227491	1.027436
H16	-4.094643	1.192271	0.004191
C17	-1.602558	1.864945	0.044592
O18	-2.265702	2.852418	0.179492
N19	-0.238199	1.714894	0.037205
H20	0.345486	2.524782	-0.106116
H21	0.474373	0.364508	-1.422801
H22	4.007282	-0.179592	-0.267487
H23	4.538843	2.019291	-0.963945
H24	4.174397	1.930017	0.777164
N25	3.265799	0.479420	-0.512699
C26	3.752571	1.815802	-0.226489
H27	2.956249	2.546673	-0.378590

Zero-point correction= 0.216447
Thermal correction to Energy= 0.231126
Thermal correction to Enthalpy= 0.232070
Thermal correction to Gibbs Free Energy= 0.173246
Sum of electronic and zero-point Energies= -752.224895
Sum of electronic and thermal Energies= -752.210216
Sum of electronic and thermal Enthalpies= -752.209271
Sum of electronic and thermal Free Energies= -752.268096

193 O6-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	-2.173787	0.403568	0.097929
C2	0.001357	0.342917	-0.411648
C3	1.351755	-0.259536	-0.527824
O4	2.179412	0.086883	0.572751
N5	1.174438	-1.693606	-0.494026
H6	2.019200	-2.232085	-0.627230
C7	0.058830	-2.335766	-0.061351
N8	0.111117	-3.655663	0.113937
H9	0.951988	-4.199947	0.006118
H10	-0.739403	-4.125113	0.388252
N11	-1.123105	-1.742298	0.163383
C12	-1.116973	-0.434564	-0.034451
C13	-3.533791	0.034714	0.467739
H14	-4.126288	0.948789	0.487218
H15	-3.940871	-0.658353	-0.269620
H16	-3.533760	-0.431397	1.453954

C17	-1.767319	1.723911	-0.161989
O18	-2.431205	2.723721	-0.123820
N19	-0.394778	1.625574	-0.478217
H20	0.201064	2.427976	-0.637756
H21	1.854064	0.028445	-1.459033
H22	2.325920	1.825861	1.391368
H23	4.172721	2.665574	0.188789
H24	4.553802	1.052288	0.857897
N25	2.498511	1.480538	0.449807
C26	3.924852	1.601928	0.150022
H27	4.116873	1.244715	-0.864088

Zero-point correction= 0.220881
Thermal correction to Energy= 0.235273
Thermal correction to Enthalpy= 0.236217
Thermal correction to Gibbs Free Energy= 0.178659
Sum of electronic and zero-point Energies= -752.254777
Sum of electronic and thermal Energies= -752.240384
Sum of electronic and thermal Enthalpies= -752.239440
Sum of electronic and thermal Free Energies= -752.296999

194 $TS^{via\ PT\ in\ adduct}$_O6-NHCH$_3$[9MOG + H_{C6}]$^{\bullet+}$

N1	2.374366	-0.143958	-0.032496
C2	0.160622	-0.486354	-0.100881
C3	-1.214184	-0.114718	-0.203531
O4	-2.107127	-0.819714	0.724503
N5	-1.330407	1.310781	-0.068236
H6	-2.243763	1.702179	-0.245865
C7	-0.287312	2.178470	-0.011270
N8	-0.548005	3.494430	0.010918
H9	-1.470813	3.872436	0.147195
H10	0.240863	4.120335	0.068173
N11	0.992941	1.806352	-0.005587
C12	1.175876	0.491301	-0.061975
C13	3.684324	0.481525	0.061502
H14	4.430339	-0.307165	-0.031170
H15	3.802734	1.206420	-0.744520
H16	3.792717	0.981732	1.025537
C17	2.174355	-1.534452	-0.023212
O18	3.011563	-2.398174	0.028598
N19	0.784257	-1.700545	-0.081773
H20	0.365967	-2.614421	-0.007371
H21	-2.248622	-0.914418	-1.046214
H22	-2.857591	-2.464579	-0.103095
H23	-4.969220	-1.627309	-0.751781
H24	-4.697631	-1.235964	0.974734
N25	-2.968432	-1.453706	-0.209167
C26	-4.369807	-1.046529	-0.048390
H27	-4.456748	0.014934	-0.279500

Zero-point correction= 0.215095
Thermal correction to Energy= 0.229560
Thermal correction to Enthalpy= 0.230504
Thermal correction to Gibbs Free Energy= 0.173237
Sum of electronic and zero-point Energies= -752.191334
Sum of electronic and thermal Energies= -752.176869
Sum of electronic and thermal Enthalpies= -752.175925
Sum of electronic and thermal Free Energies= -752.233192

195 $TS^{via\ HA_NH2\ products}$_O6-NHCH$_3$[9MOG + H_{C6}]$^{\bullet+}$

N1	-2.121519	-0.417554	0.390075
C2	-0.455703	0.641588	-0.687370
C3	0.946023	0.745027	-1.088066
O4	1.068536	1.290980	0.162223
N5	1.536530	-0.578290	-1.217484
H6	2.499418	-0.577153	-1.529280
C7	1.113283	-1.595374	-0.435568
N8	1.879222	-2.670716	-0.278676
H9	2.788230	-2.766866	-0.703559
H10	1.501328	-3.447847	0.243860
N11	-0.094564	-1.630656	0.175002
C12	-0.843734	-0.570750	0.004538
C13	-2.933044	-1.385087	1.117380
H14	-3.924458	-0.950845	1.241178
H15	-2.997314	-2.313198	0.547749
H16	-2.484618	-1.577780	2.092700
C17	-2.617058	0.834401	-0.058838
O18	-3.716439	1.274573	0.108236
N19	-1.555187	1.425288	-0.764218
H20	-1.629322	2.347783	-1.168452
H21	1.242688	1.368570	-1.932105
H22	3.011554	2.572712	0.346531
H23	4.444111	1.258502	1.807751
H24	2.795024	1.516717	2.399994
N25	3.089338	1.553510	0.285089
C26	3.382772	1.048402	1.602523
H27	3.244621	-0.035337	1.633852

Zero-point correction= 0.215417
Thermal correction to Energy= 0.230354
Thermal correction to Enthalpy= 0.231298
Thermal correction to Gibbs Free Energy= 0.172444
Sum of electronic and zero-point Energies= -752.195673
Sum of electronic and thermal Energies= -752.180736
Sum of electronic and thermal Enthalpies= -752.179792
Sum of electronic and thermal Free Energies= -752.238645

196 O6-NHCH$_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	2.119287	-0.560066	0.091180
C2	-0.156202	-0.268156	-0.048339
C3	-1.278279	0.473576	-0.202226
O4	-2.551511	0.112530	-0.418727
N5	-1.127743	1.857980	-0.122010
H6	-1.907139	2.374925	0.268969
C7	0.160401	2.418681	0.003009
N8	0.171689	3.773493	0.057830
N9	1.252131	1.722648	0.109218
C10	1.081576	0.382148	0.183100
C11	3.532456	-0.232058	0.256790
H12	3.821547	0.495932	-0.501770
H13	3.689355	0.192350	1.249514
H14	4.109203	-1.148685	0.142562
C15	1.687075	-1.809542	-0.106351
O16	2.197499	-2.890218	-0.186670
N17	0.119888	-1.683410	-0.208138
H18	-0.305408	-2.273906	0.512578
H19	-0.527438	4.293295	-0.451467
H20	-0.187558	-2.067000	-1.105737
H21	1.084986	4.199933	0.115520
H22	-3.243814	-1.501618	-1.193970
H23	-3.777898	-2.672582	0.788660
H24	-4.495210	-1.037219	0.804821
N25	-2.711639	-1.314902	-0.345639
C26	-3.558168	-1.602145	0.814940
H27	-3.006973	-1.379143	1.730872

Zero-point correction= 0.219549
Thermal correction to Energy= 0.234521
Thermal correction to Enthalpy= 0.235465
Thermal correction to Gibbs Free Energy= 0.176511
Sum of electronic and zero-point Energies= -752.190373
Sum of electronic and thermal Energies= -752.175401
Sum of electronic and thermal Enthalpies= -752.174457

Sum of electronic and thermal Free Energies= -752.233411

197 TS$^{\text{via async add + PT}}$_O6-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	1.218198	1.634171	0.067339
C2	-0.104651	0.029660	-0.804060
C3	-0.669482	-1.269219	-0.753534
O4	-1.968229	-1.397197	-0.354328
N5	0.278321	-2.217334	-0.275627
H6	0.038231	-3.193868	-0.382777
C7	1.566306	-1.886511	0.059606
N8	2.412583	-2.882106	0.354953
N9	2.016310	-0.639146	0.140146
C10	1.111217	0.278603	-0.229850
C11	2.405570	2.295798	0.594862
H12	2.727924	1.792763	1.507077
H13	3.205171	2.261595	-0.146398
H14	2.143705	3.331476	0.808439
C15	0.037464	2.277701	-0.176568
O16	-0.271486	3.427946	-0.066565
N17	-0.906644	1.223502	-0.672844
H18	-1.378269	1.557542	-1.516517
H19	2.161069	-3.855762	0.316788
H20	-1.692228	0.791694	0.100682
H21	3.357990	-2.634304	0.603463
H22	-1.994559	-0.757107	1.560310
H23	-4.122620	0.328084	1.497242
H24	-4.228762	-1.344878	0.873430
N25	-2.350801	-0.377761	0.681915
C26	-3.813683	-0.350176	0.698245
H27	-4.172145	0.032354	-0.257971

Zero-point correction= 0.215334
Thermal correction to Energy= 0.229473
Thermal correction to Enthalpy= 0.230417
Thermal correction to Gibbs Free Energy= 0.174325
Sum of electronic and zero-point Energies= -752.192419
Sum of electronic and thermal Energies= -752.178281
Sum of electronic and thermal Enthalpies= -752.177337
Sum of electronic and thermal Free Energies= -752.233429

198 TS$^{\text{via async HA_NH2 + add}}$_O6-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	1.940486	0.658998	0.126796
C2	0.100963	-0.249720	-0.829668
C3	-1.293409	-0.468010	-0.927589
O4	-1.817289	-1.669433	-0.763959
N5	-2.010042	0.689139	-0.500242
H6	-3.010601	0.678672	-0.647319
C7	-1.405344	1.831892	-0.056760
N8	-2.180656	2.883861	0.235818
N9	-0.092321	1.954873	0.129401
C10	0.598869	0.861252	-0.215293
C11	2.821154	1.664620	0.713826
H12	3.016184	2.451821	-0.015840
H13	2.342933	2.089954	1.596291
H14	3.753641	1.173857	0.989606
C15	2.330982	-0.612436	-0.138594
O16	3.366702	-1.188243	-0.009547
N17	1.093540	-1.298244	-0.738263
H18	0.665403	-2.030968	-0.104196
H19	-3.177087	2.894961	0.094159
H20	1.357903	-1.743038	-1.622964
H21	-1.726880	3.726051	0.555008
H22	-1.435457	-3.390238	0.177761
H23	-1.393030	-2.685024	2.477656
H24	-2.871842	-2.165049	1.625281
N25	-1.122451	-2.455900	0.438214
C26	-1.784386	-2.053057	1.673541
H27	-1.529346	-1.015927	1.903755

Zero-point correction= 0.217539
Thermal correction to Energy= 0.231948
Thermal correction to Enthalpy= 0.232892
Thermal correction to Gibbs Free Energy= 0.175676
Sum of electronic and zero-point Energies= -752.192054
Sum of electronic and thermal Energies= -752.177645
Sum of electronic and thermal Enthalpies= -752.176701
Sum of electronic and thermal Free Energies= -752.233917

199 O6-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-2.132866	-0.374787	-0.045733
C2	0.091726	-0.287244	0.076775
C3	1.358145	0.324111	-0.003358
O4	2.505118	-0.127859	0.591008
N5	1.269899	1.735314	-0.001227
C6	0.075846	2.418466	-0.032614
N7	0.156471	3.765533	-0.111198
H8	0.990196	4.255578	0.170095
H9	-0.714509	4.270269	-0.054558
N10	-1.106240	1.844148	-0.023111
C11	-1.036658	0.490085	0.005419
C12	-3.531351	0.032205	-0.125727
H13	-4.064685	-0.246812	0.785978
H14	-3.541925	1.117543	-0.222408
H15	-4.004196	-0.406598	-1.006996
C16	-1.662876	-1.629160	0.016742
O17	-2.344838	-2.756246	0.024899
N18	-0.329083	-1.610663	0.082341
H19	0.291892	-2.406489	0.159212
H20	-3.299964	-2.622443	0.056446
H21	2.114598	2.234061	-0.246591
H22	3.035120	-1.847917	1.244206
H23	3.730494	-2.839929	-0.800051
H24	4.529797	-1.261117	-0.547201
C25	3.571351	-1.761460	-0.719682
N26	2.616231	-1.543997	0.367927
H27	3.132962	-1.404144	-1.653689

Zero-point correction= 0.218780
Thermal correction to Energy= 0.234009
Thermal correction to Enthalpy= 0.234954
Thermal correction to Gibbs Free Energy= 0.176181
Sum of electronic and zero-point Energies= -752.216691
Sum of electronic and thermal Energies= -752.201461
Sum of electronic and thermal Enthalpies= -752.200517
Sum of electronic and thermal Free Energies= -752.259290

200 TS$^{\text{via HA_NH2 products}}$_O6-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	2.225617	0.161235	0.179613
C2	0.167297	-0.443501	-0.425307
C3	-1.198128	-0.266604	-0.724489
O4	-2.094469	-1.188930	-0.867202
N5	-1.606966	1.074202	-0.465905
C6	-0.759035	2.083539	-0.093233
N7	-1.282275	3.315056	0.052536
H8	-2.244419	3.532292	-0.143068
H9	-0.659297	4.063310	0.310765
N10	0.528760	1.907722	0.141449
C11	0.927114	0.630143	-0.031499
C12	3.362993	0.973960	0.597983
H13	4.135246	0.974052	-0.174078
H14	2.993076	1.990131	0.731966
H15	3.759478	0.613953	1.550151
C16	2.226029	-1.157199	-0.067562

O17	3.231920	-2.001190	0.010733
N18	1.004789	-1.551053	-0.436619
H19	0.742778	-2.507001	-0.632447
H20	4.044834	-1.598517	0.340470
H21	-2.563148	1.287870	-0.715795
H22	-2.671977	-2.846555	0.135305
H23	-4.028932	-1.954837	1.866721
H24	-4.463555	-1.295103	0.270710
C25	-3.673893	-1.341888	1.029715
N26	-2.439935	-1.945354	0.554350
H27	-3.467873	-0.341997	1.419447

Zero-point correction= 0.215536
Thermal correction to Energy= 0.231100
Thermal correction to Enthalpy= 0.232044
Thermal correction to Gibbs Free Energy= 0.171751
Sum of electronic and zero-point Energies= -752.214124
Sum of electronic and thermal Energies= -752.198560
Sum of electronic and thermal Enthalpies= -752.197616
Sum of electronic and thermal Free Energies= -752.257909

201 O6-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	2.158228	0.481814	-0.290071
C2	-0.101587	0.251414	0.180463
C3	-1.247405	-0.466504	0.236506
O4	-2.532056	-0.088464	0.350810
N5	-1.110532	-1.855607	0.189969
H6	-1.894081	-2.415303	0.497145
C7	0.103265	-2.452909	-0.117801
N8	0.082411	-3.800095	-0.258084
H9	-0.750446	-4.265590	-0.583722
H10	0.962018	-4.232220	-0.498195
N11	1.217883	-1.782356	-0.221348
C12	1.116724	-0.466459	0.106834
C13	3.432209	0.413787	0.495412
H14	3.188473	0.565017	1.546117
H15	3.859404	-0.576594	0.343870
H16	4.099858	1.196178	0.135538
C17	1.480255	1.872063	-0.166692
O18	2.110889	2.877020	-0.286736
N19	0.180429	1.620365	0.073832
H20	-0.510584	2.342412	0.228051
H21	2.401565	0.361509	-1.285036
H22	-3.122932	1.447869	1.353743
H23	-3.755033	2.833208	-0.448410
H24	-4.506009	1.221161	-0.611618
N25	-2.654842	1.340884	0.455159
C26	-3.559305	1.770329	-0.611497
H27	-3.062880	1.648566	-1.575621

Zero-point correction= 0.220255
Thermal correction to Energy= 0.234765
Thermal correction to Enthalpy= 0.235709
Thermal correction to Gibbs Free Energy= 0.178541
Sum of electronic and zero-point Energies= -752.197910
Sum of electronic and thermal Energies= -752.183400
Sum of electronic and thermal Enthalpies= -752.182456
Sum of electronic and thermal Free Energies= -752.239624

202 TS$^{\text{via async HA_NH2 + add}}$_O6-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	2.402601	0.079000	0.394899
C2	0.246095	-0.476905	-0.147443
C3	-1.092776	-0.234363	-0.463309
O4	-2.007995	-1.095162	-0.729067
N5	-1.437700	1.134890	-0.318715
H6	-2.380632	1.376186	-0.591598
C7	-0.556601	2.115373	0.060090
N8	-1.018882	3.376207	0.140575
H9	-1.999001	3.599440	0.094697
H10	-0.383511	4.085720	0.470293
N11	0.714235	1.874916	0.325746
C12	1.043126	0.574615	0.194218
C13	3.448080	0.695134	-0.492759
H14	3.147871	0.534391	-1.527777
H15	3.484187	1.760299	-0.269110
H16	4.399494	0.206793	-0.284484
C17	2.288687	-1.456121	0.154859
O18	3.238857	-2.165660	0.253933
N19	0.994065	-1.664722	-0.158538
H20	0.644141	-2.581297	-0.400286
H21	2.698786	0.207010	1.370388
H22	-2.731288	-2.431049	0.672890
H23	-4.969442	-1.695329	0.947056
H24	-4.509364	-1.835537	-0.767574
N25	-2.951535	-1.433846	0.648545
C26	-4.312193	-1.295533	0.165054
H27	-4.554142	-0.238360	0.034730

Zero-point correction= 0.216016
Thermal correction to Energy= 0.231051
Thermal correction to Enthalpy= 0.231995
Thermal correction to Gibbs Free Energy= 0.172839
Sum of electronic and zero-point Energies= -752.186537
Sum of electronic and thermal Energies= -752.171502
Sum of electronic and thermal Enthalpies= -752.170558
Sum of electronic and thermal Free Energies= -752.229714

203 N7-NHCH$_3$[9MOG + H$_{N1}$]$^{+}$

N1	-0.592604	1.653146	-0.067206
C2	0.055383	-0.521437	-0.300840
C3	0.848139	-1.641633	-0.293607
O4	0.659696	-2.836585	-0.358430
N5	2.360843	-1.202729	-0.124806
H6	2.845942	-1.623283	-0.925617
C7	2.693822	0.256229	0.006302
N8	3.967881	0.452436	0.487727
H9	4.122998	1.398040	0.815477
N10	1.749003	1.179200	0.083717
C11	0.511030	0.799172	-0.070628
C12	-0.516122	3.099326	0.118287
H13	-0.163683	3.316882	1.127481
H14	0.176509	3.516887	-0.613241
H15	-1.512681	3.513342	-0.027840
C16	-1.751863	0.996956	-0.273556
O17	-2.881267	1.358317	-0.398829
N18	-1.387828	-0.519286	-0.349001
H19	-1.761239	-0.890049	-1.236826
H20	2.711004	-1.709321	0.701734
H21	4.740679	0.118176	-0.077508
H22	-1.444993	-2.043502	0.902672
H23	-4.013243	-0.654214	0.476816
H24	-3.521675	-2.133802	-0.407442
N25	-2.001460	-1.196799	0.789748
C26	-3.398994	-1.552465	0.517408
H27	-3.726261	-2.161677	1.360913

Zero-point correction= 0.219546
Thermal correction to Energy= 0.234485
Thermal correction to Enthalpy= 0.235429
Thermal correction to Gibbs Free Energy= 0.176724
Sum of electronic and zero-point Energies= -752.185576
Sum of electronic and thermal Energies= -752.170637
Sum of electronic and thermal Enthalpies= -752.169693

Sum of electronic and thermal Free Energies= -752.228398

204 TS$^{via\ HA_NH2\ products}$_N7-NHCH$_3$[9MOG + H$_{N1}$]$^+$

N1	-0.627952	1.590930	-0.140498
C2	0.077416	-0.514625	-0.471791
C3	0.917007	-1.612581	-0.451548
O4	0.818621	-2.801664	-0.570929
N5	2.435586	-1.084381	-0.233674
H6	2.904717	-1.277413	-1.126731
C7	2.668659	0.324636	0.199869
N8	3.909807	0.528981	0.721624
H9	4.063756	1.461994	1.082282
N10	1.714900	1.195528	0.213337
C11	0.485388	0.792358	-0.114315
C12	-0.662879	3.022853	0.127470
H13	-0.427344	3.205795	1.176928
H14	0.058902	3.533305	-0.510849
H15	-1.670238	3.373975	-0.092810
C16	-1.746969	0.865499	-0.475147
O17	-2.876660	1.231043	-0.667859
N18	-1.319243	-0.530793	-0.521888
H19	-1.794847	-1.089788	-1.229064
H20	2.840592	-1.734776	0.450519
H21	4.719879	0.121048	0.273121
H22	-1.507097	-2.116720	1.010631
H23	-3.961339	-0.536884	0.797282
H24	-3.665161	-2.148412	0.065083
N25	-2.004185	-1.223180	1.089927
C26	-3.421346	-1.478464	0.900132
H27	-3.763562	-1.964803	1.824086

Zero-point correction= 0.215579
Thermal correction to Energy= 0.230593
Thermal correction to Enthalpy= 0.231537
Thermal correction to Gibbs Free Energy= 0.172804
Sum of electronic and zero-point Energies= -752.162896
Sum of electronic and thermal Energies= -752.147882
Sum of electronic and thermal Enthalpies= -752.146937
Sum of electronic and thermal Free Energies= -752.205671

205 N7-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	-0.969554	1.479459	0.036107
C2	0.153925	-0.498512	-0.272981
C3	1.257437	-1.463325	-0.175732
O4	1.168116	-2.627601	-0.507724
N5	2.328530	-0.860162	0.423884
H6	3.135234	-1.458409	0.558850
C7	2.553844	0.587410	0.472347
N8	3.202325	1.017159	-0.755527
H9	4.108713	0.571053	-0.862371
H10	3.346783	2.023077	-0.747115
N11	1.351044	1.401370	0.573717
C12	0.277041	0.839940	0.156794
C13	-1.203898	2.881779	0.381708
H14	-2.253789	3.103459	0.195711
H15	-0.966141	3.035642	1.434770
H16	-0.567157	3.515511	-0.236831
C17	-1.909066	0.666998	-0.479864
O18	-3.064953	0.781177	-0.734946
N19	-1.200459	-0.727212	-0.711275
H20	3.131832	0.774933	1.385794
H21	-1.220951	-0.938771	-1.718796
H22	-2.824529	-1.815041	-0.472411
H23	-2.514136	-2.550348	1.733846
H24	-0.909612	-1.829360	1.780367
C25	-1.916769	-1.711317	1.375972
N26	-1.882835	-1.839134	-0.080635
H27	-2.369992	-0.778556	1.736187

Zero-point correction= 0.219979
Thermal correction to Energy= 0.234379
Thermal correction to Enthalpy= 0.235323
Thermal correction to Gibbs Free Energy= 0.177839
Sum of electronic and zero-point Energies= -752.191730
Sum of electronic and thermal Energies= -752.177329
Sum of electronic and thermal Enthalpies= -752.176385
Sum of electronic and thermal Free Energies= -752.233869

206 TS$^{via\ async\ HA_NH2\ +\ add}$_N7-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	-1.041321	1.411326	0.071293
C2	0.139873	-0.472159	-0.415750
C3	1.278892	-1.406146	-0.404908
O4	1.199278	-2.537198	-0.841868
N5	2.325580	-0.844966	0.260506
H6	3.145515	-1.433167	0.354532
C7	2.494387	0.589721	0.538574
N8	3.190408	1.210201	-0.572322
H9	4.119088	0.816445	-0.690354
H10	3.287253	2.209547	-0.417116
N11	1.264762	1.353391	0.691988
C12	0.219178	0.824316	0.197964
C13	-1.356236	2.790262	0.439445
H14	-2.414505	2.957943	0.243942
H15	-1.142063	2.935207	1.498287
H16	-0.751170	3.474717	-0.157273
C17	-1.876178	0.609216	-0.645885
O18	-2.990833	0.758789	-1.042851
N19	-1.127116	-0.688983	-0.814525
H20	3.017941	0.648644	1.501266
H21	-1.335119	-1.291342	-1.611813
H22	-3.003586	-1.369411	0.313282
H23	-2.140747	-2.504499	2.246098
H24	-0.516077	-2.176789	1.652096
C25	-1.540045	-1.796420	1.653030
N26	-2.109543	-1.877342	0.338170
H27	-1.612712	-0.818145	2.144219

Zero-point correction= 0.216126
Thermal correction to Energy= 0.230713
Thermal correction to Enthalpy= 0.231657
Thermal correction to Gibbs Free Energy= 0.173481
Sum of electronic and zero-point Energies= -752.172526
Sum of electronic and thermal Energies= -752.157938
Sum of electronic and thermal Enthalpies= -752.156994
Sum of electronic and thermal Free Energies= -752.215171

207 N7-[9MOG + H$_{N2}$]$^+$

N1	-0.870501	1.497964	-0.119329
C2	0.019775	-0.600119	-0.229265
C3	1.056091	-1.566833	-0.372511
O4	0.971452	-2.732057	-0.703625
N5	2.321824	-0.979725	-0.074413
H6	3.017313	-1.681082	0.155433
C7	2.445414	0.314761	0.457768
N8	3.775108	0.930045	0.130049
H9	3.948343	0.974934	-0.885206
H10	3.751036	1.888326	0.491145
N11	1.467228	1.250339	0.310404
C12	0.299548	0.737035	0.021442
C13	-0.970492	2.934660	0.111638
H14	-0.685472	3.156754	1.140785
H15	-0.310185	3.463935	-0.576386
H16	-2.004134	3.231246	-0.062336

C17	-1.909955	0.727536	-0.497814
O18	-3.062285	0.954265	-0.713189
N19	-1.371912	-0.734089	-0.577703
H20	4.556437	0.438811	0.569429
H21	-1.490785	-1.072000	-1.540622
H22	-3.106510	-1.563274	-0.123178
H23	-2.744055	-2.069874	2.142867
H24	-1.073610	-1.511618	2.013776
C25	-2.088846	-1.350685	1.650312
N26	-2.152556	-1.661045	0.224517
H27	-2.425260	-0.336381	1.904703

Zero-point correction= 0.221803
Thermal correction to Energy= 0.236318
Thermal correction to Enthalpy= 0.237262
Thermal correction to Gibbs Free Energy= 0.179704
Sum of electronic and zero-point Energies= -752.188502
Sum of electronic and thermal Energies= -752.173987
Sum of electronic and thermal Enthalpies= -752.173043
Sum of electronic and thermal Free Energies= -752.230601

208 $TS^{\text{via async add + PT}}$_N7-[9MOG + H_{N2}]$^+$

N1	1.501937	-1.066286	-0.309564
C2	-0.411076	-0.037972	-1.061330
C3	-1.809450	0.300730	-0.996370
O4	-2.277107	1.389380	-1.309582
N5	-2.532808	-0.732383	-0.383626
H6	-3.528006	-0.570763	-0.279430
C7	-1.814284	-1.305951	0.692854
N8	-1.521894	-0.296145	1.755416
H9	-2.384286	0.132914	2.094312
H10	-1.084208	-0.768449	2.547470
N11	-0.590751	-1.949613	0.416375
C12	0.085591	-1.162062	-0.343005
C13	2.412587	-2.138120	0.085221
H14	1.901661	-2.748150	0.831532
H15	2.662676	-2.747972	-0.784153
H16	3.318087	-1.699626	0.503660
C17	1.878913	0.199403	-0.529691
O18	2.916626	0.783706	-0.560842
N19	0.522831	0.987765	-0.715015
H20	-0.621241	0.708827	1.212017
H21	0.660218	1.758373	-1.378678
H22	-0.667152	2.263626	0.287699
H23	0.570821	2.814610	2.217959
H24	1.793910	1.585224	1.809870
C25	1.090068	2.308882	1.401265
N26	0.055777	1.607237	0.609735
H27	1.621630	3.043210	0.794212

Zero-point correction= 0.216774
Thermal correction to Energy= 0.229978
Thermal correction to Enthalpy= 0.230923
Thermal correction to Gibbs Free Energy= 0.177062
Sum of electronic and zero-point Energies= -752.115711
Sum of electronic and thermal Energies= -752.102506
Sum of electronic and thermal Enthalpies= -752.101562
Sum of electronic and thermal Free Energies= -752.155423

209 $TS^{\text{via async HA_NH2 + add}}$_N7-$NHCH_3$[9MOG + H_{N2}]$^{\bullet+}$

N1	-0.977312	1.444583	-0.106704
C2	0.016428	-0.547547	-0.463924
C3	1.087636	-1.495303	-0.544947
O4	1.046081	-2.664697	-0.859225
N5	2.321280	-0.874051	-0.188106
H6	3.063566	-1.546118	-0.027284
C7	2.383575	0.405819	0.346987
N8	3.721151	1.039517	0.284859
H9	4.081298	1.121736	-0.677878
H10	3.608550	1.987305	0.661662
N11	1.393661	1.290161	0.302296
C12	0.233030	0.773194	-0.048830
C13	-1.196339	2.855775	0.173400
H14	-0.943594	3.068840	1.213122
H15	-0.583654	3.468490	-0.490115
H16	-2.250816	3.067343	-0.001194
C17	-1.952422	0.605402	-0.581411
O18	-3.106574	0.822582	-0.832266
N19	-1.334682	-0.730058	-0.666994
H20	4.425150	0.553239	0.847621
H21	-1.653227	-1.328163	-1.426360
H22	-3.123219	-1.280344	0.541723
H23	-2.042305	-2.127851	2.608448
H24	-0.533419	-1.682363	1.835776
C25	-1.600281	-1.440343	1.876293
N26	-2.217115	-1.755022	0.612239
H27	-1.743032	-0.413084	2.237865

Zero-point correction= 0.217614
Thermal correction to Energy= 0.232450
Thermal correction to Enthalpy= 0.233394
Thermal correction to Gibbs Free Energy= 0.174362
Sum of electronic and zero-point Energies= -752.171669
Sum of electronic and thermal Energies= -752.156833
Sum of electronic and thermal Enthalpies= -752.155889
Sum of electronic and thermal Free Energies= -752.214921

210 N7-$NHCH_3$[9MOG + H_{N3}]$^{\bullet+}$

N1	-0.549127	1.558999	-0.065101
C2	0.061238	-0.615204	0.262528
C3	0.924129	-1.602108	-0.223423
O4	0.674006	-2.678056	-0.735075
N5	2.319355	-1.194465	-0.112895
H6	2.983458	-1.908447	-0.386970
C7	2.725862	0.061929	0.102240
N8	4.031609	0.352223	0.126756
H9	4.727031	-0.367400	0.004206
H10	4.363760	1.300437	0.207566
N11	1.818971	1.030301	0.319696
C12	0.443626	0.732082	0.523284
C13	-0.559442	3.013774	-0.016210
H14	-1.496530	3.365038	-0.447753
H15	-0.486457	3.351800	1.020785
H16	0.269373	3.414803	-0.604928
C17	-1.621332	0.852279	-0.487385
O18	-2.664935	1.191993	-0.969806
N19	-1.326924	-0.622121	-0.130745
H20	2.165468	1.912179	0.672601
H21	-1.467136	-1.221824	-0.955740
H22	-2.050455	-0.623844	1.726018
H23	-4.099986	-0.301344	0.336909
H24	-3.694913	-1.873677	-0.404544
C25	-3.611166	-1.264931	0.499534
N26	-2.201635	-1.185230	0.890941
H27	-4.109411	-1.804075	1.306938

Zero-point correction= 0.220035
Thermal correction to Energy= 0.234933
Thermal correction to Enthalpy= 0.235877
Thermal correction to Gibbs Free Energy= 0.177481
Sum of electronic and zero-point Energies= -752.203223
Sum of electronic and thermal Energies= -752.188325
Sum of electronic and thermal Enthalpies= -752.187381

Sum of electronic and thermal Free Energies= -752.245777

211 TS$^{via\ HA_NH2\ products}$_N7-NHCH$_3$[9MOG + H$_{N3}$]$^{•+}$

N1	-0.571957	1.600122	-0.074914
C2	0.058549	-0.552998	-0.105582
C3	0.955777	-1.619708	-0.315003
O4	0.767032	-2.762016	-0.659700
N5	2.331621	-1.170001	-0.111378
H6	3.018086	-1.901141	-0.256929
C7	2.736580	0.084481	0.141177
N8	4.036404	0.357329	0.313918
H9	4.731742	-0.370382	0.255361
H10	4.373397	1.302569	0.409102
N11	1.820089	1.061387	0.249681
C12	0.460251	0.741254	0.235211
C13	-0.594287	3.046610	0.072234
H14	-1.587195	3.390995	-0.217469
H15	-0.408399	3.324110	1.112800
H16	0.144425	3.509163	-0.587761
C17	-1.675940	0.883507	-0.495437
O18	-2.771965	1.281680	-0.810389
N19	-1.322819	-0.537350	-0.322972
H20	2.115325	1.969257	0.582297
H21	-1.678409	-1.148094	-1.060610
H22	-2.145556	-0.460593	1.664241
H23	-4.104758	-0.602481	0.286424
H24	-3.569241	-2.249592	-0.181757
C25	-3.551255	-1.491251	0.606580
N26	-2.170203	-1.246416	1.008705
H27	-4.049943	-1.927989	1.478657

Zero-point correction= 0.216403
Thermal correction to Energy= 0.231586
Thermal correction to Enthalpy= 0.232531
Thermal correction to Gibbs Free Energy= 0.173756
Sum of electronic and zero-point Energies= -752.194121
Sum of electronic and thermal Energies= -752.178938
Sum of electronic and thermal Enthalpies= -752.177994
Sum of electronic and thermal Free Energies= -752.236768

212 N7-[9MOG + H$_{C4}$]$^{+}$

N1	-0.785285	1.428929	-0.087909
C2	0.032655	-0.691311	0.168633
C3	1.117927	-1.561310	-0.260362
O4	0.925593	-2.634191	-0.800895
N5	2.356038	-1.014050	0.001856
H6	3.152044	-1.607373	-0.198481
C7	2.526110	0.373297	0.169031
N8	3.805867	0.795550	0.095688
H9	4.526947	0.252609	-0.350825
H10	3.965142	1.785989	0.200381
N11	1.568805	1.205602	0.395741
C12	0.260578	0.700884	0.656426
C13	-0.877731	2.885048	-0.038319
H14	-1.132091	3.203428	0.975915
H15	0.084825	3.307317	-0.326522
H16	-1.654126	3.205825	-0.731761
C17	-1.687551	0.672825	-0.707888
O18	-2.691473	0.881415	-1.321516
N19	-1.256852	-0.815774	-0.449677
H20	0.042041	0.802903	1.733000
H21	-1.170366	-1.322390	-1.341898
H22	-3.064045	-1.588777	-0.281043
H23	-2.894615	0.059256	1.547912
H24	-3.310089	-1.592132	2.055988
N25	-2.233220	-1.583090	0.311463
C26	-2.531040	-0.974392	1.608029
H27	-1.651792	-1.034866	2.253192

Zero-point correction= 0.219443
Thermal correction to Energy= 0.234169
Thermal correction to Enthalpy= 0.235114
Thermal correction to Gibbs Free Energy= 0.176670
Sum of electronic and zero-point Energies= -752.210215
Sum of electronic and thermal Energies= -752.195489
Sum of electronic and thermal Enthalpies= -752.194545
Sum of electronic and thermal Free Energies= -752.252989

213 TS$^{via\ async\ add\ +\ PT}$_N7-[9MOG + H$_{C4}$]$^{+}$

N1	-1.003950	1.351882	-0.198452
C2	0.192495	-0.535465	-0.722007
C3	1.278741	-1.448687	-0.538871
O4	1.264599	-2.661260	-0.662720
N5	2.440362	-0.743068	-0.156662
H6	3.277626	-1.308557	-0.081451
C7	2.463538	0.588715	0.220674
N8	3.663700	1.112575	0.522621
H9	4.528615	0.664807	0.266713
H10	3.691555	2.087255	0.780399
N11	1.385852	1.335857	0.333934
C12	0.233498	0.669526	0.063516
C13	-1.246476	2.773630	0.011364
H14	-1.038105	3.024813	1.052532
H15	-0.594070	3.354538	-0.641804
H16	-2.290838	2.979179	-0.221189
C17	-1.911311	0.484424	-0.667469
O18	-3.048965	0.541388	-1.025056
N19	-1.170327	-0.893392	-0.538189
H20	-0.362764	-0.184813	1.126147
H21	-1.577873	-1.636271	-1.114109
H22	-0.798283	-2.123367	1.071508
H23	-3.286150	-1.979191	0.999655
H24	-2.536840	-1.631777	2.580295
N25	-1.292720	-1.232074	0.983335
C26	-2.645094	-1.285225	1.550190
H27	-3.090713	-0.291609	1.553024

Zero-point correction= 0.213764
Thermal correction to Energy= 0.228129
Thermal correction to Enthalpy= 0.229073
Thermal correction to Gibbs Free Energy= 0.172549
Sum of electronic and zero-point Energies= -752.152255
Sum of electronic and thermal Energies= -752.137891
Sum of electronic and thermal Enthalpies= -752.136946
Sum of electronic and thermal Free Energies= -752.193471

214 TS$^{via\ HA_NH2\ products}$_N7-NHCH$_3$[9MOG + H$_{C4}$]$^{•+}$

N1	-0.850018	1.494001	0.093939
C2	0.030940	-0.592717	-0.094996
C3	1.119141	-1.557964	-0.298696
O4	0.943270	-2.699890	-0.664569
N5	2.340828	-0.985168	-0.015701
H6	3.146556	-1.596722	-0.070975
C7	2.508834	0.410362	0.111005
N8	3.791535	0.827052	0.029853
H9	4.485244	0.296186	-0.472929
H10	3.945470	1.821325	0.108960
N11	1.547887	1.243899	0.317529
C12	0.255983	0.697613	0.615773
C13	-1.011183	2.909230	0.403788
H14	-1.194805	3.037880	1.473085
H15	-0.102515	3.440837	0.118450
H16	-1.860891	3.289576	-0.162174

C17	-1.684774	0.818038	-0.705625
O18	-2.683204	1.106702	-1.298758
N19	-1.155082	-0.610829	-0.714862
H20	0.134404	0.597449	1.708329
H21	-1.283599	-1.166048	-1.561469
H22	-3.284725	-0.914917	0.011688
H23	-2.204679	-0.671701	2.094157
H24	-2.955781	-2.277073	2.011409
N25	-2.516866	-1.579926	0.168920
C26	-2.183471	-1.633026	1.566099
H27	-1.226014	-2.143701	1.706256

Zero-point correction= 0.215969
Thermal correction to Energy= 0.230589
Thermal correction to Enthalpy= 0.231533
Thermal correction to Gibbs Free Energy= 0.173644
Sum of electronic and zero-point Energies= -752.193083
Sum of electronic and thermal Energies= -752.178464
Sum of electronic and thermal Enthalpies= -752.177519
Sum of electronic and thermal Free Energies= -752.235409

215 N7-[9MOG + H_{C5}]$^{+}$

N1	-0.377561	1.765346	-0.011761
C2	-0.086563	-0.517507	0.460165
C3	0.722597	-1.562159	-0.288500
O4	0.212749	-2.470571	-0.911882
N5	2.075103	-1.340468	-0.187350
H6	2.659281	-2.036472	-0.638034
C7	2.635208	-0.095429	0.132724
N8	3.985735	-0.040833	0.205638
H9	4.522609	-0.861302	0.439995
H10	4.388027	0.849730	0.457614
N11	1.894558	0.983933	0.248097
C12	0.586773	0.795125	0.262618
C13	-0.084026	3.192188	-0.139636
H14	0.310821	3.562121	0.807129
H15	0.656829	3.334171	-0.927684
H16	-1.009628	3.708035	-0.390036
C17	-1.595647	1.252716	-0.229101
O18	-2.671289	1.717506	-0.470382
N19	-1.442399	-0.296703	-0.122128
H20	-0.244905	-0.791336	1.514108
N21	-2.512713	-0.806937	0.687510
H22	-3.317191	-0.224586	0.451216
C23	-2.779705	-2.220056	0.404394
H24	-3.642969	-2.496145	1.010668
H25	-3.000801	-2.415369	-0.652826
H26	-1.929635	-2.831744	0.709240
H27	-1.474988	-0.692218	-1.079313

Zero-point correction= 0.220268
Thermal correction to Energy= 0.234537
Thermal correction to Enthalpy= 0.235481
Thermal correction to Gibbs Free Energy= 0.178949
Sum of electronic and zero-point Energies= -752.239831
Sum of electronic and thermal Energies= -752.225562
Sum of electronic and thermal Enthalpies= -752.224618
Sum of electronic and thermal Free Energies= -752.281150

216 $TS^{via\ async\ add\ +\ PT}$_N7-[9MOG + H_{C5}]$^{+}$

N1	0.385655	1.780062	0.026781
C2	0.078530	-0.482564	-0.319146
C3	-0.728601	-1.584604	0.213609
O4	-0.273631	-2.614192	0.687758
N5	-2.086562	-1.338547	0.101439
H6	-2.687907	-2.093774	0.408681
C7	-2.631433	-0.067234	-0.107655
N8	-3.984955	0.008304	-0.132157
H9	-4.537399	-0.790676	-0.401268
H10	-4.375452	0.914298	-0.343289
N11	-1.892325	1.012125	-0.189945
C12	-0.575979	0.803341	-0.205855
C13	0.112991	3.217677	0.039645
H14	-0.274467	3.514916	-0.935175
H15	-0.629358	3.430264	0.809429
H16	1.043980	3.740225	0.253513
C17	1.608936	1.283650	0.260137
O18	2.717882	1.738924	0.396246
N19	1.429120	-0.270428	0.293572
H20	1.237002	-0.911268	-1.360702
N21	2.287576	-0.903578	-0.701673
H22	3.030318	-0.238669	-0.957275
C23	2.829855	-2.224585	-0.296980
H24	3.299579	-2.647389	-1.185372
H25	3.572049	-2.106701	0.494383
H26	1.994723	-2.850575	0.024716
H27	1.637554	-0.648164	1.231683

Zero-point correction= 0.214263
Thermal correction to Energy= 0.228490
Thermal correction to Enthalpy= 0.229435
Thermal correction to Gibbs Free Energy= 0.173328
Sum of electronic and zero-point Energies= -752.167526
Sum of electronic and thermal Energies= -752.153299
Sum of electronic and thermal Enthalpies= -752.152354
Sum of electronic and thermal Free Energies= -752.208461

217 $TS^{via\ HA_NH2\ products}$_N7-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$

N1	0.330689	1.697797	0.006007
C2	0.095413	-0.567554	-0.254940
C3	-0.756897	-1.470635	0.612333
O4	-0.315371	-2.275397	1.392877
N5	-2.105145	-1.281919	0.347616
H6	-2.736014	-1.911228	0.831880
C7	-2.612323	-0.135321	-0.268483
N8	-3.921693	-0.121700	-0.534445
H9	-4.514609	-0.928767	-0.425887
H10	-4.314286	0.715845	-0.938630
N11	-1.873398	0.927629	-0.525224
C12	-0.570282	0.766639	-0.327719
C13	0.072755	3.133181	0.092226
H14	-0.080550	3.531473	-0.911375
H15	-0.817469	3.303499	0.698368
H16	0.945344	3.596064	0.550730
C17	1.541844	1.142476	0.433871
O18	2.538460	1.708412	0.824385
N19	1.438892	-0.272730	0.226414
H20	0.176436	-1.014334	-1.254790
N21	2.534074	-0.775297	-1.111956
H22	3.300760	-0.126515	-0.906937
H23	1.769660	-0.835416	1.015203
C24	2.963899	-2.125766	-0.789721
H25	2.111613	-2.811437	-0.815969
H26	3.648680	-2.430021	-1.590100
H27	3.495340	-2.227856	0.165121

Zero-point correction= 0.216356
Thermal correction to Energy= 0.230919
Thermal correction to Enthalpy= 0.231863
Thermal correction to Gibbs Free Energy= 0.173728
Sum of electronic and zero-point Energies= -752.207921
Sum of electronic and thermal Energies= -752.193358
Sum of electronic and thermal Enthalpies= -752.192414

Sum of electronic and thermal Free Energies= -752.250549

218 N7-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	0.461423	1.607409	0.067831
C2	-0.033412	-0.601519	-0.161935
C3	-0.911059	-1.763438	0.134427
O4	-0.692836	-1.765802	1.465794
N5	-2.262416	-1.324916	-0.285313
H6	-2.965589	-2.049525	-0.332640
C7	-2.671733	-0.040285	-0.226186
N8	-3.971588	0.244183	-0.319018
H9	-4.690298	-0.460540	-0.353785
H10	-4.243336	1.215745	-0.316687
N11	-1.833096	1.011597	-0.118171
C12	-0.562325	0.672353	-0.079103
C13	0.274703	3.057123	0.078451
H14	1.247229	3.519444	0.241335
H15	-0.138605	3.377142	-0.878760
H16	-0.409917	3.323645	0.883940
C17	1.667495	1.004814	0.194588
O18	2.773809	1.430041	0.306264
N19	1.383322	-0.532489	0.120022
H20	1.563936	-0.933044	1.052754
H21	-0.684089	-2.701742	-0.381620
H22	2.153860	-0.800214	-1.692963
H23	4.146010	-0.583547	-0.198611
H24	3.540008	-2.069065	0.600442
C25	3.568561	-1.500630	-0.333344
N26	2.192882	-1.290309	-0.802013
H27	4.045935	-2.131052	-1.084623

Zero-point correction= 0.220094
Thermal correction to Energy= 0.234543
Thermal correction to Enthalpy= 0.235487
Thermal correction to Gibbs Free Energy= 0.178082
Sum of electronic and zero-point Energies= -752.184765
Sum of electronic and thermal Energies= -752.170317
Sum of electronic and thermal Enthalpies= -752.169373
Sum of electronic and thermal Free Energies= -752.226778

219 TS$^{via\ HA_NH2\ products}$_N7-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	0.490628	1.572897	0.067181
C2	-0.052466	-0.581837	0.523868
C3	-0.932866	-1.705468	0.224867
O4	-0.621313	-1.308218	1.573288
N5	-2.207520	-1.345268	-0.258040
H6	-2.879824	-2.086284	-0.394027
C7	-2.635111	-0.033810	-0.290099
N8	-3.932806	0.190320	-0.534572
H9	-4.618906	-0.542598	-0.606595
H10	-4.243022	1.148573	-0.587484
N11	-1.828321	1.008597	-0.157874
C12	-0.569287	0.753116	0.167613
C13	0.427243	2.993267	-0.264888
H14	1.447496	3.372966	-0.291756
H15	-0.052714	3.112474	-1.237181
H16	-0.151362	3.516811	0.496978
C17	1.702029	0.927177	0.323086
O18	2.824419	1.392259	0.367214
N19	1.391777	-0.486401	0.418046
H20	1.882313	-0.946603	1.187921
H21	-0.555355	-2.672340	-0.085242
H22	1.743779	-0.820996	-1.671072
H23	3.926744	-0.714385	-0.723042
H24	3.574859	-2.262007	0.114306
C25	3.361529	-1.650257	-0.766367
N26	1.916463	-1.478632	-0.904925
H27	3.683167	-2.221651	-1.644029

Zero-point correction= 0.215826
Thermal correction to Energy= 0.230354
Thermal correction to Enthalpy= 0.231298
Thermal correction to Gibbs Free Energy= 0.173613
Sum of electronic and zero-point Energies= -752.158991
Sum of electronic and thermal Energies= -752.144464
Sum of electronic and thermal Enthalpies= -752.143519
Sum of electronic and thermal Free Energies= -752.201204

220 N7-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-0.564207	1.677714	-0.018633
C2	0.079833	-0.479109	-0.312490
C3	0.972928	-1.571379	-0.466694
O4	0.618037	-2.768722	0.127572
N5	2.309660	-1.118558	-0.236983
H6	3.047620	-1.797590	-0.361508
C7	2.651300	0.168690	0.061697
N8	3.945431	0.450309	0.260869
H9	4.671346	-0.246781	0.263580
H10	4.186887	1.402315	0.489281
N11	1.776369	1.167995	0.151563
C12	0.512577	0.783785	-0.045953
C13	-0.457796	3.110814	0.239320
H14	-0.086035	3.271715	1.251963
H15	0.228709	3.556459	-0.481008
H16	-1.450033	3.546625	0.130625
C17	-1.728717	1.044194	-0.263492
O18	-2.854786	1.413486	-0.378957
N19	-1.360578	-0.470748	-0.398323
H20	-1.711913	-0.806836	-1.309147
H21	0.823188	-3.512835	-0.449107
H22	-1.402624	-1.995775	0.856480
H23	-4.005176	-0.705805	0.283946
H24	-3.425964	-2.178007	-0.558984
N25	-1.998795	-1.182742	0.703099
C26	-3.366314	-1.584555	0.365288
H27	-3.720052	-2.194027	1.197756

Zero-point correction= 0.219533
Thermal correction to Energy= 0.234589
Thermal correction to Enthalpy= 0.235533
Thermal correction to Gibbs Free Energy= 0.177102
Sum of electronic and zero-point Energies= -752.210112
Sum of electronic and thermal Energies= -752.195056
Sum of electronic and thermal Enthalpies= -752.194112
Sum of electronic and thermal Free Energies= -752.252543

221 TS$^{via\ HA_NH2\ products}$_N7-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-0.503896	1.707244	0.032222
C2	0.070426	-0.420180	-0.491507
C3	0.918545	-1.554952	-0.463747
O4	0.530800	-2.797957	-0.117336
N5	2.245652	-1.199744	-0.130920
H6	2.921525	-1.953967	-0.135442
C7	2.652251	0.066733	0.101856
N8	3.953449	0.319947	0.277995
H9	4.667327	-0.389040	0.237311
H10	4.225644	1.274181	0.458028
N11	1.808089	1.118795	0.175176
C12	0.553084	0.813213	-0.083234
C13	-0.398706	3.139130	0.292963
H14	0.383136	3.297771	1.034745
H15	-0.152522	3.674654	-0.626120
H16	-1.356347	3.488325	0.677665

C17	-1.669784	1.084349	-0.321771
O18	-2.782690	1.501189	-0.437860
N19	-1.325139	-0.372930	-0.511513
H20	-1.813462	-0.762631	-1.323349
H21	-0.347131	-2.750097	0.314297
H22	-1.731103	-0.861263	1.516672
H23	-3.937774	-0.661873	0.560154
H24	-3.554845	-2.097670	-0.442261
N25	-1.919408	-1.409197	0.673425
C26	-3.361376	-1.590224	0.506816
H27	-3.687218	-2.261465	1.306922

Zero-point correction= 0.216753
Thermal correction to Energy= 0.231467
Thermal correction to Enthalpy= 0.232411
Thermal correction to Gibbs Free Energy= 0.174863
Sum of electronic and zero-point Energies= -752.193911
Sum of electronic and thermal Energies= -752.179197
Sum of electronic and thermal Enthalpies= -752.178252
Sum of electronic and thermal Free Energies= -752.235801

222 N7-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-0.672087	1.665864	0.086132
C2	0.012703	-0.483165	0.154169
C3	0.967051	-1.511288	0.370912
O4	0.795922	-2.665334	0.716974
N5	2.275256	-1.008470	0.127517
C6	2.570618	0.290500	-0.168415
N7	3.847127	0.617512	-0.393995
H8	4.599080	-0.051902	-0.381832
H9	4.059106	1.583013	-0.593874
N10	1.652498	1.252158	-0.224656
C11	0.406990	0.830021	-0.021655
C12	-0.639583	3.119805	-0.023827
H13	-0.768186	3.576739	0.959833
H14	0.331670	3.395731	-0.431368
H15	-1.432295	3.451949	-0.694719
C16	-1.779447	0.966858	0.551443
O17	-2.949661	1.357803	0.045633
N18	-1.418780	-0.526714	0.401288
H19	-1.619812	-1.004942	1.286797
H20	-3.698050	1.034612	0.562139
H21	3.011179	-1.695158	0.245619
H22	-2.165775	-0.648763	-1.435047
H23	-2.121839	-3.103377	0.211018
H24	-2.762952	-2.963920	-1.431693
N25	-2.308962	-1.158963	-0.564864
C26	-2.008038	-2.583149	-0.742157
H27	-1.009337	-2.780930	-1.140499

Zero-point correction= 0.221155
Thermal correction to Energy= 0.235608
Thermal correction to Enthalpy= 0.236552
Thermal correction to Gibbs Free Energy= 0.179683
Sum of electronic and zero-point Energies= -752.219452
Sum of electronic and thermal Energies= -752.204999
Sum of electronic and thermal Enthalpies= -752.204055
Sum of electronic and thermal Free Energies= -752.260924

223 TS$^{\text{via async HA_NH2 + add}}$_N7-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	0.470935	1.733445	-0.071067
C2	-0.033980	-0.433185	-0.297302
C3	-0.858792	-1.588996	-0.332136
O4	-0.545192	-2.750379	-0.513838
N5	-2.208161	-1.212024	-0.105772
C6	-2.642646	0.063315	0.143618
N7	-3.949532	0.253753	0.357865
H8	-4.629614	-0.487908	0.327392
H9	-4.267288	1.196039	0.526009
N10	-1.834964	1.117198	0.184588
C11	-0.553819	0.825539	-0.038284
C12	0.372959	3.173509	0.134582
H13	0.386840	3.693969	-0.824858
H14	-0.568273	3.369902	0.645658
H15	1.211419	3.504081	0.748215
C16	1.610782	1.076559	-0.482461
O17	2.833015	1.532174	-0.293248
N18	1.374419	-0.324596	-0.441045
H19	1.793350	-0.855018	-1.210317
H20	3.303050	0.881363	0.272972
H21	-2.863620	-1.984730	-0.129056
H22	1.662308	-0.929850	1.588712
H23	3.426146	-2.311892	-0.323326
H24	3.244659	-2.706906	1.382485
N25	2.356221	-0.929228	0.837907
C26	2.718160	-2.307188	0.510065
H27	1.860030	-2.950563	0.286983

Zero-point correction= 0.217805
Thermal correction to Energy= 0.232354
Thermal correction to Enthalpy= 0.233298
Thermal correction to Gibbs Free Energy= 0.175883
Sum of electronic and zero-point Energies= -752.215364
Sum of electronic and thermal Energies= -752.200815
Sum of electronic and thermal Enthalpies= -752.199871
Sum of electronic and thermal Free Energies= -752.257286

224 N7-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	-0.587115	1.645775	-0.249211
C2	0.066773	-0.523533	0.210624
C3	0.992566	-1.608255	0.356934
O4	0.739381	-2.765959	0.617471
N5	2.317905	-1.157219	0.149750
H6	3.025353	-1.877433	0.249749
C7	2.666000	0.122930	-0.172977
N8	3.956929	0.414412	-0.345575
H9	4.695893	-0.261900	-0.239512
H10	4.200608	1.363874	-0.584610
N11	1.765778	1.094488	-0.328343
C12	0.510864	0.712901	-0.134543
C13	-0.326335	3.038932	0.197492
H14	-0.003314	3.009389	1.237564
H15	0.446186	3.480711	-0.430179
H16	-1.264224	3.586804	0.112493
C17	-1.785861	0.951155	0.670607
O18	-2.911277	1.305647	0.445116
N19	-1.352862	-0.624651	0.351063
H20	-0.938479	1.647613	-1.214364
H21	-1.615431	-1.185068	1.173396
H22	-1.428265	-1.937012	-1.129360
H23	-3.731792	-1.961807	-1.549737
H24	-3.453111	-2.281747	0.178705
C25	-3.366180	-1.529488	-0.617489
N26	-1.976984	-1.120193	-0.862480
H27	-3.970772	-0.657065	-0.375149

Zero-point correction= 0.220356
Thermal correction to Energy= 0.234828
Thermal correction to Enthalpy= 0.235772
Thermal correction to Gibbs Free Energy= 0.178834
Sum of electronic and zero-point Energies= -752.194690
Sum of electronic and thermal Energies= -752.180217
Sum of electronic and thermal Enthalpies= -752.179273

Sum of electronic and thermal Free Energies= -752.236211

225 TS$^{\text{via async HA_NH2 + add}}$_N7-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	0.593783	1.647355	0.252095
C2	-0.075392	-0.450005	-0.342916
C3	-0.973582	-1.556692	-0.482643
O4	-0.707107	-2.697889	-0.795455
N5	-2.295974	-1.143071	-0.187694
H6	-2.989780	-1.877265	-0.281802
C7	-2.661255	0.105939	0.232503
N8	-3.950147	0.348372	0.484885
H9	-4.674687	-0.342647	0.375303
H10	-4.206756	1.271409	0.801175
N11	-1.777870	1.089842	0.403963
C12	-0.534240	0.735771	0.119059
C13	0.386518	3.031751	-0.271251
H14	0.096532	2.955535	-1.318432
H15	-0.395559	3.512476	0.313960
H16	1.337214	3.555388	-0.179700
C17	1.751573	0.905758	-0.500231
O18	2.882286	1.351773	-0.480770
N19	1.345317	-0.462450	-0.459413
H20	0.862871	1.700279	1.244408
H21	1.729058	-1.002196	-1.239649
H22	1.407337	-2.193993	0.843533
H23	3.664389	-2.206299	1.617229
H24	3.568295	-2.152055	-0.151017
C25	3.342456	-1.593562	0.767485
N26	1.924022	-1.317613	0.973480
H27	3.909271	-0.662508	0.781547

Zero-point correction= 0.218152
Thermal correction to Energy= 0.232446
Thermal correction to Enthalpy= 0.233390
Thermal correction to Gibbs Free Energy= 0.176636
Sum of electronic and zero-point Energies= -752.179075
Sum of electronic and thermal Energies= -752.164781
Sum of electronic and thermal Enthalpies= -752.163836
Sum of electronic and thermal Free Energies= -752.220591

226 C8-NHCH$_3$[9MOG + H$_{N1}$]$^{+}$

N1	-0.353771	-1.681981	-0.593549
C2	0.036257	0.579854	-0.087477
C3	0.942993	1.654376	-0.185691
O4	0.787050	2.854030	-0.165279
N5	2.419970	1.183692	-0.403586
H6	2.985458	1.896815	0.070590
C7	2.724028	-0.200795	0.089329
N8	3.990024	-0.332885	0.534133
H9	4.252762	-1.249816	0.869916
N10	1.837547	-1.096317	0.103526
C11	0.495048	-0.816616	-0.218327
C12	-0.009033	-3.079219	-0.701449
H13	-0.225845	-3.405374	-1.722646
H14	1.028855	-3.309944	-0.447522
H15	-0.685197	-3.632192	-0.042235
C16	-2.192802	0.020845	0.797412
O17	-1.813717	-0.587139	1.770313
N18	-1.265171	0.878863	0.061941
H19	-1.511521	1.862512	-0.006348
H20	2.623531	1.253984	-1.407905
H21	4.740141	0.274698	0.242109
H22	-4.118214	-0.430529	0.866066
H23	-4.810826	0.216239	-1.242106
H24	-3.132300	0.465916	-1.731212
C25	-3.865279	0.671494	-0.948549
N26	-3.442984	0.075962	0.311534
H27	-4.020086	1.751589	-0.858465

Zero-point correction= 0.217565
Thermal correction to Energy= 0.233295
Thermal correction to Enthalpy= 0.234240
Thermal correction to Gibbs Free Energy= 0.173273
Sum of electronic and zero-point Energies= -752.236181
Sum of electronic and thermal Energies= -752.220450
Sum of electronic and thermal Enthalpies= -752.219506
Sum of electronic and thermal Free Energies= -752.280473

227 TS$^{\text{via HA_NH2 products}}$_C8-NHCH$_3$[9MOG + H$_{N1}$]$^{+}$

N1	-0.783697	-1.127018	0.069408
C2	0.266343	0.838753	0.028755
C3	1.328328	1.714949	0.085641
O4	1.560177	2.878943	0.197736
N5	2.747389	0.795753	-0.083495
H6	3.313200	1.088802	0.719475
C7	2.670776	-0.675108	-0.168872
N8	3.851457	-1.290377	-0.286183
H9	3.856057	-2.299607	-0.349609
N10	1.555399	-1.300184	-0.133915
C11	0.399165	-0.572654	-0.028883
C12	-1.082129	-2.542121	0.178184
H13	-1.545264	-2.899201	-0.744739
H14	-0.163026	-3.097098	0.359682
H15	-1.767328	-2.673510	1.019494
C16	-1.878085	-0.076299	0.316084
O17	-2.343067	-0.116983	1.517059
N18	-1.075094	1.153904	0.096092
H19	-1.371850	1.965149	0.629526
H20	3.189528	1.188705	-0.920698
H21	4.736357	-0.808034	-0.300807
H22	-3.326931	-1.130893	-0.622341
H23	-4.450977	0.594849	-1.762894
H24	-3.269443	1.763825	-1.180127
C25	-3.808032	0.851516	-0.920055
N26	-2.850558	-0.239381	-0.729720
H27	-4.429670	1.028230	-0.035756

Zero-point correction= 0.215308
Thermal correction to Energy= 0.230366
Thermal correction to Enthalpy= 0.231311
Thermal correction to Gibbs Free Energy= 0.172357
Sum of electronic and zero-point Energies= -752.196366
Sum of electronic and thermal Energies= -752.181307
Sum of electronic and thermal Enthalpies= -752.180363
Sum of electronic and thermal Free Energies= -752.239316

228 C8-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	-0.834516	-1.211391	-0.094074
C2	0.364694	0.693819	0.104759
C3	1.560020	1.586801	0.021981
O4	1.468255	2.772406	0.266319
N5	2.614018	0.889349	-0.446259
H6	3.465398	1.423878	-0.580895
C7	2.737116	-0.587755	-0.498676
N8	3.414670	-1.028604	0.702583
H9	4.383526	-0.724909	0.722249
H10	3.398695	-2.042322	0.758014
N11	1.501013	-1.330569	-0.566424
C12	0.427035	-0.727220	-0.245381
C13	-1.186362	-2.623414	-0.127472
H14	-1.980304	-2.802309	0.599746
H15	-1.505593	-2.926214	-1.128120
H16	-0.307811	-3.205963	0.154185

C17	-1.769292	-0.190631	0.355236
O18	-2.466584	-0.418694	1.417023
N19	-0.825852	1.012506	0.435948
H20	-1.091379	1.931088	0.789889
H21	3.276478	-0.790862	-1.432902
H22	-3.349059	-0.733269	-0.841170
H23	-4.067651	1.531273	0.296361
H24	-2.880017	2.181377	-0.880531
N25	-2.803941	0.100423	-0.635572
C26	-3.552910	1.351740	-0.652027
H27	-4.295183	1.286488	-1.447496

Zero-point correction= 0.218265
Thermal correction to Energy= 0.232959
Thermal correction to Enthalpy= 0.233903
Thermal correction to Gibbs Free Energy= 0.175582
Sum of electronic and zero-point Energies= -752.194159
Sum of electronic and thermal Energies= -752.179465
Sum of electronic and thermal Enthalpies= -752.178521
Sum of electronic and thermal Free Energies= -752.236842

229 TS$^{\text{via async HA_NH2 + add}}$_C8-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	-0.805854	-1.279978	0.096981
C2	0.366130	0.648249	0.286688
C3	1.520774	1.581785	0.113993
O4	1.425238	2.754443	0.409737
N5	2.534868	0.936159	-0.498939
H6	3.348854	1.502778	-0.710576
C7	2.690954	-0.531844	-0.616079
N8	3.457494	-1.001308	0.519623
H9	4.411618	-0.653959	0.497791
H10	3.489443	-2.016398	0.524970
N11	1.468164	-1.304810	-0.625455
C12	0.424490	-0.748634	-0.158720
C13	-1.174258	-2.673440	-0.098762
H14	-2.069423	-2.873050	0.490722
H15	-1.358613	-2.881102	-1.155928
H16	-0.358936	-3.306718	0.253543
C17	-1.709821	-0.304923	0.582018
O18	-2.650561	-0.496796	1.329361
N19	-0.798788	0.904665	0.738797
H20	-1.092982	1.795621	1.136447
H21	3.167121	-0.688497	-1.592223
H22	-3.174406	-0.531276	-1.258459
H23	-4.264131	1.353434	-0.147212
H24	-2.852312	2.337587	-0.639826
N25	-2.640840	0.274247	-0.917685
C26	-3.455543	1.460623	-0.882979
H27	-3.925308	1.606690	-1.862238

Zero-point correction= 0.215706
Thermal correction to Energy= 0.230467
Thermal correction to Enthalpy= 0.231411
Thermal correction to Gibbs Free Energy= 0.172961
Sum of electronic and zero-point Energies= -752.185259
Sum of electronic and thermal Energies= -752.170498
Sum of electronic and thermal Enthalpies= -752.169553
Sum of electronic and thermal Free Energies= -752.228004

230 C8-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	-0.976452	-0.958601	-0.289312
C2	0.415100	1.044424	-0.238153
C3	1.790983	1.593607	-0.020777
O4	2.062066	2.769504	0.020613
N5	2.801063	0.620426	0.108543
H6	3.739282	0.982660	0.239766
C7	2.491456	-0.701304	0.033158
N8	3.606251	-1.661310	0.141218
H9	4.094996	-1.609005	1.043989
H10	3.176141	-2.592217	0.065870
N11	1.325097	-1.224796	-0.098439
C12	0.249256	-0.400706	-0.189976
C13	-1.112068	-2.416431	-0.345147
H14	-0.475598	-2.815734	-1.135212
H15	-0.841730	-2.873891	0.611973
H16	-2.152509	-2.647772	-0.571297
C17	-2.113546	-0.267887	0.351437
O18	-2.075652	-0.022446	1.534573
N19	-0.579738	1.821649	-0.486930
H20	-0.278507	2.799390	-0.468423
H21	4.302147	-1.565964	-0.609011
H22	-2.941869	-0.109016	-1.470848
H23	-4.678705	0.162263	0.912952
H24	-4.148511	1.660598	0.119698
N25	-3.149453	-0.099601	-0.483636
C26	-4.345597	0.595061	-0.030827
H27	-5.127325	0.467275	-0.779333

Zero-point correction= 0.218653
Thermal correction to Energy= 0.234077
Thermal correction to Enthalpy= 0.235021
Thermal correction to Gibbs Free Energy= 0.175289
Sum of electronic and zero-point Energies= -752.243371
Sum of electronic and thermal Energies= -752.227947
Sum of electronic and thermal Enthalpies= -752.227003
Sum of electronic and thermal Free Energies= -752.286735

231 TS$^{\text{via async HA_NH2 + add}}$_C8-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	-0.805130	-1.172308	0.150837
C2	0.291704	0.780270	0.220379
C3	1.416258	1.645661	0.155533
O4	1.500976	2.850506	0.265960
N5	2.625118	0.866731	-0.060796
H6	3.469430	1.427186	-0.108087
C7	2.601493	-0.469047	-0.187611
N8	3.900984	-1.153173	-0.392872
H9	4.552355	-1.010692	0.388281
H10	3.681822	-2.156395	-0.452604
N11	1.588210	-1.252690	-0.146457
C12	0.398082	-0.601640	0.061986
C13	-1.151657	-2.573850	0.190508
H14	-1.859251	-2.797361	-0.613794
H15	-0.251320	-3.175352	0.065536
H16	-1.627799	-2.796692	1.148130
C17	-1.841125	-0.147901	0.464393
O18	-2.686856	-0.348167	1.334503
N19	-1.029186	1.080738	0.415872
H20	-1.351782	1.902011	0.910472
H21	4.367927	-0.871250	-1.262863
H22	-2.009353	0.307132	-1.843772
H23	-4.325244	0.623430	-0.043854
H24	-3.712240	1.908773	-1.143842
N25	-2.596442	0.114761	-1.031083
C26	-3.841670	0.828317	-1.000921
H27	-4.470890	0.461220	-1.821413

Zero-point correction= 0.215331
Thermal correction to Energy= 0.230412
Thermal correction to Enthalpy= 0.231357
Thermal correction to Gibbs Free Energy= 0.172491
Sum of electronic and zero-point Energies= -752.187077
Sum of electronic and thermal Energies= -752.171996
Sum of electronic and thermal Enthalpies= -752.171052

Sum of electronic and thermal Free Energies= -752.229918

232 C8-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	0.814689	1.161359	0.034352
C2	-0.291964	-0.787399	0.161684
C3	-1.437415	-1.620779	0.169370
O4	-1.556863	-2.811043	0.335575
N5	-2.654076	-0.828460	-0.031875
H6	-3.495961	-1.394373	-0.022877
C7	-2.741559	0.487165	-0.215307
N8	-3.916305	1.094773	-0.415715
H9	-4.776531	0.569073	-0.439600
H10	-3.989207	2.095446	-0.512475
N11	-1.599685	1.205982	-0.200695
C12	-0.388177	0.563228	0.000175
C13	1.070478	2.565821	0.298520
H14	2.047388	2.638311	0.781211
H15	1.074991	3.154268	-0.623802
H16	0.340348	2.976233	1.004488
C17	1.848393	0.098363	0.305216
O18	2.614549	0.314237	1.337843
N19	1.058220	-1.132057	0.291225
H20	-1.620081	2.198677	-0.390231
H21	1.293232	-1.755419	1.057097
H22	3.345271	0.984679	-0.834757
H23	4.411047	-1.240294	-0.337629
H24	2.958071	-1.940677	-1.113036
N25	2.835926	0.106726	-0.782187
C26	3.622987	-1.078038	-1.079773
H27	4.082088	-0.939895	-2.060796

Zero-point correction= 0.217998
Thermal correction to Energy= 0.232880
Thermal correction to Enthalpy= 0.233825
Thermal correction to Gibbs Free Energy= 0.176341
Sum of electronic and zero-point Energies= -752.243148
Sum of electronic and thermal Energies= -752.228266
Sum of electronic and thermal Enthalpies= -752.227321
Sum of electronic and thermal Free Energies= -752.284805

233 TS$^{\text{via PT in adduct}}$_C8-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	-0.158041	2.118908	-1.056654
C2	-0.091693	-0.273169	-1.144130
C3	0.998065	-1.237835	-1.232202
O4	1.021350	-2.285472	-1.829716
N5	2.115352	-0.816089	-0.433740
H6	2.942926	-1.397210	-0.510340
C7	1.913758	-0.028238	0.663761
N8	2.724600	-0.142300	1.712620
H9	3.428650	-0.861519	1.782566
H10	2.688187	0.566383	2.430871
N11	0.898137	0.843534	0.706526
C12	0.256751	1.034342	-0.570681
C13	0.129998	3.390843	-0.426526
H14	-0.821880	3.897058	-0.244645
H15	0.701802	3.317508	0.503267
H16	0.675116	4.003087	-1.149687
C17	-2.207534	-0.316848	0.011753
O18	-3.404781	-0.319713	0.017175
N19	-1.413585	-0.666458	-1.064257
H20	-0.195928	0.462985	1.213212
H21	-1.855862	-1.213985	-1.795430
H22	-2.061996	0.564243	1.809359
H23	-2.253466	-1.808649	2.191954
H24	-0.649463	-2.001728	1.437228
N25	-1.452121	-0.050745	1.268411
C26	-1.286698	-1.332647	2.019342
H27	-0.806923	-1.113335	2.973712

Zero-point correction= 0.214174
Thermal correction to Energy= 0.228586
Thermal correction to Enthalpy= 0.229530
Thermal correction to Gibbs Free Energy= 0.172458
Sum of electronic and zero-point Energies= -752.231531
Sum of electronic and thermal Energies= -752.217119
Sum of electronic and thermal Enthalpies= -752.216174
Sum of electronic and thermal Free Energies= -752.273247

234 TS$^{\text{via HA_NH2 products}}$_C8-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	0.828039	-1.182547	-0.338718
C2	-0.286213	0.752890	-0.372372
C3	-1.419381	1.594099	-0.256005
O4	-1.548326	2.786535	-0.394366
N5	-2.614451	0.802795	0.055261
H6	-3.452121	1.371040	0.124096
C7	-2.686025	-0.509452	0.269652
N8	-3.836840	-1.109750	0.591248
H9	-4.691033	-0.581650	0.684340
H10	-3.903737	-2.109491	0.702205
N11	-1.551669	-1.233209	0.160287
C12	-0.368243	-0.597749	-0.174782
C13	1.184029	-2.578756	-0.230937
H14	2.173924	-2.689709	-0.678138
H15	1.218335	-2.911683	0.812364
H16	0.492584	-3.201360	-0.806359
C17	1.827598	-0.124447	-0.525565
O18	2.874026	-0.330538	-1.173692
N19	1.050001	1.064078	-0.618826
H20	-1.556527	-2.223400	0.363443
H21	1.315315	1.736109	-1.325676
H22	3.326729	-0.771631	1.121049
H23	4.118383	1.468679	0.818706
H24	2.475236	2.041418	1.245368
N25	2.635947	-0.019784	1.058274
C26	3.214995	1.254461	1.401657
H27	3.499565	1.226354	2.460487

Zero-point correction= 0.215294
Thermal correction to Energy= 0.230432
Thermal correction to Enthalpy= 0.231376
Thermal correction to Gibbs Free Energy= 0.172944
Sum of electronic and zero-point Energies= -752.237255
Sum of electronic and thermal Energies= -752.222117
Sum of electronic and thermal Enthalpies= -752.221173
Sum of electronic and thermal Free Energies= -752.279605

235 C8-NHCH$_3$[9MOG + H$_{C4}$]$^{\bullet+}$

N1	-1.090585	-0.829626	-0.280205
C2	0.453293	0.868835	-0.128767
C3	1.815732	1.500656	-0.141761
O4	1.990440	2.693873	-0.108429
N5	2.777624	0.527734	-0.198839
H6	3.739131	0.843140	-0.261579
C7	2.479942	-0.852407	-0.044618
N8	3.564082	-1.620055	0.209534
H9	4.368684	-1.242720	0.685977
H10	3.390109	-2.607479	0.327745
N11	1.303878	-1.354676	-0.164998
C12	0.264319	-0.495846	-0.683610
C13	-1.366258	-2.203829	0.146841
H14	-1.049323	-2.880387	-0.647417
H15	-0.847804	-2.468091	1.071825
H16	-2.440140	-2.317546	0.293763

C17	-1.720953	0.228837	0.457017
O18	-2.225098	0.016493	1.625646
N19	-0.587464	1.299458	0.456689
H20	-0.637607	2.170316	0.984047
H21	0.341647	-0.457683	-1.784777
H22	-3.293661	1.589551	0.299611
H23	-3.246160	-0.677715	-1.607848
H24	-4.446145	-0.573940	-0.281496
N25	-2.866525	0.837953	-0.238062
C26	-3.805156	-0.002328	-0.961212
H27	-4.434047	0.650596	-1.569757

Zero-point correction= 0.218315
Thermal correction to Energy= 0.232493
Thermal correction to Enthalpy= 0.233437
Thermal correction to Gibbs Free Energy= 0.177111
Sum of electronic and zero-point Energies= -752.205640
Sum of electronic and thermal Energies= -752.191462
Sum of electronic and thermal Enthalpies= -752.190518
Sum of electronic and thermal Free Energies= -752.246844

236 $TS^{via\ HA_NH2\ products}$_C8-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	1.007440	-0.897827	-0.211467
C2	-0.430137	0.845659	-0.033513
C3	-1.771068	1.501593	0.108925
O4	-1.925235	2.697963	0.088185
N5	-2.744030	0.550047	0.262488
H6	-3.686101	0.893385	0.413287
C7	-2.507531	-0.843141	0.117811
N8	-3.638647	-1.578086	0.017352
H9	-4.481524	-1.185435	-0.372659
H10	-3.510693	-2.573137	-0.095656
N11	-1.344212	-1.387486	0.118286
C12	-0.225126	-0.550628	0.452368
C13	1.499533	-2.259881	-0.332835
H14	1.873455	-2.647944	0.619952
H15	0.691248	-2.899769	-0.689784
H16	2.305022	-2.259455	-1.067754
C17	1.703868	0.204970	-0.677002
O18	2.556993	0.230501	-1.563669
N19	0.592192	1.283573	-0.643312
H20	0.675416	2.192135	-1.097256
H21	-0.102295	-0.518819	1.554280
H22	3.322856	1.610173	0.241121
H23	2.822886	-0.794687	1.872355
H24	4.221687	-0.598430	0.773889
N25	2.726890	0.876469	0.634892
C26	3.491204	-0.071808	1.402572
H27	4.052090	0.466844	2.174475

Zero-point correction= 0.215255
Thermal correction to Energy= 0.229908
Thermal correction to Enthalpy= 0.230852
Thermal correction to Gibbs Free Energy= 0.173009
Sum of electronic and zero-point Energies= -752.200129
Sum of electronic and thermal Energies= -752.185476
Sum of electronic and thermal Enthalpies= -752.184531
Sum of electronic and thermal Free Energies= -752.242375

237 C8-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$

N1	0.746812	1.145580	0.213193
C2	-0.248859	-0.852782	-0.288636
C3	-1.490910	-1.567285	0.205742
O4	-1.529241	-2.684234	0.637627
N5	-2.654888	-0.802181	0.004461
H6	-3.525582	-1.280935	0.207402
C7	-2.646403	0.545748	-0.259573
N8	-3.812095	1.146492	-0.465634
H9	-4.693114	0.656668	-0.486235
H10	-3.807793	2.144704	-0.620704
N11	-1.543581	1.292415	-0.275832
C12	-0.404682	0.633217	-0.124219
C13	1.027451	2.545644	0.487242
H14	1.358011	3.050894	-0.424002
H15	0.120233	3.024579	0.854468
H16	1.807479	2.587384	1.248059
C17	1.792083	0.068103	0.369815
O18	2.659554	0.259289	1.324823
N19	0.961064	-1.099071	0.436236
H20	1.406787	-2.002192	0.365184
H21	-0.198597	-1.065590	-1.374265
H22	3.178372	1.038442	-0.844380
H23	4.114074	-0.721679	-2.035148
H24	4.215754	-1.269730	-0.347288
N25	2.691885	0.146343	-0.804665
C26	3.530699	-0.993168	-1.154249
H27	2.901236	-1.846899	-1.413722

Zero-point correction= 0.218800
Thermal correction to Energy= 0.233196
Thermal correction to Enthalpy= 0.234140
Thermal correction to Gibbs Free Energy= 0.176775
Sum of electronic and zero-point Energies= -752.259168
Sum of electronic and thermal Energies= -752.244772
Sum of electronic and thermal Enthalpies= -752.243828
Sum of electronic and thermal Free Energies= -752.301192

238 $TS^{via\ HA_NH2\ products}$_C8-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$

N1	-0.741764	1.156836	-0.327730
C2	0.226414	-0.849334	0.186798
C3	1.491022	-1.554346	-0.259570
O4	1.550753	-2.658905	-0.719623
N5	2.641642	-0.795754	0.023767
H6	3.521922	-1.269235	-0.148275
C7	2.620103	0.545750	0.321916
N8	3.772840	1.138025	0.606997
H9	4.650970	0.645879	0.665135
H10	3.761018	2.132482	0.785051
N11	1.518611	1.294669	0.295264
C12	0.391206	0.641107	0.063754
C13	-1.037673	2.559360	-0.564393
H14	-1.280275	3.056650	0.377817
H15	-0.168460	3.038992	-1.014266
H16	-1.888180	2.603062	-1.245211
C17	-1.750588	0.082153	-0.554835
O18	-2.746118	0.289730	-1.258919
N19	-0.953819	-1.076766	-0.588648
H20	-1.407413	-1.978681	-0.592390
H21	0.112727	-1.081159	1.263604
H22	-3.197774	0.948778	1.039272
H23	-3.889324	-0.909111	2.318098
H24	-4.231040	-1.205557	0.607365
N25	-2.625244	0.100877	1.020779
C26	-3.425423	-1.058433	1.336809
H27	-2.797475	-1.951462	1.376255

Zero-point correction= 0.216555
Thermal correction to Energy= 0.230870
Thermal correction to Enthalpy= 0.231814
Thermal correction to Gibbs Free Energy= 0.174747
Sum of electronic and zero-point Energies= -752.253766
Sum of electronic and thermal Energies= -752.239451
Sum of electronic and thermal Enthalpies= -752.238506

Sum of electronic and thermal Free Energies= -752.295573

239 C8-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	0.863975	0.732925	-0.374144
C2	-0.485519	-1.084052	-0.097066
C3	-1.753174	-1.558003	0.469577
O4	-1.440757	-1.728557	-0.911851
N5	-2.730964	-0.556719	0.730433
H6	-3.638059	-0.859085	1.057858
C7	-2.594146	0.694577	0.214381
N8	-3.656349	1.496468	0.183584
H9	-4.582236	1.201246	0.449181
H10	-3.525389	2.438916	-0.153229
N11	-1.429389	1.209892	-0.205939
C12	-0.396419	0.394420	-0.230613
C13	1.326501	2.069500	-0.721823
H14	2.319562	1.977099	-1.161345
H15	0.643105	2.496201	-1.457103
H16	1.351195	2.715523	0.158564
C17	1.768484	-0.457290	-0.239307
O18	2.653790	-0.612462	-1.181218
N19	0.834160	-1.563127	-0.006168
H20	1.027772	-2.343305	-0.626712
H21	-1.841758	-2.456985	1.068418
H22	2.954300	-1.256555	1.223178
H23	4.108908	0.519521	2.102082
H24	3.027274	1.686596	1.333439
N25	2.628391	-0.335911	0.943846
C26	3.566808	0.750847	1.184668
H27	4.287074	0.864273	0.370046

Zero-point correction= 0.219314
Thermal correction to Energy= 0.233107
Thermal correction to Enthalpy= 0.234051
Thermal correction to Gibbs Free Energy= 0.178763
Sum of electronic and zero-point Energies= -752.218543
Sum of electronic and thermal Energies= -752.204750
Sum of electronic and thermal Enthalpies= -752.203806
Sum of electronic and thermal Free Energies= -752.259093

240 TS$^{via\ HA_NH2\ products}$_C8-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	0.844012	0.682219	-0.579196
C2	-0.505578	-1.097642	-0.141915
C3	-1.738249	-1.534713	0.522615
O4	-1.511824	-1.768147	-0.867355
N5	-2.689020	-0.513438	0.803441
H6	-3.579309	-0.794218	1.190943
C7	-2.567608	0.721898	0.246666
N8	-3.617620	1.539341	0.260282
H9	-4.528189	1.268187	0.595672
H10	-3.494720	2.469446	-0.112317
N11	-1.424527	1.208666	-0.260111
C12	-0.409474	0.376079	-0.336985
C13	1.356599	2.003611	-0.897026
H14	2.367811	1.879142	-1.284566
H15	0.724030	2.456973	-1.661076
H16	1.357274	2.637983	-0.007670
C17	1.712263	-0.506929	-0.444802
O18	2.730452	-0.647952	-1.118326
N19	0.816981	-1.571909	-0.113649
H20	1.009051	-2.438613	-0.601713
H21	-1.796964	-2.406609	1.163858
H22	2.839550	-1.136789	1.478940
H23	4.004962	0.662517	2.364573
H24	3.182101	1.778108	1.239993
N25	2.531823	-0.208168	1.176885
C26	3.576657	0.769108	1.362458
H27	4.386188	0.607218	0.639180

Zero-point correction= 0.216133
Thermal correction to Energy= 0.230259
Thermal correction to Enthalpy= 0.231203
Thermal correction to Gibbs Free Energy= 0.174814
Sum of electronic and zero-point Energies= -752.210522
Sum of electronic and thermal Energies= -752.196397
Sum of electronic and thermal Enthalpies= -752.195452
Sum of electronic and thermal Free Energies= -752.251841

241 C8-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-0.994713	-0.814986	0.308543
C2	0.475067	0.871997	0.177018
C3	1.720945	1.337544	-0.059144
O4	2.155627	2.590035	-0.136813
N5	2.731190	0.404462	-0.208623
H6	3.660514	0.765948	-0.384522
C7	2.490926	-0.938714	-0.132828
N8	3.527207	-1.777834	-0.250958
H9	4.482411	-1.474629	-0.346190
H10	3.335654	-2.766693	-0.197923
N11	1.274845	-1.438719	0.036423
C12	0.297737	-0.540402	0.159694
C13	-1.544504	-2.129871	0.600686
H14	-1.618091	-2.736405	-0.304934
H15	-0.901872	-2.641235	1.319414
H16	-2.530987	-1.987121	1.042380
C17	-1.786528	0.448731	0.356254
O18	-2.701344	0.523793	1.282376
N19	-0.760596	1.511867	0.374565
H20	-0.841927	2.018686	1.253584
H21	1.419935	3.213478	-0.193360
H22	-2.951179	1.560124	-0.918890
H23	-3.960797	-0.032041	-2.269211
H24	-4.232458	-0.729546	-0.658664
C25	-3.467852	-0.427568	-1.380621
N26	-2.597665	0.609900	-0.854484
H27	-2.872093	-1.294329	-1.670790

Zero-point correction= 0.219134
Thermal correction to Energy= 0.233619
Thermal correction to Enthalpy= 0.234563
Thermal correction to Gibbs Free Energy= 0.178040
Sum of electronic and zero-point Energies= -752.261946
Sum of electronic and thermal Energies= -752.247461
Sum of electronic and thermal Enthalpies= -752.246517
Sum of electronic and thermal Free Energies= -752.303039

242 TS$^{via\ async\ add\ +\ PT}$_C8-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-0.857209	1.164754	-0.210911
C2	0.287951	-0.507954	-1.164530
C3	0.991460	-1.381241	-0.330865
O4	0.425606	-2.378248	0.238987
N5	2.232856	-0.938145	0.094852
H6	2.762324	-1.552614	0.702830
C7	2.497187	0.425219	0.083226
N8	3.738629	0.821015	0.365793
H9	4.511562	0.177784	0.427736
H10	3.928351	1.811955	0.395570
N11	1.529961	1.306784	-0.100952
C12	0.396633	0.766227	-0.552710
C13	-1.221065	2.412277	0.446609
H14	-0.448526	2.666598	1.175386
H15	-1.311999	3.216464	-0.285618
H16	-2.181475	2.279035	0.942980

C17	-1.754069	-0.006787	-0.475224
O18	-2.943441	0.473951	-0.770929
N19	-1.067699	-0.759681	-1.516999
H20	-1.295335	-0.382343	-2.434008
H21	-0.616487	-1.911637	0.464593
H22	-2.503425	-1.625881	0.459861
H23	-1.934895	-1.291394	2.731632
H24	-2.775864	0.146097	2.110051
C25	-1.871317	-0.462410	2.026335
N26	-1.713188	-1.010429	0.666492
H27	-0.995686	0.138236	2.279546

Zero-point correction= 0.214625
Thermal correction to Energy= 0.227728
Thermal correction to Enthalpy= 0.228672
Thermal correction to Gibbs Free Energy= 0.175689
Sum of electronic and zero-point Energies= -752.191590
Sum of electronic and thermal Energies= -752.178488
Sum of electronic and thermal Enthalpies= -752.177543
Sum of electronic and thermal Free Energies= -752.230526

243 $TS^{via\ HA_NH2\ products}$_C8-$NHCH_3$[9MOG + H_{O6}]$^{\bullet+}$

N1	0.976786	-0.806816	-0.499860
C2	-0.482812	0.871682	-0.275213
C3	-1.711480	1.336492	0.045790
O4	-2.143192	2.586745	0.163531
N5	-2.709634	0.401669	0.248654
H6	-3.628507	0.763055	0.473894
C7	-2.472405	-0.942324	0.173044
N8	-3.498235	-1.781537	0.359361
H9	-4.445048	-1.479185	0.519375
H10	-3.308747	-2.770596	0.301460
N11	-1.267206	-1.441460	-0.063930
C12	-0.306051	-0.542038	-0.264667
C13	1.565022	-2.118886	-0.701783
H14	1.529947	-2.705314	0.219011
H15	1.022317	-2.648729	-1.486687
H16	2.597364	-1.966878	-1.017430
C17	1.738358	0.438191	-0.572054
O18	2.781960	0.535534	-1.220710
N19	0.749374	1.491438	-0.514995
H20	0.829641	2.108543	-1.316566
H21	-1.410415	3.215300	0.182941
H22	2.878761	1.521502	1.136488
H23	3.819672	-0.085263	2.556019
H24	4.289809	-0.483315	0.899494
C25	3.432983	-0.400593	1.580761
N26	2.489149	0.575548	1.098349
H27	2.951730	-1.374393	1.681113

Zero-point correction= 0.216014
Thermal correction to Energy= 0.230856
Thermal correction to Enthalpy= 0.231800
Thermal correction to Gibbs Free Energy= 0.174128
Sum of electronic and zero-point Energies= -752.253866
Sum of electronic and thermal Energies= -752.239024
Sum of electronic and thermal Enthalpies= -752.238080
Sum of electronic and thermal Free Energies= -752.295751

244 C8-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	-0.787971	-1.144118	-0.019116
C2	0.407248	0.784716	0.078769
C3	1.563026	1.596689	0.111713
O4	1.644393	2.802084	0.264244
N5	2.718569	0.786704	-0.062631
H6	3.593571	1.297688	-0.058775
C7	2.698927	-0.571620	-0.194002
N8	3.865816	-1.212367	-0.334407
N9	1.581889	-1.293787	-0.191695
C10	0.461273	-0.582755	-0.054356
C11	-1.020987	-2.545908	0.323813
H12	-1.929065	-2.904823	-0.163958
H13	-0.172497	-3.116623	-0.050941
H14	-1.114095	-2.683208	1.403220
C15	-1.807622	-0.154279	0.260712
O16	-2.544696	-0.309521	1.306598
N17	-0.958197	1.207182	0.283400
H18	-1.109783	1.660331	1.192736
H19	4.756541	-0.743510	-0.340797
H20	-1.281813	1.850741	-0.445368
H21	3.843884	-2.215900	-0.428643
H22	-2.963249	-0.961769	-1.241462
H23	-4.105270	1.131988	-1.873772
H24	-3.618332	1.794637	-0.293260
C25	-3.884295	0.884465	-0.832815
N26	-2.767135	-0.054056	-0.827260
H27	-4.773678	0.455198	-0.366753

Zero-point correction= 0.219452
Thermal correction to Energy= 0.234107
Thermal correction to Enthalpy= 0.235051
Thermal correction to Gibbs Free Energy= 0.177362
Sum of electronic and zero-point Energies= -752.247686
Sum of electronic and thermal Energies= -752.233031
Sum of electronic and thermal Enthalpies= -752.232087
Sum of electronic and thermal Free Energies= -752.289776

245 $TS^{via\ async\ HA_NH2\ +\ add}$_C8-$NHCH_3$[9MOG + H_{N7}]$^{\bullet+}$

N1	-0.943488	0.911116	-0.526432
C2	0.450890	-0.847802	-0.242869
C3	1.694101	-1.500171	-0.042080
O4	1.946901	-2.688277	-0.078148
N5	2.702908	-0.533263	0.229500
H6	3.623457	-0.926670	0.388463
C7	2.510043	0.817751	0.230079
N8	3.559791	1.609938	0.475645
N9	1.327749	1.389214	0.009397
C10	0.339832	0.527065	-0.238337
C11	-1.417503	2.274796	-0.704479
H12	-1.617411	2.757637	0.256176
H13	-0.650753	2.841860	-1.232601
H14	-2.328525	2.236821	-1.302355
C15	-1.837155	-0.209049	-0.545610
O16	-2.882211	-0.273274	-1.149850
N17	-0.801188	-1.432773	-0.662666
H18	-0.802798	-1.743017	-1.641325
H19	4.489958	1.259772	0.636424
H20	-1.118356	-2.214246	-0.085788
H21	3.412571	2.607433	0.458262
H22	-1.444900	0.069338	1.837928
H23	-3.644740	-0.621045	2.567022
H24	-4.162018	-0.527313	0.835858
C25	-3.492855	-0.126562	1.598596
N26	-2.138111	-0.316504	1.192194
H27	-3.711744	0.941571	1.750661

Zero-point correction= 0.216777
Thermal correction to Energy= 0.231463
Thermal correction to Enthalpy= 0.232407
Thermal correction to Gibbs Free Energy= 0.174334
Sum of electronic and zero-point Energies= -752.243204
Sum of electronic and thermal Energies= -752.228518
Sum of electronic and thermal Enthalpies= -752.227574

Sum of electronic and thermal Free Energies= -752.285647

246 C8-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	0.778160	1.152955	-0.112179
C2	-0.340239	-0.781339	-0.122480
C3	-1.520167	-1.599103	-0.116438
O4	-1.579945	-2.805441	-0.231622
N5	-2.678549	-0.801790	0.049148
C6	-2.680387	0.559670	0.173307
N7	-3.851087	1.178359	0.331072
H8	-4.734602	0.695438	0.364045
H9	-3.844028	2.183705	0.418917
N10	-1.577533	1.308970	0.143809
C11	-0.444732	0.636471	-0.011615
C12	1.125052	2.561067	-0.062809
H13	1.841766	2.778018	-0.856870
H14	0.216376	3.139789	-0.225313
H15	1.542992	2.820143	0.914062
C16	1.794014	0.095761	-0.259175
O17	2.380723	0.258515	-1.512001
N18	0.950998	-1.112436	-0.241382
H19	1.278426	-2.014088	-0.561772
H20	3.315430	0.025977	-1.480674
H21	-3.546179	-1.325153	0.071403
H22	3.196959	0.970942	0.895918
H23	4.171487	-1.318569	0.172429
H24	4.211123	-0.858927	1.881087
C25	3.546845	-1.065974	1.042300
N26	2.680516	0.098816	0.855780
H27	2.944162	-1.935304	1.313478

Zero-point correction= 0.219275
Thermal correction to Energy= 0.234148
Thermal correction to Enthalpy= 0.235092
Thermal correction to Gibbs Free Energy= 0.177266
Sum of electronic and zero-point Energies= -752.310979
Sum of electronic and thermal Energies= -752.296107
Sum of electronic and thermal Enthalpies= -752.295162
Sum of electronic and thermal Free Energies= -752.352989

247 TS$^{via\ async\ add+PT}$_C8-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-0.803866	-1.153672	-0.089747
C2	0.335115	0.768846	-0.179027
C3	1.526362	1.572304	-0.203210
O4	1.603253	2.766946	-0.397263
N5	2.671799	0.776221	0.039523
C6	2.657473	-0.577185	0.231352
N7	3.818452	-1.199572	0.435053
H8	4.708448	-0.727234	0.441933
H9	3.799282	-2.200063	0.567274
N10	1.546001	-1.315671	0.227547
C11	0.421902	-0.642287	0.020290
C12	-1.138983	-2.565104	-0.187185
H13	-1.898836	-2.676766	-0.963230
H14	-0.242289	-3.118031	-0.466987
H15	-1.507898	-2.951870	0.767015
C16	-1.797107	-0.096991	-0.414105
O17	-2.565268	-0.283507	-1.464188
N18	-0.945574	1.100723	-0.395744
H19	-1.234583	1.945977	-0.873614
H20	-3.439096	-0.234761	-0.484236
H21	3.545403	1.290367	0.039791
H22	-2.899859	-0.848550	1.262586
H23	-3.336792	2.015660	0.680326
H24	-4.065101	1.069148	1.985971
C25	-3.164886	1.201856	1.385780
N26	-2.922636	-0.043141	0.637151
H27	-2.321051	1.445749	2.034921

Zero-point correction= 0.215570
Thermal correction to Energy= 0.229707
Thermal correction to Enthalpy= 0.230651
Thermal correction to Gibbs Free Energy= 0.174338
Sum of electronic and zero-point Energies= -752.268208
Sum of electronic and thermal Energies= -752.254071
Sum of electronic and thermal Enthalpies= -752.253127
Sum of electronic and thermal Free Energies= -752.309440

248 TS$^{via\ HA_NH2\ products}$_C8-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-0.849959	-1.239090	-0.402058
C2	0.287861	0.665648	-0.504428
C3	1.419849	1.531730	-0.369997
O4	1.473830	2.730880	-0.548582
N5	2.548721	0.774743	0.022766
C6	2.560387	-0.576803	0.264818
N7	3.720072	-1.136055	0.635214
H8	4.581849	-0.622505	0.716688
H9	3.729425	-2.129410	0.807801
N10	1.487452	-1.346925	0.159009
C11	0.390758	-0.688759	-0.221211
C12	-1.228986	-2.594348	-0.033575
H13	-2.119192	-2.879383	-0.592607
H14	-0.403661	-3.256432	-0.291460
H15	-1.415820	-2.649864	1.042700
C16	-1.738177	-0.201852	-0.578937
O17	-2.927390	-0.494793	-1.110765
N18	-1.008692	0.918047	-0.873973
H19	-1.380040	1.827384	-1.110285
H20	-3.548833	0.240869	-1.060695
H21	3.393194	1.322990	0.138763
H22	-2.937170	-0.469062	1.553813
H23	-3.627711	1.752863	1.082231
H24	-2.865443	1.630704	2.659191
C25	-2.673063	1.524262	1.582818
N26	-2.178819	0.188847	1.342933
H27	-1.921319	2.266915	1.304473

Zero-point correction= 0.215330
Thermal correction to Energy= 0.230522
Thermal correction to Enthalpy= 0.231466
Thermal correction to Gibbs Free Energy= 0.172801
Sum of electronic and zero-point Energies= -752.255355
Sum of electronic and thermal Energies= -752.240163
Sum of electronic and thermal Enthalpies= -752.239219
Sum of electronic and thermal Free Energies= -752.297884

249 C8-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	-0.232807	1.828295	0.783442
C2	0.279492	-0.525280	0.278757
C3	1.414473	-1.456682	0.198963
O4	1.300178	-2.654699	0.354020
N5	2.635034	-0.861089	-0.105544
H6	3.421666	-1.494304	-0.191259
C7	2.751386	0.479155	-0.353249
N8	3.919954	0.939141	-0.805044
H9	4.705497	0.343463	-1.012317
H10	4.016106	1.934203	-0.942796
N11	1.771696	1.331724	-0.134461
C12	0.580191	0.886347	0.314270
C13	-1.450354	1.708940	1.577365
H14	-1.489988	0.747504	2.088556
H15	-1.433361	2.496356	2.330995
H16	-2.339046	1.830383	0.955059

C17	-2.228914	-0.707147	-0.031351
O18	-3.203952	-1.107988	0.557965
N19	-0.922586	-1.128083	0.410505
H20	0.164120	2.756954	0.694109
H21	-0.878401	-2.113746	0.671267
H22	-1.396707	0.154874	-1.681001
H23	-3.279324	1.380702	-2.371861
H24	-3.985230	-0.249928	-2.197783
N25	-2.217142	0.128617	-1.094071
C26	-3.482034	0.567839	-1.674897
H27	-4.139637	0.925766	-0.881784

Zero-point correction= 0.220347
Thermal correction to Energy= 0.235290
Thermal correction to Enthalpy= 0.236235
Thermal correction to Gibbs Free Energy= 0.178111
Sum of electronic and zero-point Energies= -752.323901
Sum of electronic and thermal Energies= -752.308958
Sum of electronic and thermal Enthalpies= -752.308014
Sum of electronic and thermal Free Energies= -752.366138

250 $TS^{via\ async\ HA_NH2\ +\ add}$_C8-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$

N1	0.916099	1.265588	-0.153960
C2	-0.308710	-0.629704	-0.508994
C3	-1.485836	-1.462518	-0.483977
O4	-1.584325	-2.617504	-0.837015
N5	-2.586586	-0.737305	0.029923
H6	-3.448308	-1.270928	0.063364
C7	-2.554085	0.554980	0.484772
N8	-3.686546	1.092031	0.961895
H9	-4.568620	0.607038	0.965911
H10	-3.659542	2.048114	1.280687
N11	-1.446046	1.281573	0.475172
C12	-0.391343	0.636190	-0.023143
C13	0.994355	2.283996	-1.242437
H14	0.644278	1.825605	-2.167192
H15	0.363445	3.130255	-0.972397
H16	2.039011	2.577390	-1.344772
C17	1.900168	0.009006	-0.463681
O18	3.012206	0.235156	-0.869645
N19	0.973861	-0.944970	-0.917378
H20	1.215382	1.673376	0.733534
H21	1.255160	-1.797084	-1.381043
H22	1.424091	-1.375122	1.513006
C23	3.342817	-0.700612	1.797048
H24	3.960092	0.129289	1.451063
H25	3.295454	-0.716200	2.894364
H26	3.805996	-1.645738	1.482610
N27	2.010121	-0.567665	1.286722

Zero-point correction= 0.215599
Thermal correction to Energy= 0.230564
Thermal correction to Enthalpy= 0.231508
Thermal correction to Gibbs Free Energy= 0.173183
Sum of electronic and zero-point Energies= -752.235343
Sum of electronic and thermal Energies= -752.220378
Sum of electronic and thermal Enthalpies= -752.219433
Sum of electronic and thermal Free Energies= -752.277759

251 O8-$NHCH_3$[9MOG + H_{N1}]$^+$

N1	0.881828	-0.649825	0.007530
C2	-0.737945	0.927452	0.019305
C3	-1.983709	1.521822	0.008998
O4	-2.430230	2.646969	0.080263
N5	-3.091643	0.372854	-0.117736
H6	-3.608235	0.607343	-0.974246
C7	-2.673542	-1.062047	-0.104821
N8	-3.725411	-1.908901	0.166806
H9	-3.426630	-2.854310	0.370590
N10	-1.417251	-1.420719	-0.077372
C11	-0.512495	-0.458343	-0.035954
C12	1.517175	-1.964616	0.072945
H13	2.247306	-1.980643	0.881549
H14	0.726138	-2.683797	0.281516
H15	2.002118	-2.197046	-0.873196
C16	1.453589	0.557645	0.069053
O17	2.730338	0.868967	0.182501
N18	0.530783	1.521494	0.082228
H19	0.737194	2.510282	0.099129
H20	-3.755910	0.540747	0.651192
H21	-4.513943	-1.893623	-0.471011
H22	3.898145	0.621418	-1.338836
H23	5.213796	0.556919	0.682817
H24	4.425585	-1.005533	1.047896
N25	3.593265	-0.008651	-0.597303
C26	4.737267	-0.328705	0.250802
H27	5.450550	-0.852242	-0.390557

Zero-point correction= 0.218858
Thermal correction to Energy= 0.233846
Thermal correction to Enthalpy= 0.234790
Thermal correction to Gibbs Free Energy= 0.175974
Sum of electronic and zero-point Energies= -752.175481
Sum of electronic and thermal Energies= -752.160493
Sum of electronic and thermal Enthalpies= -752.159548
Sum of electronic and thermal Free Energies= -752.218365

252 $TS^{via\ HA_NH2\ products}$_O8-$NHCH_3$[9MOG + H_{N1}]$^+$

N1	-0.784469	-0.726939	-0.371175
C2	0.679580	0.939111	-0.132539
C3	1.878118	1.592802	0.046452
O4	2.330098	2.709741	0.096544
N5	3.050819	0.412952	0.255549
H6	3.449594	0.633439	1.174772
C7	2.687431	-1.018513	0.163711
N8	3.736670	-1.857562	0.237075
H9	3.550306	-2.849604	0.196609
N10	1.479728	-1.411149	-0.009061
C11	0.520843	-0.457550	-0.145238
C12	-1.413829	-2.042216	-0.384971
H13	-2.172376	-2.054054	-1.166707
H14	-0.648059	-2.788810	-0.586793
H15	-1.877164	-2.227556	0.585442
C16	-1.483026	0.443391	-0.513057
O17	-2.741287	0.526446	-0.653961
N18	-0.595605	1.470500	-0.328061
H19	-0.815585	2.441040	-0.490665
H20	3.770205	0.650608	-0.436397
H21	4.656988	-1.563950	0.523055
H22	-3.781448	1.348408	0.971583
H23	-5.290887	0.059945	-0.291057
H24	-4.483499	-1.413941	0.326640
N25	-3.533183	0.359629	0.892990
C26	-4.731388	-0.373494	0.544838
H27	-5.372659	-0.358232	1.436455

Zero-point correction= 0.214246
Thermal correction to Energy= 0.229792
Thermal correction to Enthalpy= 0.230736
Thermal correction to Gibbs Free Energy= 0.170786
Sum of electronic and zero-point Energies= -752.160558
Sum of electronic and thermal Energies= -752.145012
Sum of electronic and thermal Enthalpies= -752.144068

Sum of electronic and thermal Free Energies= -752.204017

253 O8-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	-0.888319	-0.688672	-0.176387
C2	0.728974	0.885153	-0.137160
C3	2.064622	1.463601	0.028159
O4	2.262701	2.655519	0.172223
N5	2.993329	0.466086	0.065760
H6	3.958148	0.744683	0.200984
C7	2.803298	-0.956624	-0.268740
N8	3.720302	-1.697582	0.532724
H9	3.864548	-2.635640	0.179591
H10	3.439240	-1.735357	1.506693
N11	1.415082	-1.429215	-0.187047
C12	0.519870	-0.493727	-0.176746
C13	-1.488918	-2.030177	-0.187184
H14	-2.172004	-2.141690	0.652003
H15	-2.014917	-2.198917	-1.123796
H16	-0.657718	-2.728103	-0.088877
C17	-1.448695	0.525080	-0.146681
O18	-2.697862	0.907186	-0.125660
N19	-0.498547	1.485013	-0.115326
H20	-0.676391	2.482403	-0.076714
H21	3.077772	-1.115569	-1.323023
H22	-4.154867	0.218503	-1.174777
H23	-5.364765	-0.869369	0.525080
H24	-4.040805	-0.553628	1.660838
N25	-3.663150	-0.153668	-0.362880
C26	-4.567240	-0.168972	0.785609
H27	-4.999303	0.811299	1.008044

Zero-point correction= 0.220151
Thermal correction to Energy= 0.234512
Thermal correction to Enthalpy= 0.235456
Thermal correction to Gibbs Free Energy= 0.177659
Sum of electronic and zero-point Energies= -752.207677
Sum of electronic and thermal Energies= -752.193315
Sum of electronic and thermal Enthalpies= -752.192371
Sum of electronic and thermal Free Energies= -752.250168

254 TS$^{\text{via async HA_NH2 + add}}$_O8-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	-0.795160	-0.818191	0.354652
C2	0.683535	0.846505	0.077569
C3	2.000075	1.496813	-0.099950
O4	2.146745	2.698402	0.001326
N5	2.949870	0.552422	-0.310282
H6	3.907014	0.878397	-0.393064
C7	2.773554	-0.893708	-0.558967
N8	3.861249	-1.557011	0.082261
H9	4.005245	-2.490986	-0.282182
H10	3.754128	-1.595230	1.090473
N11	1.459073	-1.430237	-0.215272
C12	0.532911	-0.573993	0.040332
C13	-1.414560	-2.134337	0.436176
H14	-2.386028	-2.021076	0.915589
H15	-1.532206	-2.552059	-0.565081
H16	-0.778387	-2.787416	1.034175
C17	-1.437166	0.368509	0.571333
O18	-2.623949	0.569802	0.844877
N19	-0.481600	1.379598	0.379740
H20	-0.669040	2.372774	0.493082
H21	2.868081	-1.067566	-1.640528
H22	-4.056640	1.517562	-0.609499
H23	-5.453232	-0.225715	-1.432548
H24	-4.316474	-1.387556	-0.728543
N25	-3.685188	0.595959	-0.863031
C26	-4.711872	-0.375647	-0.628261
H27	-5.241398	-0.249393	0.322633

Zero-point correction= 0.214843
Thermal correction to Energy= 0.229551
Thermal correction to Enthalpy= 0.230495
Thermal correction to Gibbs Free Energy= 0.171852
Sum of electronic and zero-point Energies= -752.178130
Sum of electronic and thermal Energies= -752.163422
Sum of electronic and thermal Enthalpies= -752.162478
Sum of electronic and thermal Free Energies= -752.221122

255 O8-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	-0.862420	-0.648241	-0.149659
C2	0.728936	0.912192	-0.044482
C3	2.045823	1.476017	-0.026718
O4	2.347893	2.653768	0.002591
N5	3.012696	0.448543	-0.057158
H6	3.917750	0.796847	-0.353476
C7	2.705866	-0.915870	-0.299605
N8	3.653948	-1.818238	0.469099
H9	3.627159	-1.644959	1.484627
H10	3.335907	-2.776248	0.301015
N11	1.441776	-1.404423	-0.169084
C12	0.524177	-0.452036	-0.122780
C13	-1.511669	-1.942897	-0.325240
H14	-2.241289	-1.879782	-1.133347
H15	-0.729784	-2.651781	-0.595388
H16	-2.002974	-2.247077	0.597762
C17	-1.447106	0.564337	-0.073190
O18	-2.733663	0.856679	-0.146968
N19	-0.521778	1.514151	-0.002025
H20	-0.709894	2.506351	0.055656
H21	4.620562	-1.735686	0.149814
H22	-3.793897	0.623598	1.458766
H23	-5.238147	0.529614	-0.472604
H24	-4.475896	-1.039734	-0.861318
C25	-4.734469	-0.349077	-0.057297
N26	-3.536765	-0.014701	0.706168
H27	-5.404871	-0.860362	0.638001

Zero-point correction= 0.221821
Thermal correction to Energy= 0.236132
Thermal correction to Enthalpy= 0.237076
Thermal correction to Gibbs Free Energy= 0.180146
Sum of electronic and zero-point Energies= -752.180501
Sum of electronic and thermal Energies= -752.166190
Sum of electronic and thermal Enthalpies= -752.165246
Sum of electronic and thermal Free Energies= -752.222176

256 TS$^{\text{via async HA_NH2 + add}}$_O8-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	-0.819626	-0.689705	-0.429885
C2	0.699389	0.900153	-0.102915
C3	2.008883	1.489745	0.043556
O4	2.279811	2.672377	0.088799
N5	2.985079	0.481130	0.122116
H6	3.925877	0.844165	0.011342
C7	2.725084	-0.874520	-0.133140
N8	3.660229	-1.789806	0.594122
H9	3.611725	-1.683865	1.619222
H10	3.357841	-2.741497	0.363572
N11	1.487166	-1.391722	-0.162409
C12	0.526862	-0.477971	-0.226284
C13	-1.482490	-1.973989	-0.576610
H14	-2.296839	-1.868775	-1.293906
H15	-0.753770	-2.692729	-0.951279
H16	-1.876875	-2.308432	0.385213

C17	-1.466769	0.526079	-0.429950
O18	-2.706773	0.717108	-0.548166
N19	-0.521775	1.482279	-0.208143
H20	-0.713642	2.475457	-0.174035
H21	4.634390	-1.682695	0.302720
H22	-3.744766	1.164714	1.261836
H23	-5.305562	0.216325	-0.192332
H24	-4.518067	-1.375420	0.051629
C25	-4.740206	-0.408698	0.506851
N26	-3.528115	0.199500	1.000120
H27	-5.369840	-0.589648	1.390453

Zero-point correction= 0.216713
Thermal correction to Energy= 0.231414
Thermal correction to Enthalpy= 0.232359
Thermal correction to Gibbs Free Energy= 0.174325
Sum of electronic and zero-point Energies= -752.161182
Sum of electronic and thermal Energies= -752.146481
Sum of electronic and thermal Enthalpies= -752.145537
Sum of electronic and thermal Free Energies= -752.203570

257 O8-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	-0.646113	-1.082630	0.010005
C2	0.514307	0.823075	-0.020446
C3	1.680477	1.628486	-0.036331
O4	1.820853	2.828556	-0.073036
N5	2.882540	0.788670	-0.039202
H6	3.738052	1.333315	-0.065607
C7	2.946984	-0.540535	0.000207
N8	4.116675	-1.189764	0.008848
H9	4.990906	-0.687289	-0.004584
H10	4.168408	-2.196134	0.031754
N11	1.787836	-1.232968	0.026082
C12	0.585979	-0.543605	0.018530
C13	-0.986372	-2.488951	-0.114639
H14	-2.066614	-2.579550	-0.012316
H15	-0.685727	-2.885253	-1.090313
H16	-0.526821	-3.064360	0.693823
C17	-1.589176	-0.023225	-0.142136
O18	-2.703953	-0.213055	0.629684
N19	-0.830585	1.164705	0.016758
H20	1.797293	-2.242561	0.069804
H21	-1.172184	2.031017	-0.375031
H22	-4.018025	1.091311	1.150308
H23	-5.521230	0.858461	-0.666851
H24	-5.175940	-0.737602	0.061076
C25	-4.745312	0.110565	-0.484181
N26	-3.673796	0.778835	0.245675
H27	-4.360537	-0.228143	-1.448425

Zero-point correction= 0.218367
Thermal correction to Energy= 0.233714
Thermal correction to Enthalpy= 0.234658
Thermal correction to Gibbs Free Energy= 0.175042
Sum of electronic and zero-point Energies= -752.190683
Sum of electronic and thermal Energies= -752.175336
Sum of electronic and thermal Enthalpies= -752.174392
Sum of electronic and thermal Free Energies= -752.234008

258 TS$^{\text{via async add + PT}}$_O8-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	-1.498159	-0.154456	-1.183410
C2	0.291580	1.130027	-0.727765
C3	1.647929	1.328281	-0.301178
O4	2.231169	2.331602	0.025118
N5	2.357220	0.057749	-0.273910
H6	3.346683	0.153142	-0.070984
C7	1.754470	-1.142400	-0.176991
N8	2.418282	-2.212864	0.266334
H9	3.367748	-2.160831	0.601812
H10	2.009441	-3.125035	0.128695
N11	0.449302	-1.282457	-0.495007
C12	-0.120410	-0.132686	-1.037145
C13	-2.281907	-1.349998	-1.443174
H14	-3.312709	-1.046060	-1.622086
H15	-1.894589	-1.832484	-2.340887
H16	-2.260581	-2.072224	-0.619213
C17	-1.909217	0.881440	-0.340546
O18	-2.290210	0.384828	0.907015
N19	-0.860155	1.847283	-0.359471
H20	-0.380848	-1.194481	0.495452
H21	-1.039985	2.807113	-0.622628
H22	-1.930845	-1.345455	1.748421
H23	0.078473	-0.772250	2.951656
H24	-1.275830	0.349492	3.283411
C25	-0.578834	-0.008876	2.525302
N26	-1.304790	-0.620164	1.398031
H27	0.011800	0.827272	2.150300

Zero-point correction= 0.214890
Thermal correction to Energy= 0.228481
Thermal correction to Enthalpy= 0.229425
Thermal correction to Gibbs Free Energy= 0.175155
Sum of electronic and zero-point Energies= -752.125859
Sum of electronic and thermal Energies= -752.112268
Sum of electronic and thermal Enthalpies= -752.111324
Sum of electronic and thermal Free Energies= -752.165594

259 TS$^{\text{via HA_NH2 products}}$_O8-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	0.798153	-0.760576	-0.304711
C2	-0.656235	0.901949	0.079204
C3	-1.898559	1.527895	0.052985
O4	-2.239850	2.703981	-0.025155
N5	-2.976696	0.492886	0.090806
H6	-3.902955	0.893997	-0.003761
C7	-2.823129	-0.818185	0.117571
N8	-3.870240	-1.651771	0.190569
H9	-4.809567	-1.293642	0.270207
H10	-3.769085	-2.632126	-0.021861
N11	-1.572901	-1.362909	0.097545
C12	-0.473636	-0.483496	0.116161
C13	1.414493	-2.076832	-0.398838
H14	2.355160	-1.972867	-0.936777
H15	1.605147	-2.473284	0.600239
H16	0.755419	-2.740647	-0.961181
C17	1.459975	0.401893	-0.469624
O18	2.769145	0.514359	-0.606629
N19	0.614003	1.431901	-0.168629
H20	-1.478461	-2.261165	0.553967
H21	0.786726	2.398246	-0.406395
H22	3.629553	1.322081	0.967545
H23	5.288428	-0.277365	1.355023
H24	5.286745	0.197430	-0.366900
C25	4.715017	-0.299321	0.424192
N26	3.443393	0.352122	0.711580
H27	4.540998	-1.342359	0.154135

Zero-point correction= 0.216681
Thermal correction to Energy= 0.231660
Thermal correction to Enthalpy= 0.232604
Thermal correction to Gibbs Free Energy= 0.174287
Sum of electronic and zero-point Energies= -752.185689
Sum of electronic and thermal Energies= -752.170710
Sum of electronic and thermal Enthalpies= -752.169766

Sum of electronic and thermal Free Energies= -752.228083

260 O8-NHCH$_3$[9MOG + H$_{C4}$]$^{\bullet+}$

N1	0.874550	-0.724194	0.176163
C2	-0.731426	0.907229	0.416729
C3	-2.038124	1.442138	0.137715
O4	-2.288338	2.615552	-0.070609
N5	-2.996070	0.426619	0.126598
H6	-3.953926	0.730762	0.006526
C7	-2.649610	-0.910650	-0.102337
N8	-3.671341	-1.706191	-0.496109
H9	-4.477733	-1.327609	-0.966413
H10	-3.445495	-2.672358	-0.676039
N11	-1.465197	-1.401238	0.071234
C12	-0.516854	-0.539418	0.695387
C13	1.473460	-2.062200	0.191057
H14	2.201227	-2.150431	0.998423
H15	0.648002	-2.757335	0.343774
H16	1.951565	-2.273410	-0.760924
C17	1.374975	0.452759	-0.135279
O18	2.557364	0.819476	-0.553910
N19	0.465541	1.449886	0.017658
H20	-0.466226	-0.748815	1.779422
H21	0.606959	2.400785	-0.300929
H22	3.903719	-0.112878	-1.557423
H23	5.387385	-0.632282	0.202302
H24	4.200201	-0.021593	1.366636
N25	3.547317	-0.239910	-0.611311
C26	4.590551	0.100117	0.354619
H27	4.990679	1.110281	0.223820

Zero-point correction= 0.219934
Thermal correction to Energy= 0.234409
Thermal correction to Enthalpy= 0.235353
Thermal correction to Gibbs Free Energy= 0.177043
Sum of electronic and zero-point Energies= -752.214957
Sum of electronic and thermal Energies= -752.200483
Sum of electronic and thermal Enthalpies= -752.199538
Sum of electronic and thermal Free Energies= -752.257849

261 TS$^{via\ HA_NH2\ products}$_O8-NHCH$_3$[9MOG + H$_{C4}$]$^{\bullet+}$

N1	0.727017	-1.036541	-0.017976
C2	-0.563000	0.818306	0.165321
C3	-1.819263	1.581399	0.130545
O4	-1.883250	2.785855	0.019503
N5	-2.898033	0.725690	0.236625
H6	-3.810032	1.164621	0.281512
C7	-2.792939	-0.669019	0.034840
N8	-3.974771	-1.286003	-0.196716
H9	-4.744234	-0.794075	-0.623318
H10	-3.932459	-2.282477	-0.350781
N11	-1.690910	-1.333422	0.094702
C12	-0.544013	-0.616828	0.572265
C13	1.237916	-2.393069	0.083820
H14	1.649032	-2.573504	1.080034
H15	0.419351	-3.083799	-0.121715
H16	2.020466	-2.526062	-0.662663
C17	1.396532	0.003493	-0.533234
O18	2.519682	0.055694	-1.060507
N19	0.589452	1.147459	-0.378846
H20	-0.474631	-0.716558	1.671912
H21	0.816127	2.044588	-0.799892
H22	4.370535	-0.907050	-0.294938
H23	5.312061	0.753549	1.214857
H24	3.822499	1.663787	0.967889
N25	3.832046	-0.328296	0.356754
C26	4.490899	0.936587	0.500203
H27	4.929426	1.337163	-0.419231

Zero-point correction= 0.214244
Thermal correction to Energy= 0.229066
Thermal correction to Enthalpy= 0.230010
Thermal correction to Gibbs Free Energy= 0.171205
Sum of electronic and zero-point Energies= -752.183929
Sum of electronic and thermal Energies= -752.169106
Sum of electronic and thermal Enthalpies= -752.168162
Sum of electronic and thermal Free Energies= -752.226967

262 O8-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	0.509157	-1.256578	0.049110
C2	-0.454694	0.770707	0.736426
C3	-1.462434	1.613158	-0.039860
O4	-1.223204	2.709587	-0.487256
N5	-2.692740	0.989024	-0.142260
H6	-3.411978	1.536623	-0.600381
C7	-2.893616	-0.385423	0.023888
N8	-4.167849	-0.822938	-0.108149
H9	-4.946321	-0.202629	0.049059
H10	-4.326969	-1.804935	0.058718
N11	-1.903944	-1.224114	0.205813
C12	-0.713254	-0.679572	0.451171
C13	0.681649	-2.660386	-0.308291
H14	-0.081155	-2.931325	-1.039171
H15	1.673727	-2.800478	-0.733986
H16	0.567612	-3.276552	0.584468
C17	1.411276	-0.285030	-0.047618
O18	2.637996	-0.532362	-0.442391
N19	0.922215	0.906513	0.290216
H20	1.471659	1.753631	0.244869
H21	-0.545108	1.028956	1.805116
H22	3.752636	0.717902	-1.402221
H23	4.272332	0.337546	1.467691
H24	5.138898	-0.512746	0.150393
C25	4.602009	0.398859	0.429665
N26	3.451014	0.671169	-0.429865
H27	5.265741	1.260798	0.326285

Zero-point correction= 0.218900
Thermal correction to Energy= 0.233826
Thermal correction to Enthalpy= 0.234770
Thermal correction to Gibbs Free Energy= 0.175739
Sum of electronic and zero-point Energies= -752.231617
Sum of electronic and thermal Energies= -752.216692
Sum of electronic and thermal Enthalpies= -752.215748
Sum of electronic and thermal Free Energies= -752.274779

263 TS$^{via\ async\ add\ +\ PT}$_O8-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	1.014097	-0.915785	-0.889011
C2	-0.202108	0.858175	-0.258946
C3	-1.509581	1.484362	-0.137735
O4	-1.792400	2.648041	-0.284062
N5	-2.488973	0.538974	0.272717
H6	-3.408338	0.934847	0.433329
C7	-2.310343	-0.815123	0.265087
N8	-3.336142	-1.590104	0.617618
H9	-4.236526	-1.227368	0.887184
H10	-3.208565	-2.590235	0.574436
N11	-1.165900	-1.410884	-0.076758
C12	-0.191424	-0.574172	-0.408181
C13	1.540849	-2.258607	-1.075882
H14	2.491885	-2.355336	-0.547285
H15	0.818605	-2.970210	-0.676569
H16	1.696850	-2.449936	-2.138626

C17	1.779144	0.279414	-1.077553
O18	2.758536	0.457523	-0.089648
N19	0.843076	1.305042	-1.160101
H20	1.198571	2.246445	-1.044019
H21	0.739057	0.874576	0.819841
H22	2.426836	1.638656	1.461298
H23	1.830198	-1.231898	1.794836
H24	3.369721	-0.451205	2.264146
C25	2.295844	-0.307263	2.136395
N26	2.033191	0.749322	1.152694
H27	1.842896	0.000486	3.081877

Zero-point correction= 0.216271
Thermal correction to Energy= 0.229656
Thermal correction to Enthalpy= 0.230601
Thermal correction to Gibbs Free Energy= 0.176462
Sum of electronic and zero-point Energies= -752.166566
Sum of electronic and thermal Energies= -752.153181
Sum of electronic and thermal Enthalpies= -752.152236
Sum of electronic and thermal Free Energies= -752.206375

264 $TS^{via\ HA_NH2\ products}$_O8-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	-0.699440	0.897683	-0.281927
C2	0.540190	-0.890672	0.487455
C3	1.835612	-1.507363	-0.027210
O4	1.970004	-2.642209	-0.394695
N5	2.902757	-0.605222	0.054038
H6	3.811645	-0.996658	-0.165856
C7	2.756748	0.762205	0.209923
N8	3.870221	1.487300	0.339797
H9	4.787849	1.079356	0.418274
H10	3.777471	2.489338	0.415291
N11	1.585059	1.374690	0.175882
C12	0.527758	0.572742	0.149448
C13	-1.112443	2.227488	-0.720478
H14	-0.600834	2.482709	-1.649845
H15	-2.189163	2.208055	-0.880015
H16	-0.851285	2.948614	0.053156
C17	-1.448013	-0.249754	-0.470806
O18	-2.664335	-0.259408	-0.823316
N19	-0.682351	-1.331793	-0.132158
H20	-1.122376	-2.210793	0.097324
H21	0.542269	-1.038598	1.584623
H22	-4.250482	-1.361340	-0.105987
H23	-3.734741	1.145755	1.311468
H24	-4.918175	0.897316	-0.017768
C25	-4.398729	0.427563	0.824313
N26	-3.656083	-0.765175	0.473255
H27	-5.145400	0.113555	1.565339

Zero-point correction= 0.215845
Thermal correction to Energy= 0.230513
Thermal correction to Enthalpy= 0.231457
Thermal correction to Gibbs Free Energy= 0.173227
Sum of electronic and zero-point Energies= -752.214617
Sum of electronic and thermal Energies= -752.199949
Sum of electronic and thermal Enthalpies= -752.199004
Sum of electronic and thermal Free Energies= -752.257234

265 O8-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	0.509734	1.197915	0.052503
C2	-0.442426	-0.904322	0.067141
C3	-1.579687	-1.745532	-0.284880
O4	-0.954986	-1.834664	1.014716
N5	-2.822345	-1.066288	-0.356344
H6	-3.649489	-1.631056	-0.215533
C7	-2.933315	0.288389	-0.076728
N8	-4.190520	0.781949	-0.016385
H9	-4.960536	0.305799	-0.458056
H10	-4.277978	1.778306	0.111626
N11	-1.915689	1.099373	0.112783
C12	-0.711723	0.527491	0.207934
C13	0.696543	2.638685	0.193887
H14	-0.112644	3.138153	-0.338764
H15	0.663012	2.909835	1.250187
H16	1.657050	2.918522	-0.235476
C17	1.441225	0.293449	-0.223056
O18	2.708514	0.620923	-0.356419
N19	0.930881	-0.947528	-0.317606
H20	1.522308	-1.761361	-0.414388
H21	-1.510045	-2.640026	-0.894872
H22	3.998629	-0.330520	-1.430906
H23	5.217683	-1.374070	0.300356
H24	4.025178	-0.788767	1.474302
C25	4.524175	-0.561642	0.531176
N26	3.538492	-0.553066	-0.549455
H27	5.075991	0.379539	0.613839

Zero-point correction= 0.218786
Thermal correction to Energy= 0.233377
Thermal correction to Enthalpy= 0.234322
Thermal correction to Gibbs Free Energy= 0.176405
Sum of electronic and zero-point Energies= -752.185017
Sum of electronic and thermal Energies= -752.170426
Sum of electronic and thermal Enthalpies= -752.169482
Sum of electronic and thermal Free Energies= -752.227398

266 $TS^{via\ HA_NH2\ products}$_O8-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	0.670928	0.882176	-0.343389
C2	-0.555087	-1.027430	-0.125793
C3	-1.871341	-1.653850	-0.212880
O4	-1.092675	-1.736838	0.985924
N5	-2.975319	-0.756481	-0.169160
H6	-3.898801	-1.160246	-0.096904
C7	-2.810876	0.565502	0.138317
N8	-3.898083	1.288701	0.417227
H9	-4.828198	0.904081	0.448100
H10	-3.773861	2.272643	0.602099
N11	-1.637699	1.201267	0.126934
C12	-0.566884	0.451844	-0.073515
C13	1.081216	2.280095	-0.418555
H14	0.540866	2.777516	-1.225450
H15	0.855492	2.767415	0.529895
H16	2.152038	2.306001	-0.613615
C17	1.470821	-0.190137	-0.724803
O18	2.731375	-0.136371	-0.876348
N19	0.699563	-1.335402	-0.687552
H20	1.139269	-2.237909	-0.573113
H21	-2.066629	-2.587195	-0.729321
H22	4.263361	-1.208137	-0.053398
H23	4.739436	0.066916	1.918513
H24	3.298801	1.027004	1.571948
C25	4.095090	0.437327	1.111310
N26	3.528404	-0.735497	0.475433
H27	4.696446	1.064134	0.443713

Zero-point correction= 0.215794
Thermal correction to Energy= 0.230279
Thermal correction to Enthalpy= 0.231223
Thermal correction to Gibbs Free Energy= 0.173490
Sum of electronic and zero-point Energies= -752.174492
Sum of electronic and thermal Energies= -752.160007
Sum of electronic and thermal Enthalpies= -752.159063

Sum of electronic and thermal Free Energies= -752.216796

267 O8-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	0.787710	-0.933883	-0.331550
C2	-0.602041	0.811426	-0.248940
C3	-1.849139	1.446372	-0.212669
O4	-2.014982	2.744531	0.156073
N5	-2.890267	0.542118	0.143158
H6	-3.774369	0.953181	0.407482
C7	-2.721321	-0.816298	0.221327
N8	-3.807719	-1.554440	0.529652
H9	-4.743222	-1.195657	0.434105
H10	-3.687991	-2.555145	0.548655
N11	-1.565272	-1.422834	0.044036
C12	-0.535008	-0.568520	-0.156223
C13	1.288539	-2.306097	-0.335534
H14	1.764657	-2.527392	0.618984
H15	0.433447	-2.961124	-0.495436
H16	2.005497	-2.423131	-1.148195
C17	1.512335	0.185121	-0.485405
O18	2.809530	0.288772	-0.717565
N19	0.693412	1.253988	-0.439421
H20	1.008106	2.211167	-0.508115
H21	-2.432415	3.254865	-0.547413
H22	4.280511	-0.863401	-0.221500
H23	4.814810	1.369729	0.504055
H24	3.488039	1.210519	1.700869
N25	3.582503	-0.375775	0.337584
C26	4.236582	0.671012	1.117389
H27	4.904292	0.157659	1.814564

Zero-point correction= 0.218012
Thermal correction to Energy= 0.233459
Thermal correction to Enthalpy= 0.234403
Thermal correction to Gibbs Free Energy= 0.174920
Sum of electronic and zero-point Energies= -752.214506
Sum of electronic and thermal Energies= -752.199059
Sum of electronic and thermal Enthalpies= -752.198115
Sum of electronic and thermal Free Energies= -752.257598

268 TS$^{\text{via HA_NH2 products}}$_O8-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	0.679977	-1.114987	-0.412449
C2	-0.491290	0.782307	-0.259432
C3	-1.653924	1.473779	-0.112410
O4	-1.806304	2.810728	-0.097898
N5	-2.788879	0.706111	0.193048
H6	-3.625382	1.220271	0.435824
C7	-2.749444	-0.654542	0.297166
N8	-3.881283	-1.303898	0.608398
H9	-4.772082	-0.848695	0.716704
H10	-3.838047	-2.308284	0.684292
N11	-1.643475	-1.358643	0.105194
C12	-0.549082	-0.637883	-0.157522
C13	1.093927	-2.510934	-0.349961
H14	1.581102	-2.701172	0.607818
H15	0.206839	-3.134647	-0.449342
H16	1.787662	-2.708684	-1.166429
C17	1.546049	-0.067357	-0.700448
O18	2.821286	-0.156344	-0.725433
N19	0.812780	1.100160	-0.545895
H20	1.187716	2.019791	-0.716470
H21	-2.060357	3.160918	-0.962057
H22	4.139731	-0.956137	0.596455
H23	4.833314	1.275609	0.192793
H24	3.402527	1.825895	1.123565
N25	3.444302	-0.239347	0.808488
C26	4.133833	1.024251	0.997433
H27	4.692745	0.936569	1.937048

Zero-point correction= 0.214529
Thermal correction to Energy= 0.230335
Thermal correction to Enthalpy= 0.231280
Thermal correction to Gibbs Free Energy= 0.170421
Sum of electronic and zero-point Energies= -752.213191
Sum of electronic and thermal Energies= -752.197384
Sum of electronic and thermal Enthalpies= -752.196440
Sum of electronic and thermal Free Energies= -752.257298

269 O8-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	0.837657	-0.954983	0.526439
C2	-0.515282	0.824230	0.264205
C3	-1.715924	1.530158	0.014245
O4	-1.918932	2.728499	0.018184
N5	-2.755401	0.596218	-0.261900
H6	-3.655909	1.022009	-0.449134
C7	-2.608599	-0.761310	-0.276576
N8	-3.679459	-1.512382	-0.558439
N9	-1.455296	-1.377487	-0.023547
C10	-0.447122	-0.548005	0.239638
C11	1.247173	-2.335776	0.747486
H12	0.658808	-2.972487	0.088069
H13	2.306851	-2.431956	0.509842
H14	1.075365	-2.625676	1.787009
C15	1.599897	0.139357	0.941130
O16	2.898531	0.245449	0.656479
N17	0.791823	1.355728	0.596398
H18	1.283392	1.787279	-0.212819
H19	-4.590112	-1.126833	-0.746950
H20	0.773116	2.030777	1.367981
H21	-3.567889	-2.514523	-0.553735
H22	3.927363	1.348651	-0.562175
H23	4.219383	-0.945359	-1.246311
H24	2.502956	-0.924666	-1.763840
N25	3.089953	0.786854	-0.704383
C26	3.397975	-0.319597	-1.608655
H27	3.676240	0.129217	-2.566051

Zero-point correction= 0.220689
Thermal correction to Energy= 0.235079
Thermal correction to Enthalpy= 0.236024
Thermal correction to Gibbs Free Energy= 0.178823
Sum of electronic and zero-point Energies= -752.199357
Sum of electronic and thermal Energies= -752.184967
Sum of electronic and thermal Enthalpies= -752.184023
Sum of electronic and thermal Free Energies= -752.241223

270 TS$^{\text{via async add + PT}}$_O8-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	-0.793907	-1.169182	-0.524375
C2	0.372303	0.739907	-0.384585
C3	1.505848	1.568149	-0.188632
O4	1.609036	2.774664	-0.302450
N5	2.619050	0.761719	0.186768
H6	3.472955	1.284747	0.342023
C7	2.599286	-0.597145	0.326309
N8	3.731242	-1.214597	0.694538
N9	1.515132	-1.335076	0.117408
C10	0.443942	-0.623839	-0.243727
C11	-1.103568	-2.590206	-0.572536
H12	-0.431798	-3.106791	0.112073
H13	-2.137868	-2.740169	-0.259697
H14	-0.965113	-2.981494	-1.583316
C15	-1.640178	-0.171038	-1.006066
O16	-2.932820	-0.086219	-0.507211

N17	-0.958695	1.098847	-0.789260
H18	-1.803778	1.409742	0.109173
H19	4.601044	-0.730637	0.842733
H20	-0.995655	1.736984	-1.587120
H21	3.716525	-2.219801	0.767716
H22	-3.786865	1.412218	0.424062
H23	-3.772742	-0.493734	1.957052
H24	-1.990523	-0.328625	2.005083
N25	-2.934813	0.873944	0.576202
C26	-2.935117	0.201535	1.881168
H27	-3.017077	0.976241	2.646963

Zero-point correction= 0.216397
Thermal correction to Energy= 0.230402
Thermal correction to Enthalpy= 0.231346
Thermal correction to Gibbs Free Energy= 0.174841
Sum of electronic and zero-point Energies= -752.194367
Sum of electronic and thermal Energies= -752.180361
Sum of electronic and thermal Enthalpies= -752.179417
Sum of electronic and thermal Free Energies= -752.235923

271 TS$^{\text{via async HA_NH2 + add}}$_O8-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	-0.810736	-0.941962	-0.511078
C2	0.552805	0.830284	-0.230732
C3	1.761861	1.525783	0.008448
O4	1.974344	2.722260	0.004961
N5	2.796369	0.582868	0.272487
H6	3.701214	1.001231	0.455687
C7	2.639873	-0.773433	0.280831
N8	3.706351	-1.534053	0.552116
N9	1.480403	-1.379903	0.030245
C10	0.476608	-0.542085	-0.219522
C11	-1.232089	-2.319016	-0.734495
H12	-0.648289	-2.961183	-0.076363
H13	-2.292215	-2.406219	-0.496341
H14	-1.062956	-2.608417	-1.774426
C15	-1.574323	0.156163	-0.888004
O16	-2.835875	0.284141	-0.779694
N17	-0.751527	1.370356	-0.555365
H18	-1.240786	1.805548	0.251661
H19	4.620158	-1.156242	0.741273
H20	-0.737433	2.050527	-1.323296
H21	3.586761	-2.535286	0.545065
H22	-4.041061	1.345067	0.494060
H23	-4.429023	-0.941491	0.984988
H24	-2.789847	-1.010006	1.716053
N25	-3.218031	0.808958	0.772429
C26	-3.648794	-0.371651	1.499647
H27	-4.049727	-0.014870	2.456610

Zero-point correction= 0.218092
Thermal correction to Energy= 0.232535
Thermal correction to Enthalpy= 0.233480
Thermal correction to Gibbs Free Energy= 0.176040
Sum of electronic and zero-point Energies= -752.197446
Sum of electronic and thermal Energies= -752.183003
Sum of electronic and thermal Enthalpies= -752.182059
Sum of electronic and thermal Free Energies= -752.239498

272 O8-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	0.897870	-0.832086	-0.342244
C2	-0.609186	0.869771	-0.191797
C3	-1.902812	1.480022	-0.017844
O4	-2.189244	2.654634	-0.086593
N5	-2.871385	0.483960	0.256301
H6	-3.807018	0.851984	0.387805
C7	-2.640736	-0.864756	0.341541
N8	-3.678363	-1.670894	0.615556
H9	-4.613034	-1.331952	0.771408
H10	-3.506355	-2.661869	0.679521
N11	-1.438783	-1.390538	0.161053
C12	-0.505486	-0.474570	-0.100288
C13	1.534733	0.457410	-0.791119
O14	2.829328	0.540502	-0.478405
N15	0.628040	1.456742	-0.443289
H16	0.708936	2.391790	-0.823123
H17	2.980498	1.150224	1.393008
H18	4.438671	-1.266395	0.579618
H19	5.131559	0.377548	0.658421
C20	4.377973	-0.296877	1.075971
N21	3.021604	0.229470	0.954794
H22	4.564493	-0.437424	2.143726
C23	1.113065	-1.977768	-1.278657
H24	1.377394	-1.025867	0.562972
H25	2.186913	-2.107769	-1.406757
H26	0.657066	-2.863647	-0.839064
H27	0.642022	-1.733672	-2.229591

Zero-point correction= 0.220133
Thermal correction to Energy= 0.234417
Thermal correction to Enthalpy= 0.235361
Thermal correction to Gibbs Free Energy= 0.178764
Sum of electronic and zero-point Energies= -752.189238
Sum of electronic and thermal Energies= -752.174954
Sum of electronic and thermal Enthalpies= -752.174010
Sum of electronic and thermal Free Energies= -752.230606

273 TS$^{\text{via async add + PT}}$_O8-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	0.970993	-0.971740	-0.400222
C2	-0.426565	0.809792	-0.384864
C3	-1.671330	1.509644	-0.233294
O4	-1.902209	2.685120	-0.422968
N5	-2.679098	0.607388	0.189064
H6	-3.588523	1.038797	0.308838
C7	-2.515328	-0.735071	0.407970
N8	-3.584285	-1.447713	0.801267
H9	-4.500949	-1.048607	0.914240
H10	-3.466903	-2.438559	0.941914
N11	-1.351830	-1.346350	0.251759
C12	-0.373984	-0.524564	-0.139888
C13	1.112502	-2.271396	-1.107747
H14	0.646430	-3.041741	-0.494933
H15	0.623202	-2.211751	-2.080116
H16	2.175111	-2.476145	-1.239080
C17	1.660194	0.182726	-0.993701
O18	2.957147	0.209087	-0.511525
N19	0.827447	1.276933	-0.773058
H20	1.755595	-0.928335	0.575063
H21	0.962334	2.166435	-1.235265
H22	3.769259	-0.868739	0.909397
H23	3.026705	0.358343	2.817777
H24	2.039281	1.380306	1.741125
N25	2.931819	-0.291539	0.850446
C26	2.962851	0.807627	1.823936
H27	3.823592	1.454945	1.647733

Zero-point correction= 0.215841
Thermal correction to Energy= 0.229749
Thermal correction to Enthalpy= 0.230693
Thermal correction to Gibbs Free Energy= 0.175135
Sum of electronic and zero-point Energies= -752.185795
Sum of electronic and thermal Energies= -752.171887
Sum of electronic and thermal Enthalpies= -752.170943

Sum of electronic and thermal Free Energies= -752.226502

274 $TS^{via\ async\ HA_NH2\ +\ add}$_O8-$NHCH_3$[9MOG + H_{N9}]$^{\bullet+}$

N1	-0.884582	-0.809927	0.325041
C2	0.639272	0.874761	0.171568
C3	1.940051	1.471412	0.004336
O4	2.236671	2.643693	0.069235
N5	2.900584	0.464558	-0.256973
H6	3.840647	0.822770	-0.384101
C7	2.657820	-0.882879	-0.333971
N8	3.690022	-1.700964	-0.592897
H9	4.628087	-1.371839	-0.749398
H10	3.507989	-2.690244	-0.655474
N11	1.449838	-1.395765	-0.158993
C12	0.522437	-0.468880	0.085903
C13	-1.522790	0.497966	0.722333
O14	-2.785496	0.555589	0.557741
N15	-0.592157	1.476751	0.418870
H16	-0.679125	2.423686	0.764493
H17	-3.172849	1.156213	-1.399788
H18	-4.500259	-1.295778	-0.498046
H19	-5.197821	0.350314	-0.483198
C20	-4.497692	-0.321447	-0.988964
N21	-3.143194	0.196795	-1.049661
H22	-4.825863	-0.458105	-2.026229
C23	-1.118128	-1.933202	1.285692
H24	-1.367997	-1.023561	-0.573089
H25	-2.194043	-2.040690	1.416525
H26	-0.677613	-2.834908	0.863022
H27	-0.639956	-1.678631	2.230377

Zero-point correction= 0.217335
Thermal correction to Energy= 0.231817
Thermal correction to Enthalpy= 0.232761
Thermal correction to Gibbs Free Energy= 0.175468
Sum of electronic and zero-point Energies= -752.187372
Sum of electronic and thermal Energies= -752.172891
Sum of electronic and thermal Enthalpies= -752.171947
Sum of electronic and thermal Free Energies= -752.229239

275 N9-$NHCH_3$[9MOG + H_{N1}]$^{+}$

N1	-1.372415	-0.557191	-0.326811
C2	0.298841	1.023887	-0.022024
C3	1.556552	1.576321	0.098707
O4	2.048549	2.681069	0.140314
N5	2.633866	0.367181	0.239737
H6	3.016081	0.463193	1.188236
C7	2.194658	-1.028412	-0.035401
N8	3.231950	-1.880796	-0.291535
H9	2.947058	-2.819814	-0.538119
N10	0.946959	-1.334717	-0.156602
C11	0.054978	-0.345082	-0.096566
C12	-1.644049	-1.180261	-1.664032
H13	-1.172734	-0.563087	-2.429061
H14	-1.215010	-2.180229	-1.640939
H15	-2.723781	-1.210337	-1.814051
C16	-1.967011	0.897199	-0.312794
O17	-3.147063	1.054887	-0.404976
N18	-0.921588	1.719768	-0.159985
H19	-1.029846	2.722816	-0.088983
H20	3.396634	0.626383	-0.397955
H21	4.052314	-1.849779	0.300456
H22	-2.988928	-1.386641	0.438703
H23	-2.138095	0.139012	2.188006
H24	-2.392686	-1.547244	2.684424
C25	-1.803799	-0.895648	2.037943
N26	-1.997167	-1.396141	0.676825
H27	-0.755155	-0.996683	2.320180

Zero-point correction= 0.218906
Thermal correction to Energy= 0.233480
Thermal correction to Enthalpy= 0.234424
Thermal correction to Gibbs Free Energy= 0.177467
Sum of electronic and zero-point Energies= -752.181887
Sum of electronic and thermal Energies= -752.167314
Sum of electronic and thermal Enthalpies= -752.166370
Sum of electronic and thermal Free Energies= -752.223327

276 $TS^{via\ HA_NH2\ products}$_N9-$NHCH_3$[9MOG + H_{N1}]$^{+}$

N1	-1.331797	-0.556212	-0.379939
C2	0.262625	1.041020	-0.126679
C3	1.501159	1.612617	0.045436
O4	2.007498	2.696406	0.152083
N5	2.608991	0.366663	0.131835
H6	3.011618	0.457051	1.071061
C7	2.176243	-1.028268	-0.131368
N8	3.194636	-1.905136	-0.261662
H9	2.947078	-2.871412	-0.425235
N10	0.943367	-1.335696	-0.284781
C11	0.031419	-0.331413	-0.272596
C12	-1.821861	-1.597776	-1.310744
H13	-1.497884	-1.346282	-2.321751
H14	-1.408652	-2.549366	-0.986064
H15	-2.908731	-1.613015	-1.256644
C16	-1.964078	0.796985	-0.518331
O17	-3.130841	0.944057	-0.753982
N18	-0.975670	1.688504	-0.266460
H19	-1.123868	2.686647	-0.308224
H20	3.343492	0.649131	-0.526461
H21	4.110939	-1.728306	0.120480
H22	-2.995475	-0.818086	1.042504
H23	-1.537042	0.561701	2.313091
H24	-1.896149	-0.941598	3.183160
C25	-1.420454	-0.529430	2.284661
N26	-2.051769	-1.199671	1.168845
H27	-0.363187	-0.801743	2.332140

Zero-point correction= 0.215847
Thermal correction to Energy= 0.230696
Thermal correction to Enthalpy= 0.231640
Thermal correction to Gibbs Free Energy= 0.174110
Sum of electronic and zero-point Energies= -752.166770
Sum of electronic and thermal Energies= -752.151922
Sum of electronic and thermal Enthalpies= -752.150977
Sum of electronic and thermal Free Energies= -752.208508

277 N9-$NHCH_3$[9MOG + H_{C2}]$^{\bullet+}$

N1	1.438848	-0.221862	-0.223555
C2	-0.466454	1.041212	0.183884
C3	-1.898795	1.351644	0.244487
O4	-2.321398	2.490449	0.300223
N5	-2.636742	0.208263	0.147764
H6	-3.644493	0.315848	0.155846
C7	-2.164582	-1.182083	0.225536
N8	-3.021508	-1.963321	-0.595267
H9	-2.963466	-2.954180	-0.397407
H10	-2.893755	-1.789506	-1.585878
N11	-0.725792	-1.343002	-0.074622
C12	-0.034792	-0.271834	-0.011174
C13	1.849137	-0.783300	-1.552373
H14	2.929509	-0.672641	-1.645425
H15	1.542467	-1.827089	-1.589713
H16	1.339230	-0.218838	-2.334773

C17	1.761541	1.303735	-0.158815
O18	2.874898	1.692829	-0.296547
N19	0.579499	1.921569	0.082758
H20	0.492454	2.929171	0.172844
H21	-2.261257	-1.547026	1.258620
H22	3.073239	-0.379577	0.879167
H23	2.656191	-2.436419	1.972232
H24	1.131793	-2.602757	1.092526
N25	2.125184	-0.751327	0.947623
C26	2.147941	-2.215022	1.032586
H27	2.689689	-2.701566	0.214864

Zero-point correction= 0.219650
Thermal correction to Energy= 0.233709
Thermal correction to Enthalpy= 0.234653
Thermal correction to Gibbs Free Energy= 0.178682
Sum of electronic and zero-point Energies= -752.206227
Sum of electronic and thermal Energies= -752.192168
Sum of electronic and thermal Enthalpies= -752.191224
Sum of electronic and thermal Free Energies= -752.247196

278 TS$^{\text{via async HA_NH2 + add}}$_N9-NHCH$_3$[9MOG + H$_{C2}$]$^{\bullet+}$

N1	-1.276843	-0.354111	0.683475
C2	0.437879	0.952458	0.104780
C3	1.760289	1.253700	-0.449922
O4	2.118530	2.372615	-0.757378
N5	2.479125	0.097754	-0.628886
H6	3.427604	0.230992	-0.960220
C7	2.196132	-1.203093	-0.025761
N8	2.888274	-1.347136	1.227278
H9	2.933374	-2.299899	1.569666
H10	2.595187	-0.702888	1.953774
N11	0.775741	-1.473321	0.207305
C12	0.044799	-0.377322	0.349479
C13	-2.050226	-1.446952	1.245765
H14	-3.107456	-1.197074	1.166391
H15	-1.806755	-2.362747	0.706938
H16	-1.783193	-1.567015	2.299919
C17	-1.719141	1.037927	0.737262
O18	-2.813106	1.384933	1.073800
N19	-0.613847	1.772175	0.356888
H20	-0.628124	2.776519	0.224987
H21	2.563509	-1.974320	-0.704543
H22	-3.146356	-0.283568	-1.467066
H23	-1.712554	-1.151191	-3.336654
H24	-0.580155	-1.534776	-2.051159
N25	-2.125903	-0.227311	-1.571942
C26	-1.647174	-1.378896	-2.256342
H27	-2.219650	-2.297688	-2.083803

Zero-point correction= 0.212209
Thermal correction to Energy= 0.227563
Thermal correction to Enthalpy= 0.228508
Thermal correction to Gibbs Free Energy= 0.168995
Sum of electronic and zero-point Energies= -752.156598
Sum of electronic and thermal Energies= -752.141244
Sum of electronic and thermal Enthalpies= -752.140300
Sum of electronic and thermal Free Energies= -752.199812

279 N9-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	-1.366122	-0.575287	-0.336107
C2	0.273242	1.011565	-0.044183
C3	1.594551	1.544019	0.104134
O4	1.910142	2.714072	0.191922
N5	2.557572	0.502892	0.141173
H6	3.425954	0.817169	0.560753
C7	2.198862	-0.861307	0.265727
N8	3.239482	-1.764839	-0.330062
H9	4.122748	-1.739352	0.183643
H10	2.864291	-2.716447	-0.276297
N11	0.962722	-1.304671	-0.062387
C12	0.076028	-0.341626	-0.123471
C13	-1.630408	-1.190679	-1.673753
H14	-1.175271	-0.558786	-2.436884
H15	-1.185895	-2.184078	-1.660828
H16	-2.710398	-1.236659	-1.818157
C17	-1.986678	0.878904	-0.312827
O18	-3.171306	1.012144	-0.397724
N19	-0.945802	1.704768	-0.170369
H20	-1.045061	2.709573	-0.103976
H21	3.435364	-1.550957	-1.319677
H22	-2.950282	-1.415693	0.463432
H23	-2.046374	0.100164	2.195407
H24	-2.293478	-1.587822	2.690206
N25	-1.951556	-1.426166	0.671623
C26	-1.719407	-0.934709	2.032355
H27	-0.663497	-1.040731	2.283796

Zero-point correction= 0.220877
Thermal correction to Energy= 0.235105
Thermal correction to Enthalpy= 0.236049
Thermal correction to Gibbs Free Energy= 0.180013
Sum of electronic and zero-point Energies= -752.179608
Sum of electronic and thermal Energies= -752.165380
Sum of electronic and thermal Enthalpies= -752.164436
Sum of electronic and thermal Free Energies= -752.220472

280 TS$^{\text{via async add + PT}}$_N9-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	1.244474	-0.109327	0.535440
C2	-0.740221	1.018835	0.318612
C3	-2.153517	1.013234	-0.052968
O4	-2.777053	1.949424	-0.509006
N5	-2.676216	-0.272074	0.125763
H6	-3.652895	-0.391104	-0.112704
C7	-1.854869	-1.397482	0.378189
N8	-1.310169	-2.018918	-0.860816
H9	-1.896477	-1.830440	-1.673405
H10	0.150402	-1.487402	-0.781570
N11	-0.765500	-1.236740	1.247099
C12	-0.231433	-0.090602	0.908748
C13	2.218002	-0.334700	1.634563
H14	2.153229	0.523512	2.303849
H15	1.918940	-1.239391	2.168021
H16	3.224623	-0.401515	1.220120
C17	1.493385	1.310221	-0.168477
O18	2.608766	1.666775	-0.397871
N19	0.271167	1.818597	-0.273894
H20	0.121915	2.769484	-0.591220
H21	-1.263326	-3.031344	-0.745810
H22	1.500703	-2.043061	0.123011
H23	3.216071	-0.854564	-1.231590
H24	2.191491	-2.030774	-2.107857
N25	1.263308	-1.222906	-0.444267
C26	2.208121	-1.075371	-1.581229
H27	1.855367	-0.288217	-2.245729

Zero-point correction= 0.216117
Thermal correction to Energy= 0.229144
Thermal correction to Enthalpy= 0.230088
Thermal correction to Gibbs Free Energy= 0.177037
Sum of electronic and zero-point Energies= -752.104152
Sum of electronic and thermal Energies= -752.091125
Sum of electronic and thermal Enthalpies= -752.090181

Sum of electronic and thermal Free Energies= -752.143232

281 TS$^{via\ async\ HA_NH2\ +\ add}$_N9-NHCH$_3$[9MOG + H$_{N2}$]$^{\bullet+}$

N1	-1.347173	-0.579522	-0.366916
C2	0.265721	1.032628	-0.128480
C3	1.559451	1.564998	0.054250
O4	1.938870	2.711831	0.183437
N5	2.534840	0.482692	0.072940
H6	3.492640	0.791036	0.186006
C7	2.170676	-0.818957	-0.115946
N8	3.257339	-1.818981	-0.116078
H9	3.774042	-1.845146	0.771589
H10	2.803276	-2.730766	-0.252912
N11	0.992776	-1.290758	-0.288111
C12	0.029399	-0.336467	-0.294309
C13	-1.834735	-1.545629	-1.380324
H14	-1.512321	-1.211353	-2.367052
H15	-1.418740	-2.519729	-1.133087
H16	-2.922447	-1.570277	-1.333617
C17	-1.963782	0.789127	-0.468079
O18	-3.142038	0.946863	-0.656607
N19	-0.959213	1.673640	-0.238540
H20	-1.106614	2.673346	-0.235313
H21	3.932902	-1.676520	-0.876926
H22	-2.971718	-1.098379	0.937665
H23	-1.791192	0.525382	2.226555
H24	-1.974722	-1.000929	3.110790
N25	-1.978593	-1.302873	1.084423
C26	-1.517519	-0.537923	2.230049
H27	-0.434863	-0.642276	2.334669

Zero-point correction= 0.217440
Thermal correction to Energy= 0.232000
Thermal correction to Enthalpy= 0.232944
Thermal correction to Gibbs Free Energy= 0.176037
Sum of electronic and zero-point Energies= -752.164277
Sum of electronic and thermal Energies= -752.149717
Sum of electronic and thermal Enthalpies= -752.148773
Sum of electronic and thermal Free Energies= -752.205680

282 N9-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	-1.392154	-0.641081	-0.288942
C2	0.224279	1.015910	-0.464056
C3	1.462035	1.548016	-0.087824
O4	1.784203	2.685099	0.210413
N5	2.488410	0.502005	-0.049681
H6	3.407215	0.845820	0.202742
C7	2.261981	-0.814196	-0.134478
N8	3.271042	-1.685547	-0.000069
H9	4.216746	-1.368191	0.144197
N10	1.021448	-1.257635	-0.382820
C11	-0.010873	-0.346822	-0.725813
C12	-2.161693	-1.448768	-1.283058
H13	-2.035091	-0.986643	-2.260130
H14	-1.760049	-2.461729	-1.273395
H15	-3.214308	-1.444092	-0.995482
C16	-2.036762	0.796253	-0.197216
O17	-3.215371	0.908397	-0.028902
N18	-1.013933	1.651939	-0.293141
H19	-1.140696	2.654289	-0.237815
H20	3.117607	-2.681354	-0.014738
H21	-2.463318	-1.543173	1.119324
H22	0.912540	-2.228506	-0.640403
C23	-0.971858	-0.567163	2.123867
H24	0.101844	-0.405521	2.023263
H25	-1.478284	0.394778	2.264193
H26	-1.140021	-1.181136	3.009606
N27	-1.471599	-1.347094	0.988656

Zero-point correction= 0.219346
Thermal correction to Energy= 0.233965
Thermal correction to Enthalpy= 0.234909
Thermal correction to Gibbs Free Energy= 0.178414
Sum of electronic and zero-point Energies= -752.206819
Sum of electronic and thermal Energies= -752.192200
Sum of electronic and thermal Enthalpies= -752.191256
Sum of electronic and thermal Free Energies= -752.247751

283 TS$^{via\ HA_NH2\ products}$_N9-NHCH$_3$[9MOG + H$_{N3}$]$^{\bullet+}$

N1	-1.358039	-0.552007	-0.385938
C2	0.277317	1.050065	-0.234479
C3	1.573110	1.532923	0.004692
O4	1.988791	2.650845	0.231973
N5	2.542106	0.428086	-0.071389
H6	3.504185	0.737119	0.005568
C7	2.266018	-0.880781	-0.139704
N8	3.235339	-1.797199	-0.018068
H9	4.179443	-1.528058	0.210927
N10	0.997604	-1.265673	-0.337571
C11	0.007197	-0.285552	-0.502427
C12	-2.003513	-1.413189	-1.416677
H13	-1.729909	-1.039895	-2.402644
H14	-1.665533	-2.438239	-1.269574
H15	-3.083228	-1.346959	-1.281483
C16	-1.981248	0.844485	-0.326036
O17	-3.171467	0.993124	-0.363577
N18	-0.949615	1.704168	-0.164809
H19	-1.080132	2.705781	-0.128410
H20	3.074413	-2.766774	-0.241819
H21	-2.714256	-1.476780	0.969384
H22	0.724567	-2.227319	-0.182504
C23	-1.362265	-0.580530	2.190313
H24	-0.287250	-0.386555	2.214812
H25	-1.910124	0.366780	2.257974
H26	-1.607624	-1.179205	3.072701
N27	-1.696372	-1.399685	1.031175

Zero-point correction= 0.216384
Thermal correction to Energy= 0.231285
Thermal correction to Enthalpy= 0.232229
Thermal correction to Gibbs Free Energy= 0.174758
Sum of electronic and zero-point Energies= -752.202411
Sum of electronic and thermal Energies= -752.187510
Sum of electronic and thermal Enthalpies= -752.186566
Sum of electronic and thermal Free Energies= -752.244037

284 N9-NHCH$_3$[9MOG + H$_{C4}$]$^{\bullet+}$

N1	-1.287855	-0.418678	0.338226
C2	0.426598	0.986183	-0.382248
C3	1.805665	1.367976	-0.255089
O4	2.213247	2.510624	-0.163119
N5	2.644065	0.247501	-0.246851
H6	3.634247	0.452496	-0.201016
C7	2.179008	-1.050436	-0.046572
N8	3.121962	-1.971033	0.223291
H9	4.087669	-1.739780	0.385157
H10	2.835831	-2.933868	0.303296
N11	0.930443	-1.407695	-0.120904
C12	0.009199	-0.428659	-0.527774
C13	-1.773546	1.049837	0.250542
O14	-2.879889	1.384417	0.515395
N15	-0.667452	1.764544	-0.108734
H16	-0.369624	-0.617864	-1.542695

H17	-0.656404	2.778642	-0.071029
H18	-1.957650	-2.253594	0.121468
H19	-2.141101	-1.347097	-2.190953
H20	-3.661850	-1.906559	-1.473447
C21	-2.864046	-1.167836	-1.386655
N22	-2.333750	-1.320956	-0.032967
H23	-3.318859	-0.182695	-1.498611
C24	-0.986729	-0.670054	1.789577
H25	-1.925978	-0.563731	2.329088
H26	-0.578311	-1.675980	1.875712
H27	-0.243620	0.051862	2.129701

Zero-point correction= 0.220063
Thermal correction to Energy= 0.234231
Thermal correction to Enthalpy= 0.235175
Thermal correction to Gibbs Free Energy= 0.179118
Sum of electronic and zero-point Energies= -752.230794
Sum of electronic and thermal Energies= -752.216626
Sum of electronic and thermal Enthalpies= -752.215682
Sum of electronic and thermal Free Energies= -752.271739

285 $TS^{via\ async\ add\ +\ PT}$_N9-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.268393	-0.438630	0.294435
C2	0.504176	0.975444	-0.286228
C3	1.867297	1.381526	-0.215362
O4	2.302105	2.518177	-0.148712
N5	2.715786	0.250175	-0.218123
H6	3.704524	0.466447	-0.218667
C7	2.283476	-1.048111	-0.022401
N8	3.245164	-1.985388	0.141402
H9	4.187287	-1.741705	0.398390
H10	2.944871	-2.933338	0.302004
N11	1.024293	-1.397011	-0.034883
C12	0.150101	-0.384372	-0.378240
C13	-1.712395	1.072462	0.319935
O14	-2.825937	1.368075	0.645805
N15	-0.618306	1.760840	-0.023103
H16	-0.978407	-0.910707	-1.435113
H17	-0.614857	2.774497	-0.023155
H18	-1.841684	-2.183390	-0.511164
H19	-3.389524	0.111906	-1.580441
H20	-3.635841	-1.630652	-1.864681
C21	-3.346836	-0.877771	-1.130627
N22	-1.946333	-1.195484	-0.764966
H23	-4.000475	-0.923555	-0.259307
C24	-1.409512	-1.045547	1.642210
H25	-2.461061	-1.047991	1.932285
H26	-0.975662	-2.045899	1.611994
H27	-0.831847	-0.428929	2.332052

Zero-point correction= 0.213660
Thermal correction to Energy= 0.228044
Thermal correction to Enthalpy= 0.228988
Thermal correction to Gibbs Free Energy= 0.172597
Sum of electronic and zero-point Energies= -752.157361
Sum of electronic and thermal Energies= -752.142977
Sum of electronic and thermal Enthalpies= -752.142033
Sum of electronic and thermal Free Energies= -752.198423

286 $TS^{via\ HA_NH2\ products}$_N9-$NHCH_3$[9MOG + H_{C4}]$^{\bullet+}$

N1	1.202061	-0.778877	-0.038332
C2	-0.358046	0.896514	0.022334
C3	-1.699447	1.494310	0.119483
O4	-1.950292	2.667419	-0.028199
N5	-2.635847	0.503075	0.382651
H6	-3.589555	0.816389	0.519995
C7	-2.360747	-0.852289	0.120930
N8	-3.445824	-1.634213	-0.044046
H9	-4.334983	-1.254881	-0.328350
H10	-3.282331	-2.614790	-0.216096
N11	-1.165774	-1.348210	0.062746
C12	-0.123518	-0.478513	0.538075
C13	1.507649	0.151864	-1.052908
O14	2.401340	0.106186	-1.855048
N15	0.571039	1.191861	-0.875223
H16	-0.021821	-0.510971	1.628357
H17	0.553921	2.000020	-1.492184
N18	2.310962	-0.109261	1.551798
C19	1.596361	-2.174758	-0.243017
H20	2.610855	-2.191404	-0.640896
H21	1.534691	-2.700700	0.709985
H22	0.904440	-2.638374	-0.949868
H23	2.818289	-0.995909	1.637113
C24	3.245453	0.894269	1.117594
H25	3.976543	0.568584	0.369983
H26	2.722441	1.795785	0.786358
H27	3.796583	1.178400	2.029476

Zero-point correction= 0.214907
Thermal correction to Energy= 0.229432
Thermal correction to Enthalpy= 0.230376
Thermal correction to Gibbs Free Energy= 0.172540
Sum of electronic and zero-point Energies= -752.180403
Sum of electronic and thermal Energies= -752.165878
Sum of electronic and thermal Enthalpies= -752.164934
Sum of electronic and thermal Free Energies= -752.222769

287 N9-$NHCH_3$[9MOG + H_{C5}]$^{\bullet+}$

N1	1.389144	-0.245310	-0.210015
C2	-0.435022	0.950427	0.812529
C3	-1.828047	1.288577	0.286274
O4	-2.228863	2.417560	0.158747
N5	-2.601807	0.168779	0.019433
H6	-3.559168	0.366871	-0.248772
C7	-2.078562	-1.104922	-0.175965
N8	-2.950758	-2.093252	-0.429761
H9	-3.947988	-1.975664	-0.354237
H10	-2.586794	-3.021538	-0.580455
N11	-0.785645	-1.343815	-0.167289
C12	0.008119	-0.356123	0.239493
C13	1.661611	-0.855879	-1.547035
H14	1.434106	-1.917880	-1.495743
H15	1.011044	-0.376598	-2.277574
H16	2.710577	-0.671206	-1.769946
C17	1.617793	1.302804	-0.305824
O18	2.566286	1.749995	-0.862960
N19	0.587170	1.862199	0.349727
H20	0.496211	2.869049	0.403251
H21	-0.494842	0.955852	1.912320
H22	2.314299	-0.124153	1.561941
H23	2.938946	-2.306424	1.927118
H24	1.210006	-2.353436	1.492309
N25	2.407484	-0.722631	0.742548
C26	2.217537	-2.122653	1.129259
H27	2.474516	-2.780492	0.298610

Zero-point correction= 0.219494
Thermal correction to Energy= 0.233875
Thermal correction to Enthalpy= 0.234819
Thermal correction to Gibbs Free Energy= 0.177569
Sum of electronic and zero-point Energies= -752.231120
Sum of electronic and thermal Energies= -752.216739
Sum of electronic and thermal Enthalpies= -752.215795

Sum of electronic and thermal Free Energies= -752.273045

288 $TS^{via\ HA_NH2\ products}$_N9-NHCH$_3$[9MOG + H$_{C5}$]$^{\bullet+}$

N1	1.242891	0.457959	0.465712
C2	-0.311920	-0.914437	-0.652282
C3	-1.678676	-1.411466	-0.193659
O4	-1.969641	-2.567502	-0.045583
N5	-2.590228	-0.365931	-0.040025
H6	-3.543810	-0.650546	0.154485
C7	-2.220575	0.964163	0.091036
N8	-3.196275	1.871950	0.166943
H9	-4.170470	1.646704	0.042727
H10	-2.936427	2.837697	0.304808
N11	-0.961775	1.349346	0.197902
C12	-0.049800	0.403766	0.001460
C13	1.513758	1.219060	1.709050
H14	1.267532	2.260208	1.517494
H15	0.901865	0.806374	2.512334
H16	2.570668	1.108921	1.943563
C17	1.737603	-0.967088	0.461249
O18	2.775917	-1.276355	0.965951
N19	0.818342	-1.687327	-0.217833
H20	0.924008	-2.682444	-0.360024
H21	-0.356612	-0.840948	-1.750383
H22	3.233507	0.837122	-0.400245
H23	2.705067	1.582153	-2.647555
H24	2.113181	-0.051198	-2.292146
N25	2.371456	1.332736	-0.651892
C26	2.016345	1.007523	-2.016844
H27	1.009997	1.376559	-2.233715

Zero-point correction= 0.217247
Thermal correction to Energy= 0.231367
Thermal correction to Enthalpy= 0.232312
Thermal correction to Gibbs Free Energy= 0.176352
Sum of electronic and zero-point Energies= -752.223956
Sum of electronic and thermal Energies= -752.209835
Sum of electronic and thermal Enthalpies= -752.208891
Sum of electronic and thermal Free Energies= -752.264851

289 N9-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	1.329013	0.329027	0.243921
C2	-0.396085	-1.303972	-0.009658
C3	-1.736555	-1.563963	-0.521965
O4	-1.303939	-2.060616	0.762748
N5	-2.614717	-0.452551	-0.508175
H6	-3.602193	-0.652097	-0.587659
C7	-2.239349	0.761075	0.030580
N8	-3.198711	1.692727	0.170988
H9	-4.129986	1.579124	-0.193384
H10	-2.933227	2.593440	0.536343
N11	-1.003338	1.065880	0.379390
C12	-0.105841	0.078857	0.370704
H13	2.639615	0.959283	-1.103362
C14	1.900905	-1.054763	-0.170064
O15	3.078029	-1.201709	-0.281920
N16	0.853241	-1.869630	-0.375703
H17	0.998593	-2.846320	-0.595454
H18	-1.967466	-2.319607	-1.265060
H19	3.024284	0.924160	1.366146
N20	1.654976	1.160396	-0.924586
C21	1.472392	2.600318	-0.717216
H22	0.431027	2.807919	-0.478953
H23	2.130767	3.030346	0.045456
H24	1.707608	3.059606	-1.678844
C25	1.956791	0.778655	1.532462
H26	1.466247	1.700888	1.838482
H27	1.785224	0.003683	2.279771

Zero-point correction= 0.219645
Thermal correction to Energy= 0.233567
Thermal correction to Enthalpy= 0.234511
Thermal correction to Gibbs Free Energy= 0.179215
Sum of electronic and zero-point Energies= -752.186512
Sum of electronic and thermal Energies= -752.172591
Sum of electronic and thermal Enthalpies= -752.171646
Sum of electronic and thermal Free Energies= -752.226942

290 $TS^{via\ HA_NH2\ products}$_N9-NHCH$_3$[9MOG + H$_{C6}$]$^{\bullet+}$

N1	1.272818	0.285603	0.380662
C2	-0.356841	-1.311701	-0.094887
C3	-1.671891	-1.501096	-0.703602
O4	-1.332171	-2.096049	0.557536
N5	-2.537616	-0.377885	-0.630622
H6	-3.495326	-0.513535	-0.922207
C7	-2.234949	0.706730	0.154192
N8	-3.209800	1.587419	0.411899
H9	-4.168320	1.447392	0.137482
H10	-2.982205	2.392496	0.974789
N11	-1.016630	0.972928	0.611991
C12	-0.089473	0.041131	0.421863
H13	2.692509	0.971604	-1.155814
C14	1.916776	-1.032588	0.050224
O15	3.096434	-1.196828	0.125820
N16	0.918815	-1.847077	-0.377495
H17	1.099930	-2.816249	-0.598820
H18	-1.875067	-2.182265	-1.522403
H19	2.947973	1.217661	1.243938
N20	1.674416	1.089870	-1.188780
C21	1.363225	2.503782	-1.093981
H22	0.299794	2.642088	-0.891719
H23	1.963769	3.072553	-0.375032
H24	1.564536	2.909538	-2.093728
C25	1.898295	1.053068	1.482154
H26	1.362457	1.994831	1.584508
H27	1.810972	0.474945	2.402808

Zero-point correction= 0.217011
Thermal correction to Energy= 0.230942
Thermal correction to Enthalpy= 0.231886
Thermal correction to Gibbs Free Energy= 0.176757
Sum of electronic and zero-point Energies= -752.175382
Sum of electronic and thermal Energies= -752.161452
Sum of electronic and thermal Enthalpies= -752.160508
Sum of electronic and thermal Free Energies= -752.215636

291 N9-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-1.445458	-0.223880	-0.223087
C2	0.480262	1.049186	0.048478
C3	1.813527	1.241850	0.186584
O4	2.421595	2.435679	0.297371
N5	2.622650	0.087361	0.094838
H6	3.555396	0.238680	-0.272617
C7	2.048841	-1.162471	-0.147296
N8	2.928036	-2.178636	-0.318226
H9	3.832661	-2.143485	0.125885
H10	2.529789	-3.095517	-0.453784
N11	0.763317	-1.364853	-0.246884
C12	0.005446	-0.245104	-0.171069
C13	-2.003822	-0.789136	-1.495518
H14	-1.603659	-0.209868	-2.327971
H15	-1.677753	-1.824370	-1.577590
H16	-3.090398	-0.708099	-1.459969

C17	-1.776741	1.300330	-0.117207
O18	-2.906767	1.671358	-0.189652
N19	-0.604620	1.932509	0.070774
H20	-0.553464	2.936515	0.172137
H21	2.969303	2.486643	1.092477
H22	-3.027858	-0.435813	0.959758
H23	-2.522775	-2.753624	0.340308
H24	-0.953055	-2.530127	1.169954
C25	-1.992992	-2.209001	1.129914
N26	-2.058243	-0.751576	1.005281
H27	-2.463709	-2.437627	2.087477

Zero-point correction= 0.218599
Thermal correction to Energy= 0.233327
Thermal correction to Enthalpy= 0.234271
Thermal correction to Gibbs Free Energy= 0.177027
Sum of electronic and zero-point Energies= -752.216936
Sum of electronic and thermal Energies= -752.202209
Sum of electronic and thermal Enthalpies= -752.201264
Sum of electronic and thermal Free Energies= -752.258509

292 TS$^{\text{via HA_NH2 products}}$_N9-NHCH$_3$[9MOG + H$_{O6}$]$^{\bullet+}$

N1	-1.391206	0.211609	0.339298
C2	0.464450	-1.066923	-0.020895
C3	1.782800	-1.240552	-0.237727
O4	2.388114	-2.418525	-0.453067
N5	2.589032	-0.100967	-0.104289
H6	3.578940	-0.261764	0.030502
C7	2.055297	1.128931	0.238433
N8	2.929367	2.142721	0.407289
H9	3.854970	2.118073	0.010795
H10	2.541364	3.047690	0.625550
N11	0.771959	1.326968	0.423242
C12	0.001594	0.223762	0.329790
C13	-2.090216	0.998559	1.382427
H14	-1.839832	0.584046	2.359566
H15	-1.744172	2.028412	1.317260
H16	-3.163543	0.927490	1.212700
C17	-1.771961	-1.248804	0.273985
O18	-2.894546	-1.620798	0.442434
N19	-0.633056	-1.920903	-0.035367
H20	-0.615924	-2.924086	-0.145557
H21	2.843375	-2.446900	-1.305254
H22	-2.997545	0.413318	-1.103572
H23	-2.483954	2.705602	-0.757970
H24	-0.833431	2.378000	-1.375509
C25	-1.883395	2.086852	-1.434899
N26	-2.011239	0.651429	-1.246011
H27	-2.224200	2.277758	-2.459268

Zero-point correction= 0.215810
Thermal correction to Energy= 0.230833
Thermal correction to Enthalpy= 0.231777
Thermal correction to Gibbs Free Energy= 0.174244
Sum of electronic and zero-point Energies= -752.209902
Sum of electronic and thermal Energies= -752.194879
Sum of electronic and thermal Enthalpies= -752.193935
Sum of electronic and thermal Free Energies= -752.251468

293 N9-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	-1.341574	-0.654705	-0.369668
C2	0.309073	0.988761	-0.107705
C3	1.657920	1.472680	0.024340
O4	2.016544	2.627707	0.098086
N5	2.573141	0.396385	0.063154
C6	2.228277	-0.922306	-0.029243
N7	3.191743	-1.845400	0.024120
H8	2.920711	-2.815160	-0.041472
N9	0.967912	-1.323138	-0.170557
C10	0.073171	-0.343144	-0.204418
C11	-1.578737	-1.527336	-1.556424
H12	-1.155584	-1.037886	-2.432844
H13	-1.110373	-2.491540	-1.367611
H14	-2.657554	-1.630041	-1.679346
C15	-2.081436	0.804702	-0.677142
O16	-3.159010	0.967006	-0.163798
N17	-0.848574	1.827252	-0.182608
H18	-1.098286	2.271438	0.707387
H19	4.168777	-1.621909	0.124559
H20	-2.871331	-1.365820	0.624632
H21	-1.961463	0.372065	2.092409
H22	-2.135807	-1.233420	2.817656
C23	-1.601403	-0.663492	2.056576
N24	-1.864716	-1.342538	0.788598
H25	-0.537417	-0.713525	2.294542
H26	3.543838	0.675262	0.159568
H27	-0.752513	2.568648	-0.880962

Zero-point correction= 0.220178
Thermal correction to Energy= 0.234476
Thermal correction to Enthalpy= 0.235420
Thermal correction to Gibbs Free Energy= 0.179444
Sum of electronic and zero-point Energies= -752.194859
Sum of electronic and thermal Energies= -752.180561
Sum of electronic and thermal Enthalpies= -752.179617
Sum of electronic and thermal Free Energies= -752.235593

294 TS$^{\text{via async HA_NH2 + add}}$_N9-NHCH$_3$[9MOG + H$_{N7}$]$^{\bullet+}$

N1	-1.312496	-0.611859	-0.365704
C2	0.344028	0.968047	-0.090253
C3	1.677771	1.466549	0.030427
O4	2.045883	2.619786	0.088986
N5	2.588784	0.379348	0.079640
C6	2.247652	-0.938179	-0.039921
N7	3.212310	-1.859444	0.001695
H8	2.942463	-2.828899	-0.073491
N9	0.987942	-1.346713	-0.198621
C10	0.104060	-0.364929	-0.218173
C11	-1.678517	-1.725637	-1.287756
H12	-1.198777	-1.558628	-2.251303
H13	-1.331866	-2.651914	-0.834466
H14	-2.762327	-1.711493	-1.401323
C15	-1.904951	0.648585	-0.732021
O16	-3.093536	0.906184	-0.764891
N17	-0.864446	1.728399	-0.264415
H18	-1.187135	2.203185	0.587144
H19	4.187781	-1.636233	0.117090
H20	-2.739611	-1.540878	0.924677
H21	-2.577375	0.598522	1.896885
H22	-2.206407	-0.661375	3.081065
C23	-1.865203	-0.198225	2.149274
N24	-1.783466	-1.270733	1.169854
H25	-0.869662	0.209518	2.347237
H26	3.559645	0.655421	0.181375
H27	-0.784929	2.444763	-0.994272

Zero-point correction= 0.218496
Thermal correction to Energy= 0.232462
Thermal correction to Enthalpy= 0.233406
Thermal correction to Gibbs Free Energy= 0.178154
Sum of electronic and zero-point Energies= -752.179963
Sum of electronic and thermal Energies= -752.165997
Sum of electronic and thermal Enthalpies= -752.165053

Sum of electronic and thermal Free Energies= -752.220306

295 O8-NHCH$_3$[9MOG + H$_{N9}$]$^{\bullet+}$

N1	-1.347857	-0.499147	-0.307673
C2	0.317783	1.035397	0.038075
C3	1.674243	1.503533	0.185494
O4	2.055924	2.632975	0.394340
N5	2.574752	0.417752	0.053277
C6	2.236967	-0.891449	-0.178441
N7	3.225932	-1.795468	-0.274527
H8	4.201111	-1.549668	-0.236618
H9	2.977841	-2.753001	-0.466766
N10	0.979586	-1.283990	-0.298823
C11	0.107341	-0.280262	-0.169170
C12	-1.683148	-0.795648	-1.744161
H13	-1.384357	0.063130	-2.344793
H14	-1.120653	-1.682465	-2.037962
H15	-2.756141	-0.961170	-1.810863
C16	-1.929107	0.844954	0.151793
O17	-3.097473	1.196958	-0.398025
N18	-0.879387	1.739758	0.055334
H19	-0.957991	2.689605	0.393004
H20	-3.834998	0.820905	0.098835
H21	3.548303	0.684213	0.149769
H22	-1.571739	-2.421417	0.101831
N23	-1.921011	-1.554177	0.507034
C24	-1.527495	-1.469054	1.916443
H25	-1.916296	-0.546494	2.350543
H26	-2.010749	-2.311193	2.413630
H27	-0.445545	-1.529827	2.076320

Zero-point correction= 0.219790
Thermal correction to Energy= 0.234149
Thermal correction to Enthalpy= 0.235093
Thermal correction to Gibbs Free Energy= 0.179353
Sum of electronic and zero-point Energies= -752.212109
Sum of electronic and thermal Energies= -752.197750
Sum of electronic and thermal Enthalpies= -752.196806
Sum of electronic and thermal Free Energies= -752.252546

296 TS$^{\text{via async HA_NH2 + add}}$_N9-NHCH$_3$[9MOG + H$_{O8}$]$^{\bullet+}$

N1	-1.335779	-0.497614	-0.349475
C2	0.329034	1.036840	-0.075441
C3	1.681520	1.496452	0.107423
O4	2.069172	2.626533	0.303160
N5	2.569961	0.397612	0.029137
C6	2.221025	-0.915862	-0.178665
N7	3.206891	-1.828663	-0.220202
H8	4.182541	-1.585361	-0.180024
H9	2.957976	-2.786519	-0.409734
N10	0.967338	-1.303954	-0.321836
C11	0.092534	-0.290343	-0.259097
C12	-1.792097	-1.283026	-1.541495
H13	-1.594820	-0.693828	-2.436916
H14	-1.218095	-2.208670	-1.564526
H15	-2.854578	-1.485664	-1.428407
C16	-1.868085	0.816609	-0.226173
O17	-3.107673	1.124806	-0.584074
N18	-0.868124	1.723441	-0.092657
H19	-0.998712	2.709200	0.085754
H20	-3.758788	0.675222	-0.025997
H21	3.543731	0.653270	0.148228
H22	-1.514763	-2.320193	0.729507
C23	-1.426157	-0.894047	2.174365
H24	-1.914252	-1.463091	2.970774
H25	-0.340329	-0.986512	2.291086
H26	-1.726158	0.151272	2.295644
N27	-1.952056	-1.415047	0.921664

Zero-point correction= 0.216275
Thermal correction to Energy= 0.231140
Thermal correction to Enthalpy= 0.232084
Thermal correction to Gibbs Free Energy= 0.174930
Sum of electronic and zero-point Energies= -752.202780
Sum of electronic and thermal Energies= -752.187914
Sum of electronic and thermal Enthalpies= -752.186970
Sum of electronic and thermal Free Energies= -752.244124

Cartesian coordinates for products and TSs in Scheme S2 and Table S2

1 [9MOG + H_{N1}]$^+$···$^{\bullet}CH_2NH_2$

N1	-2.339951	0.703419	0.137395
C2	-0.814653	-0.879079	-0.159711
C3	0.436749	-1.433589	-0.390326
O4	0.899504	-2.537050	-0.496779
N5	1.494225	-0.264316	-0.573061
H6	1.880466	-0.401424	-1.513149
C7	1.102423	1.144337	-0.401603
N8	2.126239	1.995669	-0.520700
H9	1.933471	2.981259	-0.407202
N10	-0.109410	1.498885	-0.176098
C11	-1.032481	0.495501	-0.083390
C12	-3.038781	1.970511	0.290883
H13	-2.312931	2.777566	0.207158
H14	-3.797438	2.059877	-0.487806
H15	-3.525133	1.997562	1.266816
C16	-3.027694	-0.545974	0.214338
O17	-4.209773	-0.679556	0.401753
N18	-2.047205	-1.495032	0.031062
H19	-2.235762	-2.485402	0.018233
H20	2.315681	-0.505141	0.099649
H21	3.087870	1.672809	-0.479948
C22	3.854675	-0.744977	0.991280
H23	3.507964	-0.642295	2.015149
H24	4.011287	-1.745768	0.598009
N25	4.648301	0.274004	0.488072
H26	4.962094	0.979326	1.143172
H27	5.367766	0.015699	-0.175383

Zero-point correction= 0.215617
Thermal correction to Energy= 0.231448
Thermal correction to Enthalpy= 0.232392
Thermal correction to Gibbs Free Energy= 0.170866
Sum of electronic and zero-point Energies= -752.249027
Sum of electronic and thermal Energies= -752.233196
Sum of electronic and thermal Enthalpies= -752.232251
Sum of electronic and thermal Free Energies= -752.293777

2 TS_[9MOG + H_{N1}]$^+$···$^{\bullet}CH_2NH_2$

N1	-2.298742	0.670984	0.201140
C2	-0.749906	-0.860005	-0.219258
C3	0.499918	-1.364048	-0.559115
O4	0.972021	-2.453444	-0.757319
N5	1.527824	-0.182375	-0.663306
H6	2.023478	-0.327440	-1.548314
C7	1.096384	1.207020	-0.522863
N8	2.073405	2.101591	-0.724481
H9	1.843964	3.081590	-0.636220
N10	-0.107144	1.531891	-0.216639
C11	-0.997469	0.503692	-0.086704
C12	-3.020977	1.913905	0.425673
H13	-2.307549	2.736096	0.408436
H14	-3.770180	2.046304	-0.356395
H15	-3.521308	1.864613	1.393477
C16	-2.952184	-0.596603	0.257503
O17	-4.120290	-0.768659	0.496586
N18	-1.960193	-1.512997	-0.013301
H19	-2.121988	-2.507756	-0.039706
H20	2.298274	-0.416326	0.132612
H21	3.044197	1.834198	-0.792275
C22	3.523433	-0.743374	1.199538
H23	3.027178	-0.497145	2.135455
H24	3.613500	-1.796411	0.941479
N25	4.555166	0.081916	0.814632
H26	4.802642	0.866032	1.401892
H27	5.326551	-0.307506	0.290463

Zero-point correction= 0.214297
Thermal correction to Energy= 0.229436
Thermal correction to Enthalpy= 0.230380
Thermal correction to Gibbs Free Energy= 0.171178
Sum of electronic and zero-point Energies= -752.250189
Sum of electronic and thermal Energies= -752.235049
Sum of electronic and thermal Enthalpies= -752.234105
Sum of electronic and thermal Free Energies= -752.293308

3 [9MOG + H_{N1}]$^+$

N1	1.508662	-0.792513	-0.001418
C2	0.129398	0.945290	-0.000539
C3	-1.051923	1.654278	0.001333
O4	-1.473867	2.762941	0.003347
N5	-2.310931	0.484689	-0.003037
H6	-2.861105	0.738401	-0.830136
C7	-1.995369	-0.956360	-0.000603
N8	-3.054795	-1.767624	0.000743
H9	-2.888704	-2.765683	0.002928
N10	-0.785191	-1.379715	0.000120
C11	0.215388	-0.452779	-0.000341
C12	2.072659	-2.135887	0.002734
H13	1.863623	-2.627728	0.953802
H14	1.652853	-2.715710	-0.819407
H15	3.148987	-2.024795	-0.126695
C16	2.331038	0.383381	-0.000410
O17	3.532715	0.395596	-0.002107
N18	1.436574	1.427843	0.000967
H19	1.725157	2.394275	-0.001821
H20	-2.869335	0.740458	0.817857
H21	-4.009642	-1.443809	-0.001113

Zero-point correction= 0.162167
Thermal correction to Energy= 0.174412
Thermal correction to Enthalpy= 0.175356
Thermal correction to Gibbs Free Energy= 0.123089
Sum of electronic and zero-point Energies= -657.086907
Sum of electronic and thermal Energies= -657.074662
Sum of electronic and thermal Enthalpies= -657.073718
Sum of electronic and thermal Free Energies= -657.125985

4 $^{\bullet}CH_2NH_2$

C1	0.728229	0.000011	0.081610
H2	1.240296	-0.932245	-0.126071
H3	1.240498	0.932082	-0.126447
N4	-0.654341	0.000031	-0.092898
H5	-1.134872	-0.836146	0.206351
H6	-1.134909	0.836027	0.206791

Zero-point correction= 0.050737
Thermal correction to Energy= 0.054181
Thermal correction to Enthalpy= 0.055125
Thermal correction to Gibbs Free Energy= 0.027564
Sum of electronic and zero-point Energies= -95.128413
Sum of electronic and thermal Energies= -95.124968
Sum of electronic and thermal Enthalpies= -95.124024
Sum of electronic and thermal Free Energies= -95.151585

5 C2-CH_2NH_2-[9MOG + H_{N1}]$^{\bullet+}$

N1	1.841101	-0.840713	-0.073579
C2	0.495961	0.961484	-0.199085
C3	-0.700178	1.694050	-0.379447

O4	-0.912749	2.877854	-0.353319
N5	-1.823294	0.750234	-0.751528
H6	-1.896644	0.700450	-1.774251
C7	-1.795833	-0.791645	-0.271069
N8	-2.619565	-1.463221	-1.200977
H9	-2.133398	-2.196850	-1.700277
N10	-0.466814	-1.304004	-0.296667
C11	0.523658	-0.489083	-0.202931
C12	2.352815	-2.202485	-0.023807
H13	1.876224	-2.746972	0.792934
H14	2.153883	-2.709120	-0.969430
H15	3.427540	-2.142520	0.144853
C16	2.648147	0.293608	0.052494
O17	3.835855	0.350833	0.195926
N18	1.757930	1.395126	-0.018551
H19	2.074149	2.355669	0.019944
H20	-2.689866	1.190760	-0.429260
H21	-3.507126	-1.788500	-0.840344
C22	-2.366604	-0.766406	1.161607
H23	-3.425935	-0.489964	1.103235
H24	-2.315913	-1.797776	1.528100
N25	-1.651470	0.197186	1.973457
H26	-2.256017	0.685238	2.622759
H27	-0.904752	-0.229304	2.509236

Zero-point correction= 0.220995
Thermal correction to Energy= 0.235405
Thermal correction to Enthalpy= 0.236349
Thermal correction to Gibbs Free Energy= 0.179831
Sum of electronic and zero-point Energies= -752.285337
Sum of electronic and thermal Energies= -752.270927
Sum of electronic and thermal Enthalpies= -752.269983
Sum of electronic and thermal Free Energies= -752.326501

6 TS_C2-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	1.994032	-0.747050	0.052869
C2	0.562509	0.917845	-0.307045
C3	-0.656153	1.539903	-0.535529
O4	-1.083659	2.665914	-0.520252
N5	-1.713086	0.435347	-0.965053
H6	-1.790468	0.469191	-1.988945
C7	-1.474228	-0.976012	-0.545736
N8	-2.449861	-1.814381	-1.012786
H9	-2.225922	-2.799118	-0.948769
N10	-0.252918	-1.414752	-0.364221
C11	0.706790	-0.475477	-0.242367
C12	2.596015	-2.060381	0.221093
H13	2.134759	-2.580767	1.062099
H14	2.472539	-2.646535	-0.690476
H15	3.655712	-1.900425	0.419388
C16	2.730314	0.464145	0.199216
O17	3.905681	0.551399	0.446439
N18	1.800831	1.465967	0.005955
H19	2.055206	2.440859	-0.036099
H20	-2.606375	0.769602	-0.570076
H21	-3.419996	-1.588425	-0.841422
C22	-2.111344	-0.457277	1.597410
H23	-2.338208	-1.492302	1.823889
H24	-1.149890	-0.060115	1.906418
N25	-3.151228	0.423747	1.519583
H26	-4.090021	0.099039	1.707849
H27	-2.991318	1.391874	1.769966

Zero-point correction= 0.217538
Thermal correction to Energy= 0.232176
Thermal correction to Enthalpy= 0.233120
Thermal correction to Gibbs Free Energy= 0.175857
Sum of electronic and zero-point Energies= -752.237959
Sum of electronic and thermal Energies= -752.223320
Sum of electronic and thermal Enthalpies= -752.222376
Sum of electronic and thermal Free Energies= -752.279640

7 N2-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	1.751512	-1.216762	0.055848
C2	1.228214	0.951320	-0.030472
C3	0.477957	2.102502	-0.009762
O4	0.591219	3.286609	-0.120674
N5	-1.157542	1.625397	0.116926
H6	-1.497240	1.766952	-0.843971
C7	-1.390358	0.292924	0.678622
N8	-2.791720	-0.154399	0.659211
H9	-2.827074	-0.969080	1.281267
N10	-0.537766	-0.704299	0.445511
C11	0.715247	-0.350445	0.164919
C12	1.695590	-2.657798	0.214682
H13	1.335883	-2.912365	1.213480
H14	1.036346	-3.094713	-0.537831
H15	2.709240	-3.034864	0.078436
C16	2.961364	-0.516153	-0.191262
O17	4.049857	-1.013956	-0.339026
N18	2.603094	0.814087	-0.219029
H19	3.260932	1.550207	-0.421801
H20	-1.543259	2.376141	0.693244
H21	-3.431519	0.527482	1.075977
C22	-3.394945	-0.631323	-0.697996
H23	-2.660659	-1.350749	-1.064530
H24	-3.408525	0.250455	-1.342311
N25	-4.672594	-1.165195	-0.460272
H26	-4.768656	-2.164508	-0.565289
H27	-5.457390	-0.664157	-0.848809

Zero-point correction= 0.221033
Thermal correction to Energy= 0.236135
Thermal correction to Enthalpy= 0.237079
Thermal correction to Gibbs Free Energy= 0.177726
Sum of electronic and zero-point Energies= -752.220399
Sum of electronic and thermal Energies= -752.205297
Sum of electronic and thermal Enthalpies= -752.204353
Sum of electronic and thermal Free Energies= -752.263706

8 TS_N2-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	1.559385	-1.317782	0.123302
C2	1.341869	0.892477	-0.082863
C3	0.763720	2.134876	-0.102568
O4	1.036957	3.286791	-0.285040
N5	-0.892885	1.917015	0.164776
H6	-1.306031	2.200837	-0.733159
C7	-1.365165	0.608687	0.624334
N8	-2.732139	0.478232	0.782381
H9	-2.958857	-0.315539	1.376533
N10	-0.632296	-0.483676	0.501355
C11	0.655722	-0.311658	0.194947
C12	1.307759	-2.726297	0.356792
H13	0.892218	-2.873695	1.355480
H14	0.614677	-3.116509	-0.391646
H15	2.265588	-3.239751	0.272239
C16	2.850357	-0.809155	-0.188403
O17	3.853263	-1.467915	-0.319597
N18	2.680362	0.549718	-0.296859
H19	3.431502	1.176263	-0.538071
H20	-1.098622	2.667096	0.830241
H21	-3.231219	1.307758	1.087440
C22	-3.827413	-0.552973	-0.952495
H23	-2.858683	-0.711764	-1.408094

H24	-4.414689	0.314098	-1.225273
N25	-4.464451	-1.613604	-0.460949
H26	-4.002638	-2.506813	-0.372418
H27	-5.441946	-1.578045	-0.212669

Zero-point correction= 0.216194
Thermal correction to Energy= 0.231788
Thermal correction to Enthalpy= 0.232732
Thermal correction to Gibbs Free Energy= 0.171297
Sum of electronic and zero-point Energies= -752.211901
Sum of electronic and thermal Energies= -752.196307
Sum of electronic and thermal Enthalpies= -752.195363
Sum of electronic and thermal Free Energies= -752.256798

9 N3-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	-1.374983	-1.049880	-0.014009
C2	-0.830488	1.105169	0.017061
C3	-0.060419	2.263008	-0.078821
O4	-0.300204	3.437355	-0.123707
N5	1.470504	1.878377	-0.174889
H6	1.945580	2.629594	0.333997
C7	1.837602	0.556221	0.407481
N8	3.190394	0.308851	0.402354
H9	3.405397	-0.663630	0.635435
N10	1.003468	-0.492067	-0.025132
C11	-0.332308	-0.192149	-0.020560
C12	-1.397243	-2.496301	0.142588
H13	-1.287647	-3.004118	-0.817878
H14	-0.616569	-2.808751	0.838820
H15	-2.373338	-2.751425	0.557165
C16	-2.605414	-0.306663	0.047524
O17	-3.701577	-0.802188	0.102870
N18	-2.221790	1.005795	0.053540
H19	-2.873859	1.769527	0.146028
H20	1.755913	1.975032	-1.162907
H21	3.768674	0.975150	0.899990
C22	1.568010	-1.648172	-0.753613
H23	0.724946	-2.186792	-1.192211
H24	2.184222	-1.270232	-1.575442
N25	2.415627	-2.423712	0.123676
H26	1.888509	-2.990995	0.779489
H27	3.031454	-3.032916	-0.404530

Zero-point correction= 0.221934
Thermal correction to Energy= 0.236020
Thermal correction to Enthalpy= 0.236964
Thermal correction to Gibbs Free Energy= 0.181138
Sum of electronic and zero-point Energies= -752.240715
Sum of electronic and thermal Energies= -752.226629
Sum of electronic and thermal Enthalpies= -752.225685
Sum of electronic and thermal Free Energies= -752.281511

10 TS_N3-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	1.451114	-0.889786	-0.388265
C2	0.726613	1.141139	0.145032
C3	-0.144960	2.206525	0.294055
O4	-0.084022	3.347367	0.662510
N5	-1.623003	1.737295	-0.137853
H6	-1.939684	2.493470	-0.753896
C7	-1.816568	0.410762	-0.777907
N8	-3.151875	0.099694	-0.958281
H9	-3.271021	-0.827939	-1.348433
N10	-0.896285	-0.522488	-0.707495
C11	0.344450	-0.114131	-0.337027
C12	1.577972	-2.227755	-0.939487
H13	1.846409	-2.938256	-0.154319
H14	0.630249	-2.502505	-1.402133
H15	2.370760	-2.229573	-1.688926
C16	2.590155	-0.153256	0.049604
O17	3.717463	-0.579230	0.090684
N18	2.099504	1.085792	0.386501
H19	2.688557	1.846677	0.687166
H20	-2.198677	1.820495	0.713282
H21	-3.710354	0.778205	-1.465272
C22	-1.183520	-1.908273	1.309879
H23	-0.251980	-2.420624	1.114276
H24	-1.182259	-1.020880	1.930171
N25	-2.319194	-2.589810	1.180524
H26	-2.336689	-3.501934	0.750112
H27	-3.199518	-2.217177	1.501595

Zero-point correction= 0.215145
Thermal correction to Energy= 0.230920
Thermal correction to Enthalpy= 0.231865
Thermal correction to Gibbs Free Energy= 0.171307
Sum of electronic and zero-point Energies= -752.216508
Sum of electronic and thermal Energies= -752.200733
Sum of electronic and thermal Enthalpies= -752.199789
Sum of electronic and thermal Free Energies= -752.260347

11 C4-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	1.589883	-0.291655	-0.411515
C2	-0.067297	1.094763	0.286592
C3	-1.371896	1.580611	0.367201
O4	-1.860147	2.682503	0.479840
N5	-2.390917	0.393567	0.192471
H6	-3.227576	0.846221	-0.191791
C7	-1.894593	-0.743372	-0.669847
N8	-2.901919	-1.396719	-1.293310
H9	-2.623967	-2.157231	-1.899271
N10	-0.675376	-1.060009	-0.700025
C11	0.261554	-0.370244	0.164841
C12	2.382391	-1.422546	-0.868664
H13	3.045480	-1.798335	-0.084578
H14	1.705054	-2.209002	-1.201385
H15	2.994767	-1.094755	-1.709784
C16	2.115749	0.965559	-0.351130
O17	3.210166	1.360394	-0.647396
N18	1.053237	1.806271	0.138057
H19	1.127091	2.816581	0.134134
H20	-2.659281	0.025531	1.113073
H21	-3.771833	-0.943775	-1.529639
C22	0.267573	-1.055508	1.583812
H23	0.990735	-0.514376	2.201015
H24	-0.719835	-0.885789	2.038486
N25	0.559948	-2.453768	1.625203
H26	1.538560	-2.682696	1.527028
H27	-0.004244	-3.024942	1.010175

Zero-point correction= 0.220542
Thermal correction to Energy= 0.234933
Thermal correction to Enthalpy= 0.235877
Thermal correction to Gibbs Free Energy= 0.179589
Sum of electronic and zero-point Energies= -752.247878
Sum of electronic and thermal Energies= -752.233488
Sum of electronic and thermal Enthalpies= -752.232544
Sum of electronic and thermal Free Energies= -752.288832

12 TS_C4-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	-1.270142	0.539647	-0.779261
C2	0.163881	-1.067182	-0.222327
C3	1.353586	-1.684980	0.062175

O4	1.830398	-2.752854	0.294470
N5	2.531331	-0.433044	0.124921
H6	3.296801	-0.806676	-0.443846
C7	2.179028	0.940795	-0.271744
N8	3.212090	1.791662	-0.344533
H9	3.024455	2.743492	-0.627768
N10	0.968276	1.283792	-0.505651
C11	0.007159	0.315293	-0.435407
C12	-1.875747	1.825249	-1.068307
H13	-1.730630	2.502645	-0.223675
H14	-1.428770	2.260394	-1.963208
H15	-2.938549	1.648439	-1.232795
C16	-2.022717	-0.667106	-0.707796
O17	-3.205470	-0.774908	-0.916170
N18	-1.106291	-1.632305	-0.359869
H19	-1.334327	-2.613743	-0.330265
H20	2.845163	-0.457028	1.100649
H21	4.166169	1.529897	-0.154663
C22	-0.715607	0.917179	2.245363
H23	-0.040563	0.197352	2.691458
H24	-0.462946	1.969767	2.245620
N25	-2.027311	0.569015	2.123212
H26	-2.347501	-0.336304	2.429471
H27	-2.741893	1.276991	2.059133

Zero-point correction= 0.213504
Thermal correction to Energy= 0.230156
Thermal correction to Enthalpy= 0.231100
Thermal correction to Gibbs Free Energy= 0.168334
Sum of electronic and zero-point Energies= -752.231069
Sum of electronic and thermal Energies= -752.214418
Sum of electronic and thermal Enthalpies= -752.213473
Sum of electronic and thermal Free Energies= -752.276240

13 C5-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	-1.537845	-1.108783	0.089857
C2	-0.100465	0.710707	0.033926
C3	0.974914	0.980980	-0.975727
O4	1.014135	1.679696	-1.930992
N5	2.232181	0.149043	-0.639931
H6	2.804490	0.665014	0.044073
C7	2.004270	-1.267467	-0.092714
N8	3.121313	-1.744568	0.552572
H9	2.907851	-2.452997	1.244777
N10	0.767472	-1.640898	0.205892
C11	-0.223474	-0.800819	0.129666
C12	-2.097193	-2.449547	0.157566
H13	-1.689972	-3.066136	-0.646688
H14	-1.861263	-2.901805	1.121884
H15	-3.176732	-2.353322	0.044965
C16	-2.312187	0.035623	-0.238143
O17	-3.505208	0.059794	-0.364601
N18	-1.413409	1.074661	-0.395072
H19	-1.742181	2.026895	-0.449263
H20	2.777516	0.118257	-1.508804
H21	3.909972	-2.015735	-0.024942
C22	0.288739	1.340166	1.439850
H23	-0.416895	0.904703	2.153066
H24	1.283794	0.979689	1.733808
N25	0.225261	2.756902	1.522889
H26	-0.689952	3.169254	1.618950
H27	0.849530	3.307916	0.952933

Zero-point correction= 0.218431
Thermal correction to Energy= 0.233413
Thermal correction to Enthalpy= 0.234357
Thermal correction to Gibbs Free Energy= 0.176385
Sum of electronic and zero-point Energies= -752.242999
Sum of electronic and thermal Energies= -752.228017
Sum of electronic and thermal Enthalpies= -752.227073
Sum of electronic and thermal Free Energies= -752.285045

14 TS_C5-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	1.744633	-0.947432	-0.055319
C2	0.090862	0.510996	0.425120
C3	-1.161593	0.931548	0.857345
O4	-1.647021	1.990509	1.191692
N5	-2.163094	-0.303832	0.826528
H6	-3.058010	0.056720	0.475674
C7	-1.767780	-1.518454	0.051117
N8	-2.839415	-2.168659	-0.518265
H9	-2.551099	-2.869244	-1.190883
N10	-0.509391	-1.785514	-0.194726
C11	0.383252	-0.850148	0.083717
C12	2.484445	-2.147785	-0.403017
H13	2.223936	-2.956236	0.282775
H14	2.255977	-2.450043	-1.426998
H15	3.545252	-1.914839	-0.312893
C16	2.356870	0.262795	0.300505
O17	3.538581	0.480790	0.380331
N18	1.314862	1.177033	0.529434
H19	1.477138	1.952627	1.156043
H20	-2.320092	-0.532155	1.817004
H21	-3.552989	-2.531265	0.106553
C22	-0.628368	1.460027	-1.600741
H23	0.253583	0.978502	-2.005124
H24	-1.596151	1.000452	-1.768849
N25	-0.585403	2.757915	-1.389746
H26	0.304962	3.233486	-1.325651
H27	-1.396465	3.261163	-1.053445

Zero-point correction= 0.216804
Thermal correction to Energy= 0.231871
Thermal correction to Enthalpy= 0.232816
Thermal correction to Gibbs Free Energy= 0.174183
Sum of electronic and zero-point Energies= -752.226115
Sum of electronic and thermal Energies= -752.211048
Sum of electronic and thermal Enthalpies= -752.210104
Sum of electronic and thermal Free Energies= -752.268736

15 C6-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	-0.103065	1.869593	-0.026835
C2	0.713171	-0.228001	0.018616
C3	0.939498	-1.668522	0.123161
O4	0.016095	-2.459581	-0.033709
N5	-2.441633	-1.634593	-0.923783
H6	-1.490853	-1.990594	-0.995593
C7	-2.643305	-0.650296	-0.042165
N8	-3.830238	-0.545390	0.568088
H9	-4.020837	0.278072	1.117422
N10	-1.793492	0.348991	0.200619
C11	-0.521661	0.569015	0.033348
C12	-0.979044	3.029764	-0.009793
H13	-1.674834	2.983105	-0.848369
H14	-1.536400	3.057805	0.928310
H15	-0.348503	3.914139	-0.095406
C16	1.292100	1.971583	-0.072108
O17	1.957181	2.970534	-0.136634
N18	1.738907	0.651750	-0.028993
H19	2.709375	0.309856	-0.104901
H20	-3.181416	-2.296527	-1.106725
H21	-4.534777	-1.262847	0.508600
C22	2.325241	-2.187107	0.497585
H23	2.412767	-2.058738	1.583558

H24	2.313477	-3.263397	0.296882
N25	3.421317	-1.459520	-0.144607
H26	3.579520	-1.796565	-1.089414
H27	4.287707	-1.596357	0.365091

Zero-point correction= 0.219213
Thermal correction to Energy= 0.234392
Thermal correction to Enthalpy= 0.235336
Thermal correction to Gibbs Free Energy= 0.175869
Sum of electronic and zero-point Energies= -752.318950
Sum of electronic and thermal Energies= -752.303771
Sum of electronic and thermal Enthalpies= -752.302827
Sum of electronic and thermal Free Energies= -752.362294

16 TS_C6-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	-1.702269	-0.832302	0.158929
C2	-0.212786	0.744715	0.664186
C3	1.039249	1.389943	0.626429
O4	1.536119	2.443919	0.879460
N5	2.147291	0.034180	0.969182
H6	2.107824	-0.037421	1.991420
C7	1.801418	-1.232484	0.344087
N8	2.838132	-2.012008	-0.021482
H9	2.612880	-2.920235	-0.404664
N10	0.574924	-1.552944	0.136145
C11	-0.377488	-0.600574	0.362166
C12	-2.334716	-2.111049	-0.116474
H13	-1.914383	-2.552986	-1.021607
H14	-2.192062	-2.793708	0.722922
H15	-3.398402	-1.918246	-0.255519
C16	-2.422920	0.374713	0.267739
O17	-3.618228	0.512458	0.174572
N18	-1.457370	1.347078	0.499513
H19	-1.718501	2.249802	0.869530
H20	3.070134	0.383322	0.707581
H21	3.752094	-1.908949	0.392985
C22	1.256768	1.267643	-1.801742
H23	1.152359	2.341593	-1.710520
H24	2.254918	0.846464	-1.861348
N25	0.266879	0.588149	-2.405317
H26	0.388318	-0.361389	-2.719865
H27	-0.628566	1.018217	-2.580314

Zero-point correction= 0.215786
Thermal correction to Energy= 0.231340
Thermal correction to Enthalpy= 0.232284
Thermal correction to Gibbs Free Energy= 0.172908
Sum of electronic and zero-point Energies= -752.233122
Sum of electronic and thermal Energies= -752.217567
Sum of electronic and thermal Enthalpies= -752.216623
Sum of electronic and thermal Free Energies= -752.275999

17 O6-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	2.351377	0.256885	0.118867
C2	0.299074	-0.620499	-0.247644
C3	-1.044896	-0.572762	-0.361413
O4	-1.909803	-1.563627	-0.639153
N5	-1.644390	0.780518	-0.516423
H6	-2.549788	0.686610	0.013386
C7	-0.792516	1.915005	-0.048511
N8	-1.453366	3.109949	-0.115209
H9	-0.867892	3.910314	0.088104
N10	0.484748	1.794735	0.112046
C11	1.035631	0.589949	-0.039706
C12	3.451515	1.169626	0.372975
H13	3.507487	1.916325	-0.421109
H14	3.313979	1.665908	1.335754
H15	4.367260	0.578920	0.389789
C16	2.505131	-1.132469	0.011429
O17	3.528427	-1.761875	0.079235
N18	1.212732	-1.640848	-0.190553
H19	1.048596	-2.616611	-0.383045
H20	-1.904767	0.947584	-1.504413
H21	-2.377421	3.176433	0.292284
C22	-2.858024	-1.847772	0.409756
H23	-2.309825	-2.155917	1.303695
H24	-3.441201	-2.680625	0.016344
N25	-3.654771	-0.668015	0.710048
H26	-3.835146	-0.582101	1.704653
H27	-4.550068	-0.681866	0.231163

Zero-point correction= 0.221038
Thermal correction to Energy= 0.235235
Thermal correction to Enthalpy= 0.236180
Thermal correction to Gibbs Free Energy= 0.179815
Sum of electronic and zero-point Energies= -752.250969
Sum of electronic and thermal Energies= -752.236772
Sum of electronic and thermal Enthalpies= -752.235827
Sum of electronic and thermal Free Energies= -752.292192

18 TS_O6-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	2.230336	-0.867345	0.027107
C2	0.043251	-0.319623	-0.042586
C3	-1.055202	0.476929	-0.028619
O4	-2.298227	0.273224	-0.033922
N5	-0.666872	1.953302	-0.159280
H6	-1.327200	2.466233	0.430182
C7	0.747414	2.360212	0.193343
N8	0.957704	3.697685	-0.131825
H9	1.931472	3.871578	-0.353507
N10	1.724501	1.462679	0.110070
C11	1.376236	0.202729	0.013632
C12	3.676787	-0.798238	0.091428
H13	4.069949	-0.289245	-0.791143
H14	3.984988	-0.258042	0.988831
H15	4.051579	-1.821174	0.124106
C16	1.510997	-2.068530	-0.031049
O17	1.969989	-3.184597	-0.099511
N18	0.165128	-1.713822	0.010119
H19	-0.514267	-2.365113	-0.346867
H20	-0.873661	2.262996	-1.123662
H21	0.631132	4.371451	0.552544
C22	-4.176034	-1.464168	0.101300
H23	-3.393588	-1.499829	0.848038
H24	-4.319042	-2.269182	-0.613123
N25	-4.963037	-0.458354	0.072541
H26	-4.790795	0.333808	0.685688
H27	-5.699673	-0.367393	-0.619444

Zero-point correction= 0.217491
Thermal correction to Energy= 0.233178
Thermal correction to Enthalpy= 0.234122
Thermal correction to Gibbs Free Energy= 0.171685
Sum of electronic and zero-point Energies= -752.216755
Sum of electronic and thermal Energies= -752.201068
Sum of electronic and thermal Enthalpies= -752.200124
Sum of electronic and thermal Free Energies= -752.262561

19 N7-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	-0.572972	1.647403	-0.092688
C2	0.066596	-0.528764	-0.280549
C3	0.861487	-1.647108	-0.309926

O4	0.691920	-2.840642	-0.430420
N5	2.378136	-1.205464	-0.111972
H6	2.870096	-1.622966	-0.910088
C7	2.712099	0.248397	0.032930
N8	3.981175	0.441759	0.532695
H9	4.132593	1.388516	0.858733
N10	1.769768	1.174501	0.092279
C11	0.531995	0.791569	-0.072423
C12	-0.500222	3.094427	0.070783
H13	-0.110503	3.329456	1.062310
H14	0.161596	3.510262	-0.690073
H15	-1.504802	3.499237	-0.043802
C16	-1.727961	0.976577	-0.308573
O17	-2.862888	1.353433	-0.402486
N18	-1.373793	-0.499680	-0.380343
H19	-1.736121	-0.870441	-1.264980
H20	2.717705	-1.719753	0.713840
H21	4.759208	0.109839	-0.026882
C22	-2.154010	-1.317042	0.799079
H23	-1.604191	-2.257930	0.819613
H24	-1.930838	-0.708068	1.676653
N25	-3.497314	-1.490459	0.570230
H26	-4.115484	-0.695442	0.623887
H27	-3.806431	-2.249798	-0.015290

Zero-point correction= 0.219640
Thermal correction to Energy= 0.234781
Thermal correction to Enthalpy= 0.235725
Thermal correction to Gibbs Free Energy= 0.176733
Sum of electronic and zero-point Energies= -752.232472
Sum of electronic and thermal Energies= -752.217332
Sum of electronic and thermal Enthalpies= -752.216387
Sum of electronic and thermal Free Energies= -752.275379

20 TS_N7-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	0.499033	1.552037	-0.150942
C2	-0.214751	-0.575916	-0.370377
C3	-1.041884	-1.671893	-0.306341
O4	-0.910374	-2.875695	-0.423554
N5	-2.529353	-1.171842	-0.133201
H6	-2.963725	-1.876195	0.470030
C7	-2.763728	0.209210	0.407069
N8	-4.113566	0.531133	0.395179
H9	-4.261229	1.532909	0.421704
N10	-1.825588	1.145352	0.283342
C11	-0.635303	0.742498	-0.084075
C12	0.516225	2.985466	0.083191
H13	-0.147616	3.481301	-0.627044
H14	0.179442	3.199355	1.099282
H15	1.537942	3.336436	-0.057986
C16	1.596667	0.804078	-0.474242
O17	2.753025	1.190125	-0.612848
N18	1.193162	-0.548890	-0.541792
H19	1.595274	-1.078504	-1.307854
H20	-3.000361	-1.273881	-1.046510
H21	-4.692963	0.062398	1.082966
C22	2.961222	-1.302375	1.169661
H23	2.426315	-0.519284	1.690495
H24	2.682818	-2.341342	1.312577
N25	4.012084	-1.001411	0.494532
H26	4.183245	-0.019666	0.257016
H27	4.558558	-1.710019	0.017383

Zero-point correction= 0.217509
Thermal correction to Energy= 0.232633
Thermal correction to Enthalpy= 0.233577
Thermal correction to Gibbs Free Energy= 0.174270
Sum of electronic and zero-point Energies= -752.226119
Sum of electronic and thermal Energies= -752.210995
Sum of electronic and thermal Enthalpies= -752.210051
Sum of electronic and thermal Free Energies= -752.269358

21 C8-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	0.159075	-1.877055	-0.735497
C2	-0.036150	0.406125	-0.181685
C3	0.646170	1.640730	-0.286354
O4	0.275513	2.786591	-0.334853
N5	2.206903	1.444160	-0.400603
H6	2.600039	2.306872	-0.009291
C7	2.721815	0.212901	0.281203
N8	3.911266	0.401636	0.891659
H9	4.572083	1.098730	0.582944
H10	4.300536	-0.407382	1.357471
N11	2.034942	-0.843290	0.294576
C12	0.722795	-0.859285	-0.229209
C13	0.828771	-3.153541	-0.795715
H14	1.799136	-3.181721	-0.292463
H15	0.153868	-3.893624	-0.356398
H16	0.949116	-3.423718	-1.849526
C17	-2.245748	-0.455662	0.535002
O18	-1.861349	-1.357574	1.230916
N19	-1.379782	0.458414	-0.116067
H20	-1.887032	1.304164	-0.408024
C21	-3.713281	-0.129328	0.277157
H22	-4.071487	-0.899613	-0.414065
H23	-4.240259	-0.285255	1.222599
N24	-3.891508	1.202757	-0.286125
H25	-4.467514	1.200611	-1.117842
H26	-4.300614	1.849490	0.377077
H27	2.446302	1.421323	-1.398977

Zero-point correction= 0.218022
Thermal correction to Energy= 0.233476
Thermal correction to Enthalpy= 0.234420
Thermal correction to Gibbs Free Energy= 0.174290
Sum of electronic and zero-point Energies= -752.227076
Sum of electronic and thermal Energies= -752.211622
Sum of electronic and thermal Enthalpies= -752.210677
Sum of electronic and thermal Free Energies= -752.270807

22 TS_C8-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	0.733640	1.067869	0.227004
C2	-0.130391	-0.992660	0.272523
C3	-1.040608	-1.923294	0.581452
O4	-1.822477	-2.759965	0.741330
N5	-2.804474	-0.372663	-1.305786
H6	-3.694417	-0.707477	-1.641378
C7	-2.717266	0.592916	-0.366314
N8	-3.849871	1.106238	0.124492
H9	-4.756844	0.913106	-0.269081
H10	-3.777719	1.800900	0.852019
N11	-1.572951	1.092268	0.078090
C12	-0.429600	0.427976	0.139784
C13	0.896995	2.511417	0.210925
H14	0.991096	2.882733	-0.813439
H15	0.027979	2.973230	0.679758
H16	1.794900	2.754023	0.779789
C17	1.881912	0.152589	0.394488
O18	2.746268	0.501805	1.313727
N19	1.262401	-1.153381	0.511870
H20	1.758308	-1.830413	-0.066016
C21	2.829261	0.210371	-0.963319
H22	2.097462	0.343129	-1.765107
H23	3.454989	1.101273	-0.882918

N24	3.516493	-1.023452	-1.111603
H25	3.525777	-1.392290	-2.051968
H26	4.440622	-1.046859	-0.701547
H27	-1.990983	-0.620120	-1.846251

Zero-point correction= 0.215268
Thermal correction to Energy= 0.230861
Thermal correction to Enthalpy= 0.231806
Thermal correction to Gibbs Free Energy= 0.171958
Sum of electronic and zero-point Energies= -752.209048
Sum of electronic and thermal Energies= -752.193455
Sum of electronic and thermal Enthalpies= -752.192511
Sum of electronic and thermal Free Energies= -752.252358

23 O8-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	0.570745	-1.362815	-0.067337
C2	-0.341311	0.698523	-0.030381
C3	-1.277941	1.710298	0.001804
O4	-1.277181	2.920479	0.081407
N5	-2.735268	1.053657	-0.083804
H6	-3.155496	1.469201	-0.923623
C7	-2.882657	-0.434604	-0.076436
N8	-4.164290	-0.827920	0.250580
H9	-4.221944	-1.813322	0.475581
N10	-1.846029	-1.236030	-0.069045
C11	-0.652392	-0.673251	-0.069077
C12	0.710902	-2.812651	-0.066272
H13	0.166102	-3.222353	0.785255
H14	0.297079	-3.216830	-0.991050
H15	1.767803	-3.061519	0.009380
C16	1.555643	-0.456216	-0.032689
O17	2.812596	-0.813649	-0.073450
N18	1.061296	0.783855	0.014338
H19	1.654180	1.591689	-0.146980
H20	-3.264076	1.450741	0.705625
H21	-4.908276	-0.548054	-0.379970
C22	3.854773	0.098331	0.408411
H23	3.710263	0.216309	1.484715
H24	4.754342	-0.485074	0.209226
N25	3.788652	1.367547	-0.239231
H26	4.307655	1.408689	-1.108420
H27	4.081211	2.125241	0.365948

Zero-point correction= 0.220112
Thermal correction to Energy= 0.235123
Thermal correction to Enthalpy= 0.236067
Thermal correction to Gibbs Free Energy= 0.176942
Sum of electronic and zero-point Energies= -752.242113
Sum of electronic and thermal Energies= -752.227103
Sum of electronic and thermal Enthalpies= -752.226158
Sum of electronic and thermal Free Energies= -752.285283

24 TS_O8-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	0.501820	-1.471358	-0.228764
C2	-0.316841	0.623588	-0.391335
C3	-1.188464	1.679070	-0.299417
O4	-1.116233	2.890761	-0.387420
N5	-2.641582	1.127963	0.017826
H6	-3.233369	1.523144	-0.719535
C7	-2.870178	-0.350786	0.156219
N8	-4.054235	-0.617852	0.830549
H9	-4.060760	-1.554102	1.217232
N10	-1.850545	-1.202134	0.164797
C11	-0.669560	-0.718491	-0.131221
C12	0.584102	-2.908974	-0.046455
H13	0.311660	-3.172465	0.977756
H14	-0.099537	-3.405428	-0.737188
H15	1.608600	-3.215553	-0.255469
C16	1.556413	-0.665275	-0.555874
O17	2.725918	-0.996877	-0.735597
N18	1.094242	0.667219	-0.586213
H19	1.439286	1.201248	-1.377719
H20	-2.941523	1.600505	0.883182
H21	-4.910303	-0.438523	0.316341
C22	4.147456	0.407634	0.998843
H23	3.591331	-0.448418	1.357175
H24	5.220243	0.338085	0.847874
N25	3.546550	1.515304	0.782178
H26	4.045487	2.329087	0.435694
H27	2.520079	1.556764	0.791630

Zero-point correction= 0.217174
Thermal correction to Energy= 0.232634
Thermal correction to Enthalpy= 0.233578
Thermal correction to Gibbs Free Energy= 0.172907
Sum of electronic and zero-point Energies= -752.222403
Sum of electronic and thermal Energies= -752.206943
Sum of electronic and thermal Enthalpies= -752.205998
Sum of electronic and thermal Free Energies= -752.266670

25 N9-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	-1.363241	-0.557547	-0.358804
C2	0.303744	1.031429	-0.084464
C3	1.554047	1.587165	0.078571
O4	2.040503	2.691332	0.171242
N5	2.644147	0.383980	0.159417
H6	3.105809	0.528350	1.065254
C7	2.199913	-1.024690	-0.012042
N8	3.239295	-1.897108	-0.210429
H9	2.947927	-2.840059	-0.432666
N10	0.947590	-1.330813	-0.159020
C11	0.067418	-0.335585	-0.184573
C12	-1.699936	-1.198771	-1.669913
H13	-1.263824	-0.604509	-2.472734
H14	-1.271427	-2.200911	-1.673291
H15	-2.785006	-1.231715	-1.770523
C16	-1.966579	0.864548	-0.306534
O17	-3.149832	1.026285	-0.378144
N18	-0.929338	1.706674	-0.188071
H19	-1.057364	2.705131	-0.100421
H20	3.353004	0.614362	-0.549156
H21	4.024796	-1.865925	0.428146
C22	-1.991639	-1.375266	0.812116
H23	-3.045599	-1.458682	0.541812
H24	-1.497464	-2.346022	0.741713
N25	-1.779268	-0.711061	2.031003
H26	-2.602369	-0.337242	2.478943
H27	-1.149960	-1.155571	2.680494

Zero-point correction= 0.219375
Thermal correction to Energy= 0.234143
Thermal correction to Enthalpy= 0.235087
Thermal correction to Gibbs Free Energy= 0.177820
Sum of electronic and zero-point Energies= -752.226830
Sum of electronic and thermal Energies= -752.212063
Sum of electronic and thermal Enthalpies= -752.211118
Sum of electronic and thermal Free Energies= -752.268385

26 TS_N9-CH_2NH_2[9MOG + H_{N1}]$^{\bullet+}$

N1	-1.090240	-0.508977	-0.512363
C2	0.559427	0.988915	-0.131897
C3	1.798336	1.502683	0.176016

O4	2.294872	2.596186	0.349278
N5	2.851155	0.291422	0.245862
H6	3.372440	0.469029	1.110981
C7	2.364377	-1.115830	0.179295
N8	3.398528	-2.021767	0.041836
H9	3.075473	-2.941942	-0.229257
N10	1.118143	-1.399063	-0.112075
C11	0.283098	-0.383404	-0.266718
C12	-1.665741	-1.665564	-1.185988
H13	-1.237882	-1.776232	-2.185884
H14	-1.452188	-2.566958	-0.609934
H15	-2.740432	-1.508798	-1.280982
C16	-1.640770	0.782925	-0.668879
O17	-2.814676	1.013674	-0.937091
N18	-0.655865	1.667419	-0.347373
H19	-0.763720	2.664534	-0.456979
H20	3.529859	0.459166	-0.511792
H21	4.075999	-2.069429	0.794661
C22	-2.506762	-0.538172	1.689682
H23	-1.931854	0.370006	1.828185
H24	-2.137052	-1.483889	2.070514
N25	-3.695312	-0.461959	1.200458
H26	-3.995278	0.393104	0.727312
H27	-4.273598	-1.286305	1.082200

Zero-point correction= 0.216676
Thermal correction to Energy= 0.231909
Thermal correction to Enthalpy= 0.232853
Thermal correction to Gibbs Free Energy= 0.173870
Sum of electronic and zero-point Energies= -752.220906
Sum of electronic and thermal Energies= -752.205672
Sum of electronic and thermal Enthalpies= -752.204728
Sum of electronic and thermal Free Energies= -752.263711

27 [9MOG + H_{C2}]$^{\bullet}\cdots^{+}CH_2NH_2$

N1	0.980782	-1.473212	-0.003427
C2	1.377314	0.727578	0.094670
C3	1.061452	2.145239	0.016595
O4	1.888728	3.031766	-0.074912
N5	-0.304296	2.334824	-0.013887
H6	-0.584597	3.307838	0.011327
C7	-1.331371	1.355773	0.372377
N8	-2.574172	1.582289	-0.332263
H9	-2.393022	1.704173	-1.326372
H10	-3.037725	2.419895	0.006669
N11	-0.927698	-0.030609	0.151918
C12	0.352913	-0.260645	0.092552
C13	0.355020	-2.777660	-0.020889
H14	1.146044	-3.522611	-0.112874
H15	-0.186706	-2.950108	0.913762
H16	-0.315517	-2.864092	-0.880494
C17	2.376603	-1.293551	-0.056086
O18	3.215483	-2.149979	-0.135950
N19	2.567298	0.094289	0.006768
H20	3.476570	0.535115	-0.044606
H21	-1.548844	1.467305	1.445225
C22	-4.182069	-1.151652	-0.117744
H23	-5.077506	-1.768148	-0.131054
H24	-4.212974	-0.075637	-0.289505
N25	-3.037713	-1.662808	0.105819
H26	-2.963567	-2.662319	0.276912
H27	-2.124416	-1.029608	0.124560

Zero-point correction= 0.217831
Thermal correction to Energy= 0.232929
Thermal correction to Enthalpy= 0.233873
Thermal correction to Gibbs Free Energy= 0.174460
Sum of electronic and zero-point Energies= -752.287219
Sum of electronic and thermal Energies= -752.272122
Sum of electronic and thermal Enthalpies= -752.271178
Sum of electronic and thermal Free Energies= -752.330591

28 TS_[9MOG + H_{C2}]$^{\bullet}\cdots^{+}CH_2NH_2$

N1	1.641088	-0.998429	-0.214672
C2	0.763558	1.037536	0.121836
C3	-0.287222	2.020135	0.300784
O4	-0.123897	3.163135	0.678692
N5	-1.532118	1.460880	0.038562
H6	-2.283756	2.139698	0.013857
C7	-1.736436	0.208485	-0.660445
N8	-2.116962	0.397312	-2.014658
H9	-2.929601	0.981587	-2.168117
H10	-2.154320	-0.462958	-2.546983
N11	-0.711630	-0.771349	-0.566267
C12	0.460970	-0.307157	-0.252281
C13	1.842567	-2.382487	-0.603664
H14	2.915469	-2.546150	-0.703934
H15	1.447858	-3.060105	0.157018
H16	1.347568	-2.568289	-1.558318
C17	2.692341	-0.140275	0.148765
O18	3.856794	-0.412906	0.258502
N19	2.088524	1.114731	0.358925
H20	2.603229	1.937585	0.644774
H21	-2.632518	-0.278285	-0.055353
C22	-3.246252	-1.397036	0.936565
H23	-3.811473	-0.666532	1.507525
H24	-3.704159	-1.878809	0.077825
N25	-2.232496	-1.987261	1.510073
H26	-1.841655	-1.638788	2.375961
H27	-1.711816	-2.707185	1.025096

Zero-point correction= 0.216216
Thermal correction to Energy= 0.230890
Thermal correction to Enthalpy= 0.231834
Thermal correction to Gibbs Free Energy= 0.173265
Sum of electronic and zero-point Energies= -752.249666
Sum of electronic and thermal Energies= -752.234992
Sum of electronic and thermal Enthalpies= -752.234048
Sum of electronic and thermal Free Energies= -752.292617

29 [9MOG + H_{C2}]$^{\bullet}$

N1	-1.608887	-0.648936	-0.121328
C2	0.084947	0.815490	0.054127
C3	1.429037	1.323135	-0.144818
O4	1.741548	2.506312	-0.090557
N5	2.273794	0.301181	-0.495924
H6	3.234922	0.572673	-0.649765
C7	1.991723	-1.122233	-0.275357
N8	2.385999	-1.490939	1.082225
H9	3.394852	-1.452615	1.192583
H10	2.078163	-2.438973	1.276147
N11	0.602049	-1.511476	-0.422722
C12	-0.228155	-0.555421	-0.182518
C13	-2.373914	-1.868049	-0.266248
H14	-3.424743	-1.620129	-0.115604
H15	-2.230194	-2.287551	-1.264407
H16	-2.053009	-2.600214	0.478163
C17	-2.167541	0.593242	0.156319
O18	-3.338976	0.869277	0.289949
N19	-1.082737	1.477676	0.254812
H20	-1.187742	2.469450	0.407419
H21	2.559064	-1.656871	-1.048136

Zero-point correction= 0.162490
Thermal correction to Energy= 0.173942
Thermal correction to Enthalpy= 0.174887
Thermal correction to Gibbs Free Energy= 0.124467
Sum of electronic and zero-point Energies= -657.340113
Sum of electronic and thermal Energies= -657.328660
Sum of electronic and thermal Enthalpies= -657.327716
Sum of electronic and thermal Free Energies= -657.378136

30 $CH_2NH_2^+$

C1	-0.675347	0.000000	-0.000026
H2	-1.212087	0.944942	0.000036
H3	-1.212087	-0.944942	0.000036
N4	0.600448	0.000000	0.000030
H5	1.136561	0.866543	-0.000064
H6	1.136562	-0.866543	-0.000064

Zero-point correction= 0.054920
Thermal correction to Energy= 0.057900
Thermal correction to Enthalpy= 0.058844
Thermal correction to Gibbs Free Energy= 0.032714
Sum of electronic and zero-point Energies= -94.896708
Sum of electronic and thermal Energies= -94.893728
Sum of electronic and thermal Enthalpies= -94.892784
Sum of electronic and thermal Free Energies= -94.918914

31 C5-$^+NH_2\dot{C}H_2$_[9MOG+H_{C2}]

N1	1.690013	0.821330	0.259544
C2	0.094043	-0.811847	-0.035474
C3	-1.196537	-1.085603	-0.795468
O4	-1.343101	-2.157188	-1.356517
N5	-2.080587	-0.079095	-0.698488
H6	-2.968505	-0.191586	-1.176740
C7	-1.953401	1.173106	0.083481
N8	-0.566824	1.546598	0.343899
C9	0.324567	0.653844	0.246098
C10	2.344298	2.116144	0.401945
H11	2.126434	2.527461	1.387580
H12	3.416238	1.958180	0.290061
H13	1.987432	2.805788	-0.366752
C14	2.303439	-0.253687	-0.410374
O15	3.441844	-0.329261	-0.770057
N16	1.305927	-1.236546	-0.574109
H17	1.399726	-1.988415	-1.245723
H18	-0.198384	-2.591248	1.059052
H19	0.805317	-1.538899	1.838791
H20	-2.144786	-1.692425	2.049282
H21	-1.001667	-0.428482	2.922388
C22	-1.182142	-1.234015	2.225112
N23	-0.098621	-1.614073	1.360547
H24	-2.447574	1.034748	1.053580
N25	-2.687169	2.162002	-0.633742
H26	-2.179864	2.495904	-1.447387
H27	-2.929086	2.951401	-0.047025

Zero-point correction= 0.219252
Thermal correction to Energy= 0.233878
Thermal correction to Enthalpy= 0.234822
Thermal correction to Gibbs Free Energy= 0.177964
Sum of electronic and zero-point Energies= -752.232728
Sum of electronic and thermal Energies= -752.218101
Sum of electronic and thermal Enthalpies= -752.217157
Sum of electronic and thermal Free Energies= -752.274015

32 TS_C5-$^+NH_2\dot{C}H_2$_[9MOG+H_{C2}]

N1	1.702500	0.907003	0.110918
C2	0.126577	-0.785090	0.123040
C3	-0.971018	-1.196214	-0.873958
O4	-0.946772	-2.284655	-1.407525
N5	-1.895339	-0.217401	-1.002387
H6	-2.748405	-0.418087	-1.512754
C7	-1.886023	0.949830	-0.131517
N8	-0.581023	1.570170	-0.030917
C9	0.354450	0.713989	0.085779
C10	2.353791	2.204911	-0.012019
H11	1.991705	2.865943	0.775599
H12	3.426497	2.047038	0.091867
H13	2.136028	2.644884	-0.987782
C14	2.377989	-0.308309	-0.120445
O15	3.545759	-0.449190	-0.332966
N16	1.407450	-1.329365	-0.046900
H17	1.553502	-2.189623	-0.563967
H18	-0.468609	-2.228205	1.505213
H19	0.380730	-1.006817	2.184273
H20	-2.493610	-1.299128	1.999202
H21	-1.520593	-0.046184	2.962656
C22	-1.657732	-0.609713	2.046796
N23	-0.395591	-1.204573	1.544834
H24	-2.042577	0.466106	0.983561
N25	-2.981285	1.775236	-0.446140
H26	-2.887711	2.200054	-1.365550
H27	-3.104049	2.510859	0.239700

Zero-point correction= 0.216012
Thermal correction to Energy= 0.229601
Thermal correction to Enthalpy= 0.230545
Thermal correction to Gibbs Free Energy= 0.175879
Sum of electronic and zero-point Energies= -752.217801
Sum of electronic and thermal Energies= -752.204212
Sum of electronic and thermal Enthalpies= -752.203268
Sum of electronic and thermal Free Energies= -752.257934

33 N1-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	2.129651	0.381116	-0.368852
C2	0.291988	-0.671038	0.410628
C3	-1.081877	-0.865449	0.693977
O4	-1.630991	-1.801691	1.230128
N5	-1.900676	0.253326	0.139342
H6	-2.705943	0.337866	0.767926
C7	-1.226670	1.673717	0.133578
N8	-1.377116	2.208576	1.441176
H9	-1.808200	3.123445	1.461737
H10	-0.518041	2.219147	1.977064
N11	0.124445	1.653502	-0.341491
C12	0.792397	0.574872	-0.139042
C13	3.053621	1.385305	-0.878476
H14	4.016709	0.899815	-1.032029
H15	2.677992	1.778970	-1.823550
H16	3.158384	2.197915	-0.157231
C17	2.524215	-0.887253	0.058364
O18	3.613949	-1.382236	0.030554
N19	1.338965	-1.504614	0.548265
H20	1.326497	-2.450295	0.909130
H21	-1.843163	2.231547	-0.575140
C22	-2.449294	-0.149351	-1.311021
H23	-1.545009	-0.202311	-1.920383
H24	-3.041920	0.721882	-1.595679
N25	-3.193885	-1.312536	-1.365766
H26	-2.725779	-2.201524	-1.280727
H27	-4.131160	-1.305456	-0.993344

Zero-point correction= 0.220732
Thermal correction to Energy= 0.235426
Thermal correction to Enthalpy= 0.236371
Thermal correction to Gibbs Free Energy= 0.178473
Sum of electronic and zero-point Energies= -752.272870
Sum of electronic and thermal Energies= -752.258175
Sum of electronic and thermal Enthalpies= -752.257231
Sum of electronic and thermal Free Energies= -752.315129

34 TS_N1-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	-2.257113	0.198609	0.352387
C2	-0.285231	-0.565955	-0.418783
C3	1.107298	-0.522196	-0.739304
O4	1.756203	-1.439307	-1.250440
N5	1.713588	0.662841	-0.333485
H6	2.481463	0.927495	-0.945489
C7	0.976706	1.895939	0.107525
N8	1.177844	2.884732	-0.919327
H9	1.061246	3.822189	-0.550688
H10	0.518490	2.763800	-1.683203
N11	-0.410421	1.700065	0.469746
C12	-0.941028	0.567361	0.173008
C13	-3.301360	1.040472	0.911068
H14	-4.246170	0.507372	0.808737
H15	-3.101153	1.240090	1.965395
H16	-3.344636	1.983882	0.364559
C17	-2.470049	-1.096568	-0.110201
O18	-3.491143	-1.731036	-0.121139
N19	-1.207775	-1.541754	-0.576007
H20	-1.080024	-2.436821	-1.026942
H21	1.489786	2.255764	1.004921
C22	3.467706	-0.583678	1.221568
H23	3.135147	-0.130837	2.149130
H24	4.112603	-0.039019	0.544111
N25	3.196825	-1.811873	0.977758
H26	2.613984	-2.363290	1.599076
H27	3.423898	-2.228476	0.076244

Zero-point correction= 0.219086
Thermal correction to Energy= 0.233893
Thermal correction to Enthalpy= 0.234837
Thermal correction to Gibbs Free Energy= 0.175791
Sum of electronic and zero-point Energies= -752.266015
Sum of electronic and thermal Energies= -752.251208
Sum of electronic and thermal Enthalpies= -752.250264
Sum of electronic and thermal Free Energies= -752.309310

35 N2-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	2.065667	-1.026251	0.073383
C2	0.982734	0.935335	-0.062051
C3	-0.091719	1.870993	0.171125
O4	-0.036054	3.074092	0.023752
N5	-1.239268	1.218340	0.641507
H6	-1.892443	1.840930	1.100592
C7	-1.363925	-0.193493	0.878029
N8	-2.362736	-0.774488	-0.150705
H9	-2.339155	-1.794726	-0.053355
H10	-2.009926	-0.580904	-1.093042
N11	-0.213731	-1.026539	0.760651
C12	0.851533	-0.444949	0.300334
C13	2.408679	-2.418246	0.316679
H14	3.465279	-2.542646	0.081233
H15	2.230381	-2.663821	1.364810
H16	1.808694	-3.068925	-0.321959
C17	2.976365	-0.074845	-0.411518
O18	4.126431	-0.241020	-0.710552
N19	2.249894	1.133902	-0.478512
H20	2.661281	2.010902	-0.770552
H21	-1.851308	-0.364645	1.844334
C22	-3.809988	-0.297209	-0.072087
H23	-3.771140	0.784434	-0.212673
H24	-4.137473	-0.521123	0.946643
N25	-4.560515	-0.957755	-1.071969
H26	-4.949898	-0.366047	-1.791145
H27	-5.234548	-1.633988	-0.744035

Zero-point correction= 0.222972
Thermal correction to Energy= 0.237280
Thermal correction to Enthalpy= 0.238224
Thermal correction to Gibbs Free Energy= 0.180596
Sum of electronic and zero-point Energies= -752.293396
Sum of electronic and thermal Energies= -752.279088
Sum of electronic and thermal Enthalpies= -752.278144
Sum of electronic and thermal Free Energies= -752.335772

36 TS_N2-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	-1.231335	-1.371586	-0.039450
C2	-1.264298	0.867911	-0.091295
C3	-0.718644	2.207170	0.045487
O4	-1.379989	3.219094	0.175898
N5	0.664109	2.164907	0.080910
H6	1.095658	3.081338	0.058978
C7	1.483319	1.042668	-0.394969
N8	2.804875	1.077175	0.218173
H9	2.715082	1.126810	1.231351
H10	3.326798	1.893510	-0.088616
N11	0.888238	-0.268638	-0.167047
C12	-0.411027	-0.275290	-0.112216
C13	-0.823389	-2.760603	-0.053239
H14	-1.726444	-3.369298	-0.108219
H15	-0.199066	-2.960575	-0.927692
H16	-0.285656	-3.012945	0.865257
C17	-2.577044	-0.969533	0.018577
O18	-3.547207	-1.676411	0.078752
N19	-2.541314	0.433762	-0.012732
H20	-3.368074	1.012666	0.054101
H21	1.645141	1.147813	-1.480407
C22	3.798176	-1.175803	-0.335709
H23	4.860331	-1.057755	-0.148329
H24	3.364895	-0.813636	-1.256969
N25	3.070078	-1.883610	0.448097
H26	3.432258	-2.274636	1.309569
H27	2.051525	-1.797947	0.298298

Zero-point correction= 0.219299
Thermal correction to Energy= 0.233648
Thermal correction to Enthalpy= 0.234592
Thermal correction to Gibbs Free Energy= 0.177244
Sum of electronic and zero-point Energies= -752.275611
Sum of electronic and thermal Energies= -752.261262
Sum of electronic and thermal Enthalpies= -752.260318
Sum of electronic and thermal Free Energies= -752.317666

37 N3-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	1.351332	1.043461	-0.102518
C2	0.651166	-1.082995	0.008813
C3	-0.224205	-2.237925	-0.231282
O4	0.187206	-3.377494	-0.283054
N5	-1.504873	-1.819101	-0.497258
H6	-2.182086	-2.536826	-0.720962
C7	-1.980160	-0.535156	-0.033548
N8	-2.071995	-0.517547	1.404854
H9	-2.585175	-1.321297	1.752496

H10	-2.521910	0.339582	1.717432
N11	-1.031102	0.543528	-0.428797
C12	0.244738	0.268748	-0.186696
C13	1.506120	2.493809	-0.136798
H14	2.525398	2.707263	0.186029
H15	1.372795	2.877281	-1.149785
H16	0.807566	2.965108	0.556764
C17	2.481916	0.215276	0.167389
O18	3.610454	0.584476	0.321606
N19	1.977978	-1.085589	0.219269
H20	2.555059	-1.909076	0.346637
H21	-2.911184	-0.315010	-0.567432
C22	-1.616042	1.852897	-0.773944
H23	-0.804349	2.495885	-1.118673
H24	-2.274687	1.679069	-1.628340
N25	-2.387562	2.364035	0.326217
H26	-1.860212	2.957814	0.955328
H27	-3.220129	2.854910	0.026114

Zero-point correction= 0.222749
Thermal correction to Energy= 0.236650
Thermal correction to Enthalpy= 0.237595
Thermal correction to Gibbs Free Energy= 0.181731
Sum of electronic and zero-point Energies= -752.296486
Sum of electronic and thermal Energies= -752.282585
Sum of electronic and thermal Enthalpies= -752.281641
Sum of electronic and thermal Free Energies= -752.337505

38 TS_N3-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	-1.734455	-0.511651	0.319684
C2	-0.142762	1.023038	-0.081271
C3	1.207034	1.479486	-0.361986
O4	1.489373	2.512186	-0.937380
N5	2.142068	0.491575	-0.011235
H6	3.082896	0.872335	0.040050
C7	1.791435	-0.436154	1.092711
N8	1.692186	0.296579	2.337184
H9	2.595813	0.623588	2.665447
H10	1.274440	-0.279304	3.061238
N11	0.517757	-1.116247	0.873045
C12	-0.385774	-0.288931	0.441886
C13	-2.457842	-1.665129	0.826688
H14	-3.521860	-1.475118	0.686664
H15	-2.174499	-2.565598	0.277816
H16	-2.239621	-1.805450	1.886947
C17	-2.369079	0.629993	-0.191446
O18	-3.542859	0.793524	-0.389349
N19	-1.331701	1.551729	-0.441128
H20	-1.490884	2.468955	-0.837139
H21	2.582969	-1.198883	1.094864
C22	1.192233	-2.452688	-1.373489
H23	1.881834	-2.604173	-0.553946
H24	0.430071	-3.195108	-1.587376
N25	1.327688	-1.434552	-2.139582
H26	1.984158	-0.692657	-1.871243
H27	0.716298	-1.273988	-2.933825

Zero-point correction= 0.219029
Thermal correction to Energy= 0.233596
Thermal correction to Enthalpy= 0.234540
Thermal correction to Gibbs Free Energy= 0.176865
Sum of electronic and zero-point Energies= -752.259778
Sum of electronic and thermal Energies= -752.245211
Sum of electronic and thermal Enthalpies= -752.244266
Sum of electronic and thermal Free Energies= -752.301942

39 C4-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	1.572954	0.143467	-0.275154
C2	-0.510741	0.697149	0.453519
C3	-1.977069	0.518081	0.740095
O4	-2.558323	1.147423	1.591436
N5	-2.429703	-0.507688	-0.033877
H6	-3.400486	-0.781973	0.057638
C7	-1.677985	-0.864944	-1.237174
N8	-1.557974	0.332035	-2.055675
H9	-2.470006	0.724717	-2.274055
H10	-1.065708	0.147021	-2.925253
N11	-0.288495	-1.248153	-0.991939
C12	0.311542	-0.485988	0.067569
C13	2.726606	-0.521449	-0.879155
H14	3.214226	0.191593	-1.545342
H15	3.427564	-0.857599	-0.115496
H16	2.368444	-1.380024	-1.444091
C17	1.591956	1.461117	0.028104
O18	2.433801	2.304181	-0.059256
N19	0.218193	1.745774	0.528630
H20	-0.089969	2.681881	0.785683
H21	-2.183682	-1.715543	-1.702318
C22	0.445301	-1.457001	1.332982
H23	0.780194	-0.832551	2.166815
H24	-0.562477	-1.824987	1.560813
N25	1.410082	-2.472242	1.059917
H26	2.020332	-2.673776	1.838995
H27	1.024685	-3.325731	0.680212

Zero-point correction= 0.219609
Thermal correction to Energy= 0.233976
Thermal correction to Enthalpy= 0.234921
Thermal correction to Gibbs Free Energy= 0.178494
Sum of electronic and zero-point Energies= -752.218412
Sum of electronic and thermal Energies= -752.204044
Sum of electronic and thermal Enthalpies= -752.203100
Sum of electronic and thermal Free Energies= -752.259527

40 TS_C4-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	1.570989	-0.023897	0.405113
C2	-0.424329	-0.813748	-0.299464
C3	-1.874868	-0.796738	-0.671216
O4	-2.379052	-1.649145	-1.365793
N5	-2.428304	0.359479	-0.205724
H6	-3.411104	0.507756	-0.402890
C7	-1.826776	1.045918	0.943888
N8	-1.881184	0.147768	2.086398
H9	-2.836527	-0.133999	2.289215
H10	-1.489950	0.582403	2.917234
N11	-0.407225	1.354954	0.796693
C12	0.259661	0.416122	0.029328
C13	2.607336	0.788526	1.026742
H14	3.023081	0.244659	1.876609
H15	3.413849	1.005533	0.322727
H16	2.150046	1.713556	1.376754
C17	1.728085	-1.358573	0.182399
O18	2.671857	-2.081287	0.325691
N19	0.415374	-1.801037	-0.304164
H20	0.211358	-2.766155	-0.552604
H21	-2.361647	1.993604	1.062169
C22	0.432922	1.246221	-1.609567
H23	0.789633	0.426784	-2.234555
H24	-0.595217	1.536656	-1.818235
N25	1.306098	2.287401	-1.545122
H26	2.297656	2.130122	-1.627113
H27	1.023959	3.163485	-1.133500

Zero-point correction= 0.218036
Thermal correction to Energy= 0.232363
Thermal correction to Enthalpy= 0.233307
Thermal correction to Gibbs Free Energy= 0.176685
Sum of electronic and zero-point Energies= -752.218289
Sum of electronic and thermal Energies= -752.203962
Sum of electronic and thermal Enthalpies= -752.203018
Sum of electronic and thermal Free Energies= -752.259640

41 C5-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	1.429883	1.043900	-0.099970
C2	0.044294	-0.779920	-0.101066
C3	-1.284261	-1.278294	-0.654542
O4	-1.358624	-2.330932	-1.249859
N5	-2.285316	-0.420171	-0.366010
H6	-3.214020	-0.659690	-0.696591
C7	-2.196217	0.862144	0.361732
N8	-3.226534	1.692777	-0.164889
H9	-3.477821	2.440828	0.469710
N10	-0.866512	1.469342	0.314173
C11	0.114253	0.694294	0.077403
C12	1.954268	2.402128	-0.038635
H13	1.702904	2.845231	0.924969
H14	3.035510	2.345100	-0.158917
H15	1.523126	3.006113	-0.839977
C16	2.137215	-0.015757	-0.684934
O17	3.276253	-0.029777	-1.055784
N18	1.216987	-1.083673	-0.750169
H19	1.423158	-1.957871	-1.220586
H20	-2.976636	2.086227	-1.066665
C21	0.066773	-1.512471	1.531307
H22	-0.899573	-1.217317	1.940000
H23	0.116168	-2.565509	1.252802
N24	1.123751	-1.072249	2.267481
H25	1.050102	-0.262250	2.866292
H26	2.034246	-1.505444	2.197801
H27	-2.421959	0.688032	1.424411

Zero-point correction= 0.218666
Thermal correction to Energy= 0.233482
Thermal correction to Enthalpy= 0.234426
Thermal correction to Gibbs Free Energy= 0.176828
Sum of electronic and zero-point Energies= -752.258633
Sum of electronic and thermal Energies= -752.243817
Sum of electronic and thermal Enthalpies= -752.242873
Sum of electronic and thermal Free Energies= -752.300471

42 TS_C5-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	1.424277	1.060493	-0.109040
C2	0.026727	-0.737010	-0.213482
C3	-1.304838	-1.266332	-0.668546
O4	-1.401528	-2.328319	-1.248843
N5	-2.303930	-0.422086	-0.325186
H6	-3.243730	-0.677505	-0.608779
C7	-2.202877	0.865066	0.393763
N8	-3.231554	1.700498	-0.131863
H9	-3.457358	2.464868	0.493102
N10	-0.872577	1.470326	0.353271
C11	0.104333	0.709039	0.056102
C12	1.959629	2.409311	0.024908
H13	1.716670	2.801457	1.012718
H14	3.040080	2.351084	-0.102421
H15	1.531400	3.061147	-0.739309
C16	2.130339	0.016812	-0.711066
O17	3.276105	-0.006414	-1.061282
N18	1.198764	-1.047530	-0.825362
H19	1.400373	-1.906201	-1.325382
H20	-2.990364	2.073574	-1.044672
C21	0.103391	-1.565858	1.588679
H22	-0.832757	-1.180783	1.985313
H23	0.086291	-2.584569	1.207764
N24	1.209742	-1.185929	2.235832
H25	1.219407	-0.370511	2.832553
H26	2.089919	-1.666815	2.107606
H27	-2.429837	0.695541	1.456784

Zero-point correction= 0.218570
Thermal correction to Energy= 0.232880
Thermal correction to Enthalpy= 0.233825
Thermal correction to Gibbs Free Energy= 0.177127
Sum of electronic and zero-point Energies= -752.258503
Sum of electronic and thermal Energies= -752.244193
Sum of electronic and thermal Enthalpies= -752.243249
Sum of electronic and thermal Free Energies= -752.299947

43 O6-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	1.919403	-0.921881	-0.083327
C2	-0.222963	-0.216642	-0.102304
C3	-1.226979	0.765593	-0.069830
O4	-2.526278	0.609592	0.104569
N5	-0.804819	2.019951	-0.148508
H6	-1.492322	2.760699	-0.052044
C7	0.610520	2.484268	-0.304576
N8	0.791960	3.534265	0.646070
H9	1.500685	4.192729	0.345642
H10	1.038809	3.179156	1.564263
N11	1.589094	1.425618	-0.239652
C12	1.162811	0.221677	-0.167145
C13	3.373782	-0.970595	-0.087091
H14	3.666795	-2.018356	-0.028209
H15	3.755669	-0.526564	-1.007403
H16	3.766746	-0.426227	0.773285
C17	1.106671	-2.042798	0.069259
O18	1.427759	-3.190438	0.202008
N19	-0.227003	-1.552606	0.037926
H20	-1.077156	-2.079281	0.263300
H21	0.669353	2.923810	-1.308403
C22	-3.267985	-0.532070	-0.401356
H23	-2.993167	-0.697570	-1.446280
H24	-4.293453	-0.163342	-0.341740
N25	-3.005194	-1.721883	0.363545
H26	-3.344955	-2.539147	-0.136867
H27	-3.468085	-1.699974	1.267712

Zero-point correction= 0.221726
Thermal correction to Energy= 0.235984
Thermal correction to Enthalpy= 0.236928
Thermal correction to Gibbs Free Energy= 0.179647
Sum of electronic and zero-point Energies= -752.283375
Sum of electronic and thermal Energies= -752.269118
Sum of electronic and thermal Enthalpies= -752.268174
Sum of electronic and thermal Free Energies= -752.325455

44 TS_O6-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	2.416303	0.589981	-0.003599
C2	0.176048	0.407745	0.134882
C3	-1.088981	-0.270639	0.067851
O4	-2.191877	0.303487	-0.064214
N5	-0.940877	-1.612084	0.122398
H6	-1.766977	-2.187789	0.029731
C7	0.308714	-2.372755	0.373657
N8	0.213626	-3.562779	-0.424138
H9	0.837530	-4.279894	-0.071708

H10	0.469010	-3.369886	-1.388305
N11	1.529019	-1.616898	0.174847
C12	1.400239	-0.338322	0.115073
C13	3.835127	0.284137	-0.044275
H14	4.374652	1.230291	-0.078337
H15	4.118585	-0.276132	0.848517
H16	4.066227	-0.307024	-0.932366
C17	1.898074	1.877180	-0.058331
O18	2.487544	2.924058	-0.152928
N19	0.496087	1.720277	0.022421
H20	-0.132866	2.506984	-0.005810
H21	0.299977	-2.683667	1.427934
C22	-4.769336	0.371067	-0.209509
H23	-5.428296	-0.250437	0.389025
H24	-4.234816	-0.030981	-1.060276
N25	-4.636344	1.606202	0.085475
H26	-5.103151	2.024659	0.883982
H27	-3.969223	2.180136	-0.423175

Zero-point correction= 0.218283
Thermal correction to Energy= 0.233766
Thermal correction to Enthalpy= 0.234711
Thermal correction to Gibbs Free Energy= 0.172415
Sum of electronic and zero-point Energies= -752.272962
Sum of electronic and thermal Energies= -752.257479
Sum of electronic and thermal Enthalpies= -752.256535
Sum of electronic and thermal Free Energies= -752.318830

45 O8-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	-0.680324	-0.811101	-0.060484
C2	0.809254	0.865473	-0.138431
C3	2.105179	1.524582	-0.021422
O4	2.242627	2.731169	0.099485
N5	3.103083	0.593172	0.003582
H6	4.049301	0.941890	0.093827
C7	2.995894	-0.840671	-0.312851
N8	4.002574	-1.505768	0.456041
H9	4.165801	-2.446349	0.117118
H10	3.755279	-1.543245	1.439705
N11	1.652421	-1.404881	-0.153156
C12	0.696902	-0.538175	-0.128737
C13	-1.266389	-2.135529	-0.012627
H14	-1.755729	-2.305599	0.949810
H15	-1.976548	-2.270267	-0.831970
H16	-0.456437	-2.856382	-0.127014
C17	-1.374870	0.364978	-0.022545
O18	-2.605181	0.524451	0.042487
N19	-0.450723	1.385437	-0.070228
H20	-0.684185	2.367792	-0.027224
H21	3.241275	-0.991855	-1.374993
C22	-4.534035	-0.500709	-0.094013
H23	-4.317509	-0.684688	-1.137747
H24	-4.209208	-1.199221	0.665095
N25	-5.366401	0.429931	0.219915
H26	-5.615159	0.612745	1.185102
H27	-5.712486	1.083006	-0.473435

Zero-point correction= 0.219459
Thermal correction to Energy= 0.234861
Thermal correction to Enthalpy= 0.235805
Thermal correction to Gibbs Free Energy= 0.175003
Sum of electronic and zero-point Energies= -752.271775
Sum of electronic and thermal Energies= -752.256373
Sum of electronic and thermal Enthalpies= -752.255429
Sum of electronic and thermal Free Energies= -752.316231

46 TS_O8-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	-0.599714	-0.905208	-0.085808
C2	0.813785	0.834163	-0.171007
C3	2.074604	1.552274	-0.040633
O4	2.156388	2.767087	0.058928
N5	3.113512	0.669210	0.022726
H6	4.040641	1.062256	0.125626
C7	3.076277	-0.774919	-0.262605
N8	4.093930	-1.376377	0.545848
H9	4.300979	-2.317999	0.234320
H10	3.819507	-1.404070	1.522765
N11	1.757832	-1.395413	-0.118248
C12	0.762116	-0.574490	-0.131893
C13	-1.138842	-2.249552	-0.034727
H14	-1.635404	-2.427020	0.921911
H15	-1.843151	-2.405211	-0.854792
H16	-0.304028	-2.942597	-0.139954
C17	-1.353129	0.238462	-0.089612
O18	-2.585981	0.319393	-0.056094
N19	-0.467913	1.300067	-0.140620
H20	-0.737953	2.272923	-0.125681
H21	3.355367	-0.937685	-1.314618
C22	-5.045782	-0.334360	-0.325606
H23	-4.521356	-0.036860	-1.224758
H24	-5.350281	-1.364321	-0.167777
N25	-5.328885	0.543884	0.556353
H26	-5.804531	0.306286	1.421455
H27	-4.998550	1.499843	0.453557

Zero-point correction= 0.218467
Thermal correction to Energy= 0.233751
Thermal correction to Enthalpy= 0.234696
Thermal correction to Gibbs Free Energy= 0.173144
Sum of electronic and zero-point Energies= -752.269384
Sum of electronic and thermal Energies= -752.254100
Sum of electronic and thermal Enthalpies= -752.253155
Sum of electronic and thermal Free Energies= -752.314707

47 N9-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	1.417044	-0.136642	-0.273269
C2	-0.507696	1.052086	0.159244
C3	-1.944849	1.307359	0.278240
O4	-2.414502	2.424524	0.383986
N5	-2.642474	0.137965	0.177005
H6	-3.652739	0.210512	0.207101
C7	-2.122380	-1.237170	0.190685
N8	-2.951775	-2.007018	-0.674115
H9	-2.848519	-3.003824	-0.531046
H10	-2.820401	-1.776496	-1.652976
N11	-0.680570	-1.345488	-0.106637
C12	-0.028422	-0.242883	-0.075919
C13	1.917118	-0.776223	-1.519193
H14	1.405776	-0.343038	-2.379593
H15	2.989944	-0.595500	-1.591172
H16	1.694834	-1.840691	-1.454531
C17	1.708147	1.336246	-0.227285
O18	2.801738	1.784059	-0.395464
N19	0.521421	1.950894	0.074706
H20	0.423275	2.956565	0.163024
H21	-2.223561	-1.653626	1.203579
C22	2.233936	-0.832970	1.086321
H23	3.219760	-0.389968	0.949349
H24	1.665568	-0.376698	1.896345
N25	2.219731	-2.184676	1.082462
H26	2.931938	-2.707503	0.598815
H27	1.397478	-2.692311	1.369305

Zero-point correction= 0.219891
Thermal correction to Energy= 0.234404
Thermal correction to Enthalpy= 0.235348
Thermal correction to Gibbs Free Energy= 0.178271
Sum of electronic and zero-point Energies= -752.254376
Sum of electronic and thermal Energies= -752.239863
Sum of electronic and thermal Enthalpies= -752.238919
Sum of electronic and thermal Free Energies= -752.295996

48 TS_N9-CH_2NH_2[9MOG + H_{C2}]$^{\bullet+}$

N1	-1.387245	-0.098299	0.356891
C2	0.524182	1.048321	-0.153787
C3	1.957400	1.278241	-0.333536
O4	2.442383	2.382807	-0.495715
N5	2.642801	0.101771	-0.222306
H6	3.652278	0.160850	-0.284839
C7	2.107850	-1.266106	-0.152714
N8	2.946222	-1.997140	0.740423
H9	2.818839	-2.998414	0.660428
H10	2.831353	-1.707471	1.705776
N11	0.672505	-1.347140	0.173549
C12	0.032479	-0.234732	0.136930
C13	-1.960852	-0.820573	1.508865
H14	-1.471465	-0.500508	2.430321
H15	-3.027331	-0.599118	1.560937
H16	-1.783175	-1.885986	1.360473
C17	-1.672697	1.342900	0.310841
O18	-2.757098	1.812177	0.509030
N19	-0.495903	1.954450	-0.058857
H20	-0.398901	2.957301	-0.169814
H21	2.194044	-1.735959	-1.143246
C22	-2.271850	-0.803776	-1.223184
H23	-3.215805	-0.302413	-1.024261
H24	-1.598588	-0.325683	-1.928773
N25	-2.276631	-2.126414	-1.210361
H26	-3.018806	-2.643794	-0.762284
H27	-1.476044	-2.654927	-1.527109

Zero-point correction= 0.219072
Thermal correction to Energy= 0.233250
Thermal correction to Enthalpy= 0.234194
Thermal correction to Gibbs Free Energy= 0.177257
Sum of electronic and zero-point Energies= -752.254857
Sum of electronic and thermal Energies= -752.240679
Sum of electronic and thermal Enthalpies= -752.239735
Sum of electronic and thermal Free Energies= -752.296672

49 [9MOG + H_{N2}]$^{+}$···$^{\bullet}CH_2NH_2$

N1	2.399321	-0.737561	0.096348
C2	0.878083	0.874177	-0.110925
C3	-0.421700	1.447876	-0.241067
O4	-0.773487	2.609751	-0.247929
N5	-1.394276	0.400417	-0.370267
H6	-2.367881	0.712499	-0.410039
C7	-1.080769	-0.907277	-0.312036
N8	-2.209762	-1.836674	-0.446069
H9	-2.446115	-1.998241	-1.430731
H10	-1.924480	-2.734340	-0.041231
N11	0.083658	-1.429317	-0.171669
C12	1.071377	-0.491320	-0.070715
C13	3.057666	-2.028667	0.183182
H14	2.658553	-2.602162	1.021767
H15	2.925985	-2.585445	-0.746608
H16	4.118127	-1.834243	0.344799
C17	3.095167	0.489011	0.169573
O18	4.284397	0.636927	0.312439
N19	2.109582	1.461989	0.041470
H20	2.307767	2.451207	0.050889
H21	-3.097039	-1.469578	0.053264
C22	-4.562099	-0.535465	0.741361
H23	-5.335520	-1.125537	0.256695
H24	-4.377725	-0.705324	1.798418
N25	-4.368655	0.751389	0.272469
H26	-4.144824	1.474232	0.946380
H27	-4.969538	1.081774	-0.471893

Zero-point correction= 0.218074
Thermal correction to Energy= 0.233339
Thermal correction to Enthalpy= 0.234284
Thermal correction to Gibbs Free Energy= 0.174419
Sum of electronic and zero-point Energies= -752.264090
Sum of electronic and thermal Energies= -752.248825
Sum of electronic and thermal Enthalpies= -752.247880
Sum of electronic and thermal Free Energies= -752.307745

50 TS_[9MOG + H_{N2}]$^{+}$···$^{\bullet}CH_2NH_2$

N1	2.174075	-0.891190	0.112882
C2	0.921608	0.930877	-0.132759
C3	-0.252847	1.689138	-0.406391
O4	-0.448107	2.887007	-0.365248
N5	-1.320837	0.799025	-0.766707
H6	-2.188357	1.269917	-0.997176
C7	-1.201717	-0.549093	-0.811555
N8	-2.404651	-1.284135	-1.098057
H9	-2.875949	-0.978699	-1.951877
H10	-2.155520	-2.271703	-1.191520
N11	-0.140608	-1.226782	-0.537614
C12	0.927799	-0.446809	-0.205744
C13	2.640251	-2.265184	0.159597
H14	2.112753	-2.821701	0.936915
H15	2.492682	-2.747875	-0.808146
H16	3.704516	-2.230998	0.393687
C17	3.004693	0.213692	0.402713
O18	4.169164	0.177373	0.719365
N19	2.184088	1.323962	0.242938
H20	2.509266	2.270977	0.365484
H21	-3.218781	-1.164109	-0.109708
C22	-4.008844	-0.964452	1.065684
H23	-4.930784	-1.481368	0.798968
H24	-3.367880	-1.481788	1.781390
N25	-4.145432	0.379525	1.285036
H26	-3.495093	0.887819	1.867761
H27	-4.967426	0.882637	0.982663

Zero-point correction= 0.213158
Thermal correction to Energy= 0.228293
Thermal correction to Enthalpy= 0.229237
Thermal correction to Gibbs Free Energy= 0.168297
Sum of electronic and zero-point Energies= -752.266400
Sum of electronic and thermal Energies= -752.251265
Sum of electronic and thermal Enthalpies= -752.250321
Sum of electronic and thermal Free Energies= -752.311261

51 [9MOG + H_{N2}]$^{+}$

N1	1.548495	-0.812913	-0.001284
C2	0.126583	0.900641	0.001422
C3	-1.136159	1.568797	0.000730
O4	-1.403499	2.747167	0.000475
N5	-2.198024	0.585029	0.000191
H6	-3.128432	0.990838	-0.000451
C7	-1.961489	-0.741631	-0.000100
N8	-3.139082	-1.638980	-0.001534
H9	-3.726629	-1.525373	-0.836562

H10	-2.763368	-2.596867	-0.000291
N11	-0.827965	-1.337794	0.000561
C12	0.231340	-0.474852	0.001210
C13	2.128086	-2.144979	0.002360
H14	1.894654	-2.661514	0.935477
H15	1.758319	-2.720027	-0.848350
H16	3.207692	-2.019786	-0.083098
C17	2.329466	0.365002	-0.000836
O18	3.532471	0.433947	-0.002192
N19	1.400165	1.403551	0.000206
H20	1.663651	2.378088	0.000161
H21	-3.729741	-1.524393	0.831147

Zero-point correction= 0.164670
Thermal correction to Energy= 0.176258
Thermal correction to Enthalpy= 0.177203
Thermal correction to Gibbs Free Energy= 0.126956
Sum of electronic and zero-point Energies= -657.096782
Sum of electronic and thermal Energies= -657.085194
Sum of electronic and thermal Enthalpies= -657.084250
Sum of electronic and thermal Free Energies= -657.134496

52 N1-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-2.227305	0.719891	0.055828
C2	-0.671891	-0.878240	-0.034878
C3	0.559672	-1.473066	-0.184875
O4	0.993107	-2.589527	-0.306837
N5	1.726955	-0.298642	-0.292061
H6	1.976946	-0.363772	-1.290967
C7	1.291152	1.064265	0.085040
N8	2.280480	2.079056	-0.344495
H9	2.176270	2.365871	-1.327659
H10	2.146714	2.916587	0.227191
N11	0.032718	1.473085	-0.028374
C12	-0.890682	0.513457	-0.002901
C13	-2.906864	2.001088	0.113685
H14	-2.528227	2.586506	0.953163
H15	-2.758219	2.550772	-0.817859
H16	-3.968167	1.795276	0.252569
C17	-2.917226	-0.521824	0.063849
O18	-4.113474	-0.666616	0.112101
N19	-1.927416	-1.479836	0.007314
H20	-2.124520	-2.467996	-0.010413
H21	3.232369	1.664092	-0.178426
C22	2.914302	-0.782511	0.510083
H23	3.079165	-1.815996	0.204127
H24	2.592374	-0.756007	1.551461
N25	4.056259	0.090172	0.298389
H26	4.726450	-0.310346	-0.351174
H27	4.549168	0.259062	1.169646

Zero-point correction= 0.221949
Thermal correction to Energy= 0.236222
Thermal correction to Enthalpy= 0.237166
Thermal correction to Gibbs Free Energy= 0.180354
Sum of electronic and zero-point Energies= -752.228895
Sum of electronic and thermal Energies= -752.214622
Sum of electronic and thermal Enthalpies= -752.213678
Sum of electronic and thermal Free Energies= -752.270490

53 TS_N1-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-2.089601	0.775617	0.144737
C2	-0.632754	-0.868141	-0.251956
C3	0.593945	-1.469678	-0.550231
O4	0.947455	-2.624073	-0.692220
N5	1.688498	-0.431900	-0.558380
H6	2.422905	-0.776308	-1.176955
C7	1.316030	0.897216	-0.745299
N8	2.442509	1.850430	-0.835314
H9	2.878972	1.884789	-1.761960
H10	2.049306	2.776603	-0.635267
N11	0.176451	1.429665	-0.357686
C12	-0.787639	0.516394	-0.150651
C13	-2.706636	2.077418	0.315765
H14	-2.259513	2.601038	1.163182
H15	-2.589662	2.673145	-0.591665
H16	-3.765706	1.905528	0.508929
C17	-2.812848	-0.438366	0.223094
O18	-3.989183	-0.554929	0.468355
N19	-1.879891	-1.428034	-0.035703
H20	-2.108578	-2.409814	-0.033606
H21	3.144998	1.604911	-0.109366
C22	2.579809	-0.775112	1.163816
H23	2.981051	-1.759984	0.942484
H24	1.690693	-0.761001	1.787015
N25	3.492459	0.269536	1.372378
H26	4.465398	-0.015668	1.351038
H27	3.311543	0.813185	2.209641

Zero-point correction= 0.219334
Thermal correction to Energy= 0.233662
Thermal correction to Enthalpy= 0.234606
Thermal correction to Gibbs Free Energy= 0.177770
Sum of electronic and zero-point Energies= -752.214400
Sum of electronic and thermal Energies= -752.200073
Sum of electronic and thermal Enthalpies= -752.199128
Sum of electronic and thermal Free Energies= -752.255964

54 C2-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	1.827033	-0.866608	-0.094681
C2	0.574725	0.993434	-0.100910
C3	-0.631883	1.773817	-0.221374
O4	-0.716859	2.979677	-0.129836
N5	-1.744497	0.959423	-0.496310
H6	-2.605861	1.452845	-0.284562
C7	-1.764277	-0.469353	-0.303869
N8	-2.510337	-1.045564	-1.548286
H9	-2.050470	-0.687494	-2.389460
H10	-2.418263	-2.065431	-1.540968
N11	-0.524063	-1.166084	-0.339319
C12	0.537253	-0.432516	-0.190043
C13	2.276934	-2.248116	-0.117695
H14	1.770644	-2.815717	0.665111
H15	2.070067	-2.696879	-1.090869
H16	3.351677	-2.245879	0.063048
C17	2.693669	0.227278	0.072907
O18	3.886818	0.204747	0.200712
N19	1.861441	1.364540	0.060014
H20	2.212941	2.308539	0.152617
H21	-3.500184	-0.789460	-1.583094
C22	-2.584326	-0.882457	0.943422
H23	-3.572523	-0.408915	0.892515
H24	-2.730408	-1.971247	0.915966
N25	-1.872530	-0.413909	2.104755
H26	-1.283005	-1.124389	2.518084
H27	-2.476181	-0.026470	2.816759

Zero-point correction= 0.221940
Thermal correction to Energy= 0.236457
Thermal correction to Enthalpy= 0.237401
Thermal correction to Gibbs Free Energy= 0.180118
Sum of electronic and zero-point Energies= -752.296628
Sum of electronic and thermal Energies= -752.282111

Sum of electronic and thermal Enthalpies= -752.281167
Sum of electronic and thermal Free Energies= -752.338450

55 TS_C2-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	1.818338	-0.854508	-0.123586
C2	0.542577	0.963477	-0.273328
C3	-0.661269	1.716135	-0.414264
O4	-0.851494	2.909639	-0.300918
N5	-1.747289	0.839483	-0.742679
H6	-2.646294	1.308135	-0.751749
C7	-1.642203	-0.518208	-0.669737
N8	-2.760189	-1.282222	-1.282539
H9	-2.803634	-1.139588	-2.300526
H10	-2.553850	-2.272654	-1.109111
N11	-0.534745	-1.192417	-0.606070
C12	0.547665	-0.415727	-0.349062
C13	2.299526	-2.223537	-0.145436
H14	1.781932	-2.822199	0.606816
H15	2.152847	-2.664912	-1.133256
H16	3.365002	-2.189819	0.083445
C17	2.662210	0.254200	0.106540
O18	3.848013	0.223356	0.330691
N19	1.824443	1.360753	0.023668
H20	2.158378	2.309892	0.098983
H21	-3.670872	-1.062360	-0.870094
C22	-2.524275	-0.792251	1.656341
H23	-3.509312	-0.331013	1.632878
H24	-2.472323	-1.873947	1.737569
N25	-1.554433	-0.091579	2.306354
H26	-0.748910	-0.555010	2.694783
H27	-1.693374	0.868399	2.579716

Zero-point correction= 0.217092
Thermal correction to Energy= 0.232561
Thermal correction to Enthalpy= 0.233505
Thermal correction to Gibbs Free Energy= 0.173853
Sum of electronic and zero-point Energies= -752.242094
Sum of electronic and thermal Energies= -752.226625
Sum of electronic and thermal Enthalpies= -752.225680
Sum of electronic and thermal Free Energies= -752.285332

56 N3-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-1.397313	-1.080315	0.013812
C2	-0.856577	1.071217	-0.067494
C3	-0.039405	2.244239	-0.114948
O4	-0.388257	3.402759	-0.169914
N5	1.339868	1.903177	-0.047066
H6	1.948792	2.696768	-0.217532
C7	1.869147	0.632889	-0.154312
N8	3.058109	0.392861	0.734297
H9	2.859983	0.598109	1.722599
H10	3.256283	-0.649352	0.613217
N11	1.007393	-0.474161	-0.114563
C12	-0.353668	-0.198489	-0.067481
C13	-1.422668	-2.514183	0.246170
H14	-1.288104	-3.077475	-0.680947
H15	-0.671347	-2.797932	0.987337
H16	-2.414209	-2.744830	0.639600
C17	-2.616712	-0.341761	0.073541
O18	-3.718470	-0.826798	0.178438
N19	-2.234894	0.974949	0.010281
H20	-2.882828	1.747267	0.044968
H21	3.869196	0.941049	0.443380
C22	1.533487	-1.685001	-0.776475
H23	0.727443	-2.411224	-0.855288
H24	1.866572	-1.425784	-1.785047
N25	2.682396	-2.178899	-0.015588
H26	2.392803	-2.804362	0.732064
H27	3.318694	-2.696669	-0.614758

Zero-point correction= 0.222442
Thermal correction to Energy= 0.236282
Thermal correction to Enthalpy= 0.237226
Thermal correction to Gibbs Free Energy= 0.181508
Sum of electronic and zero-point Energies= -752.256246
Sum of electronic and thermal Energies= -752.242407
Sum of electronic and thermal Enthalpies= -752.241462
Sum of electronic and thermal Free Energies= -752.297180

57 TS_N3-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-1.443238	-1.034213	0.214689
C2	-0.831974	1.078940	-0.081994
C3	0.053464	2.208818	-0.164292
O4	-0.214769	3.363794	-0.419461
N5	1.383627	1.806445	0.122615
H6	2.028127	2.581407	0.227770
C7	1.756568	0.545361	0.516491
N8	3.122677	0.270514	0.767329
H9	3.301092	0.084104	1.752526
H10	3.213649	-1.434925	-0.127109
N11	0.957311	-0.533450	0.346522
C12	-0.378244	-0.175374	0.191115
C13	-1.467755	-2.433402	0.588693
H14	-1.302506	-3.084505	-0.275349
H15	-0.714457	-2.621702	1.356641
H16	-2.458677	-2.650030	0.990654
C17	-2.630126	-0.299349	-0.015872
O18	-3.752879	-0.748224	-0.023484
N19	-2.203938	1.003532	-0.205917
H20	-2.835032	1.776820	-0.352977
H21	3.749073	1.008458	0.461000
C22	1.445427	-1.495469	-1.142203
H23	0.656348	-2.194270	-1.400854
H24	1.722940	-0.799273	-1.929204
N25	2.634726	-2.177193	-0.585000
H26	2.353605	-2.831070	0.149197
H27	3.184694	-2.686159	-1.282022

Zero-point correction= 0.219432
Thermal correction to Energy= 0.233608
Thermal correction to Enthalpy= 0.234552
Thermal correction to Gibbs Free Energy= 0.178305
Sum of electronic and zero-point Energies= -752.233805
Sum of electronic and thermal Energies= -752.219630
Sum of electronic and thermal Enthalpies= -752.218686
Sum of electronic and thermal Free Energies= -752.274932

58 C4-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	1.644683	-0.634066	-0.354815
C2	0.158358	1.002606	0.184834
C3	-1.091127	1.666046	0.063519
O4	-1.331394	2.856986	0.155011
N5	-2.143016	0.739107	-0.261835
H6	-3.077984	1.124954	-0.285471
C7	-1.818759	-0.512227	-0.673534
N8	-2.934481	-1.266555	-1.315082
H9	-3.367868	-0.761695	-2.096077
H10	-2.517152	-2.137765	-1.665342
N11	-0.722072	-1.130731	-0.649378
C12	0.306931	-0.497602	0.174141
C13	2.329438	-1.903631	-0.518558
H14	2.672590	-2.314156	0.436629
H15	1.657786	-2.611186	-1.007816

H16	3.197899	-1.735406	-1.155626
C17	2.333230	0.556299	-0.319489
O18	3.492575	0.763436	-0.566776
N19	1.385750	1.547846	0.060860
H20	1.582349	2.535935	-0.032477
H21	-3.658325	-1.509133	-0.629238
C22	0.204775	-1.132941	1.594078
H23	1.017880	-0.700347	2.192555
H24	0.405184	-2.201598	1.476260
N25	-1.119517	-0.961537	2.167299
H26	-1.195664	-0.083294	2.670266
H27	-1.322659	-1.699432	2.831163

Zero-point correction= 0.221771
Thermal correction to Energy= 0.236272
Thermal correction to Enthalpy= 0.237216
Thermal correction to Gibbs Free Energy= 0.180314
Sum of electronic and zero-point Energies= -752.260521
Sum of electronic and thermal Energies= -752.246020
Sum of electronic and thermal Enthalpies= -752.245076
Sum of electronic and thermal Free Energies= -752.301978

59 TS_C4-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	1.640877	-0.661692	-0.453449
C2	0.238480	1.041532	-0.054342
C3	-0.986863	1.747804	-0.029961
O4	-1.223865	2.920289	0.188217
N5	-2.077404	0.846578	-0.347485
H6	-2.993564	1.278306	-0.327288
C7	-1.857316	-0.441562	-0.692050
N8	-3.039948	-1.210392	-1.148926
H9	-3.499324	-0.784749	-1.962675
H10	-2.684545	-2.135933	-1.419550
N11	-0.754764	-1.077313	-0.747849
C12	0.308298	-0.356430	-0.232121
C13	2.210124	-1.973520	-0.683189
H14	2.327045	-2.528406	0.252830
H15	1.571579	-2.533105	-1.368032
H16	3.194574	-1.834531	-1.130146
C17	2.431499	0.466285	-0.197910
O18	3.637506	0.524120	-0.206887
N19	1.526522	1.494838	0.071831
H20	1.813434	2.452257	0.212171
H21	-3.735141	-1.334111	-0.405000
C22	0.070424	-1.103957	1.858175
H23	0.727044	-0.343912	2.271215
H24	0.496012	-2.090782	1.710232
N25	-1.266359	-1.068219	2.221246
H26	-1.544033	-0.302399	2.819894
H27	-1.672560	-1.945415	2.516509

Zero-point correction= 0.218025
Thermal correction to Energy= 0.232914
Thermal correction to Enthalpy= 0.233858
Thermal correction to Gibbs Free Energy= 0.176177
Sum of electronic and zero-point Energies= -752.226446
Sum of electronic and thermal Energies= -752.211558
Sum of electronic and thermal Enthalpies= -752.210613
Sum of electronic and thermal Free Energies= -752.268295

60 C5-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	1.625757	-0.926855	0.134542
C2	0.161081	0.846340	-0.000177
C3	-1.057445	1.151741	-0.849314
O4	-1.215900	2.168031	-1.479360
N5	-2.058059	0.182198	-0.740994
H6	-2.973149	0.491937	-1.048338
C7	-1.891819	-0.975480	0.026507
N8	-2.831831	-2.066153	-0.352123
H9	-2.738540	-2.345116	-1.340612
H10	-2.576427	-2.877490	0.221514
N11	-0.665385	-1.487549	0.275882
C12	0.318961	-0.635290	0.167935
C13	2.222325	-2.243777	0.275741
H14	1.984447	-2.654213	1.257925
H15	1.851151	-2.913427	-0.503857
H16	3.300387	-2.120980	0.173904
C17	2.364937	0.206797	-0.348201
O18	3.551173	0.218337	-0.530389
N19	1.434718	1.192344	-0.570870
H20	1.732232	2.145041	-0.724799
H21	-3.812400	-1.837529	-0.168412
C22	-0.012292	1.574244	1.410403
H23	0.885727	1.311255	1.979474
H24	0.038009	2.644102	1.185272
N25	-1.174919	1.307404	2.182302
H26	-1.279647	0.381085	2.565862
H27	-2.040428	1.727217	1.881515

Zero-point correction= 0.221134
Thermal correction to Energy= 0.235732
Thermal correction to Enthalpy= 0.236676
Thermal correction to Gibbs Free Energy= 0.180000
Sum of electronic and zero-point Energies= -752.264956
Sum of electronic and thermal Energies= -752.250358
Sum of electronic and thermal Enthalpies= -752.249414
Sum of electronic and thermal Free Energies= -752.306090

61 TS_C5-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-1.917116	0.681073	0.206792
C2	-0.168825	-0.529077	-0.502986
C3	1.159509	-0.751803	-0.981937
O4	1.623930	-1.743694	-1.513592
N5	1.984392	0.370157	-0.694722
H6	2.972049	0.193549	-0.838067
C7	1.518028	1.466899	-0.010466
N8	2.392739	2.657073	-0.014826
H9	2.569339	3.018340	-0.963422
H10	1.879805	3.379675	0.504690
N11	0.267446	1.729986	0.259139
C12	-0.563653	0.714989	0.004068
C13	-2.757204	1.758936	0.692745
H14	-2.379007	2.125994	1.648563
H15	-2.790135	2.577210	-0.030678
H16	-3.759706	1.351598	0.824501
C17	-2.430461	-0.539319	-0.267489
O18	-3.586974	-0.883671	-0.280243
N19	-1.318218	-1.253988	-0.710630
H20	-1.389598	-2.157555	-1.153123
H21	3.297046	2.510217	0.444323
C22	0.771524	-1.819099	1.600973
H23	0.446398	-1.130756	2.370961
H24	0.063729	-2.523201	1.184029
N25	2.085042	-2.120149	1.532108
H26	2.752712	-1.717828	2.168975
H27	2.408222	-2.866537	0.935455

Zero-point correction= 0.216400
Thermal correction to Energy= 0.231984
Thermal correction to Enthalpy= 0.232928
Thermal correction to Gibbs Free Energy= 0.173390
Sum of electronic and zero-point Energies= -752.233160
Sum of electronic and thermal Energies= -752.217576

Sum of electronic and thermal Enthalpies= -752.216632
Sum of electronic and thermal Free Energies= -752.276170

62 C6-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-1.856675	0.834968	0.181367
C2	-0.392463	-0.853599	-0.158140
C3	0.695726	-1.841952	-0.161367
O4	0.377733	-2.994762	-0.414397
N5	1.755396	1.110244	-1.750950
H6	2.720396	1.190127	-2.062738
C7	1.538424	1.469141	-0.560611
N8	2.616513	1.859290	0.400672
H9	3.492303	2.137857	-0.042211
H10	2.286969	2.600833	1.022820
N11	0.350685	1.550190	0.081867
C12	-0.528055	0.592281	0.011161
C13	-2.454680	2.152462	0.337599
H14	-2.101301	2.612296	1.261454
H15	-2.188785	2.782637	-0.512811
H16	-3.534717	2.015661	0.380613
C17	-2.609524	-0.339634	0.039305
O18	-3.802428	-0.460548	0.092964
N19	-1.658507	-1.338512	-0.179990
H20	-1.882536	-2.321981	-0.282270
H21	2.701682	0.910037	0.950236
C22	2.159026	-1.558055	0.161637
H23	2.590538	-2.548403	0.320611
H24	2.630999	-1.128865	-0.727109
N25	2.408761	-0.667883	1.328087
H26	1.668334	-0.771213	2.020401
H27	3.249752	-0.998449	1.797596

Zero-point correction= 0.219502
Thermal correction to Energy= 0.234018
Thermal correction to Enthalpy= 0.234962
Thermal correction to Gibbs Free Energy= 0.177498
Sum of electronic and zero-point Energies= -752.262006
Sum of electronic and thermal Energies= -752.247490
Sum of electronic and thermal Enthalpies= -752.246546
Sum of electronic and thermal Free Energies= -752.304010

63 TS_C6-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-1.904175	0.763367	0.074029
C2	-0.294002	-0.715775	-0.376683
C3	1.080871	-1.279578	-0.483236
O4	1.342669	-2.308442	-1.154366
N5	1.923910	-0.018951	-0.814878
H6	2.848899	-0.233632	-1.169055
C7	1.549706	1.185637	-0.414131
N8	2.582451	2.254492	-0.373818
H9	3.063482	2.378553	-1.271444
H10	2.089736	3.125100	-0.139076
N11	0.377257	1.604311	-0.061959
C12	-0.558491	0.616659	-0.111354
C13	-2.638843	1.999012	0.281957
H14	-2.269348	2.509469	1.172843
H15	-2.539657	2.651330	-0.588140
H16	-3.686979	1.733396	0.419485
C17	-2.524377	-0.489468	-0.061723
O18	-3.701884	-0.736846	0.007455
N19	-1.469423	-1.384131	-0.309995
H20	-1.616396	-2.349221	-0.574993
H21	3.279700	2.065093	0.354646
C22	1.528007	-1.597633	1.148942
H23	0.755732	-2.309953	1.448492
H24	2.477250	-2.110141	0.997112
N25	1.670387	-0.457722	1.986357
H26	0.857211	-0.248445	2.551774
H27	2.494003	-0.491939	2.572880

Zero-point correction= 0.218215
Thermal correction to Energy= 0.232681
Thermal correction to Enthalpy= 0.233626
Thermal correction to Gibbs Free Energy= 0.176801
Sum of electronic and zero-point Energies= -752.213851
Sum of electronic and thermal Energies= -752.199385
Sum of electronic and thermal Enthalpies= -752.198440
Sum of electronic and thermal Free Energies= -752.255265

64 O6-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-2.355532	0.180790	-0.132906
C2	-0.273638	-0.628041	0.134110
C3	1.064759	-0.492650	0.258758
O4	1.889638	-1.507159	0.546202
N5	1.602390	0.787406	0.172204
H6	2.599084	0.757583	-0.071680
C7	0.786853	1.853204	-0.254303
N8	1.209308	3.156078	0.376345
H9	2.143660	3.449709	0.086201
H10	0.534714	3.859392	0.060495
N11	-0.573353	1.766977	-0.217510
C12	-1.054948	0.559335	-0.091629
C13	-3.499565	1.045122	-0.358234
H14	-3.572892	1.787890	0.438479
H15	-3.401468	1.548125	-1.322069
H16	-4.388142	0.413861	-0.356957
C17	-2.466776	-1.217921	0.069181
O18	-3.488908	-1.852407	0.095545
N19	-1.167347	-1.679311	0.222614
H20	-0.958919	-2.642162	0.432334
H21	1.179366	3.128199	1.406547
C22	2.972349	-1.778061	-0.370993
H23	2.556007	-1.912940	-1.373630
H24	3.367835	-2.725633	-0.002460
N25	3.931415	-0.698181	-0.390460
H26	4.391243	-0.626448	-1.291176
H27	4.641298	-0.803283	0.326592

Zero-point correction= 0.222441
Thermal correction to Energy= 0.236786
Thermal correction to Enthalpy= 0.237730
Thermal correction to Gibbs Free Energy= 0.180811
Sum of electronic and zero-point Energies= -752.252619
Sum of electronic and thermal Energies= -752.238274
Sum of electronic and thermal Enthalpies= -752.237330
Sum of electronic and thermal Free Energies= -752.294250

65 TS_O6-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-0.020943	1.979676	0.116166
C2	0.174013	-0.178418	-0.467197
C3	-0.175292	-1.539102	-0.464113
O4	0.544214	-2.521344	-0.713545
N5	-1.527999	-1.736827	-0.113951
H6	-1.713280	-2.699657	0.142854
C7	-2.325160	-0.721878	0.457782
N8	-3.759276	-0.797675	-0.045956
H9	-4.231223	-1.660046	0.229476
H10	-4.249923	-0.004356	0.375332
N11	-1.938467	0.582074	0.459340
C12	-0.696755	0.777184	0.059660
C13	-0.574832	3.245869	0.559619
H14	-1.332359	3.596219	-0.144925
H15	-1.025918	3.122922	1.545476

H16	0.240000	3.968007	0.605284
C17	1.261842	1.834222	-0.392235
O18	2.091349	2.695327	-0.557439
N19	1.441450	0.445221	-0.676654
H20	1.895235	0.305931	-1.575758
H21	-3.819806	-0.703187	-1.069969
C22	2.880998	-2.413640	0.453443
H23	2.773814	-2.422470	-0.623438
H24	3.098958	-3.331204	0.991056
N25	2.760473	-1.310572	1.088349
H26	2.477574	-0.453493	0.561547
H27	2.846880	-1.269225	2.098117

Zero-point correction= 0.219474
Thermal correction to Energy= 0.234029
Thermal correction to Enthalpy= 0.234973
Thermal correction to Gibbs Free Energy= 0.177358
Sum of electronic and zero-point Energies= -752.234511
Sum of electronic and thermal Energies= -752.219956
Sum of electronic and thermal Enthalpies= -752.219012
Sum of electronic and thermal Free Energies= -752.276627

66 N7-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-0.888680	1.505385	-0.116075
C2	0.055301	-0.527392	-0.447792
C3	1.040737	-1.538435	-0.348364
O4	0.902758	-2.742845	-0.506165
N5	2.301530	-0.978713	-0.011391
H6	2.942187	-1.683471	0.337984
C7	2.439684	0.345803	0.446756
N8	3.761091	0.945887	0.034669
H9	3.883117	0.962261	-0.988368
H10	3.759858	1.913154	0.371003
N11	1.459336	1.280143	0.305820
C12	0.304324	0.778633	-0.058938
C13	-1.034956	2.909644	0.241571
H14	-0.767106	3.050560	1.289817
H15	-0.384875	3.516953	-0.389308
H16	-2.075346	3.189727	0.081288
C17	-1.926620	0.713930	-0.475026
O18	-3.092777	0.937864	-0.618803
N19	-1.357140	-0.687895	-0.690795
H20	4.560123	0.459617	0.445967
H21	-1.565339	-0.962478	-1.657698
C22	-2.090036	-1.708953	0.250150
H23	-3.121813	-1.698518	-0.104473
H24	-1.596779	-2.654228	0.018417
N25	-1.947420	-1.295133	1.582382
H26	-2.795518	-1.016136	2.051529
H27	-1.349968	-1.864685	2.161181

Zero-point correction= 0.222706
Thermal correction to Energy= 0.237194
Thermal correction to Enthalpy= 0.238138
Thermal correction to Gibbs Free Energy= 0.180832
Sum of electronic and zero-point Energies= -752.238820
Sum of electronic and thermal Energies= -752.224332
Sum of electronic and thermal Enthalpies= -752.223388
Sum of electronic and thermal Free Energies= -752.280694

67 TS_N7-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-0.664969	1.772703	0.106957
C2	-0.083496	-0.310356	-0.494882
C3	0.721358	-1.461810	-0.469497
O4	0.380571	-2.646366	-0.660234
N5	2.059792	-1.169203	-0.144261
H6	2.573925	-2.004361	0.113636
C7	2.448122	0.061929	0.427195
N8	3.813921	0.500218	-0.068449
H9	3.841037	0.618269	-1.091541
H10	3.993760	1.412266	0.360335
N11	1.622698	1.141421	0.445713
C12	0.392737	0.890137	0.045688
C13	-0.606969	3.142825	0.583039
H14	-0.186857	3.166750	1.589843
H15	0.011634	3.749424	-0.081812
H16	-1.623979	3.534388	0.591262
C17	-1.806794	1.185599	-0.422640
O18	-2.891237	1.692843	-0.580817
N19	-1.470915	-0.161531	-0.741510
H20	4.559651	-0.142364	0.203305
H21	-1.828124	-0.441447	-1.649740
C22	-2.597981	-1.987990	0.517556
H23	-3.369349	-1.401271	1.005057
H24	-2.729362	-2.318342	-0.503910
N25	-1.598336	-2.447450	1.182039
H26	-1.459772	-2.211190	2.156802
H27	-0.834439	-2.909045	0.652995

Zero-point correction= 0.219674
Thermal correction to Energy= 0.234100
Thermal correction to Enthalpy= 0.235044
Thermal correction to Gibbs Free Energy= 0.177729
Sum of electronic and zero-point Energies= -752.235617
Sum of electronic and thermal Energies= -752.221191
Sum of electronic and thermal Enthalpies= -752.220247
Sum of electronic and thermal Free Energies= -752.277562

68 C8-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-0.706593	-1.341974	0.583626
C2	0.218623	0.767091	0.106092
C3	1.393103	1.607423	0.010745
O4	1.415573	2.821127	0.031445
N5	2.614570	0.877098	-0.112594
H6	3.451234	1.443503	-0.190488
C7	2.585697	-0.473776	-0.136679
N8	3.898210	-1.146909	-0.356445
H9	4.577622	-0.941852	0.385548
H10	3.696104	-2.155257	-0.343751
N11	1.603848	-1.254278	-0.004758
C12	0.330590	-0.670542	0.236600
C13	-0.724626	-2.774289	0.696298
H14	0.187631	-3.272291	0.352097
H15	-0.909536	-3.028512	1.745301
H16	-1.593603	-3.127942	0.133153
C17	-2.283738	0.855091	0.125387
O18	-3.116581	1.215774	0.915051
N19	-0.964259	1.409298	0.220774
H20	-0.925385	2.375863	0.535362
H21	4.319147	-0.908650	-1.262043
C22	-2.608500	0.049359	-1.113962
H23	-2.999323	0.809816	-1.814374
H24	-1.703270	-0.361023	-1.566707
N25	-3.544116	-1.012964	-0.801745
H26	-4.019671	-1.328487	-1.639210
H27	-4.251391	-0.674424	-0.155759

Zero-point correction= 0.218434
Thermal correction to Energy= 0.233842
Thermal correction to Enthalpy= 0.234786
Thermal correction to Gibbs Free Energy= 0.175275
Sum of electronic and zero-point Energies= -752.223767
Sum of electronic and thermal Energies= -752.208359

Sum of electronic and thermal Enthalpies= -752.207415
Sum of electronic and thermal Free Energies= -752.266926

69 TS_C8-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	0.997597	-0.819473	-0.438565
C2	-0.405447	0.907228	-0.222043
C3	-1.670814	1.538523	0.019341
O4	-1.949590	2.715791	0.076470
N5	-2.704893	0.544464	0.183281
H6	-3.628205	0.933494	0.342762
C7	-2.446097	-0.777190	0.127804
N8	-3.599064	-1.694500	0.287907
H9	-4.305490	-1.578376	-0.448856
H10	-3.210964	-2.644544	0.215935
N11	-1.321861	-1.359485	-0.054674
C12	-0.267256	-0.494846	-0.229318
C13	1.586512	-2.116345	-0.651543
H14	0.805954	-2.875139	-0.709840
H15	2.163668	-2.071298	-1.579186
H16	2.281181	-2.322545	0.169959
C17	1.893868	0.429272	-0.438230
O18	2.843102	0.476194	-1.245209
N19	0.788010	1.457285	-0.465104
H20	0.971967	2.450939	-0.493661
H21	-4.060946	-1.602527	1.200631
C22	2.450720	0.530632	1.130355
H23	2.883988	1.537738	1.127016
H24	1.622284	0.475411	1.842574
N25	3.373655	-0.523417	1.351570
H26	3.480143	-0.797697	2.317874
H27	4.265297	-0.379096	0.895613

Zero-point correction= 0.217017
Thermal correction to Energy= 0.231458
Thermal correction to Enthalpy= 0.232402
Thermal correction to Gibbs Free Energy= 0.175882
Sum of electronic and zero-point Energies= -752.199698
Sum of electronic and thermal Energies= -752.185257
Sum of electronic and thermal Enthalpies= -752.184313
Sum of electronic and thermal Free Energies= -752.240833

70 O8-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-0.553213	-1.358086	-0.023137
C2	0.342845	0.681942	-0.000941
C3	1.352722	1.691788	-0.075063
O4	1.201833	2.899682	-0.093423
N5	2.632545	1.095261	-0.137373
H6	3.326291	1.743623	-0.492873
C7	2.847120	-0.292271	-0.339505
N8	4.088697	-0.750937	0.407526
H9	4.029729	-0.565194	1.419441
H10	4.145771	-1.763516	0.271963
N11	1.861415	-1.210572	-0.142892
C12	0.659295	-0.661948	-0.058269
C13	-0.700167	-2.805571	-0.084956
H14	0.030837	-3.190201	-0.796228
H15	-0.520298	-3.244341	0.897952
H16	-1.709723	-3.044253	-0.416256
C17	-1.547757	-0.450275	0.058713
O18	-2.801819	-0.820491	0.149212
N19	-1.045115	0.780623	0.066847
H20	-1.621206	1.599400	0.232958
H21	4.943784	-0.324573	0.047340
C22	-3.859383	0.089264	-0.297264
H23	-3.748853	0.210442	-1.377484
H24	-4.752480	-0.494770	-0.071724
N25	-3.775989	1.358384	0.349007
H26	-4.272802	1.401125	1.230799
H27	-4.077583	2.118449	-0.248347

Zero-point correction= 0.222637
Thermal correction to Energy= 0.237091
Thermal correction to Enthalpy= 0.238036
Thermal correction to Gibbs Free Energy= 0.180647
Sum of electronic and zero-point Energies= -752.246786
Sum of electronic and thermal Energies= -752.232332
Sum of electronic and thermal Enthalpies= -752.231388
Sum of electronic and thermal Free Energies= -752.288776

71 TS_O8-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-0.548033	1.455121	-0.136336
C2	0.306362	-0.591177	-0.429482
C3	1.230299	-1.655857	-0.267866
O4	1.034634	-2.853458	-0.428296
N5	2.496470	-1.164247	0.138857
H6	3.070574	-1.903134	0.529342
C7	2.699002	0.154686	0.608255
N8	4.059673	0.678443	0.162307
H9	4.158648	0.679107	-0.863080
H10	4.114581	1.646045	0.489570
N11	1.779335	1.139793	0.419977
C12	0.615207	0.693909	-0.025885
C13	-0.668495	2.866519	0.177651
H14	-0.379145	3.041619	1.215519
H15	-0.022142	3.452432	-0.478484
H16	-1.707452	3.155778	0.021148
C17	-1.570454	0.672266	-0.609250
O18	-2.732933	1.011180	-0.828569
N19	-1.078240	-0.636610	-0.726544
H20	-1.384148	-1.153365	-1.544457
H21	4.835458	0.149912	0.563209
C22	-4.140275	-0.764675	0.488835
H23	-4.986059	-0.315699	0.999924
H24	-4.109637	-0.801307	-0.592416
N25	-3.184616	-1.277334	1.168991
H26	-2.330815	-1.590285	0.687174
H27	-3.175482	-1.243072	2.183148

Zero-point correction= 0.219222
Thermal correction to Energy= 0.234152
Thermal correction to Enthalpy= 0.235096
Thermal correction to Gibbs Free Energy= 0.176030
Sum of electronic and zero-point Energies= -752.226935
Sum of electronic and thermal Energies= -752.212005
Sum of electronic and thermal Enthalpies= -752.211061
Sum of electronic and thermal Free Energies= -752.270128

72 N9-CH_2NH_2[9MOG + H_{N2}]$^{\bullet+}$

N1	-1.347770	-0.594396	-0.339837
C2	0.281047	1.004264	-0.118498
C3	1.594396	1.543336	0.072926
O4	1.908330	2.714769	0.151013
N5	2.552800	0.503684	0.173560
H6	3.407216	0.831115	0.611202
C7	2.205881	-0.861973	0.312858
N8	3.252580	-1.752035	-0.313851
H9	2.903941	-2.711797	-0.244721
N10	0.968829	-1.314893	-0.022144
C11	0.086390	-0.346277	-0.148599
C12	-1.645597	-1.325480	-1.607480
H13	-1.192112	-0.787352	-2.439968
H14	-1.216420	-2.324310	-1.529568
H15	-2.727806	-1.367873	-1.732222

C16	-1.972093	0.825341	-0.388808
O17	-3.155194	0.963284	-0.510015
N18	-0.942389	1.675769	-0.280651
H19	-1.061400	2.679143	-0.251650
H20	4.150300	-1.700255	0.171349
C21	-1.966713	-1.342270	0.881238
H22	-3.018103	-1.457527	0.612898
H23	-1.455400	-2.306782	0.875175
N24	-1.773582	-0.597642	2.052700
H25	-2.600007	-0.216287	2.486169
H26	-1.099182	-0.950206	2.712932
H27	3.410753	-1.537355	-1.309837

Zero-point correction= 0.221355
Thermal correction to Energy= 0.235773
Thermal correction to Enthalpy= 0.236717
Thermal correction to Gibbs Free Energy= 0.180310
Sum of electronic and zero-point Energies= -752.225166
Sum of electronic and thermal Energies= -752.210749
Sum of electronic and thermal Enthalpies= -752.209805
Sum of electronic and thermal Free Energies= -752.266211

73 TS_N9-CH_2NH_2[9MOG + H_{N2}]$^{\cdot+}$

N1	-1.073694	-0.818332	-0.456110
C2	0.368714	0.886840	-0.299433
C3	1.597954	1.559055	-0.045228
O4	1.822404	2.758001	-0.084890
N5	2.612100	0.628178	0.294068
H6	3.385606	1.078462	0.769940
C7	2.365598	-0.740425	0.557372
N8	3.530819	-1.589638	0.070779
H9	3.263647	-2.564597	0.226383
N10	1.206362	-1.343594	0.176385
C11	0.260040	-0.481495	-0.168827
C12	-1.481534	-2.147018	-0.894770
H13	-0.961983	-2.421397	-1.816101
H14	-1.235979	-2.879079	-0.123200
H15	-2.555689	-2.128350	-1.085465
C16	-1.752855	0.347603	-0.886343
O17	-2.940183	0.387980	-1.187527
N18	-0.876863	1.376928	-0.721167
H19	-1.063412	2.319030	-1.030874
H20	4.394839	-1.400855	0.580782
C21	-2.388172	-0.602089	1.718769
H22	-2.858160	-1.470253	1.272709
H23	-1.485910	-0.701139	2.312850
N24	-2.985279	0.532591	1.643374
H25	-3.780367	0.654050	1.016622
H26	-2.583867	1.370647	2.051052
H27	3.710922	-1.462118	-0.935922

Zero-point correction= 0.218841
Thermal correction to Energy= 0.233851
Thermal correction to Enthalpy= 0.234795
Thermal correction to Gibbs Free Energy= 0.175776
Sum of electronic and zero-point Energies= -752.220748
Sum of electronic and thermal Energies= -752.205739
Sum of electronic and thermal Enthalpies= -752.204795
Sum of electronic and thermal Free Energies= -752.263814

74 [9MOG + H_{N3}]$^{+}\cdots{}^{\cdot}CH_2NH_2$

N1	0.237985	-1.583753	0.089995
C2	1.609239	0.158737	-0.052849
C3	1.982490	1.530651	-0.093930
O4	3.069025	2.047664	-0.181136
N5	0.803080	2.372534	-0.003231
H6	1.021888	3.363097	-0.012045
C7	-0.472356	1.974332	0.092961
N8	-1.469341	2.862488	0.159663
H9	-1.294054	3.854831	0.134582
H10	-2.422756	2.556152	0.276548
N11	-0.746166	0.659232	0.121415
C12	0.304991	-0.232324	0.055399
C13	-0.925366	-2.436471	0.241184
H14	-0.571172	-3.464417	0.152769
H15	-1.379619	-2.296998	1.226107
H16	-1.658042	-2.231659	-0.542106
C17	1.561683	-2.108399	0.001765
O18	1.852297	-3.278682	0.007925
N19	2.371984	-0.995591	-0.086651
H20	3.376856	-1.046111	-0.159459
H21	-1.747106	0.356686	0.123765
C22	-3.770263	0.209734	0.043597
H23	-3.971775	0.400350	1.094948
H24	-3.981409	1.006379	-0.666995
N25	-4.033532	-1.062859	-0.403626
H26	-4.323127	-1.776929	0.247258
H27	-4.310841	-1.215158	-1.361398

Zero-point correction= 0.215772
Thermal correction to Energy= 0.232253
Thermal correction to Enthalpy= 0.233197
Thermal correction to Gibbs Free Energy= 0.170353
Sum of electronic and zero-point Energies= -752.290053
Sum of electronic and thermal Energies= -752.273572
Sum of electronic and thermal Enthalpies= -752.272628
Sum of electronic and thermal Free Energies= -752.335472

75 TS_[9MOG + H_{N3}]$^{+}\cdots{}^{\cdot}CH_2NH_2$

N1	1.533282	0.315681	-0.545195
C2	0.146978	-1.271360	0.159081
C3	-1.109515	-1.922826	0.337803
O4	-1.361193	-3.022414	0.772424
N5	-2.180777	-1.068853	-0.112996
H6	-3.093317	-1.509503	-0.067929
C7	-2.049112	0.184892	-0.589803
N8	-3.140552	0.910506	-0.879913
H9	-4.069924	0.530463	-0.788371
H10	-3.030955	1.735445	-1.450185
N11	-0.846455	0.762242	-0.746759
C12	0.219588	-0.023465	-0.399995
C13	2.092250	1.485597	-1.197351
H14	3.034134	1.194401	-1.663793
H15	1.397854	1.842344	-1.959522
H16	2.301014	2.283649	-0.478483
C17	2.340709	-0.754361	-0.085508
O18	3.548369	-0.779309	-0.085492
N19	1.441768	-1.714430	0.346468
H20	1.723426	-2.627416	0.671023
H21	-0.740323	1.959530	-0.028246
C22	-0.508863	2.879473	0.854381
H23	0.093725	3.585005	0.279476
H24	-1.506686	3.240142	1.108809
N25	0.159732	2.308291	1.910414
H26	1.165183	2.210604	1.910456
H27	-0.332729	1.907371	2.695519

Zero-point correction= 0.212619
Thermal correction to Energy= 0.227714
Thermal correction to Enthalpy= 0.228658
Thermal correction to Gibbs Free Energy= 0.170125
Sum of electronic and zero-point Energies= -752.282372
Sum of electronic and thermal Energies= -752.267277

Sum of electronic and thermal Enthalpies= -752.266333
Sum of electronic and thermal Free Energies= -752.324866

76 [9MOG + H_{N3}]$^+$

N1	1.549759	-0.779025	-0.000034
C2	0.096633	0.905617	-0.000041
C3	-1.183239	1.528130	-0.000018
O4	-1.493491	2.691300	-0.000063
N5	-2.234638	0.517154	0.000076
H6	-3.166303	0.920112	0.000093
C7	-2.090779	-0.811580	0.000132
N8	-3.147312	-1.627072	0.000215
H9	-4.088114	-1.262166	0.000240
H10	-3.048361	-2.630827	0.000254
N11	-0.840007	-1.317681	0.000103
C12	0.238740	-0.450766	0.000015
C13	2.163462	-2.095288	0.000001
H14	3.242711	-1.934914	-0.000153
H15	1.892089	-2.651536	0.901302
H16	1.891857	-2.651686	-0.901138
C17	2.316317	0.428515	-0.000125
O18	3.518307	0.492233	-0.000185
N19	1.373396	1.437375	-0.000127
H20	1.613280	2.417637	-0.000182
H21	-0.690881	-2.317904	0.000150

Zero-point correction= 0.163097
Thermal correction to Energy= 0.175053
Thermal correction to Enthalpy= 0.175997
Thermal correction to Gibbs Free Energy= 0.125420
Sum of electronic and zero-point Energies= -657.136074
Sum of electronic and thermal Energies= -657.124118
Sum of electronic and thermal Enthalpies= -657.123174
Sum of electronic and thermal Free Energies= -657.173752

77 N1-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-2.078453	0.755688	0.162693
C2	-0.609777	-0.870596	-0.247876
C3	0.625727	-1.482111	-0.446528
O4	0.989909	-2.617548	-0.614036
N5	1.790154	-0.418603	-0.317563
H6	2.503111	-0.766970	-0.965746
C7	1.440220	0.931954	-0.741005
N8	2.441096	1.838773	-0.983124
H9	3.371604	1.589091	-0.670751
H10	2.401905	2.353291	-1.853775
N11	0.240130	1.383100	-0.175263
C12	-0.781790	0.496834	-0.079358
C13	-2.712748	2.045856	0.368863
H14	-3.773115	1.852246	0.535312
H15	-2.298369	2.541130	1.250409
H16	-2.601098	2.676691	-0.516835
C17	-2.818641	-0.475388	0.137846
O18	-4.005515	-0.568875	0.317763
N19	-1.880736	-1.440433	-0.127533
H20	-2.105576	-2.421010	-0.192108
H21	0.096109	2.380794	-0.094118
C22	2.400250	-0.539058	1.112608
H23	2.486640	-1.615828	1.270008
H24	1.638937	-0.123430	1.775075
N25	3.635826	0.154049	1.168394
H26	4.446005	-0.441270	1.277460
H27	3.663127	0.913683	1.834724

Zero-point correction= 0.220382
Thermal correction to Energy= 0.235218
Thermal correction to Enthalpy= 0.236163
Thermal correction to Gibbs Free Energy= 0.178877
Sum of electronic and zero-point Energies= -752.254746
Sum of electronic and thermal Energies= -752.239910
Sum of electronic and thermal Enthalpies= -752.238966
Sum of electronic and thermal Free Energies= -752.296252

78 TS_N1-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	2.187006	-0.507933	0.214813
C2	0.439580	0.736377	-0.375641
C3	-0.899397	1.026069	-0.703357
O4	-1.431556	2.085065	-0.981404
N5	-1.759614	-0.151115	-0.527392
H6	-2.581329	-0.048653	-1.121229
C7	-1.235806	-1.476593	-0.610860
N8	-2.160585	-2.501640	-0.426555
H9	-2.505091	-2.940862	-1.271403
H10	-1.933174	-3.188683	0.283013
N11	0.042113	-1.624709	-0.050128
C12	0.866787	-0.535315	-0.065719
C13	3.053623	-1.613295	0.580515
H14	4.043478	-1.190204	0.756421
H15	2.699802	-2.091984	1.497011
H16	3.121393	-2.341783	-0.232098
C17	2.666420	0.833323	0.075095
O18	3.806677	1.185136	0.250500
N19	1.558165	1.563566	-0.280110
H20	1.591796	2.549837	-0.484914
H21	0.459061	-2.543849	-0.121193
C22	-2.668175	0.275875	1.259189
H23	-1.716413	0.394054	1.765999
H24	-3.160288	-0.689414	1.313514
N25	-3.431428	1.349725	1.146924
H26	-3.023389	2.275294	1.143535
H27	-4.384602	1.280740	0.820382

Zero-point correction= 0.218797
Thermal correction to Energy= 0.233483
Thermal correction to Enthalpy= 0.234427
Thermal correction to Gibbs Free Energy= 0.176860
Sum of electronic and zero-point Energies= -752.252568
Sum of electronic and thermal Energies= -752.237882
Sum of electronic and thermal Enthalpies= -752.236938
Sum of electronic and thermal Free Energies= -752.294505

79 C2-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	1.739572	-1.006573	-0.166808
C2	0.768506	0.998392	0.071322
C3	-0.310983	1.988168	0.037915
O4	-0.124170	3.176388	0.198809
N5	-1.517416	1.407333	-0.265275
H6	-2.298973	2.044666	-0.367786
C7	-1.886623	-0.002632	-0.285356
N8	-2.826060	-0.183351	-1.332008
H9	-3.275842	-1.090855	-1.316085
H10	-2.455150	0.020258	-2.253025
N11	-0.651262	-0.839588	-0.478775
C12	0.552049	-0.371808	-0.211004
C13	2.005078	-2.419695	-0.403004
H14	3.069511	-2.582240	-0.234116
H15	1.432688	-3.032642	0.296631
H16	1.759346	-2.680771	-1.434583
C17	2.760052	-0.063264	0.138481
O18	3.929795	-0.285932	0.255008
N19	2.088407	1.162307	0.275216
H20	2.554702	2.038561	0.480508
H21	-0.851702	-1.836444	-0.483989

C22	-2.501746	-0.458125	1.060074
H23	-1.790159	-0.205661	1.851575
H24	-3.408640	0.133336	1.224644
N25	-2.736746	-1.895659	1.023826
H26	-2.460703	-2.347681	1.886875
H27	-3.713538	-2.121685	0.875007

Zero-point correction= 0.221475
Thermal correction to Energy= 0.235686
Thermal correction to Enthalpy= 0.236630
Thermal correction to Gibbs Free Energy= 0.180112
Sum of electronic and zero-point Energies= -752.311603
Sum of electronic and thermal Energies= -752.297392
Sum of electronic and thermal Enthalpies= -752.296448
Sum of electronic and thermal Free Energies= -752.352965

80 TS_C2-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-1.745513	-0.913675	0.272297
C2	-0.711507	1.032948	-0.033847
C3	0.366837	1.971948	-0.006082
O4	0.369058	3.140993	-0.316066
N5	1.567382	1.349337	0.470697
H6	2.388994	1.940831	0.410340
C7	1.763758	0.018577	0.683482
N8	2.953544	-0.363112	1.252881
H9	3.132663	-1.353537	1.330195
H10	3.288129	0.184753	2.035384
N11	0.634145	-0.751074	0.841236
C12	-0.561851	-0.259854	0.380916
C13	-2.061164	-2.282021	0.635292
H14	-3.119668	-2.429293	0.415893
H15	-1.476316	-2.988319	0.039365
H16	-1.896195	-2.450545	1.702867
C17	-2.721483	-0.004879	-0.233217
O18	-3.879969	-0.266756	-0.442501
N19	-2.033981	1.177500	-0.417491
H20	-2.469439	2.025967	-0.746816
H21	0.725951	-1.707752	1.150511
C22	2.286016	-0.624866	-1.460678
H23	1.339717	-0.302558	-1.885278
H24	3.132043	0.050862	-1.511781
N25	2.552111	-1.954990	-1.469865
H26	1.875182	-2.606772	-1.837092
H27	3.508786	-2.276577	-1.478548

Zero-point correction= 0.216574
Thermal correction to Energy= 0.231879
Thermal correction to Enthalpy= 0.232823
Thermal correction to Gibbs Free Energy= 0.173895
Sum of electronic and zero-point Energies= -752.272451
Sum of electronic and thermal Energies= -752.257146
Sum of electronic and thermal Enthalpies= -752.256202
Sum of electronic and thermal Free Energies= -752.315130

81 N2-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-1.752608	-0.964310	0.254338
C2	-0.793829	1.006243	-0.128467
C3	0.198950	2.026085	-0.002162
O4	0.115804	3.202202	-0.280041
N5	1.416588	1.498740	0.533160
H6	2.039670	2.239193	0.838406
C7	1.635203	0.219757	1.026782
N8	2.961451	-0.334076	0.552014
H9	3.684224	0.341173	0.815025
H10	3.168620	-1.197618	1.062512
N11	0.601733	-0.697271	0.850832
C12	-0.598108	-0.256973	0.354567
C13	-2.009393	-2.336412	0.646090
H14	-3.057178	-2.537014	0.417441
H15	-1.382916	-3.028807	0.076982
H16	-1.853086	-2.472747	1.719872
C17	-2.755195	-0.124613	-0.313466
O18	-3.895001	-0.451390	-0.540574
N19	-2.119388	1.077732	-0.532259
H20	-2.583358	1.889573	-0.910203
H21	0.633616	-1.570560	1.359646
C22	3.065282	-0.673666	-0.963425
H23	2.516966	0.130061	-1.459927
H24	4.127294	-0.595415	-1.202823
N25	2.551381	-1.970536	-1.178494
H26	1.662024	-2.008064	-1.655360
H27	3.206144	-2.630754	-1.573298

Zero-point correction= 0.221902
Thermal correction to Energy= 0.236527
Thermal correction to Enthalpy= 0.237472
Thermal correction to Gibbs Free Energy= 0.179362
Sum of electronic and zero-point Energies= -752.254339
Sum of electronic and thermal Energies= -752.239713
Sum of electronic and thermal Enthalpies= -752.238769
Sum of electronic and thermal Free Energies= -752.296878

82 TS_N2-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	1.892913	-0.864093	-0.145872
C2	0.599742	0.941048	-0.018543
C3	-0.512373	1.778305	-0.355293
O4	-0.609951	2.982734	-0.235594
N5	-1.592863	1.016307	-0.876243
H6	-2.338753	1.583392	-1.262280
C7	-1.614319	-0.353856	-1.054603
N8	-2.816987	-1.019153	-0.824867
H9	-3.620483	-0.574334	-1.260508
H10	-2.792169	-1.998974	-1.092861
N11	-0.440040	-1.081456	-0.845794
C12	0.644446	-0.377933	-0.366239
C13	2.395200	-2.204595	-0.376556
H14	3.390006	-2.251156	0.068703
H15	1.751139	-2.944073	0.106580
H16	2.481460	-2.414854	-1.446314
C17	2.713491	0.188786	0.354211
O18	3.878911	0.083751	0.655987
N19	1.877095	1.279227	0.420135
H20	2.185130	2.195829	0.705699
H21	-0.248172	-1.851637	-1.477330
C22	-3.207563	-0.953963	1.423365
H23	-4.076088	-0.320335	1.302316
H24	-3.343029	-2.024746	1.497294
N25	-2.107541	-0.420245	1.928123
H26	-2.010202	0.578545	2.042590
H27	-1.330311	-0.990399	2.226538

Zero-point correction= 0.216780
Thermal correction to Energy= 0.232217
Thermal correction to Enthalpy= 0.233162
Thermal correction to Gibbs Free Energy= 0.173053
Sum of electronic and zero-point Energies= -752.250177
Sum of electronic and thermal Energies= -752.234740
Sum of electronic and thermal Enthalpies= -752.233795
Sum of electronic and thermal Free Energies= -752.293904

83 C4-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	1.554765	-0.317218	-0.463629

C2	-0.014730	1.091271	0.377257
C3	-1.316637	1.650430	0.341266
O4	-1.640391	2.808305	0.516684
N5	-2.321167	0.673833	0.002148
H6	-3.262914	1.047828	-0.023465
C7	-2.051244	-0.508689	-0.582214
N8	-3.049715	-1.245985	-1.070812
H9	-3.996548	-0.899389	-1.098649
H10	-2.867923	-2.121463	-1.537999
N11	-0.789934	-0.946566	-0.667720
C12	0.263963	-0.371605	0.186380
C13	2.383444	-1.471250	-0.770171
H14	3.176208	-1.139931	-1.440821
H15	2.848796	-1.895846	0.126417
H16	1.789709	-2.233093	-1.277970
C17	2.141777	0.925943	-0.317861
O18	3.260138	1.258436	-0.603834
N19	1.145939	1.765852	0.242070
H20	1.238227	2.773695	0.257048
H21	-0.673306	-1.954994	-0.760444
C22	0.278763	-1.197081	1.511269
H23	1.156862	-0.892589	2.092081
H24	-0.608650	-0.916589	2.087002
N25	0.223163	-2.620628	1.204017
H26	1.138522	-3.055073	1.207188
H27	-0.350321	-3.125622	1.868728

Zero-point correction= 0.222020
Thermal correction to Energy= 0.236069
Thermal correction to Enthalpy= 0.237013
Thermal correction to Gibbs Free Energy= 0.181557
Sum of electronic and zero-point Energies= -752.311615
Sum of electronic and thermal Energies= -752.297566
Sum of electronic and thermal Enthalpies= -752.296622
Sum of electronic and thermal Free Energies= -752.352078

84 TS_C4-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-1.534929	0.350611	-0.585945
C2	-0.094645	-1.139609	0.248019
C3	1.158265	-1.795393	0.308720
O4	1.435421	-2.933195	0.614361
N5	2.230842	-0.905188	-0.114842
H6	3.139693	-1.355762	-0.128420
C7	2.090017	0.329172	-0.604488
N8	3.157876	1.055769	-0.955754
H9	4.089959	0.675933	-0.889009
H10	3.046297	1.895223	-1.504386
N11	0.860758	0.867357	-0.724037
C12	-0.230779	0.184927	-0.158689
C13	-2.165165	1.574615	-1.031008
H14	-3.154370	1.311605	-1.406763
H15	-2.285407	2.289048	-0.209753
H16	-1.585886	2.027007	-1.839410
C17	-2.289172	-0.782343	-0.216521
O18	-3.484318	-0.909636	-0.319868
N19	-1.360392	-1.679972	0.292842
H20	-1.600685	-2.613824	0.590654
H21	0.810463	1.885372	-0.630502
C22	-0.252436	1.471692	1.741647
H23	-1.315620	1.363987	1.929179
H24	0.417184	0.888259	2.364147
N25	0.211984	2.713847	1.320926
H26	-0.481771	3.446136	1.238058
H27	1.051838	3.054329	1.771844

Zero-point correction= 0.216994
Thermal correction to Energy= 0.231884
Thermal correction to Enthalpy= 0.232829
Thermal correction to Gibbs Free Energy= 0.175265
Sum of electronic and zero-point Energies= -752.270899
Sum of electronic and thermal Energies= -752.256009
Sum of electronic and thermal Enthalpies= -752.255064
Sum of electronic and thermal Free Energies= -752.312628

85 C5-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	1.637703	-0.896504	0.162487
C2	0.126299	0.888501	0.230901
C3	-0.855427	1.037658	-0.937166
O4	-0.898790	1.984103	-1.674266
N5	-1.769765	-0.024826	-1.097257
H6	-2.490466	0.131782	-1.792697
C7	-1.786820	-1.157556	-0.357659
N8	-2.864303	-1.942547	-0.386462
H9	-3.722222	-1.635995	-0.819269
H10	-2.873838	-2.846349	0.061014
N11	-0.712146	-1.472882	0.365302
C12	0.358804	-0.567797	0.539086
C13	2.281101	-2.185895	0.310097
H14	3.279623	-2.099170	-0.119516
H15	2.367180	-2.459616	1.365771
H16	1.724493	-2.953940	-0.234734
C17	2.348046	0.263990	-0.231725
O18	3.503680	0.289488	-0.568032
N19	1.453339	1.303561	-0.141766
H20	1.658536	2.199831	-0.557848
H21	-0.760851	-2.284275	0.968114
C22	-0.434498	1.693556	1.434093
H23	0.317126	1.634825	2.227343
H24	-0.511179	2.740752	1.125164
N25	-1.735318	1.168367	1.833033
H26	-1.689477	0.701584	2.730355
H27	-2.429643	1.900920	1.911563

Zero-point correction= 0.220325
Thermal correction to Energy= 0.235243
Thermal correction to Enthalpy= 0.236187
Thermal correction to Gibbs Free Energy= 0.178298
Sum of electronic and zero-point Energies= -752.298320
Sum of electronic and thermal Energies= -752.283403
Sum of electronic and thermal Enthalpies= -752.282458
Sum of electronic and thermal Free Energies= -752.340347

86 TS_C5-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-1.800145	0.816628	0.145615
C2	-0.148949	-0.664816	-0.297047
C3	1.102266	-0.901414	-0.982873
O4	1.450370	-1.876819	-1.603220
N5	2.027558	0.174462	-0.788220
H6	2.953663	-0.019265	-1.151702
C7	1.775689	1.368781	-0.217871
N8	2.764716	2.256880	-0.005027
H9	3.691638	2.078541	-0.359249
H10	2.559465	3.214114	0.236479
N11	0.520494	1.622497	0.182885
C12	-0.448999	0.651350	0.056300
C13	-2.540717	2.000072	0.530913
H14	-3.599321	1.761466	0.418562
H15	-2.347562	2.261046	1.575548
H16	-2.300454	2.841789	-0.126338
C17	-2.426496	-0.381735	-0.282624
O18	-3.616381	-0.574900	-0.329228
N19	-1.389620	-1.231562	-0.614762
H20	-1.546893	-2.188066	-0.891816
H21	0.296418	2.513214	0.606706

C22	0.435487	-1.890986	1.490839
H23	-0.363922	-1.512207	2.120233
H24	0.256747	-2.834973	0.984951
N25	1.726017	-1.648341	1.904915
H26	1.868288	-1.180133	2.786795
H27	2.427190	-2.343220	1.695742

Zero-point correction= 0.215698
Thermal correction to Energy= 0.231439
Thermal correction to Enthalpy= 0.232383
Thermal correction to Gibbs Free Energy= 0.172531
Sum of electronic and zero-point Energies= -752.264150
Sum of electronic and thermal Energies= -752.248409
Sum of electronic and thermal Enthalpies= -752.247465
Sum of electronic and thermal Free Energies= -752.307317

87 C6-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-2.180961	0.365317	0.034215
C2	-0.200659	-0.675589	0.112194
C3	1.254874	-0.729643	-0.210504
O4	1.127080	-0.759110	-1.530330
N5	1.809189	0.597655	0.284961
H6	2.822537	0.539397	0.420199
C7	1.192156	1.744722	0.117596
N8	1.827851	2.921680	0.126142
H9	2.835792	2.953729	0.133114
H10	1.336787	3.793104	0.251801
N11	-0.166518	1.745663	-0.040533
C12	-0.842872	0.546204	0.021864
C13	-3.236628	1.362589	-0.011657
H14	-4.180508	0.835372	0.130725
H15	-3.108315	2.089271	0.794273
H16	-3.255719	1.861072	-0.984147
C17	-2.442917	-1.030011	0.105807
O18	-3.528683	-1.546701	0.140678
N19	-1.186367	-1.622799	0.163224
H20	-1.069724	-2.623294	0.214885
H21	-0.631236	2.575206	-0.381935
C22	2.142640	-1.800217	0.436688
H23	1.951484	-1.825139	1.513847
H24	1.859836	-2.766660	0.002505
N25	3.535618	-1.426244	0.214799
H26	4.156161	-1.920757	0.844762
H27	3.824475	-1.642051	-0.734399

Zero-point correction= 0.220124
Thermal correction to Energy= 0.234595
Thermal correction to Enthalpy= 0.235539
Thermal correction to Gibbs Free Energy= 0.179322
Sum of electronic and zero-point Energies= -752.267338
Sum of electronic and thermal Energies= -752.252866
Sum of electronic and thermal Enthalpies= -752.251922
Sum of electronic and thermal Free Energies= -752.308139

88 TS_C6-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	2.173117	0.391382	-0.169523
C2	0.230261	-0.593550	0.289779
C3	-1.232356	-0.739457	0.463251
O4	-1.708636	-1.360393	1.495007
N5	-1.821942	0.620283	0.246242
H6	-2.836003	0.589434	0.195857
C7	-1.195091	1.779516	0.094299
N8	-1.876966	2.933765	0.069807
H9	-2.854217	2.963256	0.314393
H10	-1.436917	3.803534	-0.185985
N11	0.144414	1.796798	-0.055007
C12	0.828420	0.582610	0.035149
C13	3.202850	1.388542	-0.384076
H14	4.148072	0.851166	-0.473263
H15	3.022916	1.940515	-1.310551
H16	3.272553	2.074656	0.465606
C17	2.453012	-0.978296	-0.008068
O18	3.541574	-1.503040	-0.058075
N19	1.214195	-1.569201	0.220532
H20	1.145882	-2.507877	0.583637
H21	0.648648	2.667405	0.035537
C22	-1.875770	-1.683479	-0.813610
H23	-1.297032	-1.340990	-1.672991
H24	-1.614707	-2.705628	-0.541604
N25	-3.247666	-1.420226	-0.962851
H26	-3.549897	-1.156417	-1.889053
H27	-3.876827	-2.076522	-0.521785

Zero-point correction= 0.217424
Thermal correction to Energy= 0.232332
Thermal correction to Enthalpy= 0.233277
Thermal correction to Gibbs Free Energy= 0.175543
Sum of electronic and zero-point Energies= -752.255977
Sum of electronic and thermal Energies= -752.241069
Sum of electronic and thermal Enthalpies= -752.240125
Sum of electronic and thermal Free Energies= -752.297858

89 O6-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-2.398738	-0.205727	0.084687
C2	-0.319588	0.626941	-0.075100
C3	1.073994	0.565733	-0.007055
O4	1.886775	1.525770	-0.504370
N5	1.588094	-0.777327	-0.063774
H6	2.616237	-0.783168	0.014423
C7	0.861929	-1.881520	-0.030187
N8	1.433722	-3.095307	-0.072678
H9	2.434774	-3.187567	-0.143003
H10	0.912490	-3.924806	0.164088
N11	-0.490851	-1.794666	0.043977
C12	-1.070054	-0.520718	-0.027391
C13	-3.540555	-1.097643	0.089740
H14	-4.426049	-0.477813	0.236048
H15	-3.636602	-1.622829	-0.865586
H16	-3.469012	-1.811743	0.914425
C17	-2.525506	1.196247	0.028728
O18	-3.556715	1.825832	0.039016
N19	-1.221279	1.672786	-0.044974
H20	-1.010448	2.652546	-0.149442
H21	-1.042774	-2.604589	-0.203734
C22	3.080782	1.781876	0.241688
H23	2.821009	1.985802	1.284787
H24	3.494785	2.677613	-0.224362
N25	3.969676	0.629771	0.191401
H26	4.553117	0.583527	1.020128
H27	4.581612	0.668006	-0.617958

Zero-point correction= 0.220186
Thermal correction to Energy= 0.235161
Thermal correction to Enthalpy= 0.236105
Thermal correction to Gibbs Free Energy= 0.178024
Sum of electronic and zero-point Energies= -752.278813
Sum of electronic and thermal Energies= -752.263838
Sum of electronic and thermal Enthalpies= -752.262894
Sum of electronic and thermal Free Energies= -752.320975

90 T S_O6-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	2.102877	0.262464	0.182850

C2	0.081871	-0.371061	-0.560603
C3	-1.312743	-0.286932	-0.755312
O4	-2.149511	-1.146517	-1.090943
N5	-1.794314	1.066615	-0.447157
H6	-2.777818	1.200933	-0.648006
C7	-1.070983	2.091297	-0.003948
N8	-1.624669	3.293624	0.208579
H9	-2.594542	3.466379	-0.003571
H10	-1.088178	4.068847	0.564263
N11	0.243146	1.908808	0.242742
C12	0.825133	0.681453	-0.108078
C13	3.252579	1.073722	0.531216
H14	4.104367	0.396886	0.611402
H15	3.464707	1.813461	-0.247176
H16	3.102868	1.565631	1.496303
C17	2.217080	-1.087028	-0.198008
O18	3.223526	-1.757348	-0.181477
N19	0.936253	-1.463770	-0.592943
H20	0.776981	-2.314299	-1.111219
H21	0.830829	2.709251	0.427304
C22	-2.622225	-2.413107	0.548797
H23	-2.340100	-3.275543	-0.036641
H24	-3.662630	-2.124259	0.591189
N25	-1.805239	-2.005016	1.530689
H26	-0.899620	-2.427900	1.660860
H27	-2.139639	-1.417602	2.276944

Zero-point correction= 0.214658
Thermal correction to Energy= 0.230770
Thermal correction to Enthalpy= 0.231714
Thermal correction to Gibbs Free Energy= 0.170531
Sum of electronic and zero-point Energies= -752.261147
Sum of electronic and thermal Energies= -752.245035
Sum of electronic and thermal Enthalpies= -752.244091
Sum of electronic and thermal Free Energies= -752.305274

91 N7-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	0.511866	1.601420	0.070185
C2	-0.063331	-0.577964	-0.239702
C3	-0.904881	-1.604705	0.179803
O4	-0.627871	-2.703786	0.638024
N5	-2.309536	-1.231720	0.066069
H6	-2.958211	-1.973598	0.299240
C7	-2.743797	0.027441	-0.073895
N8	-4.056530	0.289721	-0.068681
H9	-4.734444	-0.448048	0.042257
H10	-4.409210	1.233047	-0.106711
N11	-1.860625	1.023667	-0.250695
C12	-0.481337	0.758846	-0.495743
C13	0.522637	3.052862	-0.032805
H14	1.465772	3.418537	0.372914
H15	0.435106	3.352345	-1.080629
H16	-0.298008	3.476326	0.551507
C17	1.615881	0.908100	0.435940
O18	2.695485	1.284591	0.809796
N19	1.317362	-0.549547	0.182938
H20	-2.229042	1.915532	-0.552366
H21	1.460629	-1.090656	1.044597
C22	2.366276	-1.158077	-0.882630
H23	1.867719	-2.079403	-1.182740
H24	2.339861	-0.422535	-1.688263
N25	3.634510	-1.375666	-0.381630
H26	4.195055	-0.573936	-0.134160
H27	3.795858	-2.198190	0.178684

Zero-point correction= 0.220502
Thermal correction to Energy= 0.235435
Thermal correction to Enthalpy= 0.236380
Thermal correction to Gibbs Free Energy= 0.178345
Sum of electronic and zero-point Energies= -752.252315
Sum of electronic and thermal Energies= -752.237381
Sum of electronic and thermal Enthalpies= -752.236437
Sum of electronic and thermal Free Energies= -752.294471

92 TS_N7-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-0.493066	1.560539	-0.146890
C2	0.158696	-0.585331	-0.064404
C3	1.061361	-1.634524	-0.259582
O4	0.879688	-2.788719	-0.611685
N5	2.434768	-1.189578	-0.018117
H6	3.126777	-1.914163	-0.164442
C7	2.823569	0.080758	0.164205
N8	4.126188	0.374187	0.309234
H9	4.828628	-0.344219	0.233029
H10	4.450813	1.327970	0.324223
N11	1.900973	1.047479	0.253820
C12	0.525430	0.715906	0.314628
C13	-0.598430	2.986156	0.099794
H14	-1.558735	3.321068	-0.293181
H15	-0.551659	3.194896	1.172937
H16	0.198282	3.523205	-0.422109
C17	-1.567339	0.807778	-0.572247
O18	-2.677437	1.199195	-0.882849
N19	-1.183472	-0.549340	-0.438399
H20	2.197879	1.953453	0.588886
H21	-1.539479	-1.214272	-1.114979
C22	-2.846738	-1.153422	1.160690
H23	-2.341957	-2.078173	1.409446
H24	-2.595945	-0.243692	1.688506
N25	-3.986157	-1.201917	0.494413
H26	-4.455317	-0.345729	0.228145
H27	-4.311226	-2.057662	0.068880

Zero-point correction= 0.216180
Thermal correction to Energy= 0.231672
Thermal correction to Enthalpy= 0.232616
Thermal correction to Gibbs Free Energy= 0.172920
Sum of electronic and zero-point Energies= -752.245126
Sum of electronic and thermal Energies= -752.229635
Sum of electronic and thermal Enthalpies= -752.228690
Sum of electronic and thermal Free Energies= -752.288386

93 C8-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	0.627643	1.461227	0.547596
C2	-0.170748	-0.744238	0.105052
C3	-1.329572	-1.609161	0.028743
O4	-1.310297	-2.819401	0.073979
N5	-2.583485	-0.941814	-0.109263
H6	-3.381412	-1.564491	-0.171148
C7	-2.740065	0.385278	-0.178257
N8	-3.944810	0.918664	-0.373788
H9	-4.760263	0.339483	-0.508725
H10	-4.086177	1.917360	-0.396627
N11	-1.658034	1.160732	-0.048731
C12	-0.330922	0.686344	0.221201
C13	0.432623	2.890532	0.678797
H14	1.332636	3.332365	1.104775
H15	0.271839	3.360096	-0.301769
H16	-0.403384	3.142394	1.347133
C17	2.355194	-0.893556	0.087720
O18	3.205595	-1.357857	0.799411
N19	1.012129	-1.374115	0.260446
H20	-1.774300	2.163909	-0.101600
H21	0.954841	-2.345658	0.561737

C22	2.640869	0.032865	-1.089377
H23	3.088041	-0.616343	-1.852047
H24	1.714799	0.420653	-1.516924
N25	3.549860	1.113047	-0.801432
H26	3.232383	1.647290	-0.000585
H27	4.481216	0.768439	-0.598410

Zero-point correction= 0.218303
Thermal correction to Energy= 0.233784
Thermal correction to Enthalpy= 0.234729
Thermal correction to Gibbs Free Energy= 0.174713
Sum of electronic and zero-point Energies= -752.276325
Sum of electronic and thermal Energies= -752.260844
Sum of electronic and thermal Enthalpies= -752.259899
Sum of electronic and thermal Free Energies= -752.319915

94 TS_C8-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	1.006506	-0.805353	-0.490512
C2	-0.412551	0.907370	-0.266428
C3	-1.674601	1.505161	0.009624
O4	-1.986700	2.669056	0.089450
N5	-2.707686	0.490928	0.184663
C6	-2.555569	-0.834075	0.145882
N7	-3.589051	-1.660301	0.324130
H8	-4.520476	-1.304558	0.478537
H9	-3.487300	-2.662040	0.267385
N10	-1.319683	-1.332958	-0.068902
C11	-0.246348	-0.476628	-0.281397
C12	1.612927	-2.098872	-0.691295
H13	0.964607	-2.735207	-1.301923
H14	2.544724	-1.919111	-1.232352
H15	1.851411	-2.574300	0.264916
C16	1.894379	0.479852	-0.450475
O17	2.893117	0.512734	-1.185717
N18	0.787861	1.472709	-0.542047
H19	0.961938	2.467817	-0.503441
C20	2.365204	0.574344	1.172469
H21	2.849889	1.555870	1.172608
H22	1.479088	0.575388	1.813853
N23	3.206755	-0.517657	1.469837
H24	3.145045	-0.875999	2.411164
H25	4.161286	-0.411804	1.154829
H26	-1.168304	-2.332839	-0.075303
H27	-3.626805	0.887990	0.349391

Zero-point correction= 0.215938
Thermal correction to Energy= 0.230654
Thermal correction to Enthalpy= 0.231599
Thermal correction to Gibbs Free Energy= 0.174970
Sum of electronic and zero-point Energies= -752.242799
Sum of electronic and thermal Energies= -752.228083
Sum of electronic and thermal Enthalpies= -752.227138
Sum of electronic and thermal Free Energies= -752.283767

95 O8-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	0.810023	0.757065	-0.018201
C2	-0.662220	-0.921203	-0.028558
C3	-1.946669	-1.512564	-0.058166
O4	-2.293607	-2.671347	-0.102347
N5	-2.986390	-0.478174	-0.017871
H6	-3.923298	-0.866096	-0.046400
C7	-2.818329	0.841344	0.018517
N8	-3.857573	1.684644	0.035040
H9	-4.805598	1.341291	0.027309
H10	-3.733064	2.684600	0.052543
N11	-1.556667	1.323848	0.039652
C12	-0.489649	0.439769	0.022775
C13	1.389729	2.087041	0.011775
H14	2.473546	1.962925	-0.058499
H15	1.049512	2.677916	-0.845374
H16	1.146797	2.593120	0.950968
C17	1.578785	-0.452874	-0.154223
O18	2.630661	-0.603193	0.693924
N19	0.601417	-1.473705	-0.143277
H20	-1.390259	2.319458	0.090723
H21	0.824830	-2.419078	0.127754
C22	3.941604	-0.627494	0.082126
H23	4.575183	-1.009276	0.883796
H24	3.918009	-1.344060	-0.742850
N25	4.349468	0.664468	-0.378613
H26	4.627286	0.684108	-1.349741
H27	5.059171	1.100276	0.194565

Zero-point correction= 0.218959
Thermal correction to Energy= 0.234440
Thermal correction to Enthalpy= 0.235384
Thermal correction to Gibbs Free Energy= 0.176057
Sum of electronic and zero-point Energies= -752.248964
Sum of electronic and thermal Energies= -752.233483
Sum of electronic and thermal Enthalpies= -752.232539
Sum of electronic and thermal Free Energies= -752.291866

96 TS_O8-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	0.670815	-1.192538	-0.318773
C2	-0.392794	0.769191	-0.083905
C3	-1.488275	1.628563	-0.128711
O4	-1.591322	2.822300	-0.377888
N5	-2.736974	0.877705	0.162236
H6	-3.564429	1.460580	0.123113
C7	-2.857274	-0.443149	0.262138
N8	-4.054199	-1.018073	0.467133
H9	-4.891458	-0.458191	0.503385
H10	-4.177793	-2.013730	0.373360
N11	-1.754807	-1.215928	0.202597
C12	-0.488012	-0.602193	0.144361
C13	1.010715	-2.600988	-0.279637
H14	2.028168	-2.703349	-0.657737
H15	0.960897	-2.979598	0.745402
H16	0.340327	-3.175935	-0.924394
C17	1.549829	-0.214537	-0.738329
O18	2.709903	-0.389799	-1.120879
N19	0.926811	1.005041	-0.507320
H20	-1.827942	-2.170227	0.525440
H21	1.165753	1.820748	-1.053465
C22	4.108936	0.684170	0.365992
H23	4.853006	-0.006977	-0.000357
H24	3.909553	1.603567	-0.163724
N25	3.626769	0.530852	1.585427
H26	2.975668	1.195090	1.977662
H27	3.871962	-0.267750	2.150881

Zero-point correction= 0.214056
Thermal correction to Energy= 0.230158
Thermal correction to Enthalpy= 0.231102
Thermal correction to Gibbs Free Energy= 0.169733
Sum of electronic and zero-point Energies= -752.239396
Sum of electronic and thermal Energies= -752.223295
Sum of electronic and thermal Enthalpies= -752.222350
Sum of electronic and thermal Free Energies= -752.283719

97 N9-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-1.372645	-0.571070	-0.382681

C2	0.274538	0.975983	-0.116602
C3	1.623498	1.518998	0.055383
O4	1.871959	2.702451	0.154827
N5	2.571314	0.511433	0.063070
H6	3.514985	0.820697	0.262719
C7	2.325351	-0.884669	0.195480
N8	3.326798	-1.772460	-0.188748
H9	3.861667	-2.182698	0.564448
N10	1.009218	-1.292426	-0.182931
C11	0.056647	-0.332197	-0.287371
C12	-1.815741	-1.210910	-1.659037
H13	-1.362447	-0.684246	-2.498994
H14	-1.507490	-2.257640	-1.655720
H15	-2.902495	-1.137522	-1.711989
C16	-1.985955	0.863320	-0.267264
O17	-3.168087	1.016753	-0.323049
N18	-0.935354	1.682219	-0.115398
H19	-1.019130	2.683699	0.001286
H20	3.919548	-1.477867	-0.958587
C21	-1.906098	-1.394431	0.866273
H22	-2.978086	-1.459402	0.673392
H23	-1.427826	-2.368553	0.746161
N24	-1.590442	-0.742118	2.053384
H25	-2.351230	-0.344218	2.581633
H26	-0.848498	-1.123697	2.618370
H27	0.974357	-2.147801	-0.724985

Zero-point correction= 0.218716
Thermal correction to Energy= 0.233816
Thermal correction to Enthalpy= 0.234760
Thermal correction to Gibbs Free Energy= 0.176800
Sum of electronic and zero-point Energies= -752.237354
Sum of electronic and thermal Energies= -752.222254
Sum of electronic and thermal Enthalpies= -752.221310
Sum of electronic and thermal Free Energies= -752.279269

98 TS_N9-CH_2NH_2[9MOG + H_{N3}]$^{\bullet+}$

N1	-1.371742	-0.577558	-0.417863
C2	0.244104	0.967996	-0.183738
C3	1.583344	1.520854	0.007517
O4	1.827970	2.704985	0.119378
N5	2.538673	0.518759	0.019724
H6	3.479968	0.834426	0.220111
C7	2.304480	-0.880014	0.140959
N8	3.316584	-1.754217	-0.250784
H9	3.863309	-2.157599	0.497329
N10	0.992183	-1.302086	-0.241224
C11	0.032290	-0.344626	-0.369054
C12	-1.925682	-1.524252	-1.408198
H13	-1.610909	-1.241913	-2.414222
H14	-1.579915	-2.533425	-1.176495
H15	-3.013251	-1.479744	-1.343521
C16	-1.995561	0.782301	-0.447309
O17	-3.176947	0.941855	-0.596516
N18	-0.982079	1.645975	-0.203397
H19	-1.088227	2.651492	-0.215262
H20	3.899431	-1.449609	-1.024355
C21	-1.869483	-1.213121	1.296493
H22	-2.937844	-1.086184	1.138466
H23	-1.463323	-2.209411	1.147359
N24	-1.323076	-0.505411	2.280612
H25	-1.768768	0.325941	2.640195
H26	-0.399967	-0.720304	2.627548
H27	0.976568	-2.141450	-0.809547

Zero-point correction= 0.217867
Thermal correction to Energy= 0.232663
Thermal correction to Enthalpy= 0.233607
Thermal correction to Gibbs Free Energy= 0.175747
Sum of electronic and zero-point Energies= -752.237062
Sum of electronic and thermal Energies= -752.222266
Sum of electronic and thermal Enthalpies= -752.221322
Sum of electronic and thermal Free Energies= -752.279182

99 [9MOG + H_{C4}]$^{\bullet\cdots+}$$CH_2NH_2$

N1	-1.326392	-1.659209	0.176711
C2	0.206208	0.014775	0.066571
C3	0.615006	1.355822	-0.115416
O4	1.774363	1.747100	-0.407224
N5	-0.411228	2.252452	0.053559
H6	-0.175129	3.235750	0.024613
C7	-1.764073	1.840218	0.003389
N8	-2.644583	2.859605	-0.204266
H9	-2.387952	3.616670	-0.820328
H10	-3.611519	2.572417	-0.256011
N11	-2.151275	0.631669	0.179037
C12	-1.144500	-0.295658	0.634345
C13	-2.510402	-2.439499	0.481081
H14	-2.611935	-2.583034	1.561368
H15	-3.392848	-1.925961	0.096107
H16	-2.408551	-3.410186	-0.004135
C17	-0.212616	-2.181441	-0.397808
O18	0.000184	-3.282744	-0.840478
N19	0.770688	-1.121018	-0.406691
H20	1.472514	-1.144384	-1.135623
H21	-1.131764	-0.284765	1.739892
C22	4.145317	-0.461613	0.726657
H23	3.252834	-0.940287	1.123768
H24	5.124277	-0.893260	0.917599
N25	4.017221	0.598834	0.036358
H26	3.037543	1.054811	-0.162036
H27	4.845502	1.055440	-0.339477

Zero-point correction= 0.217521
Thermal correction to Energy= 0.232830
Thermal correction to Enthalpy= 0.233774
Thermal correction to Gibbs Free Energy= 0.173281
Sum of electronic and zero-point Energies= -752.282254
Sum of electronic and thermal Energies= -752.266945
Sum of electronic and thermal Enthalpies= -752.266001
Sum of electronic and thermal Free Energies= -752.326494

100 TS_[9MOG + H_{C4}]$^{\bullet\cdots+}$$CH_2NH_2$

N1	-1.653003	-0.859247	-0.069757
C2	-0.041380	0.583268	0.600327
C3	1.303050	0.974763	0.938284
O4	1.635536	2.010396	1.493788
N5	2.224291	0.020575	0.492499
H6	3.192274	0.224496	0.710675
C7	1.856926	-1.276851	0.105181
N8	2.878148	-2.170143	0.049982
H9	3.658788	-2.084039	0.683236
H10	2.609669	-3.114282	-0.187692
N11	0.658857	-1.615455	-0.238256
C12	-0.275924	-0.549029	-0.311671
C13	-2.368219	-1.933238	-0.731532
H14	-2.491703	-1.724585	-1.799608
H15	-1.818397	-2.866349	-0.602041
H16	-3.351362	-2.017486	-0.268574
C17	-2.260014	0.086741	0.715596
O18	-3.411995	0.191366	1.045534
N19	-1.213871	0.991865	1.101375
H20	-1.346266	1.684241	1.828412
H21	-0.204870	-0.118250	-1.397892

C22	0.121166	1.252153	-2.556898
H23	-0.879423	1.141627	-2.960257
H24	0.946183	0.690369	-2.981013
N25	0.379022	2.258883	-1.763745
H26	-0.351950	2.880279	-1.438988
H27	1.320993	2.477702	-1.461231

Zero-point correction= 0.216092
Thermal correction to Energy= 0.230791
Thermal correction to Enthalpy= 0.231736
Thermal correction to Gibbs Free Energy= 0.173343
Sum of electronic and zero-point Energies= -752.257082
Sum of electronic and thermal Energies= -752.242382
Sum of electronic and thermal Enthalpies= -752.241438
Sum of electronic and thermal Free Energies= -752.299831

101 [9MOG + H_{C4}]$^{\bullet}$

N1	1.588367	-0.724496	0.073740
C2	0.013548	0.896474	0.310863
C3	-1.296970	1.424371	0.154745
O4	-1.607543	2.600019	-0.017033
N5	-2.259539	0.396839	0.208193
H6	-3.221914	0.698226	0.147097
C7	-1.925939	-0.924474	-0.093140
N8	-2.998249	-1.712208	-0.452931
H9	-3.683433	-1.298038	-1.068755
H10	-2.719890	-2.645011	-0.723001
N11	-0.744487	-1.420106	-0.010734
C12	0.243190	-0.555747	0.593563
C13	2.323792	-1.958894	0.214004
H14	2.489574	-2.200786	1.271144
H15	1.766833	-2.770417	-0.258678
H16	3.288531	-1.837194	-0.279643
C17	2.187457	0.470401	-0.214999
O18	3.328615	0.682900	-0.566874
N19	1.196087	1.463757	-0.033734
H20	1.311324	2.403814	-0.382584
H21	0.254679	-0.753234	1.683717

Zero-point correction= 0.162314
Thermal correction to Energy= 0.173616
Thermal correction to Enthalpy= 0.174560
Thermal correction to Gibbs Free Energy= 0.124695
Sum of electronic and zero-point Energies= -657.342022
Sum of electronic and thermal Energies= -657.330720
Sum of electronic and thermal Enthalpies= -657.329775
Sum of electronic and thermal Free Energies= -657.379640

102 C5-$^{+}NH_2\dot{C}H_2$_[9MOG+H_{C4}]

N1	-1.791848	0.221686	0.448261
C2	0.181665	-0.779700	-0.178544
C3	1.660710	-0.602337	-0.515813
O4	2.322378	-1.558908	-0.874053
N5	2.113728	0.666121	-0.395449
H6	3.093377	0.818355	-0.606936
C7	1.327650	1.714089	0.150021
N8	1.938691	2.923340	0.104686
H9	2.605350	3.134974	-0.621889
H10	1.393193	3.700418	0.448391
N11	0.178766	1.551703	0.682461
C12	-0.391436	0.242649	0.827966
C13	-2.754109	1.102343	1.097659
H14	-2.815725	0.852182	2.158357
H15	-2.466599	2.150344	0.982034
H16	-3.725209	0.937822	0.631225
C17	-1.914086	-0.073107	-0.894737
O18	-2.855014	0.082900	-1.626170
N19	-0.686467	-0.675419	-1.266413
H20	-0.486963	-0.933254	-2.222060
H21	-0.271796	-0.095225	1.865505
H22	-0.876182	-2.532772	0.329631
H23	0.653180	-2.798759	-0.293667
H24	1.710392	-2.571479	1.808339
H25	-0.061858	-2.541510	2.536109
C26	0.636948	-2.489942	1.714500
N27	0.107970	-2.258433	0.395086

Zero-point correction= 0.219375
Thermal correction to Energy= 0.233862
Thermal correction to Enthalpy= 0.234806
Thermal correction to Gibbs Free Energy= 0.178350
Sum of electronic and zero-point Energies= -752.255891
Sum of electronic and thermal Energies= -752.241405
Sum of electronic and thermal Enthalpies= -752.240460
Sum of electronic and thermal Free Energies= -752.296916

103 TS_C5-$^{+}NH_2\dot{C}H_2$_[9MOG+H_{C4}]

N1	-1.665097	0.614435	0.311507
C2	0.036597	-0.857197	-0.161631
C3	1.496277	-0.980098	-0.580531
O4	1.964328	-2.062469	-0.869343
N5	2.193041	0.188665	-0.569156
H6	3.168032	0.117453	-0.838118
C7	1.697997	1.391196	-0.018771
N8	2.566523	2.422214	-0.067205
H9	3.329639	2.446279	-0.725119
H10	2.230473	3.308129	0.280954
N11	0.536860	1.517322	0.520911
C12	-0.294635	0.400686	0.646808
C13	-2.423292	1.753999	0.807066
H14	-2.537812	1.674420	1.889674
H15	-1.920649	2.691289	0.558016
H16	-3.405296	1.726617	0.335359
C17	-1.987113	-0.003325	-0.886949
O18	-2.980381	0.126275	-1.551453
N19	-0.911151	-0.869756	-1.185322
H20	-0.867509	-1.399265	-2.043811
H21	-0.195505	-0.114995	1.785969
H22	-1.146658	-2.378306	0.709005
H23	0.449491	-2.801118	0.589813
H24	1.014326	-1.648254	2.590324
H25	-0.803216	-1.828011	2.915217
C26	-0.006293	-1.557652	2.232470
N27	-0.192194	-2.042930	0.859025

Zero-point correction= 0.215668
Thermal correction to Energy= 0.229520
Thermal correction to Enthalpy= 0.230464
Thermal correction to Gibbs Free Energy= 0.175018
Sum of electronic and zero-point Energies= -752.240020
Sum of electronic and thermal Energies= -752.226168
Sum of electronic and thermal Enthalpies= -752.225224
Sum of electronic and thermal Free Energies= -752.280671

104 N1-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.177123	0.521518	0.270573
C2	-0.375296	-0.832112	-0.066088
C3	0.919259	-1.116267	-0.517694
O4	1.400669	-2.125963	-1.004961
N5	1.825307	0.082960	-0.358800
H6	2.556249	-0.062872	-1.061053
C7	1.146244	1.388111	-0.543661

N8	1.985077	2.353189	-1.011918
H9	2.676253	2.127217	-1.713454
H10	1.552680	3.260475	-1.130991
N11	-0.045287	1.596689	-0.171804
C12	-0.752362	0.517192	0.483557
C13	-3.035518	1.591357	0.747812
H14	-2.963430	1.693031	1.835740
H15	-2.750068	2.529483	0.269812
H16	-4.062084	1.343394	0.478356
C17	-2.655514	-0.714121	-0.072342
O18	-3.784967	-1.093662	-0.216603
N19	-1.492672	-1.539870	-0.263320
H20	-1.553068	-2.452960	-0.696897
H21	-0.547799	0.586770	1.567268
C22	2.638532	0.034373	1.112957
H23	1.809461	0.092849	1.817201
H24	3.203176	0.965417	1.069882
N25	3.408587	-1.078242	1.266401
H26	2.987848	-1.964319	1.499629
H27	4.325886	-1.126377	0.851850

Zero-point correction= 0.219974
Thermal correction to Energy= 0.234701
Thermal correction to Enthalpy= 0.235645
Thermal correction to Gibbs Free Energy= 0.177821
Sum of electronic and zero-point Energies= -752.257741
Sum of electronic and thermal Energies= -752.243013
Sum of electronic and thermal Enthalpies= -752.242069
Sum of electronic and thermal Free Energies= -752.299893

105 TS_N1-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.166477	0.495613	0.297132
C2	-0.349033	-0.805106	-0.140804
C3	0.946537	-1.030720	-0.635874
O4	1.445024	-2.043877	-1.113094
N5	1.790536	0.161917	-0.501225
H6	2.534476	0.075446	-1.193798
C7	1.124523	1.449318	-0.533052
N8	1.944817	2.468279	-0.933411
H9	2.573011	2.314532	-1.710473
H10	1.489261	3.371928	-0.954211
N11	-0.056334	1.637958	-0.102317
C12	-0.736275	0.505791	0.484870
C13	-3.033124	1.528457	0.833711
H14	-2.937568	1.591291	1.923096
H15	-2.776351	2.489772	0.386460
H16	-4.061114	1.271013	0.578718
C17	-2.629201	-0.734102	-0.086708
O18	-3.757053	-1.126092	-0.222981
N19	-1.459644	-1.530353	-0.334200
H20	-1.514843	-2.417229	-0.818748
H21	-0.520008	0.508739	1.570828
C22	2.822556	-0.041771	1.211855
H23	2.009163	0.329099	1.826076
H24	3.580359	0.674689	0.914457
N25	3.185092	-1.296109	1.378111
H26	2.560643	-1.974234	1.792649
H27	4.017363	-1.667614	0.940949

Zero-point correction= 0.219402
Thermal correction to Energy= 0.233679
Thermal correction to Enthalpy= 0.234623
Thermal correction to Gibbs Free Energy= 0.177157
Sum of electronic and zero-point Energies= -752.257206
Sum of electronic and thermal Energies= -752.242930
Sum of electronic and thermal Enthalpies= -752.241985
Sum of electronic and thermal Free Energies= -752.299451

106 C2-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.768016	-1.096455	-0.124585
C2	-0.828057	0.976814	-0.247274
C3	0.252658	2.012396	-0.250645
O4	-0.014484	3.190445	-0.358209
N5	1.461855	1.422707	-0.131488
H6	2.245049	2.061741	-0.028782
C7	1.769858	0.028037	0.294059
N8	2.466707	0.105858	1.532407
H9	1.861349	0.271296	2.328543
H10	3.018401	-0.739478	1.666019
N11	0.603884	-0.834133	0.379639
C12	-0.513634	-0.462644	-0.444118
C13	-1.981188	-2.538430	-0.164386
H14	-1.931127	-2.904725	-1.192760
H15	-1.225121	-3.028384	0.450838
H16	-2.970983	-2.741649	0.243683
C17	-2.753570	-0.203703	0.133223
O18	-3.909818	-0.310547	0.396943
N19	-2.061500	1.124667	0.047213
H20	-2.520882	2.010411	0.264182
H21	-0.241259	-0.631521	-1.506217
C22	2.733453	-0.594650	-0.778747
H23	2.176386	-0.698415	-1.720925
H24	3.510021	0.158188	-0.939982
N25	3.339566	-1.799881	-0.282518
H26	2.806849	-2.638815	-0.471070
H27	4.291146	-1.924091	-0.600754

Zero-point correction= 0.218545
Thermal correction to Energy= 0.233019
Thermal correction to Enthalpy= 0.233963
Thermal correction to Gibbs Free Energy= 0.176135
Sum of electronic and zero-point Energies= -752.219610
Sum of electronic and thermal Energies= -752.205137
Sum of electronic and thermal Enthalpies= -752.204193
Sum of electronic and thermal Free Energies= -752.262021

107 TS_C2-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.758049	-1.096120	-0.165617
C2	-0.830135	0.974202	-0.259399
C3	0.245476	2.013626	-0.272978
O4	0.015062	3.177263	-0.518193
N5	1.451185	1.439323	-0.007383
H6	2.256422	2.055791	0.016017
C7	1.603731	0.091002	0.491693
N8	2.551573	0.064462	1.541875
H9	2.291326	0.691653	2.298037
H10	2.628515	-0.876555	1.913502
N11	0.525314	-0.712084	0.554533
C12	-0.489899	-0.461006	-0.434289
C13	-1.944602	-2.538450	-0.152870
H14	-1.780942	-2.951693	-1.151275
H15	-1.249166	-2.985108	0.560510
H16	-2.969334	-2.743731	0.156206
C17	-2.742954	-0.213374	0.119853
O18	-3.896619	-0.336842	0.400306
N19	-2.068162	1.114165	0.045419
H20	-2.532126	1.981628	0.310627
H21	-0.162051	-0.680585	-1.468239
C22	2.726139	-0.710614	-0.933143
H23	1.985669	-0.887632	-1.709358
H24	3.358240	0.159525	-1.086932
N25	3.387003	-1.807953	-0.504906
H26	2.953691	-2.717918	-0.515613
H27	4.243623	-1.713599	0.018961

Zero-point correction= 0.216748
Thermal correction to Energy= 0.231276
Thermal correction to Enthalpy= 0.232221
Thermal correction to Gibbs Free Energy= 0.174751
Sum of electronic and zero-point Energies= -752.211146
Sum of electronic and thermal Energies= -752.196617
Sum of electronic and thermal Enthalpies= -752.195673
Sum of electronic and thermal Free Energies= -752.253143

108 N2-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.970027	-1.147151	-0.034053
C2	-1.131898	0.957993	-0.289922
C3	-0.135705	1.955058	-0.157094
O4	-0.264424	3.157029	-0.010166
N5	1.188034	1.364897	-0.150822
H6	1.924018	2.037649	0.027021
C7	1.314143	0.044655	0.177492
N8	2.638096	-0.364731	0.670964
H9	3.000218	0.258045	1.400702
H10	2.503675	-1.284561	1.105421
N11	0.457759	-0.882573	0.091918
C12	-0.800176	-0.485085	-0.542054
C13	-2.213971	-2.563490	-0.235298
H14	-2.267205	-2.807127	-1.302392
H15	-1.419426	-3.143484	0.237189
H16	-3.166442	-2.808651	0.234476
C17	-2.998058	-0.256978	0.193685
O18	-4.139327	-0.484948	0.496093
N19	-2.441222	1.040359	0.015070
H20	-2.934901	1.879787	0.288452
H21	-0.674896	-0.695521	-1.620956
C22	3.741656	-0.522879	-0.436028
H23	3.301047	-1.235370	-1.135977
H24	3.815174	0.460221	-0.903717
N25	4.924986	-0.953244	0.169503
H26	5.208150	-1.907118	0.001967
H27	5.701266	-0.309062	0.177650

Zero-point correction= 0.221918
Thermal correction to Energy= 0.236317
Thermal correction to Enthalpy= 0.237261
Thermal correction to Gibbs Free Energy= 0.179469
Sum of electronic and zero-point Energies= -752.261929
Sum of electronic and thermal Energies= -752.247529
Sum of electronic and thermal Enthalpies= -752.246585
Sum of electronic and thermal Free Energies= -752.304377

109 TS_N2-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.568099	-1.347120	0.033158
C2	-1.273421	0.876383	-0.352561
C3	-0.573764	2.100134	-0.216584
O4	-1.027548	3.231457	-0.161442
N5	0.839569	1.878051	-0.077146
H6	1.340484	2.726889	0.154763
C7	1.299711	0.657058	0.362049
N8	2.603235	0.632579	0.918836
H9	2.988552	1.541915	1.153313
H10	2.615382	0.032630	1.738666
N11	0.705276	-0.470009	0.241311
C12	-0.565252	-0.439145	-0.469209
C13	-1.427246	-2.785267	-0.050824
H14	-1.288419	-3.109639	-1.089307
H15	-0.576888	-3.109427	0.552591
H16	-2.338448	-3.236325	0.342784
C17	-2.802666	-0.742274	0.122553
O18	-3.868672	-1.242224	0.378615
N19	-2.584408	0.635488	-0.137481
H20	-3.290004	1.335727	0.046364
H21	-0.346967	-0.680829	-1.528116
C22	3.674030	-0.796772	-0.598916
H23	2.709159	-1.287446	-0.477663
H24	3.770012	0.050074	-1.267983
N25	4.749998	-1.360873	-0.153637
H26	4.710011	-2.205560	0.405561
H27	5.669535	-0.969388	-0.322677

Zero-point correction= 0.219530
Thermal correction to Energy= 0.233849
Thermal correction to Enthalpy= 0.234793
Thermal correction to Gibbs Free Energy= 0.176810
Sum of electronic and zero-point Energies= -752.255830
Sum of electronic and thermal Energies= -752.241511
Sum of electronic and thermal Enthalpies= -752.240567
Sum of electronic and thermal Free Energies= -752.298550

110 N3-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.616360	-0.436540	-0.443985
C2	-0.114642	1.265092	-0.148330
C3	1.172075	1.835349	-0.018733
O4	1.496506	2.929647	0.399579
N5	2.175531	0.894495	-0.473539
H6	3.104172	1.285653	-0.581264
C7	2.024808	-0.444479	-0.337456
N8	3.116778	-1.204320	-0.188579
H9	4.017034	-0.787056	-0.007502
H10	3.100270	-2.191775	-0.389024
N11	0.797658	-0.973519	-0.340848
C12	-0.286007	-0.060232	-0.819525
C13	-2.429352	-1.316961	-1.282282
H14	-2.586868	-0.880138	-2.274284
H15	-1.949849	-2.290578	-1.390265
H16	-3.393442	-1.451260	-0.792602
C17	-2.258773	0.614016	0.220578
O18	-3.405589	0.666521	0.567563
N19	-1.287074	1.619980	0.412858
H20	-1.469013	2.461814	0.943879
H21	-0.179361	0.005745	-1.913221
C22	0.437622	-2.198227	0.474935
H23	-0.356380	-2.699315	-0.073770
H24	1.305706	-2.856460	0.462803
N25	0.033332	-1.956629	1.801999
H26	-0.867369	-1.517758	1.922299
H27	0.734322	-1.619832	2.445363

Zero-point correction= 0.221239
Thermal correction to Energy= 0.235537
Thermal correction to Enthalpy= 0.236481
Thermal correction to Gibbs Free Energy= 0.179178
Sum of electronic and zero-point Energies= -752.296595
Sum of electronic and thermal Energies= -752.282297
Sum of electronic and thermal Enthalpies= -752.281353
Sum of electronic and thermal Free Energies= -752.338656

111 TS_N3-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.347780	-0.010061	-1.000950
C2	0.448640	1.238149	-0.369562
C3	1.772005	1.395607	0.148090
O4	2.200689	2.337589	0.792874
N5	2.562663	0.259114	-0.151895
H6	3.523894	0.330814	0.157816
C7	1.961853	-0.991115	-0.254452
N8	2.722936	-2.057599	0.107922
H9	3.696616	-1.943886	0.339852

H10	2.451124	-2.954333	-0.263991
N11	0.727762	-1.167602	-0.621415
C12	0.092864	0.023394	-1.168982
C13	-2.218255	-0.872829	-1.775026
H14	-2.245846	-0.556409	-2.822023
H15	-1.856083	-1.904686	-1.736507
H16	-3.226926	-0.812638	-1.363230
C17	-1.788898	0.962298	-0.156300
O18	-2.899824	1.044931	0.357975
N19	-0.696526	1.774947	0.144998
H20	-0.741363	2.526702	0.819506
H21	0.347487	0.125814	-2.235505
C22	-1.163687	-1.898179	1.451398
H23	-1.411438	-2.176012	0.435361
H24	-0.363891	-2.413033	1.974193
N25	-1.832200	-0.983387	2.046942
H26	-2.552362	-0.423405	1.556756
H27	-1.613254	-0.710926	3.000771

Zero-point correction= 0.218443
Thermal correction to Energy= 0.233086
Thermal correction to Enthalpy= 0.234031
Thermal correction to Gibbs Free Energy= 0.176448
Sum of electronic and zero-point Energies= -752.273603
Sum of electronic and thermal Energies= -752.258959
Sum of electronic and thermal Enthalpies= -752.258015
Sum of electronic and thermal Free Energies= -752.315597

112 C5-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	1.724155	-0.700817	0.376559
C2	-0.087485	0.712564	0.087990
C3	-1.565731	0.802763	-0.310982
O4	-2.085069	1.851197	-0.632192
N5	-2.227386	-0.384062	-0.270599
H6	-3.215364	-0.347982	-0.494985
C7	-1.609049	-1.619240	0.030141
N8	-2.415699	-2.691760	-0.160006
H9	-3.151617	-2.668405	-0.849011
H10	-1.994139	-3.592817	0.011845
N11	-0.419231	-1.738422	0.478857
C12	0.353951	-0.579618	0.828562
C13	2.593566	-1.769662	0.838928
H14	2.765537	-1.665312	1.912378
H15	2.140108	-2.742414	0.631625
H16	3.542468	-1.684355	0.309737
C17	1.937847	-0.041345	-0.799612
O18	2.877849	-0.061370	-1.550434
N19	0.781572	0.773930	-0.982429
H20	0.677531	1.354780	-1.804735
H21	0.334472	-0.450288	1.917956
C22	0.143445	2.006494	1.192884
H23	-0.582875	1.786966	1.977653
H24	1.175721	1.846313	1.511095
N25	-0.058761	3.239411	0.632709
H26	0.673218	3.694009	0.103026
H27	-0.999119	3.591201	0.501310

Zero-point correction= 0.219574
Thermal correction to Energy= 0.233967
Thermal correction to Enthalpy= 0.234911
Thermal correction to Gibbs Free Energy= 0.178528
Sum of electronic and zero-point Energies= -752.275775
Sum of electronic and thermal Energies= -752.261381
Sum of electronic and thermal Enthalpies= -752.260437
Sum of electronic and thermal Free Energies= -752.316821

113 TS_C5-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.912789	-0.512598	-0.268446
C2	0.131879	0.420168	0.126904
C3	1.529325	0.331168	0.493161
O4	2.186294	1.247303	0.995504
N5	2.073519	-0.893368	0.169541
H6	3.062632	-1.007460	0.354298
C7	1.256852	-2.033411	-0.026650
N8	1.920411	-3.215705	0.088336
H9	2.673466	-3.305006	0.754001
H10	1.343866	-4.037081	-0.026064
N11	0.013492	-1.982647	-0.332476
C12	-0.527810	-0.684944	-0.655105
C13	-2.980997	-1.357877	-0.767180
H14	-3.113973	-1.215838	-1.843852
H15	-2.746237	-2.403788	-0.561401
H16	-3.900090	-1.079548	-0.251473
C17	-2.111854	0.526105	0.584413
O18	-3.120746	0.940076	1.096185
N19	-0.811091	1.112667	0.796046
H20	-0.642695	1.679769	1.617343
H21	-0.436110	-0.533527	-1.745188
C22	1.009910	2.488826	-1.503304
H23	1.786858	1.759560	-1.698581
H24	0.174783	2.604683	-2.186226
N25	1.155739	3.311437	-0.524495
H26	0.469024	4.032130	-0.329373
H27	1.885286	3.128363	0.170038

Zero-point correction= 0.217917
Thermal correction to Energy= 0.232675
Thermal correction to Enthalpy= 0.233619
Thermal correction to Gibbs Free Energy= 0.175439
Sum of electronic and zero-point Energies= -752.268201
Sum of electronic and thermal Energies= -752.253444
Sum of electronic and thermal Enthalpies= -752.252499
Sum of electronic and thermal Free Energies= -752.310679

114 C6-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.105523	0.315763	0.244477
C2	0.005626	-0.513305	0.083689
C3	1.505465	-0.468649	-0.001015
O4	1.911573	-0.516755	-1.314144
N5	1.881262	0.889791	0.351437
H6	2.879903	1.062697	0.374186
C7	1.039781	1.952400	-0.044244
N8	1.667438	3.103413	-0.373605
H9	2.568075	3.080191	-0.827404
H10	1.068402	3.881557	-0.609667
N11	-0.247152	1.861937	-0.012245
C12	-0.751034	0.662527	0.603492
C13	-3.248058	1.175075	0.518574
H14	-3.397307	1.279438	1.596133
H15	-3.075411	2.153462	0.067634
H16	-4.129878	0.714551	0.073816
C17	-2.209801	-0.914556	-0.304005
O18	-3.133183	-1.569346	-0.683672
N19	-0.795891	-1.388656	-0.389659
H20	-0.511855	-2.273398	-0.810392
H21	-0.647903	0.708690	1.703159
C22	2.144061	-1.559804	0.865858
H23	1.775417	-1.473661	1.892708
H24	3.228125	-1.385238	0.879274
N25	1.743040	-2.834424	0.289795
H26	2.377259	-3.124841	-0.446794
H27	1.719605	-3.571516	0.984381

Zero-point correction= 0.219744
Thermal correction to Energy= 0.233887
Thermal correction to Enthalpy= 0.234831
Thermal correction to Gibbs Free Energy= 0.178744
Sum of electronic and zero-point Energies= -752.217971
Sum of electronic and thermal Energies= -752.203827
Sum of electronic and thermal Enthalpies= -752.202883
Sum of electronic and thermal Free Energies= -752.258971

115 TS_C6-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	2.092490	0.328824	-0.253276
C2	-0.011698	-0.505847	-0.060814
C3	-1.505519	-0.454579	0.013724
O4	-1.843334	-0.638586	1.337901
N5	-1.884605	0.890773	-0.366779
H6	-2.883667	1.057140	-0.380183
C7	-1.063614	1.950411	0.052880
N8	-1.689006	3.100838	0.383885
H9	-2.608920	3.085228	0.796407
H10	-1.093150	3.874464	0.640677
N11	0.228480	1.859449	0.054303
C12	0.731614	0.676794	-0.588694
C13	3.228172	1.192248	-0.543574
H14	3.056679	2.170209	-0.091191
H15	4.117627	0.736004	-0.109786
H16	3.362732	1.295856	-1.623099
C17	2.209141	-0.898969	0.296776
O18	3.138745	-1.551418	0.664408
N19	0.796159	-1.377539	0.408656
H20	0.522033	-2.258449	0.843226
H21	0.608486	0.729388	-1.685743
C22	-2.119846	-1.550541	-0.891880
H23	-1.732900	-1.451396	-1.909692
H24	-3.203242	-1.376688	-0.928039
N25	-1.728828	-2.820085	-0.318615
H26	-2.362539	-3.119894	0.413172
H27	-1.658773	-3.554755	-1.011956

Zero-point correction= 0.217621
Thermal correction to Energy= 0.231530
Thermal correction to Enthalpy= 0.232474
Thermal correction to Gibbs Free Energy= 0.176896
Sum of electronic and zero-point Energies= -752.218165
Sum of electronic and thermal Energies= -752.204257
Sum of electronic and thermal Enthalpies= -752.203312
Sum of electronic and thermal Free Energies= -752.258890

116 O6-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.165031	-0.668054	0.184235
C2	0.094119	-0.333157	0.113034
C3	1.227742	0.481380	-0.019111
O4	2.465195	0.148688	-0.233915
N5	0.978649	1.815787	0.074063
H6	1.776357	2.438995	0.100720
C7	-0.331785	2.334832	-0.102885
N8	-0.363192	3.663828	-0.384347
H9	0.351246	4.070266	-0.970197
H10	-1.289237	4.050664	-0.500658
N11	-1.385807	1.624894	0.037128
C12	-1.183274	0.310709	0.589707
C13	-3.584321	-0.517272	0.454003
H14	-3.772393	-0.505809	1.531807
H15	-3.940680	0.411579	0.006524
H16	-4.102187	-1.365116	0.006009
C17	-1.609905	-1.822583	-0.261971
O18	-2.104371	-2.860880	-0.609758
N19	-0.178420	-1.584079	-0.275617
H20	0.429835	-2.247955	-0.735138
H21	-1.178230	0.387187	1.693441
C22	2.988752	-1.291660	0.048876
H23	2.784183	-1.819078	-0.882785
H24	2.381431	-1.644429	0.884188
N25	4.323183	-1.279342	0.342610
H26	4.981220	-1.124613	-0.405540
H27	4.618217	-0.938888	1.244597

Zero-point correction= 0.220148
Thermal correction to Energy= 0.234864
Thermal correction to Enthalpy= 0.235808
Thermal correction to Gibbs Free Energy= 0.177868
Sum of electronic and zero-point Energies= -752.277845
Sum of electronic and thermal Energies= -752.263129
Sum of electronic and thermal Enthalpies= -752.262185
Sum of electronic and thermal Free Energies= -752.320125

117 TS_O6-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-2.295748	-0.757234	0.163009
C2	-0.058365	-0.332273	0.186815
C3	1.080948	0.485930	0.006367
O4	2.255337	0.103265	-0.199509
N5	0.764597	1.835088	0.081626
H6	1.531488	2.490953	0.036822
C7	-0.554200	2.297177	-0.106241
N8	-0.637758	3.629216	-0.412947
H9	0.035275	4.015381	-1.058957
H10	-1.584593	3.951060	-0.557996
N11	-1.597587	1.570305	0.039475
C12	-1.368978	0.264428	0.607392
C13	-3.722436	-0.676216	0.401786
H14	-3.938096	-0.683176	1.475679
H15	-4.112887	0.240356	-0.043265
H16	-4.193209	-1.541599	-0.064700
C17	-1.667541	-1.900327	-0.225224
O18	-2.124607	-2.962144	-0.573512
N19	-0.263303	-1.617745	-0.164002
H20	0.394477	-2.222869	-0.631543
H21	-1.428230	0.349354	1.709389
C22	4.253169	-1.510744	-0.165970
H23	3.758968	-1.329772	-1.111881
H24	4.211851	-2.482585	0.316307
N25	4.916939	-0.568350	0.383077
H26	4.910035	0.363042	-0.024024
H27	5.383507	-0.685931	1.277134

Zero-point correction= 0.218476
Thermal correction to Energy= 0.233653
Thermal correction to Enthalpy= 0.234597
Thermal correction to Gibbs Free Energy= 0.173925
Sum of electronic and zero-point Energies= -752.267479
Sum of electronic and thermal Energies= -752.252301
Sum of electronic and thermal Enthalpies= -752.251357
Sum of electronic and thermal Free Energies= -752.312030

118 N7-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-0.802035	1.455874	-0.057352
C2	0.057822	-0.646626	0.072267
C3	1.141817	-1.557190	-0.227754
O4	0.961318	-2.687604	-0.651374
N5	2.372472	-0.989837	0.025839
H6	3.177942	-1.595197	-0.074356
C7	2.535401	0.406587	0.135514
N8	3.820329	0.824729	0.052498
H9	4.511663	0.291756	-0.451115

H10	3.967060	1.821486	0.108277
N11	1.575622	1.241970	0.328979
C12	0.273438	0.719227	0.617203
C13	-0.958709	2.895968	0.103520
H14	-1.263547	3.125033	1.128231
H15	-0.004176	3.375129	-0.114475
H16	-1.721030	3.241966	-0.593462
C17	-1.706336	0.699068	-0.678016
O18	-2.740044	0.926292	-1.238327
N19	-1.216878	-0.761448	-0.550817
H20	-1.154812	-1.189559	-1.483315
C21	-2.294087	-1.607027	0.264598
H22	-3.169403	-1.556185	-0.385126
H23	-1.861295	-2.607909	0.276059
N24	-2.477956	-1.039590	1.526396
H25	-3.357741	-0.570125	1.682050
H26	-2.180344	-1.589035	2.317967
H27	0.088539	0.761210	1.704093

Zero-point correction= 0.220435
Thermal correction to Energy= 0.235056
Thermal correction to Enthalpy= 0.236000
Thermal correction to Gibbs Free Energy= 0.178309
Sum of electronic and zero-point Energies= -752.263773
Sum of electronic and thermal Energies= -752.249152
Sum of electronic and thermal Enthalpies= -752.248207
Sum of electronic and thermal Free Energies= -752.305899

119 TS_N7-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-0.761819	1.483870	0.008466
C2	0.081272	-0.626186	0.029512
C3	1.141968	-1.584580	-0.178000
O4	0.952763	-2.731339	-0.552659
N5	2.380827	-1.037699	0.102261
H6	3.173523	-1.665634	0.056213
C7	2.577311	0.357534	0.135178
N8	3.873777	0.741075	0.034983
H9	4.540047	0.176726	-0.468911
H10	4.038358	1.736773	0.036586
N11	1.635804	1.224008	0.280836
C12	0.330795	0.722428	0.611430
C13	-0.915070	2.916087	0.213135
H14	-1.099221	3.125145	1.270355
H15	-0.002737	3.421762	-0.105801
H16	-1.760585	3.259939	-0.382031
C17	-1.622576	0.744482	-0.706711
O18	-2.646645	1.020361	-1.277374
N19	-1.143753	-0.669008	-0.635631
H20	-1.125243	-1.125229	-1.551676
C21	-2.510310	-1.639085	0.246127
H22	-3.237377	-1.497632	-0.549029
H23	-1.967001	-2.579858	0.263176
N24	-2.818908	-1.098483	1.422619
H25	-3.518952	-0.374378	1.492484
H26	-2.355040	-1.381779	2.272161
H27	0.203457	0.741550	1.707974

Zero-point correction= 0.219221
Thermal correction to Energy= 0.233593
Thermal correction to Enthalpy= 0.234537
Thermal correction to Gibbs Free Energy= 0.176889
Sum of electronic and zero-point Energies= -752.263917
Sum of electronic and thermal Energies= -752.249545
Sum of electronic and thermal Enthalpies= -752.248601
Sum of electronic and thermal Free Energies= -752.306249

120 C8-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-0.922452	-1.143077	-0.553955
C2	0.289736	0.783984	-0.352050
C3	1.528559	1.629620	-0.262939
O4	1.528972	2.830441	-0.358119
N5	2.621037	0.823243	-0.055258
H6	3.520168	1.289656	-0.008638
C7	2.525884	-0.569038	0.197984
N8	3.656770	-1.114708	0.695974
H9	4.303383	-0.564751	1.240171
H10	3.622514	-2.103490	0.897104
N11	1.483803	-1.282217	-0.050953
C12	0.423660	-0.640525	-0.774972
C13	-1.181831	-2.572225	-0.576009
H14	-0.912663	-2.949589	-1.566723
H15	-0.587015	-3.090231	0.179569
H16	-2.241689	-2.747098	-0.397500
C17	-1.753034	-0.204557	0.225236
O18	-1.628498	-0.662297	1.439326
N19	-0.871629	1.061248	0.073508
H20	0.616221	-0.702089	-1.861078
H21	-1.196280	1.942458	0.476722
C22	-3.144951	0.132539	-0.291394
H23	-3.071108	0.346311	-1.362005
H24	-3.783015	-0.749779	-0.156866
N25	-3.586291	1.326848	0.417609
H26	-4.298659	1.825474	-0.101992
H27	-3.972457	1.099830	1.327971

Zero-point correction= 0.218798
Thermal correction to Energy= 0.233057
Thermal correction to Enthalpy= 0.234001
Thermal correction to Gibbs Free Energy= 0.177618
Sum of electronic and zero-point Energies= -752.208264
Sum of electronic and thermal Energies= -752.194006
Sum of electronic and thermal Enthalpies= -752.193061
Sum of electronic and thermal Free Energies= -752.249445

121 TS_C8-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-0.946160	-1.098732	-0.698056
C2	0.310348	0.774028	-0.345353
C3	1.549950	1.620773	-0.269654
O4	1.554678	2.820316	-0.380388
N5	2.634843	0.805036	-0.064545
H6	3.544352	1.252419	-0.039007
C7	2.497896	-0.579211	0.219559
N8	3.602837	-1.143185	0.753985
H9	4.257875	-0.599041	1.293801
H10	3.542725	-2.128020	0.967689
N11	1.436259	-1.263213	-0.029509
C12	0.413789	-0.623976	-0.837734
C13	-1.157556	-2.541412	-0.603871
H14	-0.719738	-3.004487	-1.490158
H15	-0.706513	-2.977898	0.291103
H16	-2.229323	-2.744893	-0.611759
C17	-1.681346	-0.244103	0.226382
O18	-1.765138	-0.676561	1.472760
N19	-0.824200	1.007238	0.180501
H20	0.701451	-0.660703	-1.900102
H21	-1.132009	1.850733	0.666485
C22	-3.132180	0.144784	-0.248967
H23	-3.021510	0.276224	-1.328981
H24	-3.778826	-0.717320	-0.060502
N25	-3.539105	1.374217	0.381491
H26	-4.031250	1.993245	-0.249812
H27	-4.100281	1.234883	1.213024

Zero-point correction= 0.216951
Thermal correction to Energy= 0.231003
Thermal correction to Enthalpy= 0.231947
Thermal correction to Gibbs Free Energy= 0.175847
Sum of electronic and zero-point Energies= -752.204840
Sum of electronic and thermal Energies= -752.190788
Sum of electronic and thermal Enthalpies= -752.189844
Sum of electronic and thermal Free Energies= -752.245944

122 O8-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	0.765937	-0.845234	0.200185
C2	-0.707051	0.896943	0.379820
C3	-1.977058	1.517664	0.117945
O4	-2.155288	2.702285	-0.104455
N5	-3.004793	0.569872	0.142176
H6	-3.940740	0.938724	0.032426
C7	-2.756523	-0.788930	-0.082774
N8	-3.837979	-1.512309	-0.461829
H9	-4.606776	-1.079390	-0.948200
H10	-3.680298	-2.492600	-0.637874
N11	-1.607912	-1.359751	0.082992
C12	-0.601805	-0.556160	0.703210
C13	1.246959	-2.211320	0.058007
H14	1.687180	-2.577822	0.988832
H15	0.385407	-2.827243	-0.204586
H16	1.973399	-2.264579	-0.752682
C17	1.371778	0.278420	-0.168270
O18	2.556941	0.454424	-0.615254
N19	0.521669	1.340272	-0.035715
H20	-0.592813	-0.736105	1.793289
H21	0.733785	2.270805	-0.371840
C22	3.872336	-0.356716	-0.061009
H23	3.509448	-0.769835	0.877791
H24	4.004378	-1.088952	-0.851281
N25	4.912438	0.491612	0.075621
H26	5.421278	0.789863	-0.742208
H27	4.955173	1.112831	0.868403

Zero-point correction= 0.219953
Thermal correction to Energy= 0.234774
Thermal correction to Enthalpy= 0.235718
Thermal correction to Gibbs Free Energy= 0.177638
Sum of electronic and zero-point Energies= -752.276823
Sum of electronic and thermal Energies= -752.262002
Sum of electronic and thermal Enthalpies= -752.261058
Sum of electronic and thermal Free Energies= -752.319139

123 TS_O8-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	0.536557	-1.185027	0.134945
C2	-0.572691	0.788980	0.369633
C3	-1.705007	1.636539	0.137484
O4	-1.660974	2.838128	-0.080579
N5	-2.895376	0.903775	0.178213
H6	-3.746714	1.443023	0.090560
C7	-2.911948	-0.474404	-0.069418
N8	-4.126933	-0.973467	-0.426594
H9	-4.770908	-0.400839	-0.949913
H10	-4.141410	-1.960296	-0.635997
N11	-1.892030	-1.253437	0.058379
C12	-0.731982	-0.666979	0.665938
C13	0.846106	-2.599957	0.102172
H14	0.988779	-2.987944	1.115445
H15	0.016098	-3.126927	-0.371287
H16	1.754735	-2.746274	-0.481711
C17	1.354333	-0.199931	-0.258865
O18	2.501085	-0.308616	-0.740877
N19	0.709255	1.015212	-0.057256
H20	-0.748421	-0.867415	1.752976
H21	0.998652	1.862363	-0.526993
C22	4.386544	-0.156280	0.167614
H23	3.970253	-0.450081	1.122463
H24	4.653150	-0.911345	-0.558539
N25	4.855043	1.043200	0.030302
H26	5.312417	1.330898	-0.826194
H27	4.694741	1.759144	0.727570

Zero-point correction= 0.218872
Thermal correction to Energy= 0.233518
Thermal correction to Enthalpy= 0.234462
Thermal correction to Gibbs Free Energy= 0.175378
Sum of electronic and zero-point Energies= -752.274971
Sum of electronic and thermal Energies= -752.260325
Sum of electronic and thermal Enthalpies= -752.259381
Sum of electronic and thermal Free Energies= -752.318465

124 N9-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.395849	-0.106429	0.123566
C2	0.580684	1.042968	-0.373673
C3	1.992715	1.230402	-0.197503
O4	2.549465	2.307611	-0.087242
N5	2.664399	0.005474	-0.163486
H6	3.672165	0.063543	-0.090868
C7	2.006376	-1.207085	0.036230
N8	2.801104	-2.250445	0.348209
H9	3.749144	-2.133839	0.665491
H10	2.360788	-3.147044	0.481988
N11	0.725769	-1.385733	-0.086032
C12	-0.026894	-0.299597	-0.577598
C13	-1.368368	-0.568799	1.547484
H14	-1.235707	-1.648389	1.532257
H15	-0.532095	-0.094206	2.061562
H16	-2.314067	-0.284840	2.009677
C17	-1.613262	1.397265	0.122635
O18	-2.674238	1.894591	0.344681
N19	-0.399581	1.965412	-0.134203
H20	-0.246797	2.965443	-0.057034
C21	-2.574653	-0.786614	-0.648759
H22	-3.469119	-0.368407	-0.186193
H23	-2.480562	-0.397455	-1.666946
N24	-2.508742	-2.178043	-0.544204
H25	-3.294274	-2.642841	-0.118643
H26	-2.105181	-2.689636	-1.312684
H27	-0.295405	-0.442829	-1.637964

Zero-point correction= 0.220619
Thermal correction to Energy= 0.234898
Thermal correction to Enthalpy= 0.235843
Thermal correction to Gibbs Free Energy= 0.179658
Sum of electronic and zero-point Energies= -752.275350
Sum of electronic and thermal Energies= -752.261070
Sum of electronic and thermal Enthalpies= -752.260126
Sum of electronic and thermal Free Energies= -752.316311

125 TS_N9-CH_2NH_2[9MOG + H_{C4}]$^{\bullet+}$

N1	-1.051644	-0.343308	0.232694
C2	0.767188	0.952987	-0.305433
C3	2.171216	1.228954	-0.390241
O4	2.693724	2.331094	-0.347358
N5	2.903608	0.038024	-0.519955
H6	3.901969	0.153169	-0.636711
C7	2.394345	-1.172973	-0.043256
N8	3.330716	-2.121377	0.231860
H9	4.243838	-1.844433	0.557770

H10	2.972193	-2.987694	0.603884
N11	1.135779	-1.426766	0.097623
C12	0.249892	-0.442212	-0.460465
C13	-1.624897	-1.506448	0.892803
H14	-2.043904	-2.199510	0.155349
H15	-0.850861	-2.034724	1.453396
H16	-2.401710	-1.165195	1.579876
C17	-1.247126	0.931540	0.731030
O18	-2.224823	1.320250	1.354974
N19	-0.183212	1.715649	0.312995
H20	-0.054975	2.668200	0.627344
C21	-3.666093	0.202625	-0.946761
H22	-3.496614	0.761135	-0.018661
H23	-3.248094	0.536025	-1.891958
N24	-4.382922	-0.858961	-0.928175
H25	-4.796578	-1.194070	-0.061987
H26	-4.566680	-1.405276	-1.765036
H27	0.056779	-0.688035	-1.519554

Zero-point correction= 0.218654
Thermal correction to Energy= 0.233263
Thermal correction to Enthalpy= 0.234208
Thermal correction to Gibbs Free Energy= 0.176175
Sum of electronic and zero-point Energies= -752.260017
Sum of electronic and thermal Energies= -752.245408
Sum of electronic and thermal Enthalpies= -752.244464
Sum of electronic and thermal Free Energies= -752.302496

126 [9MOG + H_{C5}]$^+$···$^{\cdot}CH_2NH_2$

N1	1.308757	0.646511	0.842399
C2	-0.035332	-0.896902	-0.176706
C3	-1.346386	-1.524917	0.208385
O4	-1.565584	-2.693932	0.357002
N5	-2.370829	-0.554682	0.259065
H6	-3.306403	-0.925412	0.385917
C7	-2.138856	0.794023	0.354986
N8	-3.185259	1.612042	0.362962
H9	-4.137061	1.294558	0.263088
H10	-3.014585	2.597878	0.502257
N11	-0.922293	1.324956	0.498551
C12	0.075849	0.466581	0.401490
C13	1.854689	1.854843	1.441295
H14	1.750750	2.685403	0.741653
H15	1.326229	2.082770	2.368230
H16	2.907592	1.664331	1.647553
C17	2.071211	-0.575795	0.711332
O18	3.229722	-0.682372	1.000121
N19	1.189486	-1.506877	0.230445
H20	1.508052	-2.409460	-0.088692
H21	-0.075970	-0.761840	-1.306992
C22	0.504239	-0.037712	-3.067979
H23	1.101637	-0.890430	-3.368978
H24	-0.459994	0.122222	-3.536090
N25	1.158273	1.056169	-2.543251
H26	2.168593	1.052817	-2.552768
H27	0.758642	1.970030	-2.700181

Zero-point correction= 0.215839
Thermal correction to Energy= 0.231743
Thermal correction to Enthalpy= 0.232688
Thermal correction to Gibbs Free Energy= 0.170960
Sum of electronic and zero-point Energies= -752.290663
Sum of electronic and thermal Energies= -752.274758
Sum of electronic and thermal Enthalpies= -752.273814
Sum of electronic and thermal Free Energies= -752.335542

127 TS_[9MOG + H_{C5}]$^+$···$^{\cdot}CH_2NH_2$

N1	1.152454	-1.276570	-0.094324
C2	-0.016072	0.640110	-0.432175
C3	-1.297806	1.059222	-1.046715
O4	-1.456466	1.913327	-1.879128
N5	-2.388817	0.407034	-0.427206
H6	-3.301797	0.730525	-0.727857
C7	-2.271656	-0.709776	0.357733
N8	-3.375759	-1.225109	0.892586
H9	-4.290793	-0.819938	0.773086
H10	-3.288981	-2.081264	1.421041
N11	-1.113153	-1.332634	0.581800
C12	-0.052399	-0.733977	0.066098
C13	1.559353	-2.624173	0.276265
H14	1.367582	-2.786667	1.337302
H15	1.005394	-3.356073	-0.314212
H16	2.625419	-2.708754	0.066944
C17	1.999539	-0.386191	-0.844315
O18	3.145252	-0.607539	-1.127943
N19	1.214130	0.700012	-1.137815
H20	1.586491	1.523192	-1.586174
H21	0.099840	1.362263	0.577271
C22	0.695987	2.236368	1.761763
H23	0.755867	3.184593	1.232503
H24	-0.106509	2.135377	2.488519
N25	1.886124	1.654837	2.097425
H26	2.754420	1.970316	1.694513
H27	1.956248	1.017646	2.874434

Zero-point correction= 0.213471
Thermal correction to Energy= 0.228633
Thermal correction to Enthalpy= 0.229577
Thermal correction to Gibbs Free Energy= 0.169704
Sum of electronic and zero-point Energies= -752.291783
Sum of electronic and thermal Energies= -752.276621
Sum of electronic and thermal Enthalpies= -752.275677
Sum of electronic and thermal Free Energies= -752.335551

128 [9MOG + H_{C5}]$^+$

N1	1.452322	-0.840561	0.023328
C2	0.071599	0.899975	0.595743
C3	-1.145492	1.486875	-0.100398
O4	-1.260942	2.612107	-0.487674
N5	-2.202769	0.555494	-0.142522
H6	-3.089591	0.924446	-0.470071
C7	-2.033938	-0.795743	0.031934
N8	-3.106065	-1.570925	0.026248
H9	-4.047931	-1.215060	-0.041338
H10	-2.970174	-2.569968	0.103234
N11	-0.834071	-1.379720	0.142907
C12	0.185924	-0.557418	0.246482
C13	2.009155	-2.137532	-0.344291
H14	1.782088	-2.864388	0.435869
H15	1.584099	-2.465624	-1.294246
H16	3.086712	-2.007369	-0.439429
C17	2.252253	0.377207	0.025627
O18	3.430872	0.402417	-0.164977
N19	1.363771	1.396599	0.247157
H20	1.684892	2.334103	0.440387
H21	-0.138853	0.981275	1.676381

Zero-point correction= 0.164150
Thermal correction to Energy= 0.175267
Thermal correction to Enthalpy= 0.176211
Thermal correction to Gibbs Free Energy= 0.127180
Sum of electronic and zero-point Energies= -657.141823
Sum of electronic and thermal Energies= -657.130707

Sum of electronic and thermal Enthalpies= -657.129762
Sum of electronic and thermal Free Energies= -657.178793

129 N1-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	2.167695	0.711717	-0.139452
C2	0.493878	-0.863978	-0.450298
C3	-0.608539	-1.237622	0.505367
O4	-0.703059	-2.136969	1.274582
N5	-1.749968	-0.252166	0.387841
H6	-2.339891	-0.423177	1.211343
C7	-1.320824	1.181651	0.368629
N8	-2.366579	2.065664	0.197704
H9	-3.081999	2.062013	0.918045
H10	-2.036357	3.004734	0.008017
N11	-0.059741	1.508308	0.133794
C12	0.817610	0.590266	-0.155578
C13	2.785266	-0.558245	-0.215574
O14	3.967133	-0.767276	-0.213633
N15	1.758741	-1.493524	-0.266681
H16	1.965858	-2.433970	-0.567357
C17	-2.724707	-0.639845	-0.847076
H18	-2.547515	-1.705804	-0.998623
H19	-2.325819	-0.045431	-1.669572
N20	-4.041196	-0.360238	-0.504660
H21	-4.681645	-1.135951	-0.433736
H22	-4.444398	0.484736	-0.879725
H23	0.092471	-0.956738	-1.477164
C24	2.900668	1.933758	0.145427
H25	2.616440	2.706077	-0.570471
H26	2.685713	2.276225	1.160469
H27	3.961777	1.707001	0.045978

Zero-point correction= 0.218892
Thermal correction to Energy= 0.233794
Thermal correction to Enthalpy= 0.234738
Thermal correction to Gibbs Free Energy= 0.176543
Sum of electronic and zero-point Energies= -752.248457
Sum of electronic and thermal Energies= -752.233556
Sum of electronic and thermal Enthalpies= -752.232612
Sum of electronic and thermal Free Energies= -752.290807

130 TS_N1-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	2.173390	0.706109	-0.160196
C2	0.490246	-0.866190	-0.422798
C3	-0.622444	-1.228348	0.527054
O4	-0.735512	-2.154873	1.265116
N5	-1.733187	-0.233908	0.421137
H6	-2.340850	-0.407968	1.228961
C7	-1.304709	1.185618	0.391280
N8	-2.354944	2.077629	0.260165
H9	-3.004947	2.113868	1.040225
H10	-2.020973	3.007463	0.032760
N11	-0.047763	1.515123	0.132738
C12	0.822745	0.589286	-0.154774
C13	2.783955	-0.569053	-0.211936
O14	3.965158	-0.783299	-0.215651
N15	1.752760	-1.499664	-0.230755
H16	1.952198	-2.447955	-0.511148
C17	-2.749600	-0.627107	-0.898053
H18	-2.532431	-1.685393	-1.041382
H19	-2.318780	0.012243	-1.666797
N20	-4.054998	-0.376437	-0.608606
H21	-4.679741	-1.118272	-0.337811
H22	-4.454438	0.524996	-0.814533
H23	0.092516	-0.972872	-1.450627
C24	2.914891	1.929150	0.095584
H25	2.627027	2.690197	-0.630843
H26	2.712015	2.291212	1.106365
H27	3.973921	1.695749	-0.010433

Zero-point correction= 0.218073
Thermal correction to Energy= 0.232539
Thermal correction to Enthalpy= 0.233483
Thermal correction to Gibbs Free Energy= 0.176235
Sum of electronic and zero-point Energies= -752.249115
Sum of electronic and thermal Energies= -752.234649
Sum of electronic and thermal Enthalpies= -752.233705
Sum of electronic and thermal Free Energies= -752.290953

131 C2-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	1.855976	-0.918465	0.145799
C2	0.696427	1.010659	0.610143
C3	-0.415884	1.702708	-0.192496
O4	-0.312517	2.845143	-0.563401
N5	-1.527477	0.919955	-0.325990
H6	-2.394948	1.361143	-0.623618
C7	-1.659725	-0.490916	-0.047606
N8	-1.790686	-1.194713	-1.327583
H9	-2.003110	-2.186574	-1.297378
H10	-1.176138	-0.903768	-2.080894
N11	-0.478612	-1.166194	0.398784
C12	0.641194	-0.464261	0.376226
C13	2.249349	-2.285458	-0.161359
H14	1.640559	-2.968422	0.430944
H15	2.108881	-2.482343	-1.226756
H16	3.305779	-2.387535	0.085732
C17	2.808153	0.196786	0.076705
O18	3.974072	0.048900	-0.138654
N19	2.054705	1.312979	0.273904
H20	2.467050	2.232188	0.345385
C21	-2.887438	-0.762216	0.833550
H22	-3.001890	-1.847970	0.948832
H23	-2.665059	-0.352994	1.822531
N24	-4.030671	-0.086718	0.257253
H25	-4.593149	-0.682270	-0.336588
H26	-4.631875	0.331612	0.954578
H27	0.476356	1.222852	1.667524

Zero-point correction= 0.219158
Thermal correction to Energy= 0.233498
Thermal correction to Enthalpy= 0.234442
Thermal correction to Gibbs Free Energy= 0.177825
Sum of electronic and zero-point Energies= -752.256531
Sum of electronic and thermal Energies= -752.242191
Sum of electronic and thermal Enthalpies= -752.241247
Sum of electronic and thermal Free Energies= -752.297864

132 TS_C2-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	-1.863177	-0.933211	-0.110953
C2	-0.677548	0.975312	-0.600644
C3	0.373157	1.686875	0.263069
O4	0.223918	2.816982	0.657613
N5	1.484943	0.918722	0.455581
H6	2.268483	1.351809	0.931853
C7	1.665381	-0.481761	0.102272
N8	2.107783	-1.163302	1.316681
H9	2.513026	-2.084552	1.183896
H10	1.445273	-1.134386	2.086863
N11	0.479918	-1.188464	-0.228583
C12	-0.633675	-0.490610	-0.299997
C13	-2.281302	-2.281845	0.239299
H14	-1.553484	-2.989267	-0.156828
H15	-2.351937	-2.379572	1.325114

H16	-3.266394	-2.447183	-0.196903
C17	-2.813417	0.178987	-0.142510
O18	-3.989137	0.042366	0.024783
N19	-2.052988	1.286892	-0.365093
H20	-2.458698	2.205157	-0.472886
C21	2.779995	-0.653207	-0.974839
H22	2.865494	-1.720208	-1.202741
H23	2.438424	-0.143618	-1.880160
N24	3.994802	-0.102011	-0.461225
H25	4.745686	-0.751990	-0.285145
H26	4.328321	0.739162	-0.908615
H27	-0.386956	1.146975	-1.648365

Zero-point correction= 0.217990
Thermal correction to Energy= 0.232039
Thermal correction to Enthalpy= 0.232983
Thermal correction to Gibbs Free Energy= 0.176930
Sum of electronic and zero-point Energies= -752.256545
Sum of electronic and thermal Energies= -752.242496
Sum of electronic and thermal Enthalpies= -752.241552
Sum of electronic and thermal Free Energies= -752.297605

133 N2-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	1.879188	-1.139118	-0.015412
C2	0.908586	0.860743	0.619823
C3	0.109805	1.892589	-0.165220
O4	0.459494	3.021199	-0.395971
N5	-1.136420	1.388698	-0.555280
H6	-1.659929	2.036827	-1.136345
C7	-1.359634	0.016162	-0.687792
N8	-2.745006	-0.424891	-0.643178
H9	-3.357706	0.129105	-1.249769
H10	-2.764066	-1.378698	-1.019441
N11	-0.451162	-0.934817	-0.444996
C12	0.697851	-0.503120	0.010479
C13	2.131254	-2.464523	-0.553828
H14	1.547181	-3.203719	-0.003760
H15	1.866901	-2.498852	-1.613426
H16	3.195353	-2.664696	-0.429905
C17	2.936363	-0.234752	0.332695
O18	4.101434	-0.523198	0.352999
N19	2.334882	0.973023	0.588696
H20	2.854288	1.735706	0.995347
H21	0.510645	0.860966	1.649398
C22	-3.421825	-0.467808	0.772925
H23	-2.797868	-1.163163	1.337122
H24	-3.299190	0.544790	1.160750
N25	-4.757538	-0.864371	0.625174
H26	-4.999887	-1.788372	0.950240
H27	-5.465148	-0.179326	0.844047

Zero-point correction= 0.221512
Thermal correction to Energy= 0.236088
Thermal correction to Enthalpy= 0.237032
Thermal correction to Gibbs Free Energy= 0.178495
Sum of electronic and zero-point Energies= -752.274475
Sum of electronic and thermal Energies= -752.259899
Sum of electronic and thermal Enthalpies= -752.258954
Sum of electronic and thermal Free Energies= -752.317492

134 TS_N2-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	1.867818	-1.190466	-0.028731
C2	0.992900	0.837119	0.644074
C3	0.268904	1.932921	-0.123298
O4	0.667134	3.058863	-0.281883
N5	-0.977808	1.496453	-0.572933
H6	-1.511331	2.202940	-1.067387
C7	-1.307341	0.151565	-0.706565
N8	-2.620185	-0.179756	-0.929877
H9	-3.191366	0.505005	-1.413784
H10	-2.708618	-1.102702	-1.344410
N11	-0.428100	-0.845430	-0.522052
C12	0.723342	-0.489304	-0.016456
C13	2.059996	-2.507057	-0.610886
H14	1.417752	-3.230990	-0.107387
H15	1.824863	-2.485349	-1.677720
H16	3.106823	-2.773163	-0.466021
C17	2.962766	-0.361445	0.379210
O18	4.109401	-0.716065	0.424052
N19	2.423200	0.870556	0.657875
H20	2.970874	1.587166	1.108469
H21	0.562892	0.826510	1.661630
C22	-3.845833	-0.538964	0.954503
H23	-3.115993	-1.290211	1.228184
H24	-3.680048	0.486831	1.257830
N25	-5.096884	-0.929298	0.720609
H26	-5.337168	-1.904963	0.626422
H27	-5.855654	-0.266873	0.659086

Zero-point correction= 0.217200
Thermal correction to Energy= 0.232101
Thermal correction to Enthalpy= 0.233046
Thermal correction to Gibbs Free Energy= 0.173001
Sum of electronic and zero-point Energies= -752.268443
Sum of electronic and thermal Energies= -752.253541
Sum of electronic and thermal Enthalpies= -752.252596
Sum of electronic and thermal Free Energies= -752.312641

135 N3-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	-1.027441	-1.231292	0.109460
C2	-1.027052	0.859847	-0.901594
C3	-0.611320	2.008522	0.023623
O4	-1.326492	2.898754	0.387601
N5	0.735433	1.954316	0.438517
H6	1.039893	2.741942	1.000227
C7	1.613382	0.943579	0.189681
N8	2.909575	1.132689	0.404874
H9	3.266626	2.033101	0.687022
H10	3.480585	0.286266	0.500519
N11	1.159364	-0.225719	-0.288957
C12	-0.216705	-0.370221	-0.598640
C13	-0.673906	-2.527812	0.644952
H14	-0.414659	-3.230535	-0.153345
H15	0.156225	-2.433090	1.350998
H16	-1.547668	-2.907166	1.175970
C17	-2.374617	-0.792549	0.055157
O18	-3.313288	-1.381092	0.525393
N19	-2.360249	0.398766	-0.632465
H20	-3.156530	1.018054	-0.594750
H21	-0.901720	1.206789	-1.936661
C22	2.099959	-1.246759	-0.820581
H23	1.463671	-2.072468	-1.149692
H24	2.598596	-0.828437	-1.700927
N25	3.102456	-1.592315	0.162188
H26	2.744468	-2.211408	0.882780
H27	3.896345	-2.047108	-0.277005

Zero-point correction= 0.221892
Thermal correction to Energy= 0.235778
Thermal correction to Enthalpy= 0.236722
Thermal correction to Gibbs Free Energy= 0.180939
Sum of electronic and zero-point Energies= -752.293547
Sum of electronic and thermal Energies= -752.279661

Sum of electronic and thermal Enthalpies= -752.278717
Sum of electronic and thermal Free Energies= -752.334501

136 TS_N3-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	1.244870	-1.254112	-0.234239
C2	0.934603	0.817513	0.784227
C3	0.476262	2.118745	0.137452
O4	1.118611	3.130419	0.048899
N5	-0.848932	2.041305	-0.328653
H6	-1.215310	2.911799	-0.696453
C7	-1.552127	0.870359	-0.496336
N8	-2.872770	0.964845	-0.808637
H9	-3.273737	1.873338	-0.987398
H10	-3.252477	0.212817	-1.362640
N11	-0.978621	-0.318108	-0.381701
C12	0.294377	-0.313084	0.038318
C13	1.070963	-2.448883	-1.031914
H14	0.487256	-3.196887	-0.487545
H15	0.576393	-2.209514	-1.977229
H16	2.063454	-2.856666	-1.226787
C17	2.526787	-0.757560	0.115529
O18	3.566775	-1.342479	-0.051396
N19	2.324018	0.496778	0.643258
H20	3.075441	1.006927	1.079747
H21	0.619961	0.858792	1.844929
C22	-2.316395	-1.722712	0.886575
H23	-1.841903	-2.532476	0.351728
H24	-1.807296	-1.251786	1.715968
N25	-3.617321	-1.571546	0.779970
H26	-4.162010	-2.123725	0.132039
H27	-4.118401	-0.896548	1.340519

Zero-point correction= 0.216645
Thermal correction to Energy= 0.231746
Thermal correction to Enthalpy= 0.232690
Thermal correction to Gibbs Free Energy= 0.173484
Sum of electronic and zero-point Energies= -752.265685
Sum of electronic and thermal Energies= -752.250584
Sum of electronic and thermal Enthalpies= -752.249639
Sum of electronic and thermal Free Energies= -752.308846

137 C4-$CH_2\dot{N}H_2^+$[9MOG + H_{C5}]

N1	1.198161	-0.100583	-0.657348
C2	-0.145523	0.878392	0.940279
C3	-1.424774	1.478606	0.348647
O4	-1.650003	2.660843	0.350786
N5	-2.324525	0.539597	-0.126153
H6	-3.202843	0.916161	-0.463443
C7	-2.003678	-0.796169	-0.347947
N8	-3.012934	-1.570206	-0.779274
H9	-3.967094	-1.252850	-0.825746
H10	-2.817062	-2.538186	-0.980311
N11	-0.813181	-1.296085	-0.199672
C12	0.196107	-0.445123	0.243071
C13	1.659828	-0.924138	-1.745276
H14	2.052424	-1.872691	-1.358543
H15	0.833320	-1.150798	-2.422516
H16	2.449844	-0.380749	-2.263789
C17	1.765356	1.169929	-0.357012
O18	2.702323	1.656824	-0.931231
N19	1.028957	1.666423	0.691432
H20	1.073849	2.651878	0.912465
H21	-0.332511	0.747198	2.012486
C22	1.014758	-1.406860	1.562543
H23	1.724316	-0.689272	1.974690
H24	0.129441	-1.578767	2.173639
N25	1.590236	-2.549324	1.107025
H26	2.570898	-2.590142	0.873498
H27	1.027417	-3.359688	0.893239

Zero-point correction= 0.218741
Thermal correction to Energy= 0.233594
Thermal correction to Enthalpy= 0.234538
Thermal correction to Gibbs Free Energy= 0.176839
Sum of electronic and zero-point Energies= -752.289360
Sum of electronic and thermal Energies= -752.274507
Sum of electronic and thermal Enthalpies= -752.273563
Sum of electronic and thermal Free Energies= -752.331262

138 TS_C4- $CH_2\dot{N}H_2^+$[9MOG + H_{C5}]

N1	1.178211	0.347902	0.884867
C2	-0.146369	-0.900156	-0.521555
C3	-1.527750	-1.490372	-0.283663
O4	-1.802246	-2.655701	-0.338990
N5	-2.498712	-0.493906	-0.098730
H6	-3.454582	-0.830147	-0.055911
C7	-2.203052	0.805464	0.254778
N8	-3.217441	1.655789	0.388665
H9	-4.178482	1.403987	0.218307
H10	-3.010081	2.594246	0.698841
N11	-0.976413	1.232120	0.520154
C12	0.005459	0.378403	0.261319
C13	1.699838	1.357118	1.790498
H14	1.849168	2.297401	1.255664
H15	0.997828	1.515166	2.610731
H16	2.651905	0.989092	2.172288
C17	1.866463	-0.887503	0.619147
O18	2.976579	-1.138685	0.997974
N19	0.979475	-1.664812	-0.078694
H20	1.291028	-2.509325	-0.534369
H21	-0.095463	-0.675830	-1.597397
C22	1.101205	1.747760	-1.816755
H23	0.278985	1.833881	-2.516817
H24	1.301055	2.561052	-1.131048
N25	2.111914	0.873581	-2.113812
H26	2.134978	0.435634	-3.023050
H27	3.024999	1.020937	-1.708873

Zero-point correction= 0.216138
Thermal correction to Energy= 0.231310
Thermal correction to Enthalpy= 0.232254
Thermal correction to Gibbs Free Energy= 0.173385
Sum of electronic and zero-point Energies= -752.287522
Sum of electronic and thermal Energies= -752.272350
Sum of electronic and thermal Enthalpies= -752.271406
Sum of electronic and thermal Free Energies= -752.330276

139 C4-$^+NH_2\dot{C}H_2$[9MOG + H_{C5}]

N1	1.168733	-0.413590	-0.786987
C2	0.160615	0.612793	1.004685
C3	-0.795919	1.686768	0.474727
O4	-0.618809	2.861346	0.668976
N5	-1.902469	1.194157	-0.197160
H6	-2.567275	1.891744	-0.510739
C7	-2.042086	-0.134419	-0.577088
N8	-3.208028	-0.456787	-1.157112
H9	-3.993214	0.172173	-1.195326
H10	-3.331980	-1.402537	-1.483428
N11	-1.119003	-1.036492	-0.420296
C12	0.104897	-0.616054	0.097702
C13	1.419318	-1.171765	-2.001762
H14	1.895560	-2.135867	-1.792368
H15	0.477952	-1.330845	-2.528060

H16	2.097244	-0.584322	-2.621048
C17	2.079178	0.537215	-0.287387
O18	3.116002	0.854732	-0.806012
N19	1.547800	0.990034	0.916979
H20	1.837748	1.908777	1.229343
H21	-0.154232	0.385953	2.029483
H22	0.534152	-2.700983	0.375486
H23	1.514563	-1.784773	1.354889
H24	-1.274657	-2.652226	1.938372
H25	0.007395	-1.917074	3.147029
N26	0.547525	-1.939762	1.059961
C27	-0.303120	-2.238133	2.163282

Zero-point correction= 0.218358
Thermal correction to Energy= 0.233323
Thermal correction to Enthalpy= 0.234267
Thermal correction to Gibbs Free Energy= 0.176443
Sum of electronic and zero-point Energies= -752.269461
Sum of electronic and thermal Energies= -752.254496
Sum of electronic and thermal Enthalpies= -752.253552
Sum of electronic and thermal Free Energies= -752.311376

140 TS_ C4-$^{+}NH_2\dot{C}H_2$[9MOG + H_{C5}]

N1	1.196910	-0.421133	-0.776620
C2	0.151125	0.624210	0.985001
C3	-0.817858	1.689719	0.461632
O4	-0.652239	2.866438	0.651035
N5	-1.928629	1.180432	-0.192284
H6	-2.608913	1.868303	-0.493989
C7	-2.043360	-0.145397	-0.590438
N8	-3.207985	-0.486590	-1.160837
H9	-4.002219	0.130872	-1.198927
H10	-3.311920	-1.428329	-1.505378
N11	-1.096007	-1.027883	-0.463019
C12	0.109753	-0.595902	0.070509
C13	1.456171	-1.169649	-1.995236
H14	1.720063	-2.210901	-1.782996
H15	0.580118	-1.142267	-2.644102
H16	2.302684	-0.692284	-2.489405
C17	2.095863	0.542499	-0.269777
O18	3.143375	0.852671	-0.770243
N19	1.534481	1.013202	0.910453
H20	1.820263	1.931819	1.226027
H21	-0.169804	0.384788	2.005290
H22	0.514711	-2.713568	0.404901
H23	1.505200	-1.804864	1.384508
H24	-1.285870	-2.657529	1.962752
H25	-0.032834	-1.866876	3.161161
N26	0.538174	-1.954915	1.089991
C27	-0.321555	-2.224450	2.183313

Zero-point correction= 0.217748
Thermal correction to Energy= 0.232170
Thermal correction to Enthalpy= 0.233115
Thermal correction to Gibbs Free Energy= 0.176367
Sum of electronic and zero-point Energies= -752.270031
Sum of electronic and thermal Energies= -752.255609
Sum of electronic and thermal Enthalpies= -752.254665
Sum of electronic and thermal Free Energies= -752.311412

141 C6-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	2.013424	0.460093	-0.158319
C2	0.007934	-0.650161	-0.397592
C3	-1.199118	-0.595725	0.581945
O4	-0.927342	-0.705511	1.846068
N5	-1.901499	0.667581	0.210921
H6	-2.832299	0.775245	0.594760
C7	-1.219417	1.796065	-0.081069
N8	-1.866902	2.952620	-0.193916
H9	-2.862998	3.044154	-0.073089
H10	-1.323876	3.778593	-0.399616
N11	0.118892	1.836936	-0.247444
C12	0.710999	0.671874	-0.279268
C13	3.043262	1.474358	0.020986
H14	2.960686	2.217766	-0.772084
H15	2.924084	1.955541	0.993430
H16	4.007329	0.969617	-0.031119
C17	2.288327	-0.951153	-0.074984
O18	3.382164	-1.427854	0.025480
N19	1.063877	-1.570798	-0.127227
H20	1.020126	-2.563598	-0.294990
H21	-0.435412	-0.765790	-1.398869
C22	-2.218907	-1.846933	0.215677
H23	-1.722371	-2.733593	0.609555
H24	-3.110666	-1.644356	0.814276
N25	-2.460013	-1.924984	-1.166317
H26	-2.197916	-2.777924	-1.635953
H27	-3.318185	-1.528815	-1.516733

Zero-point correction= 0.219027
Thermal correction to Energy= 0.233594
Thermal correction to Enthalpy= 0.234538
Thermal correction to Gibbs Free Energy= 0.177831
Sum of electronic and zero-point Energies= -752.278603
Sum of electronic and thermal Energies= -752.264036
Sum of electronic and thermal Enthalpies= -752.263092
Sum of electronic and thermal Free Energies= -752.319799

142 TS_C6-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	2.066192	0.372642	-0.267775
C2	0.007036	-0.659251	-0.310652
C3	-1.097173	-0.519217	0.748231
O4	-1.049077	-0.992633	1.881255
N5	-1.748625	0.776976	0.526086
H6	-2.525460	0.955503	1.152443
C7	-1.077990	1.850766	0.036712
N8	-1.700575	3.024915	-0.046177
H9	-2.666686	3.154957	0.208669
H10	-1.163024	3.825626	-0.345129
N11	0.215709	1.820542	-0.331146
C12	0.770446	0.633877	-0.317651
C13	3.145720	1.348512	-0.204685
H14	3.033019	2.064088	-1.019147
H15	3.119449	1.870472	0.753787
H16	4.083820	0.803482	-0.302998
C17	2.284496	-1.039739	-0.040268
O18	3.359521	-1.532886	0.146383
N19	1.043719	-1.616478	-0.081474
H20	0.903152	-2.553495	0.262883
H21	-0.470700	-0.772628	-1.295614
C22	-2.582376	-1.799870	-0.100620
H23	-2.094854	-2.720395	0.202097
H24	-3.355534	-1.428464	0.563596
N25	-2.767547	-1.618211	-1.426542
H26	-2.356423	-2.241525	-2.104316
H27	-3.453370	-0.966638	-1.774578

Zero-point correction= 0.217766
Thermal correction to Energy= 0.232351
Thermal correction to Enthalpy= 0.233295
Thermal correction to Gibbs Free Energy= 0.175917
Sum of electronic and zero-point Energies= -752.277926
Sum of electronic and thermal Energies= -752.263341

Sum of electronic and thermal Enthalpies= -752.262397
Sum of electronic and thermal Free Energies= -752.319775

143 O6-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	1.895673	-0.867241	0.171611
C2	0.002371	-0.160601	-0.971126
C3	-1.097762	0.652275	-0.320631
O4	-2.078863	0.229703	0.455114
N5	-0.726781	1.976646	-0.115949
H6	-1.463580	2.621249	0.146839
C7	0.574611	2.365196	-0.029472
N8	0.877544	3.667455	-0.004402
H9	0.186024	4.394931	-0.086983
H10	1.844553	3.927910	0.117860
N11	1.564646	1.465972	0.088051
C12	1.246287	0.235898	-0.205749
C13	3.098224	-0.920075	0.991614
H14	3.917330	-0.417607	0.475644
H15	2.913438	-0.434270	1.951359
H16	3.340624	-1.971745	1.141217
C17	1.175982	-2.034008	-0.227041
O18	1.541519	-3.162979	-0.060381
N19	-0.007704	-1.586596	-0.789221
H20	-0.468596	-2.204969	-1.441196
H21	0.108795	0.133848	-2.026483
C22	-2.939181	-0.940339	0.014555
H23	-2.377759	-1.829359	0.298218
H24	-3.026738	-0.844765	-1.070601
N25	-4.179272	-0.914192	0.627482
H26	-4.201967	-1.126484	1.613829
H27	-4.805309	-0.166933	0.366527

Zero-point correction= 0.219986
Thermal correction to Energy= 0.234721
Thermal correction to Enthalpy= 0.235665
Thermal correction to Gibbs Free Energy= 0.177579
Sum of electronic and zero-point Energies= -752.284192
Sum of electronic and thermal Energies= -752.269457
Sum of electronic and thermal Enthalpies= -752.268513
Sum of electronic and thermal Free Energies= -752.326599

144 TS_O6-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	-2.256195	-0.709410	0.075244
C2	-0.023906	-0.359438	0.505539
C3	1.015151	0.423747	-0.262689
O4	2.052191	-0.012293	-0.706632
N5	0.727145	1.808450	-0.237844
H6	1.465225	2.408755	-0.588107
C7	-0.510551	2.319500	0.016000
N8	-0.676105	3.639607	0.047044
H9	0.082552	4.295926	-0.049488
H10	-1.611985	3.995398	0.178958
N11	-1.598827	1.547442	0.168435
C12	-1.369779	0.259937	0.248931
C13	-3.674001	-0.545983	-0.214965
H14	-4.140935	0.041321	0.576033
H15	-3.801763	-0.043130	-1.175382
H16	-4.112076	-1.542833	-0.254244
C17	-1.593215	-1.992637	0.010405
O18	-2.155895	-3.036113	-0.159415
N19	-0.255400	-1.724692	0.143156
H20	0.406915	-2.469368	0.295655
H21	0.221740	-0.250103	1.579993
C22	4.212228	-0.533206	0.715329
H23	3.864358	-1.139195	1.541392
H24	4.358693	0.529675	0.847346
N25	4.884474	-1.148670	-0.285001
H26	4.784116	-2.139952	-0.430895
H27	5.201600	-0.619856	-1.081414

Zero-point correction= 0.214278
Thermal correction to Energy= 0.230328
Thermal correction to Enthalpy= 0.231272
Thermal correction to Gibbs Free Energy= 0.168052
Sum of electronic and zero-point Energies= -752.274118
Sum of electronic and thermal Energies= -752.258069
Sum of electronic and thermal Enthalpies= -752.257125
Sum of electronic and thermal Free Energies= -752.320345

145 N7-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	-0.645241	1.567641	-0.097552
C2	-0.004253	-0.645436	0.299578
C3	1.027334	-1.530500	-0.367820
O4	0.726215	-2.512962	-1.016690
N5	2.309332	-1.084031	-0.161864
H6	3.038303	-1.661461	-0.566381
C7	2.625341	0.228485	0.223568
N8	3.943931	0.503914	0.388359
H9	4.579920	-0.219337	0.687724
H10	4.165881	1.441767	0.688157
N11	1.709012	1.166835	0.306594
C12	0.453909	0.766317	0.207843
C13	-0.611303	3.027096	-0.124273
H14	-0.402476	3.402562	0.878236
H15	0.172743	3.353214	-0.809131
H16	-1.582267	3.383696	-0.465101
C17	-1.730584	0.853482	-0.447675
O18	-2.846868	1.158068	-0.758930
N19	-1.303374	-0.628637	-0.420594
H20	-0.211586	-0.960853	1.333862
C21	-2.417961	-1.522899	0.165342
H22	-3.268985	-1.341426	-0.493900
H23	-2.044267	-2.539456	0.034218
N24	-2.635906	-1.180081	1.515260
H25	-3.461334	-0.623027	1.687662
H26	-2.560773	-1.942340	2.172300
H27	-1.159117	-0.932945	-1.393469

Zero-point correction= 0.220784
Thermal correction to Energy= 0.235313
Thermal correction to Enthalpy= 0.236257
Thermal correction to Gibbs Free Energy= 0.178695
Sum of electronic and zero-point Energies= -752.286269
Sum of electronic and thermal Energies= -752.271740
Sum of electronic and thermal Enthalpies= -752.270796
Sum of electronic and thermal Free Energies= -752.328358

146 TS_N7-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	-0.497732	1.390906	-0.169897
C2	0.210660	-0.751561	0.421879
C3	1.266255	-1.561845	-0.307629
O4	1.012221	-2.528030	-0.999898
N5	2.534579	-1.072928	-0.085670
H6	3.286099	-1.636035	-0.465201
C7	2.795804	0.244890	0.317518
N8	4.082438	0.547295	0.638509
H9	4.843419	-0.033298	0.323795
H10	4.286813	1.528505	0.754337
N11	1.846580	1.149632	0.388854
C12	0.604194	0.686871	0.314742
C13	-0.508961	2.820817	-0.428107
H14	-1.470503	3.075532	-0.872395
H15	-0.365907	3.365300	0.506779

H16	0.297723	3.075449	-1.118638
C17	-1.480899	0.536677	-0.565088
O18	-2.553448	0.815051	-1.087261
N19	-1.112560	-0.792065	-0.203081
H20	-1.159119	-1.448578	-0.982944
C21	-3.417609	-1.388714	0.682156
H22	-3.456863	-1.682154	-0.358313
H23	-3.063930	-2.076202	1.442094
N24	-3.947252	-0.268984	1.019338
H25	-4.206299	0.395054	0.289082
H26	-3.978060	0.042881	1.983454
H27	0.157412	-1.102433	1.466015

Zero-point correction= 0.217659
Thermal correction to Energy= 0.232508
Thermal correction to Enthalpy= 0.233452
Thermal correction to Gibbs Free Energy= 0.174910
Sum of electronic and zero-point Energies= -752.273886
Sum of electronic and thermal Energies= -752.259036
Sum of electronic and thermal Enthalpies= -752.258092
Sum of electronic and thermal Free Energies= -752.316634

147 C8-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	-0.708743	-1.188518	-0.058211
C2	0.309464	0.774057	-0.706518
C3	1.355041	1.576610	0.056716
O4	1.220844	2.690017	0.475233
N5	2.575434	0.879533	0.116051
H6	3.359478	1.402515	0.490663
C7	2.682953	-0.475809	-0.106200
N8	3.897901	-1.011232	-0.096471
H9	4.741658	-0.467256	-0.003209
H10	3.976253	-2.011922	-0.209729
N11	1.635197	-1.279015	-0.261538
C12	0.459493	-0.672287	-0.338484
C13	-0.926676	-2.533094	0.459310
H14	0.013583	-3.081089	0.420506
H15	-1.270591	-2.463424	1.494296
H16	-1.676095	-3.042115	-0.148600
C17	-1.729306	-0.099803	0.158546
O18	-1.724891	0.293304	1.440410
N19	-1.082044	1.020074	-0.508681
H20	-1.452451	1.943398	-0.316927
C21	-3.109226	-0.432562	-0.401388
H22	-2.976473	-0.754564	-1.438552
H23	-3.530704	-1.273253	0.168570
N24	-3.894947	0.783591	-0.364686
H25	-4.619038	0.791413	-1.071076
H26	-4.320630	0.937919	0.541520
H27	0.577333	0.898099	-1.769740

Zero-point correction= 0.219310
Thermal correction to Energy= 0.233700
Thermal correction to Enthalpy= 0.234644
Thermal correction to Gibbs Free Energy= 0.177861
Sum of electronic and zero-point Energies= -752.252692
Sum of electronic and thermal Energies= -752.238302
Sum of electronic and thermal Enthalpies= -752.237358
Sum of electronic and thermal Free Energies= -752.294141

148 TS_C8-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	0.703447	1.166949	-0.013940
C2	-0.311040	-0.789267	-0.667720
C3	-1.377599	-1.570901	0.084404
O4	-1.254517	-2.673537	0.536331
N5	-2.597696	-0.871441	0.099717
H6	-3.392828	-1.384807	0.463937
C7	-2.690602	0.482618	-0.138291
N8	-3.902558	1.025031	-0.166123
H9	-4.751534	0.486203	-0.093713
H10	-3.971805	2.024807	-0.292176
N11	-1.634233	1.277404	-0.274209
C12	-0.460907	0.658825	-0.315256
C13	0.931494	2.516054	0.485296
H14	-0.021486	3.041057	0.532863
H15	1.366809	2.450276	1.485092
H16	1.611608	3.047016	-0.183029
C17	1.730071	0.075822	0.198032
O18	1.855844	-0.201060	1.493615
N19	1.075596	-1.064093	-0.446378
H20	1.341267	-1.967366	-0.070550
C21	3.094549	0.414267	-0.455764
H22	2.862641	0.747792	-1.472364
H23	3.550316	1.251027	0.086812
N24	3.894522	-0.776599	-0.481884
H25	4.309094	-0.977673	-1.379720
H26	4.586384	-0.832695	0.252135
H27	-0.570413	-0.914122	-1.733352

Zero-point correction= 0.218070
Thermal correction to Energy= 0.232039
Thermal correction to Enthalpy= 0.232983
Thermal correction to Gibbs Free Energy= 0.177306
Sum of electronic and zero-point Energies= -752.253346
Sum of electronic and thermal Energies= -752.239377
Sum of electronic and thermal Enthalpies= -752.238433
Sum of electronic and thermal Free Energies= -752.294110

149 O8-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	0.481507	-1.219879	0.158324
C2	-0.577164	0.755608	0.830353
C3	-1.513466	1.591543	-0.032567
O4	-1.226636	2.682051	-0.472771
N5	-2.726988	0.964882	-0.235293
H6	-3.406307	1.501569	-0.762192
C7	-2.924128	-0.415312	-0.093363
N8	-4.182937	-0.862688	-0.321780
H9	-4.975153	-0.255594	-0.180725
H10	-4.339153	-1.848879	-0.177351
N11	-1.938450	-1.244473	0.144474
C12	-0.776802	-0.686516	0.482363
C13	0.712969	-2.604485	-0.232101
H14	0.346678	-3.262087	0.556683
H15	0.177057	-2.814537	-1.159323
H16	1.781600	-2.753143	-0.376088
C17	1.382574	-0.232359	0.137911
O18	2.608627	-0.435262	-0.202103
N19	0.834940	0.937560	0.529110
H20	1.227965	1.849016	0.343036
H21	-0.781159	0.982633	1.889726
C22	3.658630	0.711243	-0.068464
H23	3.347667	1.438697	-0.818953
H24	3.527034	1.072207	0.952557
N25	4.920979	0.240850	-0.299331
H26	5.354954	-0.335085	0.405425
H27	5.183852	0.018790	-1.247119

Zero-point correction= 0.219407
Thermal correction to Energy= 0.234525
Thermal correction to Enthalpy= 0.235470
Thermal correction to Gibbs Free Energy= 0.176449
Sum of electronic and zero-point Energies= -752.288084
Sum of electronic and thermal Energies= -752.272965

Sum of electronic and thermal Enthalpies= -752.272021
Sum of electronic and thermal Free Energies= -752.331042

150 TS_O8-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	-0.398132	1.149547	0.265861
C2	0.766989	-0.793391	0.832844
C3	1.696777	-1.592350	-0.067234
O4	1.444594	-2.695379	-0.507533
N5	2.877493	-0.917671	-0.306693
H6	3.556315	-1.414009	-0.871531
C7	3.032639	0.464675	-0.147259
N8	4.280893	0.959335	-0.421160
H9	5.078721	0.422358	-0.112137
H10	4.370596	1.953894	-0.270908
N11	2.015927	1.256398	0.108930
C12	0.887428	0.645001	0.440666
C13	-0.685330	2.497040	-0.179275
H14	-0.301885	3.215335	0.547485
H15	-0.213325	2.683779	-1.147633
H16	-1.765934	2.603828	-0.266539
C17	-1.305990	0.119522	0.290936
O18	-2.517322	0.213661	0.038297
N19	-0.645560	-1.022265	0.637554
H20	-1.052359	-1.937575	0.531792
H21	1.060203	-0.973704	1.882896
C22	-4.954070	-0.401415	0.333644
H23	-5.262727	-1.363269	0.731163
H24	-4.550118	0.367393	0.979243
N25	-5.097756	-0.164910	-0.913958
H26	-4.744534	0.701332	-1.311153
H27	-5.453841	-0.863159	-1.558451

Zero-point correction= 0.217258
Thermal correction to Energy= 0.232730
Thermal correction to Enthalpy= 0.233675
Thermal correction to Gibbs Free Energy= 0.172283
Sum of electronic and zero-point Energies= -752.276390
Sum of electronic and thermal Energies= -752.260918
Sum of electronic and thermal Enthalpies= -752.259974
Sum of electronic and thermal Free Energies= -752.321366

151 N9-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	-1.365193	0.177932	-0.211316
C2	0.497224	-0.971172	0.797993
C3	1.900365	-1.243878	0.262155
O4	2.341703	-2.354422	0.102197
N5	2.632725	-0.091287	0.027949
H6	3.593147	-0.247640	-0.255995
C7	2.059995	1.166785	-0.138129
N8	2.898534	2.190181	-0.380328
H9	3.897780	2.109196	-0.288425
H10	2.500886	3.108875	-0.499575
N11	0.761935	1.359540	-0.117856
C12	-0.001116	0.343115	0.279954
C13	-1.611896	0.805660	-1.542397
H14	-1.512054	1.882043	-1.418784
H15	-0.871182	0.435389	-2.250214
H16	-2.615705	0.527479	-1.863020
C17	-1.560320	-1.335990	-0.289141
O18	-2.543963	-1.805796	-0.780743
N19	-0.494812	-1.898480	0.303673
H20	-0.404945	-2.903777	0.371969
H21	0.558435	-1.015204	1.897078
C22	-2.448148	0.714878	0.842324
H23	-3.390092	0.328599	0.449243
H24	-2.175930	0.192412	1.762574
N25	-2.412180	2.097622	0.939468
H26	-3.202637	2.622055	0.603321
H27	-1.923311	2.517380	1.712508

Zero-point correction= 0.220042
Thermal correction to Energy= 0.234568
Thermal correction to Enthalpy= 0.235513
Thermal correction to Gibbs Free Energy= 0.178671
Sum of electronic and zero-point Energies= -752.278284
Sum of electronic and thermal Energies= -752.263758
Sum of electronic and thermal Enthalpies= -752.262814
Sum of electronic and thermal Free Energies= -752.319656

152 TS_N9-CH_2NH_2[9MOG + H_{C5}]$^{\bullet+}$

N1	1.178478	0.056644	0.449847
C2	-0.585946	-0.906790	-0.742099
C3	-2.025991	-1.160438	-0.314219
O4	-2.530663	-2.250408	-0.218408
N5	-2.720884	0.025500	-0.100892
H6	-3.704860	-0.088513	0.113307
C7	-2.112114	1.260449	0.105195
N8	-2.929830	2.320769	0.250338
H9	-3.907777	2.286238	0.014682
H10	-2.510721	3.220606	0.423909
N11	-0.810366	1.398921	0.227816
C12	-0.092424	0.299802	-0.010942
C13	1.698177	0.781544	1.607663
H14	1.816334	1.834294	1.344627
H15	1.000472	0.703555	2.444438
H16	2.655773	0.339133	1.882288
C17	1.413716	-1.375431	0.365693
O18	2.386821	-1.916127	0.825658
N19	0.381228	-1.896249	-0.347504
H20	0.309763	-2.883777	-0.543621
H21	-0.596756	-0.766814	-1.838213
C22	2.866389	0.600480	-1.074189
H23	3.551606	-0.046609	-0.538347
H24	2.261759	0.194917	-1.875555
N25	3.053004	1.906279	-1.034806
H26	3.726055	2.322671	-0.407343
H27	2.516835	2.535834	-1.614376

Zero-point correction= 0.216628
Thermal correction to Energy= 0.231615
Thermal correction to Enthalpy= 0.232559
Thermal correction to Gibbs Free Energy= 0.173471
Sum of electronic and zero-point Energies= -752.275060
Sum of electronic and thermal Energies= -752.260072
Sum of electronic and thermal Enthalpies= -752.259128
Sum of electronic and thermal Free Energies= -752.318217

153 [9MOG + H_{C6}]$^{+}$···$^{\bullet}CH_2NH_2$

N1	-0.433896	1.875746	0.026326
C2	0.206262	-0.299647	0.180796
C3	-0.142774	-1.682916	-0.159490
O4	0.140671	-1.297034	1.180072
N5	-1.519682	-1.921019	-0.432367
H6	-1.803791	-2.867938	-0.642710
C7	-2.463798	-0.994235	-0.124775
N8	-3.741663	-1.357024	-0.085456
H9	-4.052381	-2.310044	-0.190425
H10	-4.430618	-0.637960	0.082099
N11	-2.198161	0.311178	0.072873
C12	-0.935355	0.654597	0.105136
C13	-1.174848	3.122439	-0.103315
H14	-0.450189	3.934283	-0.053030
H15	-1.696803	3.147118	-1.061656

H16	-1.893484	3.203871	0.712609
C17	1.016972	1.812466	-0.048816
O18	1.720755	2.776278	-0.146764
N19	1.343722	0.481656	-0.027266
H20	2.316239	0.126882	0.018796
H21	0.556753	-2.366267	-0.630084
C22	3.431240	-2.134482	-0.362245
H23	3.557944	-2.415648	-1.399138
H24	3.233737	-2.876599	0.399738
N25	3.887031	-0.873286	0.043341
H26	4.532984	-0.426116	-0.597532
H27	4.250549	-0.835636	0.988958

Zero-point correction= 0.216306
Thermal correction to Energy= 0.231864
Thermal correction to Enthalpy= 0.232808
Thermal correction to Gibbs Free Energy= 0.172288
Sum of electronic and zero-point Energies= -752.251926
Sum of electronic and thermal Energies= -752.236368
Sum of electronic and thermal Enthalpies= -752.235423
Sum of electronic and thermal Free Energies= -752.295944

154 TS_[9MOG + H_{C6}]$^{+}$···$^{\cdot}CH_2NH_2$

N1	2.207245	-0.307520	-0.291661
C2	0.095817	-0.380518	0.446488
C3	-1.307003	0.081125	0.629076
O4	-2.017808	-0.337014	1.604376
N5	-1.226783	1.579743	0.485061
H6	-1.991473	2.058748	0.944172
C7	-0.211425	2.274194	-0.051825
N8	-0.313083	3.600390	-0.196022
H9	-1.137959	4.118760	0.057811
H10	0.498119	4.101373	-0.525469
N11	0.954456	1.721660	-0.456539
C12	1.083195	0.444760	-0.142215
C13	3.491771	0.151204	-0.798872
H14	4.159297	-0.709412	-0.830095
H15	3.364620	0.564709	-1.799936
H16	3.901294	0.914556	-0.134934
C17	1.986008	-1.598060	0.213063
O18	2.764248	-2.512850	0.274073
N19	0.641019	-1.596234	0.638794
H20	0.233088	-2.359111	1.162010
H21	-1.825696	-0.255387	-0.431662
C22	-3.457454	-0.950902	-0.643285
H23	-3.848287	-0.079228	-1.162391
H24	-3.256150	-0.922818	0.450456
N25	-3.549639	-2.090860	-1.269415
H26	-3.864707	-2.159344	-2.229108
H27	-3.281611	-2.955002	-0.814561

Zero-point correction= 0.214579
Thermal correction to Energy= 0.229205
Thermal correction to Enthalpy= 0.230149
Thermal correction to Gibbs Free Energy= 0.171866
Sum of electronic and zero-point Energies= -752.241629
Sum of electronic and thermal Energies= -752.227004
Sum of electronic and thermal Enthalpies= -752.226060
Sum of electronic and thermal Free Energies= -752.284342

155 [9MOG + H_{C6}]$^{+}$

N1	1.390948	0.838262	0.050235
C2	0.112932	-1.051831	0.060595
C3	-1.183479	-1.626099	-0.321405
O4	-0.683724	-1.718379	1.010035
N5	-2.242576	-0.694261	-0.500364
H6	-3.157321	-1.057792	-0.731879
C7	-2.119707	0.594595	-0.089735
N8	-3.205660	1.347824	0.025810
H9	-4.142398	0.995711	-0.097516
H10	-3.082115	2.319963	0.271842
N11	-0.935288	1.196171	0.140861
C12	0.128662	0.439376	0.104727
C13	1.873984	2.214035	0.037759
H14	2.957931	2.174657	-0.063910
H15	1.434250	2.748109	-0.805765
H16	1.602370	2.704487	0.973115
C17	2.269204	-0.297980	-0.105115
O18	3.459269	-0.232909	-0.176620
N19	1.444815	-1.404203	-0.192978
H20	1.819840	-2.339575	-0.128396
H21	-1.292175	-2.554384	-0.870714

Zero-point correction= 0.163943
Thermal correction to Energy= 0.174847
Thermal correction to Enthalpy= 0.175791
Thermal correction to Gibbs Free Energy= 0.127425
Sum of electronic and zero-point Energies= -657.101418
Sum of electronic and thermal Energies= -657.090514
Sum of electronic and thermal Enthalpies= -657.089570
Sum of electronic and thermal Free Energies= -657.137936

156 N1-CH_2NH_2[9MOG + H_{C6}]$^{\cdot+}$

N1	2.059513	0.616899	-0.263246
C2	0.446039	-0.814772	0.506473
C3	-0.955134	-1.192181	0.622051
O4	-0.218545	-0.960674	1.784226
N5	-1.929319	-0.111886	0.291790
H6	-2.723632	-0.216270	0.933845
C7	-1.378207	1.278306	0.436594
N8	-2.374936	2.235302	0.362820
H9	-2.984193	2.307044	1.172135
H10	-2.000842	3.145530	0.119019
N11	-0.118682	1.545235	0.111582
C12	0.748056	0.574650	0.087994
C13	2.799295	1.795124	-0.681889
H14	3.825252	1.484920	-0.877943
H15	2.356846	2.212119	-1.589006
H16	2.782576	2.543933	0.111816
C17	2.622011	-0.674813	-0.198461
O18	3.760319	-0.969034	-0.434768
N19	1.582635	-1.542979	0.162643
H20	1.792452	-2.476283	0.485183
H21	-1.377241	-2.179281	0.457544
C22	-2.523114	-0.356290	-1.142311
H23	-1.647404	-0.401718	-1.793078
H24	-3.086222	0.556451	-1.338104
N25	-3.300858	-1.529385	-1.137127
H26	-2.959418	-2.294525	-1.700195
H27	-4.294520	-1.396691	-1.258815

Zero-point correction= 0.220162
Thermal correction to Energy= 0.234318
Thermal correction to Enthalpy= 0.235262
Thermal correction to Gibbs Free Energy= 0.179325
Sum of electronic and zero-point Energies= -752.221497
Sum of electronic and thermal Energies= -752.207341
Sum of electronic and thermal Enthalpies= -752.206397
Sum of electronic and thermal Free Energies= -752.262334

157 TS_N1-CH_2NH_2[9MOG + H_{C6}]$^{\cdot+}$

N1	2.014059	0.591977	-0.374673

C2	0.479131	-0.732965	0.693319
C3	-0.918278	-1.058142	0.952821
O4	-0.054112	-0.741935	2.026886
N5	-1.867605	-0.034742	0.564910
H6	-2.737182	-0.091286	1.091496
C7	-1.384236	1.292312	0.444446
N8	-2.374101	2.255389	0.348535
H9	-2.998645	2.334311	1.144234
H10	-1.990755	3.160468	0.102164
N11	-0.144393	1.559862	0.037991
C12	0.732505	0.593392	0.083507
C13	2.704519	1.708216	-0.995346
H14	3.711417	1.373302	-1.243240
H15	2.180335	2.016732	-1.902568
H16	2.752838	2.546524	-0.298086
C17	2.585315	-0.684463	-0.213572
O18	3.704768	-1.007341	-0.506309
N19	1.582477	-1.508100	0.317489
H20	1.845475	-2.369481	0.774183
H21	-1.332642	-2.062335	0.934445
C22	-2.565966	-0.575450	-1.410011
H23	-1.543525	-0.634609	-1.763531
H24	-3.070058	0.383641	-1.446417
N25	-3.300203	-1.677333	-1.453838
H26	-2.889154	-2.581847	-1.633669
H27	-4.302937	-1.647974	-1.337502

Zero-point correction= 0.217204
Thermal correction to Energy= 0.231596
Thermal correction to Enthalpy= 0.232540
Thermal correction to Gibbs Free Energy= 0.174295
Sum of electronic and zero-point Energies= -752.215801
Sum of electronic and thermal Energies= -752.201409
Sum of electronic and thermal Enthalpies= -752.200465
Sum of electronic and thermal Free Energies= -752.258711

158 N2-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	-1.792655	-1.096472	0.192572
C2	-1.154378	1.091646	-0.072347
C3	-0.088286	2.055924	-0.320800
O4	-0.906638	2.137724	0.855698
N5	1.253177	1.599571	-0.123496
H6	1.866421	2.349328	0.184098
C7	1.407742	0.390247	0.577758
N8	2.781486	-0.106217	0.613400
H9	3.445012	0.589922	0.965820
H10	2.800316	-0.877976	1.286924
N11	0.503552	-0.597790	0.617412
C12	-0.721334	-0.280964	0.305580
C13	-1.831099	-2.520637	0.467975
H14	-2.847706	-2.862406	0.274761
H15	-1.133038	-3.051332	-0.183824
H16	-1.571949	-2.702278	1.512343
C17	-2.881313	-0.388101	-0.383470
O18	-3.966772	-0.845372	-0.612877
N19	-2.419395	0.896406	-0.649553
H20	-3.079104	1.639576	-0.827164
H21	-0.181463	2.875611	-1.025289
C22	3.352536	-0.651876	-0.736337
H23	2.659368	-1.450156	-1.006503
H24	3.249204	0.180215	-1.433774
N25	4.678453	-1.066438	-0.530180
H26	4.849312	-2.060906	-0.544769
H27	5.395371	-0.549265	-1.016415

Zero-point correction= 0.221671
Thermal correction to Energy= 0.235747
Thermal correction to Enthalpy= 0.236691
Thermal correction to Gibbs Free Energy= 0.179699
Sum of electronic and zero-point Energies= -752.230578
Sum of electronic and thermal Energies= -752.216502
Sum of electronic and thermal Enthalpies= -752.215558
Sum of electronic and thermal Free Energies= -752.272550

159 TS_N2-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	-1.780700	-1.142725	0.204359
C2	-1.271052	1.069124	-0.114234
C3	-0.254438	2.076075	-0.389645
O4	-1.079002	2.153666	0.783902
N5	1.098309	1.677759	-0.183253
H6	1.734169	2.448181	-0.015078
C7	1.347082	0.507187	0.531722
N8	2.655011	0.217183	0.835212
H9	3.261963	0.999377	1.055141
H10	2.725003	-0.517991	1.530928
N11	0.472482	-0.505062	0.652336
C12	-0.759619	-0.263868	0.304700
C13	-1.734535	-2.559008	0.514938
H14	-2.722383	-2.970971	0.309938
H15	-0.988606	-3.057101	-0.108876
H16	-1.486139	-2.699834	1.568247
C17	-2.907493	-0.515485	-0.388860
O18	-3.963953	-1.041858	-0.609120
N19	-2.522756	0.787275	-0.684805
H20	-3.223297	1.486284	-0.882989
H21	-0.383666	2.869515	-1.117934
C22	3.763962	-0.803661	-0.855861
H23	3.021999	-1.590235	-0.806431
H24	3.580628	0.040849	-1.507530
N25	5.028753	-1.105736	-0.557359
H26	5.273680	-1.983795	-0.125293
H27	5.789165	-0.481783	-0.780387

Zero-point correction= 0.217089
Thermal correction to Energy= 0.231637
Thermal correction to Enthalpy= 0.232581
Thermal correction to Gibbs Free Energy= 0.173965
Sum of electronic and zero-point Energies= -752.222613
Sum of electronic and thermal Energies= -752.208065
Sum of electronic and thermal Enthalpies= -752.207120
Sum of electronic and thermal Free Energies= -752.265737

160 N3-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	-1.360489	-0.977497	0.027164
C2	-0.799976	1.259672	0.104732
C3	0.164779	2.316962	-0.155234
O4	-0.512747	2.245486	1.094855
N5	1.536454	1.915333	-0.132515
H6	2.223657	2.606504	0.139155
C7	1.929459	0.624840	-0.160990
N8	3.226276	0.325159	-0.231909
H9	3.918681	1.042953	-0.378467
H10	3.500659	-0.608772	0.083909
N11	1.025592	-0.378011	-0.154534
C12	-0.303983	-0.126190	0.285222
C13	-1.544934	-2.335313	0.539977
H14	-2.547310	-2.411061	0.964946
H15	-1.457971	-3.077972	-0.256460
H16	-0.809940	-2.528798	1.323441
C17	-2.511525	-0.217606	-0.293336
O18	-3.620088	-0.661354	-0.430326
N19	-2.100191	1.102500	-0.402262
H20	-2.789155	1.840875	-0.400065
H21	-0.041077	3.187978	-0.769025

C22	1.462267	-1.727920	-0.561109
H23	0.556924	-2.318972	-0.691651
H24	1.943621	-1.636540	-1.538537
N25	2.428812	-2.262816	0.378678
H26	2.005321	-2.525287	1.263607
H27	2.887565	-3.083311	-0.005010

Zero-point correction= 0.222119
Thermal correction to Energy= 0.235558
Thermal correction to Enthalpy= 0.236502
Thermal correction to Gibbs Free Energy= 0.182236
Sum of electronic and zero-point Energies= -752.247745
Sum of electronic and thermal Energies= -752.234306
Sum of electronic and thermal Enthalpies= -752.233362
Sum of electronic and thermal Free Energies= -752.287628

161 TS_N3-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	1.432374	0.920479	0.415032
C2	0.843973	-1.224136	-0.158268
C3	-0.191880	-2.169993	-0.552304
O4	0.665194	-2.464746	0.546557
N5	-1.531617	-1.790789	-0.207421
H6	-2.198339	-2.546029	-0.110339
C7	-1.806360	-0.608112	0.420638
N8	-3.097583	-0.354622	0.754718
H9	-3.789346	-1.086846	0.695630
H10	-3.233422	0.317562	1.494958
N11	-0.911436	0.353721	0.648439
C12	0.389818	0.023621	0.472999
C13	1.531325	2.204805	1.083114
H14	2.513691	2.291329	1.550310
H15	1.420152	3.029136	0.371764
H16	0.755856	2.261021	1.847772
C17	2.516226	0.348607	-0.267513
O18	3.600652	0.851573	-0.420186
N19	2.076282	-0.888730	-0.746006
H20	2.760382	-1.578043	-1.022964
H21	-0.126701	-2.832365	-1.409605
C22	-1.554322	1.792560	-1.007109
H23	-0.794216	2.447808	-0.606463
H24	-1.283296	1.043483	-1.740580
N25	-2.809355	2.158200	-0.913976
H26	-3.085627	2.940702	-0.337051
H27	-3.549226	1.625688	-1.349243

Zero-point correction= 0.217294
Thermal correction to Energy= 0.231769
Thermal correction to Enthalpy= 0.232713
Thermal correction to Gibbs Free Energy= 0.175514
Sum of electronic and zero-point Energies= -752.221852
Sum of electronic and thermal Energies= -752.207377
Sum of electronic and thermal Enthalpies= -752.206433
Sum of electronic and thermal Free Energies= -752.263632

162 C5-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	1.295728	1.065143	-0.114300
C2	0.090368	-0.903173	0.027577
C3	-1.113901	-1.304606	-0.890492
N4	-2.277526	-0.552014	-0.390234
H5	-3.185560	-0.879251	-0.691849
C6	-2.170614	0.706165	0.093675
N7	-3.270705	1.384148	0.407606
H8	-4.201786	1.018406	0.284948
H9	-3.160186	2.329185	0.746054
N10	-0.996379	1.340551	0.263195
C11	0.074675	0.607366	0.083325
C12	1.714755	2.458983	-0.106902
H13	2.789699	2.473377	-0.283868
H14	1.195506	3.004867	-0.896313
H15	1.486578	2.900582	0.863605
C16	2.186615	-0.016086	-0.450356
O17	3.358166	0.107697	-0.664045
N18	1.400696	-1.139472	-0.497325
H19	1.829127	-2.049075	-0.580469
C20	-0.086647	-1.524847	1.447424
H21	-1.094968	-1.310880	1.809844
H22	-0.011642	-2.615215	1.321051
N23	0.887829	-0.963686	2.348008
H24	1.741859	-1.502165	2.412908
H25	0.525882	-0.808115	3.278750
O26	-0.864306	-1.140906	-2.194734
H27	-1.314403	-2.381556	-0.738582

Zero-point correction= 0.219492
Thermal correction to Energy= 0.233900
Thermal correction to Enthalpy= 0.234845
Thermal correction to Gibbs Free Energy= 0.178313
Sum of electronic and zero-point Energies= -752.271541
Sum of electronic and thermal Energies= -752.257132
Sum of electronic and thermal Enthalpies= -752.256188
Sum of electronic and thermal Free Energies= -752.312720

163 TS_C5-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	1.228963	0.796729	-0.620563
C2	-0.035953	-0.996962	-0.143754
C3	-1.337010	-1.660036	-0.110565
N4	-2.348399	-0.690385	0.351164
H5	-3.274752	-1.067182	0.502670
C6	-2.256618	0.614603	-0.024808
N7	-3.353219	1.377878	-0.004943
H8	-4.280383	1.002073	0.111472
H9	-3.255666	2.345577	-0.273883
N10	-1.102760	1.218529	-0.341568
C11	-0.041496	0.427136	-0.338435
C12	1.678341	2.132298	-0.981378
H13	2.760426	2.092392	-1.104857
H14	1.210053	2.440541	-1.917499
H15	1.411912	2.842256	-0.195970
C16	2.080553	-0.331538	-0.594979
O17	3.265944	-0.341915	-0.799845
N18	1.265724	-1.410524	-0.232388
H19	1.573793	-2.363613	-0.358862
C20	0.360743	0.002316	2.303791
H21	-0.272750	0.879779	2.282518
H22	-0.052372	-0.960567	2.572523
N23	1.672101	0.164201	2.353049
H24	2.298527	-0.614655	2.500318
H25	2.099360	1.071814	2.235128
O26	-1.136480	-1.706757	-1.447118
H27	-1.482097	-2.600940	0.429673

Zero-point correction= 0.216112
Thermal correction to Energy= 0.231158
Thermal correction to Enthalpy= 0.232102
Thermal correction to Gibbs Free Energy= 0.173971
Sum of electronic and zero-point Energies= -752.228867
Sum of electronic and thermal Energies= -752.213821
Sum of electronic and thermal Enthalpies= -752.212877
Sum of electronic and thermal Free Energies= -752.271008

164 O6-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	2.320242	-0.122849	0.205145

C2	0.227303	-0.458326	-0.510524
C3	-1.207392	-0.138482	-0.720159
O4	-1.935778	-0.806592	0.252879
N5	-1.301212	1.329791	-0.638025
H6	-2.176049	1.736391	-0.936414
C7	-0.375845	2.148134	-0.082630
N8	-0.682892	3.430369	0.118479
H9	-1.598788	3.816890	-0.043801
H10	0.040900	4.033623	0.480892
N11	0.869369	1.770522	0.249196
C12	1.133637	0.500077	-0.000750
C13	3.541105	0.485993	0.716057
H14	4.288550	-0.301853	0.802299
H15	3.887991	1.253943	0.023321
H16	3.349364	0.928632	1.694221
C17	2.210232	-1.479020	-0.138073
O18	3.052668	-2.332023	-0.075685
N19	0.877691	-1.634580	-0.580669
H20	0.499800	-2.538293	-0.830258
H21	-1.550195	-0.421769	-1.727700
C22	-3.385579	-0.880426	0.020441
H23	-3.533607	-1.179696	-1.025072
H24	-3.803641	0.118783	0.183212
N25	-4.006506	-1.790722	0.880790
H26	-3.732847	-2.755303	0.754786
H27	-4.004196	-1.527850	1.856377

Zero-point correction= 0.221337
Thermal correction to Energy= 0.235854
Thermal correction to Enthalpy= 0.236799
Thermal correction to Gibbs Free Energy= 0.178694
Sum of electronic and zero-point Energies= -752.303611
Sum of electronic and thermal Energies= -752.289094
Sum of electronic and thermal Enthalpies= -752.288150
Sum of electronic and thermal Free Energies= -752.346255

165 TS_O6-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	2.003502	-0.007857	0.457858
C2	0.149791	-0.291482	-0.813193
C3	-1.041937	0.268123	-1.435454
O4	-1.263233	-0.724304	-0.438135
N5	-1.336957	1.607497	-1.051756
H6	-2.124687	2.064232	-1.487556
C7	-0.746194	2.180964	0.041080
N8	-1.261094	3.323188	0.516568
H9	-2.066545	3.776119	0.117614
H10	-0.762974	3.787809	1.260398
N11	0.342155	1.696245	0.636689
C12	0.816896	0.558479	0.161084
C13	3.003317	0.508623	1.378364
H14	3.796174	-0.235446	1.448033
H15	3.409198	1.449857	1.001894
H16	2.550087	0.668861	2.357300
C17	2.216803	-1.146656	-0.360669
O18	3.175853	-1.870409	-0.333688
N19	1.107764	-1.222231	-1.198583
H20	0.946312	-2.032550	-1.776301
H21	-1.356533	0.028663	-2.447141
C22	-3.309608	-1.819071	0.496727
H23	-3.564317	-2.151377	-0.498829
H24	-3.633806	-0.856584	0.863702
N25	-2.826905	-2.709682	1.369677
H26	-2.581928	-3.644711	1.085859
H27	-2.645602	-2.461174	2.328810

Zero-point correction= 0.213273
Thermal correction to Energy= 0.229389
Thermal correction to Enthalpy= 0.230333
Thermal correction to Gibbs Free Energy= 0.167485
Sum of electronic and zero-point Energies= -752.228064
Sum of electronic and thermal Energies= -752.211949
Sum of electronic and thermal Enthalpies= -752.211005
Sum of electronic and thermal Free Energies= -752.273853

166 N7-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	0.494849	1.591429	0.148048
C2	-0.072566	-0.638199	0.447069
C3	-0.967195	-1.741096	0.104050
O4	-0.538797	-1.490333	1.465417
N5	-2.273178	-1.352453	-0.254739
H6	-3.003880	-2.029391	-0.076474
C7	-2.653614	-0.008527	-0.284038
N8	-3.967773	0.219052	-0.515831
H9	-4.528750	-0.456511	-1.010732
H10	-4.244145	1.185791	-0.599198
N11	-1.834621	0.997785	-0.113377
C12	-0.588925	0.716532	0.294633
C13	0.348864	3.035082	-0.013479
H14	-0.290235	3.232928	-0.874755
H15	-0.108750	3.452380	0.884659
H16	1.337917	3.464268	-0.165941
C17	1.687467	0.979169	0.152909
O18	2.816997	1.372875	0.054634
N19	1.394925	-0.535898	0.295616
H20	1.851651	-0.857833	1.159288
H21	-0.640571	-2.693694	-0.299535
C22	2.107761	-1.320914	-0.841569
H23	1.573427	-2.267016	-0.922605
H24	1.938115	-0.721074	-1.740465
N25	3.445448	-1.523210	-0.467980
H26	4.105505	-0.815183	-0.756385
H27	3.795818	-2.464220	-0.557868

Zero-point correction= 0.220012
Thermal correction to Energy= 0.234418
Thermal correction to Enthalpy= 0.235362
Thermal correction to Gibbs Free Energy= 0.178346
Sum of electronic and zero-point Energies= -752.224047
Sum of electronic and thermal Energies= -752.209642
Sum of electronic and thermal Enthalpies= -752.208697
Sum of electronic and thermal Free Energies= -752.265714

167 TS_N7-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	0.585142	1.486924	0.181351
C2	-0.194497	-0.639176	0.616217
C3	-1.157162	-1.700174	0.335285
O4	-0.837690	-1.309952	1.690903
N5	-2.392850	-1.264426	-0.197973
H6	-3.200054	-1.822999	0.050238
C7	-2.642895	0.091450	-0.431437
N8	-3.918281	0.384311	-0.803590
H9	-4.455764	-0.296205	-1.318560
H10	-4.090220	1.350651	-1.037550
N11	-1.755865	1.046475	-0.315091
C12	-0.580631	0.716263	0.237222
C13	0.617372	2.918467	-0.072714
H14	0.116968	3.129162	-1.019200
H15	0.102657	3.445297	0.733092
H16	1.659724	3.232448	-0.115123
C17	1.682016	0.738149	0.445160
O18	2.855077	1.059530	0.505237
N19	1.249357	-0.647037	0.559405
H20	1.688898	-1.123166	1.344821
H21	-0.884936	-2.722011	0.089013

C22	2.278097	-1.456128	-1.201425
H23	1.880740	-2.451821	-1.046778
H24	1.713272	-0.752681	-1.801016
N25	3.551730	-1.254797	-1.037581
H26	3.946746	-0.328336	-1.164044
H27	4.134442	-1.930222	-0.559517

Zero-point correction= 0.218303
Thermal correction to Energy= 0.232501
Thermal correction to Enthalpy= 0.233445
Thermal correction to Gibbs Free Energy= 0.176514
Sum of electronic and zero-point Energies= -752.221454
Sum of electronic and thermal Energies= -752.207256
Sum of electronic and thermal Enthalpies= -752.206312
Sum of electronic and thermal Free Energies= -752.263243

168 C8-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	1.288243	0.963079	-0.190248
C2	-0.307750	-0.857151	-0.557002
C3	-1.610435	-1.388144	0.063329
O4	-2.104096	-2.466324	-0.533797
N5	-2.576423	-0.293195	0.164261
H6	-3.550229	-0.564446	0.220427
C7	-2.210623	0.996837	0.168264
N8	-3.136291	1.947233	0.257868
H9	-4.124401	1.756405	0.316704
H10	-2.824845	2.907574	0.256648
N11	-0.929381	1.414363	0.123081
C12	0.023135	0.542600	-0.139316
C13	1.568393	2.408051	-0.231428
H14	2.604377	2.530880	-0.539042
H15	0.906873	2.880177	-0.956789
H16	1.402552	2.853805	0.751509
C17	2.436131	0.078607	-0.137295
O18	3.440918	0.389860	-0.710194
N19	0.403799	-1.449686	-1.409633
H20	0.031069	-2.370269	-1.654298
H21	-1.318456	-1.738315	1.082890
C22	2.392708	-1.124710	0.800053
H23	3.366553	-1.106138	1.303052
H24	2.379421	-2.018475	0.171761
N25	1.251950	-1.144788	1.709596
H26	1.371279	-0.462634	2.453286
H27	1.198576	-2.052429	2.161670

Zero-point correction= 0.217616
Thermal correction to Energy= 0.232383
Thermal correction to Enthalpy= 0.233327
Thermal correction to Gibbs Free Energy= 0.175642
Sum of electronic and zero-point Energies= -752.217233
Sum of electronic and thermal Energies= -752.202466
Sum of electronic and thermal Enthalpies= -752.201522
Sum of electronic and thermal Free Energies= -752.259207

169 TS_C8-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	1.184930	0.931897	-0.501679
C2	-0.140994	-0.827626	-0.259073
C3	-1.442811	-1.528711	-0.008457
O4	-1.740228	-2.467729	-0.935369
N5	-2.463924	-0.505441	0.177296
H6	-3.406773	-0.863714	0.247751
C7	-2.280644	0.843683	0.066070
N8	-3.362935	1.622494	0.169842
H9	-4.297328	1.266170	0.286886
H10	-3.232920	2.618060	0.071284
N11	-1.107451	1.440331	-0.105028
C12	-0.077756	0.607717	-0.287083
C13	1.744524	2.263230	-0.603728
H14	0.977696	2.939069	-0.981267
H15	2.083910	2.616239	0.375837
H16	2.595530	2.211991	-1.284342
C17	2.078024	-0.255329	-0.412210
O18	3.184201	-0.297152	-0.944343
N19	1.033841	-1.314024	-0.553889
H20	1.283202	-2.295484	-0.610918
H21	-1.367956	-2.148935	0.914426
C22	2.227233	-0.373009	1.384418
H23	2.855666	0.504156	1.526824
H24	2.789509	-1.296412	1.496538
N25	1.005514	-0.344243	2.046032
H26	0.734390	0.523960	2.487781
H27	0.758015	-1.152874	2.599264

Zero-point correction= 0.216219
Thermal correction to Energy= 0.230364
Thermal correction to Enthalpy= 0.231308
Thermal correction to Gibbs Free Energy= 0.175058
Sum of electronic and zero-point Energies= -752.183366
Sum of electronic and thermal Energies= -752.169221
Sum of electronic and thermal Enthalpies= -752.168277
Sum of electronic and thermal Free Energies= -752.224528

170 O8-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	0.487415	1.289170	0.145558
C2	-0.353423	-0.852729	0.135110
C3	-1.421871	-1.761445	-0.258447
O4	-0.875195	-1.784817	1.079242
N5	-2.692154	-1.151442	-0.421263
H6	-3.495038	-1.755844	-0.306195
C7	-2.889791	0.200430	-0.176525
N8	-4.174460	0.625050	-0.197338
H9	-4.885042	0.105406	-0.687246
H10	-4.319614	1.618113	-0.099125
N11	-1.930154	1.069149	0.054346
C12	-0.704666	0.563373	0.222868
C13	0.590730	2.740252	0.249317
H14	0.582585	3.035285	1.299941
H15	1.515397	3.066834	-0.223478
H16	-0.269572	3.174287	-0.259647
C17	1.489783	0.432905	-0.031250
O18	2.732747	0.832572	-0.032137
N19	1.043915	-0.841968	-0.164446
H20	1.685058	-1.602280	0.045491
H21	-1.268997	-2.666765	-0.836185
C22	3.793574	-0.034700	-0.551350
H23	4.672606	0.590956	-0.392695
H24	3.614073	-0.169904	-1.620320
N25	3.808702	-1.298557	0.110372
H26	4.130520	-2.044859	-0.494067
H27	4.348743	-1.301608	0.967743

Zero-point correction= 0.220320
Thermal correction to Energy= 0.234619
Thermal correction to Enthalpy= 0.235564
Thermal correction to Gibbs Free Energy= 0.178819
Sum of electronic and zero-point Energies= -752.243165
Sum of electronic and thermal Energies= -752.228866
Sum of electronic and thermal Enthalpies= -752.227921
Sum of electronic and thermal Free Energies= -752.284667

171 TS_O8-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	-0.453973	0.956444	-0.267795

C2	0.750711	-0.995767	-0.138023
C3	1.950483	-1.690942	0.306357
O4	1.474473	-1.835511	-1.049818
N5	3.089366	-0.866382	0.504549
H6	3.985809	-1.309848	0.349246
C7	3.042571	0.500893	0.243855
N8	4.246916	1.142377	0.298827
H9	4.941222	0.809902	0.951264
H10	4.192719	2.145681	0.204878
N11	1.956255	1.176253	-0.037681
C12	0.845561	0.458101	-0.249082
C13	-0.792572	2.357535	-0.402085
H14	-0.318149	2.764438	-1.296838
H15	-1.875211	2.442243	-0.491218
H16	-0.442546	2.914553	0.470286
C17	-1.345045	-0.061282	-0.101323
O18	-2.584595	0.020419	-0.129815
N19	-0.626554	-1.224976	0.113375
H20	-1.061074	-2.122442	-0.036669
H21	1.938981	-2.601355	0.897063
C22	-4.852285	0.094515	0.950399
H23	-4.275910	1.009621	0.968776
H24	-5.054270	-0.460766	1.860643
N25	-5.327809	-0.326474	-0.160382
H26	-5.855372	-1.190133	-0.228302
H27	-5.081167	0.139831	-1.028917

Zero-point correction= 0.217103
Thermal correction to Energy= 0.232234
Thermal correction to Enthalpy= 0.233179
Thermal correction to Gibbs Free Energy= 0.172633
Sum of electronic and zero-point Energies= -752.227671
Sum of electronic and thermal Energies= -752.212540
Sum of electronic and thermal Enthalpies= -752.211596
Sum of electronic and thermal Free Energies= -752.272141

172 N9-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	-1.216302	-0.298483	0.357057
C2	0.570905	1.225699	-0.020113
C3	1.909558	1.409149	-0.567667
O4	1.527968	1.972072	0.705378
N5	2.737542	0.258451	-0.537569
H6	3.735158	0.414069	-0.585966
C7	2.296907	-0.944386	-0.021059
N8	3.204053	-1.934463	0.074338
H9	4.108788	-1.885910	-0.364316
H10	2.890655	-2.825593	0.425226
N11	1.052962	-1.180614	0.350435
C12	0.226310	-0.130046	0.410817
C13	-1.622213	-1.344441	-0.862277
H14	-0.988487	-2.195603	-0.616731
H15	-1.243478	-0.812058	-1.736487
C16	-1.738406	1.058704	-0.042990
O17	-2.909096	1.305029	-0.067888
N18	-0.667200	1.815168	-0.390647
H19	-0.787327	2.797917	-0.598210
H20	2.156935	2.130668	-1.339059
C21	-1.827016	-0.755692	1.640183
N22	-2.952610	-1.663240	-0.951915
H23	-2.909548	-0.775500	1.522351
H24	-1.429792	-1.747723	1.856824
H25	-3.333234	-2.378667	-0.353883
H26	-3.611209	-0.970035	-1.273081
H27	-1.544832	-0.060027	2.430151

Zero-point correction= 0.219802
Thermal correction to Energy= 0.233931
Thermal correction to Enthalpy= 0.234876
Thermal correction to Gibbs Free Energy= 0.179397
Sum of electronic and zero-point Energies= -752.233643
Sum of electronic and thermal Energies= -752.219514
Sum of electronic and thermal Enthalpies= -752.218570
Sum of electronic and thermal Free Energies= -752.274048

173 TS_N9-CH_2NH_2[9MOG + H_{C6}]$^{\bullet+}$

N1	-1.071495	-0.261138	0.617544
C2	0.592069	1.203170	-0.051094
C3	1.875956	1.362641	-0.723081
O4	1.621781	1.974975	0.553896
N5	2.709059	0.211502	-0.719800
H6	3.695590	0.376413	-0.867863
C7	2.356606	-0.932952	-0.027221
N8	3.302966	-1.884719	0.090267
H9	4.170011	-1.857640	-0.419696
H10	3.052725	-2.736705	0.566318
N11	1.160597	-1.162232	0.479842
C12	0.300221	-0.137203	0.474514
C13	-1.976169	-1.241582	-1.305260
H14	-1.417460	-2.141409	-1.078574
H15	-1.507060	-0.448899	-1.875721
C16	-1.671467	0.992373	0.285816
O17	-2.843610	1.248110	0.423711
N18	-0.687147	1.761032	-0.300444
H19	-0.842838	2.749581	-0.441732
H20	2.052604	2.048209	-1.545247
C21	-1.680361	-1.104629	1.646785
N22	-3.287267	-1.266454	-1.227085
H23	-2.753464	-1.160096	1.465635
H24	-1.221974	-2.092332	1.595239
H25	-3.775471	-2.042921	-0.803065
H26	-3.837316	-0.442804	-1.436657
H27	-1.508833	-0.672913	2.635491

Zero-point correction= 0.217024
Thermal correction to Energy= 0.231494
Thermal correction to Enthalpy= 0.232439
Thermal correction to Gibbs Free Energy= 0.175793
Sum of electronic and zero-point Energies= -752.230607
Sum of electronic and thermal Energies= -752.216137
Sum of electronic and thermal Enthalpies= -752.215193
Sum of electronic and thermal Free Energies= -752.271838

174 [9MOG + H_{O6}]$^{+}$···$^{\bullet}CH_2NH_2$

N1	1.803034	-1.348447	-0.000101
C2	-0.065272	-0.121843	0.000201
C3	-0.729025	1.070581	0.000182
O4	-2.010123	1.334223	0.000253
N5	0.068170	2.200006	0.000121
H6	-0.426294	3.084257	0.000144
C7	1.435233	2.156091	-0.000022
N8	2.111946	3.312536	-0.000077
H9	1.672056	4.217807	0.000010
H10	3.119420	3.263686	-0.000173
N11	2.104189	1.014034	-0.000111
C12	1.349915	-0.080573	-0.000008
C13	3.194253	-1.775759	-0.000284
H14	3.697155	-1.401563	-0.893046
H15	3.697223	-1.402215	0.892716
H16	3.195312	-2.865508	-0.000676
C17	0.711444	-2.257172	0.000088
O18	0.781799	-3.457777	0.000173
N19	-0.424397	-1.461226	0.000130
H20	-1.349795	-1.857200	0.000763
H21	-2.608512	0.503993	0.000155

C22	-3.854449	-0.764520	-0.000082
H23	-3.660527	-1.297831	-0.929142
H24	-3.660971	-1.297781	0.929100
N25	-4.995430	-0.005408	-0.000362
H26	-5.387017	0.349766	0.857337
H27	-5.386633	0.349718	-0.858254

Zero-point correction= 0.215140
Thermal correction to Energy= 0.231720
Thermal correction to Enthalpy= 0.232664
Thermal correction to Gibbs Free Energy= 0.169024
Sum of electronic and zero-point Energies= -752.305072
Sum of electronic and thermal Energies= -752.288492
Sum of electronic and thermal Enthalpies= -752.287548
Sum of electronic and thermal Free Energies= -752.351188

175 TS_ [9MOG + H_{O6}]$^{+}$···$^{\bullet}CH_2NH_2$

N1	-2.225960	-0.818899	-0.159676
C2	-0.108839	-0.304713	0.332756
C3	0.957287	0.560120	0.497476
O4	2.155353	0.283927	0.805571
N5	0.605486	1.907816	0.298791
H6	1.353048	2.570364	0.464248
C7	-0.647800	2.336377	-0.023771
N8	-0.865700	3.653226	-0.163123
H9	-0.159254	4.352720	-0.008827
H10	-1.804563	3.950996	-0.379138
N11	-1.662248	1.500704	-0.213262
C12	-1.369497	0.217844	-0.029609
C13	-3.636202	-0.744732	-0.506584
H14	-4.177272	-0.174674	0.250387
H15	-3.754890	-0.268603	-1.480942
H16	-4.014761	-1.766007	-0.542188
C17	-1.557905	-2.035274	0.125217
O18	-2.042907	-3.137312	0.125398
N19	-0.241612	-1.675573	0.392878
H20	0.425998	-2.332714	0.763876
H21	3.084944	-0.246757	-0.241809
C22	3.933349	-0.688299	-0.961567
H23	3.462082	-1.533774	-1.467346
H24	4.180752	0.129739	-1.641052
N25	5.014935	-1.073795	-0.184037
H26	5.689932	-0.393156	0.135465
H27	5.017746	-1.963350	0.295071

Zero-point correction= 0.212515
Thermal correction to Energy= 0.228195
Thermal correction to Enthalpy= 0.229139
Thermal correction to Gibbs Free Energy= 0.167047
Sum of electronic and zero-point Energies= -752.297537
Sum of electronic and thermal Energies= -752.281857
Sum of electronic and thermal Enthalpies= -752.280913
Sum of electronic and thermal Free Energies= -752.343006

176 [9MOG + H_{O6}]$^{+}$

N1	1.556921	-0.766705	0.004139
C2	0.056045	0.894677	-0.008626
C3	-1.224565	1.345283	0.002801
O4	-1.713528	2.578321	0.010335
N5	-2.220414	0.391296	-0.001847
H6	-3.171344	0.742391	0.002760
C7	-1.962231	-0.951429	-0.003508
N8	-2.992277	-1.803085	-0.009695
H9	-3.957295	-1.515245	-0.015156
H10	-2.782879	-2.790326	-0.009667
N11	-0.725040	-1.429694	0.002057
C12	0.237453	-0.518570	-0.000278
C13	2.198382	-2.074705	0.016254
H14	2.010080	-2.573937	0.967883
H15	1.812277	-2.679696	-0.804674
H16	3.267820	-1.909324	-0.110514
C17	2.286201	0.454001	-0.003267
O18	3.479829	0.571810	-0.014587
N19	1.322260	1.456894	0.004088
H20	1.588616	2.426582	-0.059479
H21	-1.035544	3.262020	0.051418

Zero-point correction= 0.163088
Thermal correction to Energy= 0.175193
Thermal correction to Enthalpy= 0.176137
Thermal correction to Gibbs Free Energy= 0.124542
Sum of electronic and zero-point Energies= -657.147788
Sum of electronic and thermal Energies= -657.135683
Sum of electronic and thermal Enthalpies= -657.134738
Sum of electronic and thermal Free Energies= -657.186333

177 N1-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-2.125385	0.756848	0.152274
C2	-0.569823	-0.848725	-0.178537
C3	0.671143	-1.307429	-0.468526
O4	1.116960	-2.576110	-0.610449
N5	1.765662	-0.335232	-0.287250
H6	2.500130	-0.554265	-0.970656
C7	1.347006	1.084461	-0.533678
N8	2.340778	1.839977	-1.071517
H9	3.273456	1.724324	-0.690464
H10	2.073517	2.790132	-1.292950
N11	0.137782	1.487281	-0.314698
C12	-0.791788	0.556628	-0.068461
C13	-2.798868	2.035887	0.290600
H14	-2.380982	2.588667	1.133858
H15	-2.686655	2.619727	-0.625116
H16	-3.853744	1.829914	0.470922
C17	-2.790643	-0.476827	0.178670
O18	-3.962858	-0.671370	0.370765
N19	-1.802272	-1.443401	-0.063473
H20	-1.999372	-2.428962	0.015527
H21	0.896149	-2.939076	-1.477965
C22	2.434982	-0.493344	1.123511
H23	2.590514	-1.569196	1.219870
H24	1.662176	-0.161446	1.819053
N25	3.624750	0.269725	1.176712
H26	4.474371	-0.272127	1.257539
H27	3.616352	1.021854	1.852041

Zero-point correction= 0.220333
Thermal correction to Energy= 0.235011
Thermal correction to Enthalpy= 0.235955
Thermal correction to Gibbs Free Energy= 0.179002
Sum of electronic and zero-point Energies= -752.256049
Sum of electronic and thermal Energies= -752.241370
Sum of electronic and thermal Enthalpies= -752.240426
Sum of electronic and thermal Free Energies= -752.297379

178 TS_N1-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	2.145334	-0.746776	0.155418
C2	0.592421	0.844799	-0.208004
C3	-0.653327	1.270951	-0.548748
O4	-1.134341	2.524422	-0.709022
N5	-1.699888	0.305536	-0.482261
H6	-2.449186	0.548210	-1.133071
C7	-1.306896	-1.067137	-0.617802

N8	-2.294619	-1.902543	-1.049993
H9	-3.252936	-1.718011	-0.793712
H10	-2.035649	-2.877299	-1.109534
N11	-0.103718	-1.488440	-0.348602
C12	0.818854	-0.551852	-0.109199
C13	2.817351	-2.023425	0.317567
H14	2.382286	-2.572581	1.154756
H15	2.726533	-2.613382	-0.596443
H16	3.867608	-1.814092	0.519939
C17	2.799736	0.489871	0.235187
O18	3.961117	0.688458	0.487989
N19	1.818651	1.453613	-0.037897
H20	2.001950	2.432618	0.116039
H21	-0.611499	3.031386	-1.341635
C22	-2.622369	0.551378	1.241692
H23	-2.774306	1.620046	1.121982
H24	-1.758439	0.251975	1.828393
N25	-3.728997	-0.217617	1.346043
H26	-4.644245	0.181484	1.202437
H27	-3.698278	-1.087320	1.856003

Zero-point correction= 0.216867
Thermal correction to Energy= 0.232109
Thermal correction to Enthalpy= 0.233053
Thermal correction to Gibbs Free Energy= 0.174074
Sum of electronic and zero-point Energies= -752.252205
Sum of electronic and thermal Energies= -752.236964
Sum of electronic and thermal Enthalpies= -752.236019
Sum of electronic and thermal Free Energies= -752.294998

179 C2-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	1.729588	-1.032993	-0.170399
C2	0.763697	0.989426	0.108352
C3	-0.312511	1.884271	-0.006297
O4	-0.271218	3.200428	0.092770
N5	-1.490304	1.344777	-0.258783
H6	-2.268597	1.984364	-0.385126
C7	-1.809509	-0.153204	-0.323272
N8	-2.688754	-0.433297	-1.391093
H9	-3.616485	-0.037887	-1.323245
H10	-2.293922	-0.371416	-2.319408
N11	-0.623627	-0.947240	-0.452007
C12	0.507610	-0.404153	-0.197520
C13	1.952777	-2.449346	-0.426092
H14	1.336335	-3.045658	0.247909
H15	1.699048	-2.683876	-1.461005
H16	3.007740	-2.653408	-0.246532
C17	2.741151	-0.138993	0.151332
O18	3.915147	-0.335104	0.284982
N19	2.095229	1.125568	0.305931
H20	2.624906	1.928833	0.614711
H21	0.619600	3.567680	0.137728
C22	-2.512491	-0.482145	1.051368
H23	-1.813119	-0.195102	1.844088
H24	-3.385963	0.177241	1.129213
N25	-2.920547	-1.835292	1.227724
H26	-2.145605	-2.486511	1.213615
H27	-3.610810	-2.132654	0.549216

Zero-point correction= 0.219277
Thermal correction to Energy= 0.233990
Thermal correction to Enthalpy= 0.234935
Thermal correction to Gibbs Free Energy= 0.177819
Sum of electronic and zero-point Energies= -752.280500
Sum of electronic and thermal Energies= -752.265787
Sum of electronic and thermal Enthalpies= -752.264842
Sum of electronic and thermal Free Energies= -752.321958

180 TS_C2-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.733087	-0.939017	0.262899
C2	-0.665346	0.997928	-0.116447
C3	0.405107	1.826355	0.068187
O4	0.485178	3.144837	-0.084164
N5	1.568064	1.247897	0.474502
H6	2.339425	1.871218	0.677750
C7	1.745760	-0.163128	0.519081
N8	2.845366	-0.624660	1.247363
H9	3.607663	0.016872	1.409377
H10	2.598913	-1.172793	2.060147
N11	0.613677	-0.941337	0.651287
C12	-0.504715	-0.362081	0.299587
C13	-2.046169	-2.315703	0.608755
H14	-1.448450	-2.996609	0.000356
H15	-1.841088	-2.492547	1.665752
H16	-3.105791	-2.469017	0.405834
C17	-2.697841	-0.018718	-0.199375
O18	-3.862366	-0.236811	-0.401386
N19	-2.014775	1.186114	-0.380639
H20	-2.440401	1.921303	-0.924325
H21	-0.379906	3.570040	-0.116263
C22	2.286655	-0.526676	-1.307494
H23	1.412214	-0.149664	-1.838024
H24	3.165778	0.113721	-1.354797
N25	2.547149	-1.841438	-1.492357
H26	1.779124	-2.493373	-1.555840
H27	3.404552	-2.224135	-1.120702

Zero-point correction= 0.217431
Thermal correction to Energy= 0.232197
Thermal correction to Enthalpy= 0.233141
Thermal correction to Gibbs Free Energy= 0.176362
Sum of electronic and zero-point Energies= -752.273224
Sum of electronic and thermal Energies= -752.258458
Sum of electronic and thermal Enthalpies= -752.257514
Sum of electronic and thermal Free Energies= -752.314293

181 N2-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.847512	-1.140078	0.088002
C2	-1.038391	0.961533	0.016641
C3	-0.033406	1.863471	0.086551
O4	-0.045996	3.172367	-0.169297
N5	1.219886	1.424930	0.485026
H6	1.761548	2.147108	0.949175
C7	1.383209	0.090075	0.937732
N8	2.740337	-0.433984	0.678395
H9	3.467664	0.143834	1.107519
H10	2.791986	-1.341168	1.150886
N11	0.441588	-0.861665	0.690275
C12	-0.723024	-0.412210	0.312875
C13	-1.998615	-2.570479	0.284558
H14	-1.345123	-3.117311	-0.398018
H15	-1.753906	-2.830931	1.315932
H16	-3.039647	-2.817304	0.076720
C17	-2.901022	-0.301915	-0.334375
O18	-4.034862	-0.635546	-0.559290
N19	-2.357235	0.977332	-0.437570
H20	-2.983541	1.766956	-0.461883
H21	-0.903975	3.483662	-0.477196
C22	3.131533	-0.653509	-0.805912
H23	2.391785	-1.366431	-1.173984
H24	2.976021	0.316770	-1.280106
N25	4.465614	-1.106518	-0.863154
H26	4.598662	-2.068727	-1.137368
H27	5.124930	-0.492932	-1.318215

Zero-point correction= 0.221837
Thermal correction to Energy= 0.236658
Thermal correction to Enthalpy= 0.237603
Thermal correction to Gibbs Free Energy= 0.179327
Sum of electronic and zero-point Energies= -752.261421
Sum of electronic and thermal Energies= -752.246599
Sum of electronic and thermal Enthalpies= -752.245655
Sum of electronic and thermal Free Energies= -752.303931

182 TS_N2-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.898024	-1.182328	0.058323
C2	-1.146126	0.941037	-0.010970
C3	-0.168070	1.868812	0.065397
O4	-0.215252	3.185085	-0.151245
N5	1.104185	1.448375	0.420950
H6	1.692388	2.176835	0.808032
C7	1.329534	0.111108	0.787969
N8	2.652253	-0.305618	0.840774
H9	3.301927	0.338724	1.284329
H10	2.710173	-1.215478	1.291832
N11	0.397845	-0.850155	0.613094
C12	-0.785169	-0.426999	0.257077
C13	-2.004251	-2.618229	0.239702
H14	-1.335911	-3.135499	-0.451451
H15	-1.747671	-2.883814	1.267076
H16	-3.037979	-2.894784	0.032881
C17	-2.984871	-0.367965	-0.319602
O18	-4.116622	-0.728436	-0.515365
N19	-2.479769	0.927275	-0.420085
H20	-3.126657	1.700232	-0.417577
H21	-1.078825	3.479307	-0.459707
C22	3.621363	-0.691499	-0.941228
H23	2.958112	-1.507995	-1.203346
H24	3.402997	0.273335	-1.384606
N25	4.919925	-0.988236	-0.726546
H26	5.228225	-1.940370	-0.610278
H27	5.638834	-0.286465	-0.799943

Zero-point correction= 0.216980
Thermal correction to Energy= 0.232458
Thermal correction to Enthalpy= 0.233402
Thermal correction to Gibbs Free Energy= 0.172832
Sum of electronic and zero-point Energies= -752.252789
Sum of electronic and thermal Energies= -752.237311
Sum of electronic and thermal Enthalpies= -752.236367
Sum of electronic and thermal Free Energies= -752.296937

183 N3-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.335778	-1.147743	0.019964
C2	-0.867655	1.037622	-0.175395
C3	-0.053247	2.166690	-0.209045
O4	-0.450711	3.419721	0.116883
N5	1.307860	1.870894	0.138709
H6	1.860239	2.654954	0.464039
C7	1.850452	0.652728	0.131086
N8	3.157585	0.466571	0.312866
H9	3.798874	1.241509	0.374164
H10	3.463808	-0.489187	0.512502
N11	1.069005	-0.441751	-0.107166
C12	-0.320536	-0.226297	-0.130918
C13	-1.283883	-2.576448	0.262041
H14	-1.115499	-3.139002	-0.660617
H15	-0.513853	-2.811433	1.001169
H16	-2.257142	-2.862966	0.663279
C17	-2.564906	-0.460012	0.032562
O18	-3.659999	-0.954333	0.160184
N19	-2.236125	0.880696	-0.118732
H20	-2.921338	1.614547	-0.029208
H21	-0.503676	3.985822	-0.662378
C22	1.683237	-1.634213	-0.731379
H23	0.856999	-2.263834	-1.065372
H24	2.243324	-1.317502	-1.617106
N25	2.604694	-2.260342	0.194270
H26	2.127199	-2.761800	0.936894
H27	3.215290	-2.912926	-0.287000

Zero-point correction= 0.220203
Thermal correction to Energy= 0.234928
Thermal correction to Enthalpy= 0.235872
Thermal correction to Gibbs Free Energy= 0.178686
Sum of electronic and zero-point Energies= -752.279033
Sum of electronic and thermal Energies= -752.264308
Sum of electronic and thermal Enthalpies= -752.263364
Sum of electronic and thermal Free Energies= -752.320549

184 TS_N3-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	1.409036	-1.101967	-0.283449
C2	0.858063	1.034008	0.136737
C3	-0.011191	2.090596	0.206387
O4	0.260228	3.400784	0.382673
N5	-1.314286	1.802522	-0.246496
H6	-1.907511	2.608647	-0.404134
C7	-1.734563	0.568578	-0.577523
N8	-3.021987	0.378722	-0.940775
H9	-3.639578	1.156188	-1.116528
H10	-3.223243	-0.482098	-1.426883
N11	-0.952669	-0.523915	-0.474434
C12	0.360614	-0.216314	-0.256213
C13	1.395708	-2.481933	-0.729412
H14	1.214717	-3.167594	0.103929
H15	0.623907	-2.606093	-1.490346
H16	2.374119	-2.708085	-1.154773
C17	2.594179	-0.434879	0.061249
O18	3.706248	-0.903927	0.087771
N19	2.210867	0.875261	0.354115
H20	2.893099	1.606233	0.482032
H21	0.338045	3.631579	1.316582
C22	-1.698120	-1.634239	1.156882
H23	-0.817073	-2.263170	1.138865
H24	-1.697897	-0.796449	1.846112
N25	-2.874917	-2.229942	0.922817
H26	-2.924064	-3.134831	0.481950
H27	-3.746770	-1.778846	1.148538

Zero-point correction= 0.215765
Thermal correction to Energy= 0.231318
Thermal correction to Enthalpy= 0.232262
Thermal correction to Gibbs Free Energy= 0.173003
Sum of electronic and zero-point Energies= -752.259681
Sum of electronic and thermal Energies= -752.244128
Sum of electronic and thermal Enthalpies= -752.243184
Sum of electronic and thermal Free Energies= -752.302443

185 C4-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	1.599714	-0.280779	-0.402223
C2	-0.118226	1.065812	0.215846
C3	-1.469565	1.384025	0.276485
O4	-2.034215	2.559651	0.501931
N5	-2.329628	0.378597	-0.006516
H6	-3.318578	0.537135	0.148795
C7	-1.877015	-0.811151	-0.638729
N8	-2.877011	-1.571829	-1.155058
H9	-3.686057	-1.128388	-1.565081

H10	-2.573537	-2.419668	-1.613101
N11	-0.644397	-1.152593	-0.671786
C12	0.257253	-0.381235	0.140550
C13	2.403825	-1.396994	-0.874673
H14	3.102505	-1.743215	-0.108302
H15	1.730418	-2.201754	-1.168371
H16	2.977430	-1.068967	-1.742924
C17	2.087872	0.985093	-0.364299
O18	3.169488	1.422406	-0.650059
N19	0.982983	1.812262	0.087805
H20	1.060960	2.819772	0.030984
H21	-1.459733	3.179649	0.968106
C22	0.276751	-0.990073	1.618717
H23	0.953891	-0.372166	2.216906
H24	-0.737421	-0.869929	2.017909
N25	0.662130	-2.355691	1.718137
H26	1.647361	-2.536226	1.590149
H27	0.098660	-2.995319	1.174063

Zero-point correction= 0.220277
Thermal correction to Energy= 0.234628
Thermal correction to Enthalpy= 0.235572
Thermal correction to Gibbs Free Energy= 0.179772
Sum of electronic and zero-point Energies= -752.279500
Sum of electronic and thermal Energies= -752.265150
Sum of electronic and thermal Enthalpies= -752.264205
Sum of electronic and thermal Free Energies= -752.320005

186 TS_C4-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	1.536809	-0.295033	-0.520196
C2	-0.118019	1.089537	0.137439
C3	-1.429212	1.421202	0.214851
O4	-2.016332	2.601707	0.428232
N5	-2.341337	0.407692	-0.017067
H6	-3.318660	0.630732	0.122532
C7	-1.959357	-0.802814	-0.564609
N8	-2.960241	-1.633485	-0.948326
H9	-3.839703	-1.257244	-1.268584
H10	-2.662971	-2.490430	-1.391686
N11	-0.713287	-1.165292	-0.667962
C12	0.207229	-0.313354	-0.078620
C13	2.283187	-1.414225	-1.061604
H14	3.000136	-1.803375	-0.332632
H15	1.574607	-2.189572	-1.351014
H16	2.838664	-1.078009	-1.938570
C17	2.107075	0.958925	-0.336230
O18	3.249468	1.281315	-0.542487
N19	1.073704	1.782047	0.146002
H20	1.211277	2.779817	0.198069
H21	-1.424350	3.246627	0.830026
C22	0.325403	-0.984968	1.732011
H23	0.977017	-0.232414	2.173089
H24	-0.724246	-0.907304	2.011209
N25	0.824232	-2.246583	1.769283
H26	1.819829	-2.404107	1.763635
H27	0.246323	-3.030137	1.506410

Zero-point correction= 0.217644
Thermal correction to Energy= 0.232455
Thermal correction to Enthalpy= 0.233399
Thermal correction to Gibbs Free Energy= 0.176426
Sum of electronic and zero-point Energies= -752.278545
Sum of electronic and thermal Energies= -752.263734
Sum of electronic and thermal Enthalpies= -752.262790
Sum of electronic and thermal Free Energies= -752.319763

187 C5-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	1.293914	1.064997	-0.284936
C2	0.068327	-0.845790	0.185629
C3	-1.094817	-1.293069	-0.662562
O4	-0.964118	-1.859222	-1.867734
N5	-2.236939	-0.511477	-0.511821
H6	-3.106469	-0.863912	-0.894198
C7	-2.171406	0.750480	-0.005006
N8	-3.296921	1.383412	0.335811
H9	-4.211865	0.977358	0.221192
H10	-3.228255	2.345787	0.631649
N11	-1.003169	1.397876	0.126351
C12	0.069605	0.655092	0.024813
C13	1.714110	2.435474	-0.540653
H14	1.208407	2.820813	-1.427830
H15	1.471714	3.056096	0.322594
H16	2.791864	2.418629	-0.699623
C17	2.166498	-0.056797	-0.435672
O18	3.341647	0.008408	-0.648204
N19	1.364740	-1.193186	-0.347509
H20	1.844558	-2.008931	0.013503
H21	-0.082872	-2.250124	-1.956336
C22	-0.097180	-1.253332	1.683174
H23	-1.108932	-0.982057	2.007543
H24	-0.040644	-2.346545	1.717114
N25	0.940970	-0.643614	2.478898
H26	1.462332	-1.302120	3.040579
H27	0.610962	0.103104	3.075418

Zero-point correction= 0.219714
Thermal correction to Energy= 0.234640
Thermal correction to Enthalpy= 0.235584
Thermal correction to Gibbs Free Energy= 0.177888
Sum of electronic and zero-point Energies= -752.298209
Sum of electronic and thermal Energies= -752.283283
Sum of electronic and thermal Enthalpies= -752.282339
Sum of electronic and thermal Free Energies= -752.340035

188 TS_C5-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	1.340999	1.017474	-0.373547
C2	-0.046681	-0.750781	-0.295376
C3	-1.324856	-1.205746	-0.627085
O4	-1.702934	-2.490079	-0.803504
N5	-2.363212	-0.336230	-0.269541
H6	-3.299794	-0.718686	-0.315870
C7	-2.157958	0.965803	0.036916
N8	-3.204532	1.741901	0.351854
H9	-4.159459	1.424599	0.320591
H10	-3.024753	2.718249	0.529180
N11	-0.939733	1.522902	0.025844
C12	0.054832	0.681986	-0.200648
C13	1.904328	2.358172	-0.333071
H14	1.478270	2.966404	-1.132617
H15	1.691797	2.822782	0.630773
H16	2.980347	2.259022	-0.474207
C17	2.112168	-0.140523	-0.689151
O18	3.301703	-0.166256	-0.866579
N19	1.201098	-1.178979	-0.762512
H20	1.525765	-2.133880	-0.763459
H21	-1.515337	-2.797766	-1.698746
C22	0.266577	-1.093830	1.908796
H23	-0.501863	-0.440474	2.310352
H24	0.019071	-2.147351	1.828672
N25	1.549447	-0.795734	2.240035
H26	2.279774	-1.488071	2.202464
H27	1.797097	0.096023	2.636317

Zero-point correction= 0.215476
Thermal correction to Energy= 0.231227
Thermal correction to Enthalpy= 0.232171
Thermal correction to Gibbs Free Energy= 0.172777
Sum of electronic and zero-point Energies= -752.274761
Sum of electronic and thermal Energies= -752.259010
Sum of electronic and thermal Enthalpies= -752.258066
Sum of electronic and thermal Free Energies= -752.317459

189 C6-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.953262	0.664843	0.042461
C2	-0.159489	-0.616524	-0.340891
C3	1.285890	-0.969925	-0.404300
O4	1.629398	-1.758547	-1.501141
N5	1.990338	0.323130	-0.463055
H6	2.991872	0.241251	-0.583984
C7	1.464352	1.537926	-0.185234
N8	2.277191	2.594888	-0.130200
H9	3.274819	2.538703	-0.256952
H10	1.858288	3.497862	0.036764
N11	0.156767	1.776671	0.009851
C12	-0.603474	0.701775	-0.084678
C13	-2.829953	1.797219	0.308418
H14	-2.544769	2.268901	1.249580
H15	-2.758022	2.520854	-0.504677
H16	-3.847111	1.412822	0.376743
C17	-2.410510	-0.652208	-0.114000
O18	-3.540042	-1.057204	-0.069769
N19	-1.244687	-1.416255	-0.343214
H20	-1.282010	-2.409792	-0.527088
H21	1.370137	-1.331208	-2.326757
C22	1.723860	-1.762915	0.850124
H23	1.212161	-2.728931	0.820294
H24	2.794840	-1.972433	0.738708
N25	1.387228	-1.019594	2.046780
H26	0.901927	-1.582204	2.732779
H27	2.193922	-0.607686	2.496877

Zero-point correction= 0.220659
Thermal correction to Energy= 0.235427
Thermal correction to Enthalpy= 0.236371
Thermal correction to Gibbs Free Energy= 0.178548
Sum of electronic and zero-point Energies= -752.321253
Sum of electronic and thermal Energies= -752.306485
Sum of electronic and thermal Enthalpies= -752.305541
Sum of electronic and thermal Free Energies= -752.363364

190 TS_C6-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.774020	0.810842	-0.035900
C2	-0.128686	-0.566298	-0.658795
C3	1.198313	-0.916889	-0.717550
O4	1.744247	-2.037767	-1.232537
N5	2.090393	0.150350	-0.594484
H6	3.067723	-0.075657	-0.729434
C7	1.705504	1.396977	-0.191321
N8	2.654436	2.329042	0.001716
H9	3.621345	2.188997	-0.240828
H10	2.344668	3.266767	0.207243
N11	0.438612	1.716325	0.016557
C12	-0.433843	0.732909	-0.211910
C13	-2.530900	1.981861	0.377309
H14	-2.129598	2.370590	1.314269
H15	-2.478481	2.753731	-0.392286
H16	-3.565390	1.667412	0.513559
C17	-2.372825	-0.433055	-0.334621
O18	-3.546774	-0.698243	-0.290675
N19	-1.316398	-1.276459	-0.671969
H20	-1.484751	-2.193789	-1.053972
H21	1.375320	-2.250703	-2.099534
C22	1.270756	-1.851154	1.557308
H23	0.896964	-2.804049	1.203391
H24	2.340756	-1.724594	1.674847
N25	0.454315	-1.095653	2.335463
H26	-0.485307	-1.403089	2.533283
H27	0.835688	-0.414768	2.972954

Zero-point correction= 0.215335
Thermal correction to Energy= 0.231228
Thermal correction to Enthalpy= 0.232172
Thermal correction to Gibbs Free Energy= 0.172134
Sum of electronic and zero-point Energies= -752.283948
Sum of electronic and thermal Energies= -752.268054
Sum of electronic and thermal Enthalpies= -752.267110
Sum of electronic and thermal Free Energies= -752.327148

191 N7-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-0.512239	1.692814	-0.050635
C2	0.077733	-0.491038	-0.203148
C3	0.959146	-1.583610	-0.408373
O4	0.633996	-2.816215	0.114647
N5	2.308365	-1.154322	-0.193684
H6	3.026929	-1.857266	-0.294758
C7	2.679515	0.135299	0.053302
N8	3.983408	0.397046	0.224753
H9	4.698555	-0.310568	0.211202
H10	4.247474	1.350791	0.416789
N11	1.824626	1.149822	0.124082
C12	0.547045	0.774615	-0.025314
C13	-0.377327	3.131468	0.149312
H14	0.003214	3.328243	1.152636
H15	0.315612	3.533566	-0.590164
H16	-1.361415	3.581817	0.026224
C17	-1.693885	1.064411	-0.225983
O18	-2.822997	1.458326	-0.251323
N19	-1.360150	-0.434419	-0.347210
H20	-1.696918	-0.750799	-1.266727
H21	0.798845	-3.511545	-0.531313
C22	-2.211147	-1.258559	0.674231
H23	-1.637071	-2.171937	0.827649
H24	-2.202195	-0.653481	1.584959
N25	-3.470372	-1.507834	0.102906
H26	-4.201396	-0.846429	0.322069
H27	-3.781586	-2.466547	0.129196

Zero-point correction= 0.219950
Thermal correction to Energy= 0.235191
Thermal correction to Enthalpy= 0.236135
Thermal correction to Gibbs Free Energy= 0.177471
Sum of electronic and zero-point Energies= -752.256369
Sum of electronic and thermal Energies= -752.241127
Sum of electronic and thermal Enthalpies= -752.240183
Sum of electronic and thermal Free Energies= -752.298847

192 TS_N7-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-0.662343	1.486845	-0.188429
C2	0.265006	-0.518325	-0.546252
C3	1.286567	-1.490270	-0.606749
O4	0.991352	-2.783127	-0.217195
N5	2.514491	-0.943555	-0.119351
H6	3.346238	-1.498876	-0.261570
C7	2.678072	0.360783	0.270036
N8	3.926920	0.743584	0.625531
H9	4.631111	0.072945	0.885621

H10	4.021144	1.679548	0.987989
N11	1.711080	1.254516	0.292274
C12	0.525706	0.762428	-0.138249
C13	-0.813865	2.898202	0.123493
H14	-0.544505	3.082848	1.164890
H15	-0.167694	3.491722	-0.524930
H16	-1.856100	3.165786	-0.049077
C17	-1.674332	0.674255	-0.626372
O18	-2.866681	0.944018	-0.764300
N19	-1.113965	-0.607756	-0.778643
H20	-1.509133	-1.226900	-1.473980
H21	1.350616	-3.413335	-0.849797
C22	-2.462023	-1.356283	1.277925
H23	-2.138981	-2.391965	1.283865
H24	-1.816362	-0.589387	1.689083
N25	-3.654595	-1.051081	0.909224
H26	-3.909748	-0.071977	0.759231
H27	-4.285855	-1.750152	0.533417

Zero-point correction= 0.217205
Thermal correction to Energy= 0.232564
Thermal correction to Enthalpy= 0.233508
Thermal correction to Gibbs Free Energy= 0.174311
Sum of electronic and zero-point Energies= -752.255071
Sum of electronic and thermal Energies= -752.239713
Sum of electronic and thermal Enthalpies= -752.238768
Sum of electronic and thermal Free Energies= -752.297966

193 C8-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-0.907618	-0.882859	-0.076493
C2	0.497291	0.851433	0.014215
C3	1.745246	1.365794	-0.030033
O4	2.146348	2.635730	-0.048598
N5	2.803528	0.472974	-0.025485
H6	3.732839	0.873492	-0.051027
C7	2.609616	-0.877949	-0.019214
N8	3.686804	-1.675341	-0.005839
H9	4.632212	-1.333169	0.039347
H10	3.530999	-2.671477	0.006262
N11	1.403611	-1.424499	-0.034589
C12	0.381477	-0.567819	-0.030916
C13	-1.462113	-2.219345	0.020252
H14	-2.056707	-2.449217	-0.868459
H15	-0.644385	-2.935796	0.089712
H16	-2.084087	-2.285340	0.916408
C17	-1.766657	0.324125	0.076231
O18	-2.383973	0.363724	1.298317
N19	-0.781520	1.417981	-0.038572
H20	-0.989315	2.136943	0.648437
H21	1.421190	3.237528	-0.255243
C22	-2.933237	0.384819	-0.913057
H23	-3.067893	1.422243	-1.222645
H24	-2.778982	-0.216794	-1.814447
N25	-4.066601	-0.039317	-0.105539
H26	-4.337931	-1.010774	-0.147051
H27	-4.854106	0.587811	-0.038298

Zero-point correction= 0.218956
Thermal correction to Energy= 0.233923
Thermal correction to Enthalpy= 0.234867
Thermal correction to Gibbs Free Energy= 0.177170
Sum of electronic and zero-point Energies= -752.248617
Sum of electronic and thermal Energies= -752.233650
Sum of electronic and thermal Enthalpies= -752.232706
Sum of electronic and thermal Free Energies= -752.290403

194 TS_C8-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	0.919867	-0.872693	0.080507
C2	-0.499036	0.853696	0.007319
C3	-1.752144	1.360305	0.038287
O4	-2.167420	2.624426	0.056815
N5	-2.801022	0.458359	0.022298
H6	-3.733781	0.851792	0.041527
C7	-2.597488	-0.892173	0.014705
N8	-3.667825	-1.696552	-0.005999
H9	-4.616351	-1.361659	-0.043790
H10	-3.505202	-2.691840	-0.016021
N11	-1.387072	-1.429031	0.032289
C12	-0.372186	-0.565602	0.038698
C13	1.475673	-2.209065	-0.020176
H14	2.159220	-2.396149	0.811800
H15	0.661261	-2.931122	0.022724
H16	2.004811	-2.314446	-0.971205
C17	1.768338	0.337887	-0.071047
O18	2.290889	0.441754	-1.335094
N19	0.777060	1.416535	0.078348
H20	0.993325	2.206237	-0.521927
H21	-1.456446	3.240548	0.269138
C22	2.964016	0.384520	0.883020
H23	3.118310	1.421841	1.188448
H24	2.780951	-0.197002	1.790685
N25	4.155688	-0.083792	0.205129
H26	4.177578	-1.054316	-0.072331
H27	4.528661	0.529494	-0.505657

Zero-point correction= 0.218466
Thermal correction to Energy= 0.232708
Thermal correction to Enthalpy= 0.233652
Thermal correction to Gibbs Free Energy= 0.177930
Sum of electronic and zero-point Energies= -752.246973
Sum of electronic and thermal Energies= -752.232731
Sum of electronic and thermal Enthalpies= -752.231787
Sum of electronic and thermal Free Energies= -752.287509

195 O8-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	0.733364	-0.912892	-0.262829
C2	-0.666024	0.820484	-0.189769
C3	-1.917949	1.451294	-0.189397
O4	-2.102735	2.735560	0.221629
N5	-2.965754	0.531483	0.106751
H6	-3.861951	0.930846	0.347035
C7	-2.794447	-0.828013	0.150793
N8	-3.890045	-1.577340	0.399615
H9	-4.820868	-1.220834	0.259083
H10	-3.766446	-2.577711	0.386293
N11	-1.630335	-1.425853	0.000987
C12	-0.597792	-0.558881	-0.131860
C13	1.238888	-2.279277	-0.308380
H14	1.305193	-2.691060	0.700092
H15	0.547889	-2.881690	-0.897287
H16	2.219197	-2.270066	-0.784230
C17	1.469864	0.211271	-0.373669
O18	2.763804	0.285210	-0.531933
N19	0.633758	1.272230	-0.327517
H20	0.938816	2.232091	-0.395761
H21	-2.495733	3.269146	-0.478451
C22	3.641887	0.096770	0.738046
H23	3.282861	0.861345	1.428450
H24	3.408858	-0.908734	1.090538
N25	4.974613	0.244140	0.444527
H26	5.416666	-0.484861	-0.094990
H27	5.301210	1.171113	0.216327

Zero-point correction= 0.218468
Thermal correction to Energy= 0.234170
Thermal correction to Enthalpy= 0.235114
Thermal correction to Gibbs Free Energy= 0.174669
Sum of electronic and zero-point Energies= -752.273527
Sum of electronic and thermal Energies= -752.257825
Sum of electronic and thermal Enthalpies= -752.256881
Sum of electronic and thermal Free Energies= -752.317326

196 TS_O8-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	0.582539	-0.994603	-0.326303
C2	-0.709771	0.823901	-0.156676
C3	-1.908555	1.454125	-0.020937
O4	-2.123505	2.782903	0.048224
N5	-3.018069	0.612889	0.196838
H6	-3.861790	1.058956	0.531392
C7	-2.904513	-0.751441	0.228857
N8	-4.019674	-1.464557	0.485456
H9	-4.941079	-1.068959	0.396761
H10	-3.933749	-2.468666	0.452831
N11	-1.762814	-1.387328	0.046956
C12	-0.693570	-0.589867	-0.118150
C13	1.040013	-2.372265	-0.384006
H14	0.884029	-2.858028	0.580830
H15	0.488244	-2.912062	-1.154905
H16	2.101000	-2.354193	-0.630901
C17	1.417142	0.109309	-0.501959
O18	2.634648	0.094328	-0.667155
N19	0.592121	1.221048	-0.381136
H20	0.927436	2.164921	-0.483265
H21	-2.468210	3.137941	-0.782112
C22	4.266021	0.236709	1.054994
H23	3.841518	1.165628	1.405724
H24	3.925472	-0.708752	1.450136
N25	5.391481	0.270376	0.350261
H26	5.811831	-0.577649	0.003291
H27	5.736469	1.135411	-0.035572

Zero-point correction= 0.212883
Thermal correction to Energy= 0.229426
Thermal correction to Enthalpy= 0.230370
Thermal correction to Gibbs Free Energy= 0.167732
Sum of electronic and zero-point Energies= -752.264968
Sum of electronic and thermal Energies= -752.248425
Sum of electronic and thermal Enthalpies= -752.247481
Sum of electronic and thermal Free Energies= -752.310119

197 N9-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	-1.447896	-0.161203	-0.248081
C2	0.500293	1.077942	-0.045318
C3	1.833367	1.234648	0.133209
O4	2.455181	2.409661	0.330528
N5	2.622122	0.072787	-0.001846
H6	3.531206	0.193619	-0.435658
C7	2.013839	-1.175636	-0.154021
N8	2.870105	-2.222092	-0.231322
H9	3.760908	-2.182045	0.239200
H10	2.460821	-3.135458	-0.354185
N11	0.724578	-1.349103	-0.261910
C12	0.000952	-0.198022	-0.343748
C13	-2.151731	-0.697604	-1.449524
H14	-1.829092	-0.134796	-2.325206
H15	-1.871011	-1.744156	-1.558386
H16	-3.226454	-0.586679	-1.301886
C17	-1.765999	1.317437	-0.065019
O18	-2.891278	1.721390	-0.056950
N19	-0.581118	1.953921	0.094908
H20	-0.526455	2.957922	0.192696
H21	3.073204	2.365851	1.072292
C22	-1.984167	-0.922508	1.099417
H23	-2.989932	-0.518675	1.221736
H24	-1.300400	-0.533766	1.855944
N25	-1.969069	-2.297993	1.025379
H26	-2.732293	-2.767355	0.564625
H27	-1.072113	-2.754626	0.950341

Zero-point correction= 0.219247
Thermal correction to Energy= 0.233972
Thermal correction to Enthalpy= 0.234916
Thermal correction to Gibbs Free Energy= 0.178302
Sum of electronic and zero-point Energies= -752.261641
Sum of electronic and thermal Energies= -752.246916
Sum of electronic and thermal Enthalpies= -752.245972
Sum of electronic and thermal Free Energies= -752.302586

198 TS_N9-CH_2NH_2[9MOG + H_{O6}]$^{\bullet+}$

N1	1.353592	0.052432	-0.453948
C2	-0.573535	-1.066218	0.006676
C3	-1.902321	-1.155686	0.247012
O4	-2.560770	-2.243954	0.687466
N5	-2.646776	0.033808	0.070584
H6	-3.501633	0.095187	0.610827
C7	-2.012255	1.229601	-0.249171
N8	-2.809804	2.331395	-0.253003
H9	-3.789430	2.227926	-0.471123
H10	-2.377340	3.173942	-0.601622
N11	-0.734206	1.333740	-0.493851
C12	-0.037214	0.170629	-0.398653
C13	2.114795	0.790172	-1.466596
H14	1.756451	0.534494	-2.465760
H15	1.969939	1.858106	-1.296872
H16	3.167112	0.520642	-1.372604
C17	1.661650	-1.356669	-0.281314
O18	2.767559	-1.824051	-0.380594
N19	0.486512	-1.968720	0.069380
H20	0.429694	-2.956646	0.265098
H21	-3.225416	-2.542427	0.051803
C22	2.223880	0.799056	1.377464
H23	3.128080	0.207983	1.271808
H24	1.393273	0.391520	1.942665
N25	2.328091	2.116495	1.308496
H26	3.163746	2.559705	0.956577
H27	1.539336	2.714241	1.508113

Zero-point correction= 0.216622
Thermal correction to Energy= 0.231680
Thermal correction to Enthalpy= 0.232625
Thermal correction to Gibbs Free Energy= 0.174535
Sum of electronic and zero-point Energies= -752.258837
Sum of electronic and thermal Energies= -752.243779
Sum of electronic and thermal Enthalpies= -752.242834
Sum of electronic and thermal Free Energies= -752.300924

199 [9MOG + H_{N7}]$^{+}$

N1	1.535059	-0.800332	-0.003453
C2	0.013134	0.881065	0.002751
C3	-1.271204	1.485637	0.000549
O4	-1.562395	2.662733	-0.001265
N5	-2.264862	0.464502	0.000462
H6	-3.216849	0.814542	-0.000417
C7	-2.016339	-0.876697	0.000187
N8	-3.048028	-1.722299	-0.000159
H9	-2.849074	-2.711547	0.000618

N10	-0.781584	-1.391405	0.000290
C11	0.176461	-0.478740	0.000806
C12	2.076844	-2.160226	0.000357
H13	1.858256	-2.639441	0.955216
H14	1.620579	-2.724391	-0.812805
H15	3.153767	-2.091706	-0.146736
C16	2.314046	0.307574	0.000177
O17	3.487205	0.488165	0.001330
N18	1.314481	1.510334	-0.000291
H19	1.499335	2.093702	-0.826129
H20	-4.009734	-1.422468	0.000208
H21	1.502110	2.096859	0.822631

Zero-point correction= 0.164787
Thermal correction to Energy= 0.176196
Thermal correction to Enthalpy= 0.177140
Thermal correction to Gibbs Free Energy= 0.127359
Sum of electronic and zero-point Energies= -657.118991
Sum of electronic and thermal Energies= -657.107582
Sum of electronic and thermal Enthalpies= -657.106638
Sum of electronic and thermal Free Energies= -657.156420

200 N1-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-2.212061	0.725637	0.119121
C2	-0.551496	-0.837844	-0.106128
C3	0.689074	-1.377366	-0.347042
O4	1.109015	-2.504981	-0.532790
N5	1.779162	-0.251005	-0.312176
H6	2.368877	-0.455410	-1.130311
C7	1.300363	1.148105	-0.391322
N8	2.309769	2.070559	-0.467220
H9	2.002361	3.018088	-0.639088
N10	0.050611	1.503088	-0.185684
C11	-0.829387	0.542081	-0.034148
C12	-2.859743	2.029028	0.236527
H13	-2.432410	2.565140	1.084605
H14	-2.695314	2.597476	-0.679813
H15	-3.925188	1.866176	0.392149
C16	-2.892801	-0.432629	0.132617
O17	-4.044346	-0.724217	0.247214
N18	-1.813261	-1.553784	-0.047686
H19	-2.038083	-2.083650	-0.898414
H20	3.175230	1.804832	-0.917869
H21	-1.896113	-2.209612	0.737164
C22	2.750023	-0.505275	0.894448
H23	2.689051	-1.582964	1.046952
H24	2.297239	0.032014	1.729060
N25	4.052874	-0.072693	0.557980
H26	4.749744	-0.803813	0.534111
H27	4.381401	0.736107	1.066005

Zero-point correction= 0.220884
Thermal correction to Energy= 0.235588
Thermal correction to Enthalpy= 0.236532
Thermal correction to Gibbs Free Energy= 0.178774
Sum of electronic and zero-point Energies= -752.228504
Sum of electronic and thermal Energies= -752.213800
Sum of electronic and thermal Enthalpies= -752.212856
Sum of electronic and thermal Free Energies= -752.270614

201 TS_N1-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-2.226040	0.686330	0.171228
C2	-0.539810	-0.815565	-0.190687
C3	0.729266	-1.280350	-0.508797
O4	1.155559	-2.408361	-0.719858
N5	1.704323	-0.167265	-0.466358
H6	2.451028	-0.373874	-1.133608
C7	1.238942	1.175722	-0.527883
N8	2.242647	2.125093	-0.587842
H9	1.874278	3.068258	-0.610526
N10	-0.005726	1.534441	-0.227907
C11	-0.849431	0.544774	-0.064606
C12	-2.901812	1.965985	0.362220
H13	-2.475904	2.471361	1.229849
H14	-2.762703	2.582212	-0.526824
H15	-3.961067	1.771070	0.523563
C16	-2.869789	-0.494630	0.187811
O17	-4.004865	-0.821680	0.355952
N18	-1.770305	-1.574580	-0.081537
H19	-2.024286	-2.089707	-0.933218
H20	2.949521	1.985338	-1.301675
H21	-1.788656	-2.254217	0.687127
C22	2.835933	-0.465601	1.156361
H23	2.533704	-1.499270	1.290138
H24	2.329183	0.292899	1.743365
N25	4.131546	-0.254373	0.888647
H26	4.738917	-1.008492	0.607584
H27	4.535539	0.665221	0.975339

Zero-point correction= 0.218501
Thermal correction to Energy= 0.233282
Thermal correction to Enthalpy= 0.234226
Thermal correction to Gibbs Free Energy= 0.175580
Sum of electronic and zero-point Energies= -752.225605
Sum of electronic and thermal Energies= -752.210824
Sum of electronic and thermal Enthalpies= -752.209880
Sum of electronic and thermal Free Energies= -752.268526

202 C2-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-1.725823	-1.068574	0.138753
C2	-0.707466	0.950507	-0.189012
C3	0.305958	1.979785	0.005268
O4	0.048182	3.171419	-0.042960
N5	1.493321	1.395634	0.315602
H6	2.263020	2.008678	0.561664
C7	1.821540	-0.041358	0.316707
N8	2.751833	-0.255190	1.375118
H9	3.251870	-1.124944	1.202593
H10	2.310552	-0.276058	2.287742
N11	0.656266	-0.922603	0.393339
C12	-0.489234	-0.392010	0.133376
C13	-1.876390	-2.496892	0.419880
H14	-2.940588	-2.722622	0.469574
H15	-1.405310	-3.075291	-0.375861
H16	-1.397606	-2.721458	1.373393
C17	-2.766813	-0.255133	-0.130227
O18	-3.939490	-0.401735	-0.227883
N19	-2.121210	1.169711	-0.352404
H20	-2.501899	1.845738	0.325895
C21	2.540212	-0.390885	-1.041047
H22	1.804664	-0.244049	-1.845142
H23	3.325405	0.359539	-1.157341
N24	3.133391	-1.695862	-0.978320
H25	2.515505	-2.448758	-1.249597
H26	4.008976	-1.765695	-1.478041
H27	-2.385421	1.521552	-1.282412

Zero-point correction= 0.219999
Thermal correction to Energy= 0.234399
Thermal correction to Enthalpy= 0.235343
Thermal correction to Gibbs Free Energy= 0.178097
Sum of electronic and zero-point Energies= -752.242708
Sum of electronic and thermal Energies= -752.228309

Sum of electronic and thermal Enthalpies= -752.227364
Sum of electronic and thermal Free Energies= -752.284610

203 TS_C2-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	1.729165	-1.038294	-0.167527
C2	0.670588	0.947303	0.198784
C3	-0.333901	1.956203	-0.030122
O4	-0.144495	3.158767	0.040526
N5	-1.511131	1.345240	-0.405482
H6	-2.297554	1.949772	-0.617765
C7	-1.781354	-0.072747	-0.396961
N8	-2.831889	-0.326116	-1.331173
H9	-3.190848	-1.266385	-1.199221
H10	-2.498579	-0.240038	-2.286502
N11	-0.644750	-0.927009	-0.499754
C12	0.486480	-0.376551	-0.172230
C13	1.915557	-2.451599	-0.490400
H14	2.984945	-2.644261	-0.564565
H15	1.478091	-3.069489	0.294957
H16	1.428188	-2.663597	-1.442296
C17	2.748687	-0.212994	0.150825
O18	3.921745	-0.354081	0.273896
N19	2.082257	1.184703	0.391456
H20	2.466060	1.875362	-0.269133
C21	-2.432844	-0.412086	1.119571
H22	-1.590738	-0.259211	1.802703
H23	-3.180379	0.371333	1.247057
N24	-3.012875	-1.666233	1.218139
H25	-2.455961	-2.495795	1.337693
H26	-4.008502	-1.784059	1.134318
H27	2.332576	1.517670	1.330963

Zero-point correction= 0.218459
Thermal correction to Energy= 0.232876
Thermal correction to Enthalpy= 0.233821
Thermal correction to Gibbs Free Energy= 0.176676
Sum of electronic and zero-point Energies= -752.242104
Sum of electronic and thermal Energies= -752.227687
Sum of electronic and thermal Enthalpies= -752.226743
Sum of electronic and thermal Free Energies= -752.283887

204 N2-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	1.783891	-1.192484	0.009332
C2	1.040427	0.955779	-0.107147
C3	0.132126	2.037144	0.015823
O4	0.379605	3.230255	-0.026651
N5	-1.187294	1.552570	0.210707
H6	-1.887128	2.243355	-0.038534
C7	-1.515251	0.186089	0.082248
N8	-2.741428	-0.188167	0.837118
N9	-0.576764	-0.801629	0.170197
C10	0.646207	-0.367141	0.030327
C11	1.757351	-2.647163	0.106361
H12	1.360994	-2.941940	1.079100
H13	1.123010	-3.047167	-0.685432
H14	2.775936	-3.015592	-0.008645
C15	2.924711	-0.480701	-0.106364
O16	4.076821	-0.780356	-0.161986
N17	2.484970	1.008537	-0.172553
H18	2.858669	1.419788	-1.036402
H19	-2.482183	-0.530227	1.772594
H20	2.925387	1.517594	0.604385
H21	-3.341117	0.631681	0.956198
C22	-3.577402	-1.235697	0.090703
H23	-2.859852	-2.009636	-0.187674
H24	-4.286182	-1.629992	0.821094
N25	-4.228177	-0.590805	-0.986913
H26	-3.805179	-0.727974	-1.893227
H27	-5.229168	-0.715101	-1.021283

Zero-point correction= 0.222767
Thermal correction to Energy= 0.237438
Thermal correction to Enthalpy= 0.238382
Thermal correction to Gibbs Free Energy= 0.178180
Sum of electronic and zero-point Energies= -752.230332
Sum of electronic and thermal Energies= -752.215661
Sum of electronic and thermal Enthalpies= -752.214717
Sum of electronic and thermal Free Energies= -752.274919

205 TS_N2-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-1.849328	-1.022451	-0.111152
C2	-0.686473	0.915656	0.234299
C3	0.285004	1.872868	-0.161998
O4	0.177241	3.088865	-0.161165
N5	1.472834	1.230988	-0.592318
H6	2.102110	1.856777	-1.082752
C7	1.526255	-0.148688	-0.839700
N8	2.794932	-0.713140	-0.988640
N9	0.484189	-0.991704	-0.670644
C10	-0.588988	-0.411442	-0.204746
C11	-2.126766	-2.415424	-0.440672
H12	-1.892471	-2.595247	-1.490897
H13	-1.515473	-3.064257	0.187704
H14	-3.183425	-2.603991	-0.255280
C15	-2.808152	-0.151720	0.267564
O16	-3.979927	-0.258957	0.466315
N17	-2.093322	1.211043	0.447824
H18	-2.320902	1.571961	1.380199
H19	2.701516	-1.655465	-1.362866
H20	-2.482314	1.887305	-0.224543
H21	3.431100	-0.179284	-1.577268
C22	3.687564	-0.889257	0.800151
H23	4.090116	-1.886800	0.664070
H24	4.384771	-0.066284	0.689639
N25	2.730746	-0.741875	1.724560
H26	2.159431	-1.520568	2.010520
H27	2.436001	0.174597	2.023468

Zero-point correction= 0.219498
Thermal correction to Energy= 0.234106
Thermal correction to Enthalpy= 0.235050
Thermal correction to Gibbs Free Energy= 0.176734
Sum of electronic and zero-point Energies= -752.226289
Sum of electronic and thermal Energies= -752.211682
Sum of electronic and thermal Enthalpies= -752.210738
Sum of electronic and thermal Free Energies= -752.269054

206 N3-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-1.431378	-0.914493	0.102460
C2	-0.576524	1.186741	0.174118
C3	0.376804	2.236686	-0.039644
O4	0.093742	3.403004	-0.251933
N5	1.666711	1.733599	-0.029134
H6	2.405220	2.423849	-0.082174
C7	2.050670	0.423138	0.323395
N8	3.303469	-0.018441	-0.111080
N9	1.005073	-0.566832	0.277974
C10	-0.260981	-0.147157	0.191006
C11	-1.604251	-2.370155	-0.011301
H12	-0.826461	-2.763433	-0.666902
H13	-1.571042	-2.835082	0.975260
H14	-2.586429	-2.542878	-0.449956
C15	-2.526133	-0.110244	-0.017136

O16	-3.685145	-0.354270	-0.119938
N17	-2.002435	1.330365	-0.009942
H18	-2.470207	1.854779	0.739889
H19	3.578089	0.301658	-1.036189
H20	-2.261424	1.795594	-0.891620
H21	4.055006	0.103349	0.555000
C22	1.415507	-1.963066	0.520981
H23	0.682018	-2.431245	1.178435
H24	2.355595	-1.892940	1.071737
N25	1.491549	-2.687409	-0.724615
H26	1.581933	-3.684231	-0.553029
H27	2.307449	-2.392476	-1.253629

Zero-point correction= 0.222434
Thermal correction to Energy= 0.236679
Thermal correction to Enthalpy= 0.237623
Thermal correction to Gibbs Free Energy= 0.180795
Sum of electronic and zero-point Energies= -752.232931
Sum of electronic and thermal Energies= -752.218686
Sum of electronic and thermal Enthalpies= -752.217742
Sum of electronic and thermal Free Energies= -752.274570

207 TS_N3-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	1.451652	-1.012162	0.252059
C2	0.698750	1.125401	0.150612
C3	-0.260977	2.144828	-0.204985
O4	0.012311	3.223199	-0.707153
N5	-1.540305	1.678316	0.041759
H6	-2.305253	2.296617	-0.201631
C7	-1.778263	0.459143	0.703534
N8	-3.103466	0.187059	1.018627
N9	-0.924249	-0.606959	0.518959
C10	0.332354	-0.171854	0.341584
C11	1.499733	-2.435263	0.582670
H12	0.558318	-2.690241	1.068509
H13	1.639090	-3.031073	-0.321197
H14	2.329438	-2.618427	1.266714
C15	2.578974	-0.304432	-0.009417
O16	3.721838	-0.616348	-0.110852
N17	2.119892	1.170715	-0.130795
H18	2.328284	1.534084	-1.070847
H19	-3.194067	-0.675811	1.541692
H20	2.669958	1.737826	0.525814
H21	-3.579456	0.942039	1.500268
C22	-1.395450	-1.653695	-1.179475
H23	-0.565609	-2.350980	-1.207339
H24	-1.334761	-0.796487	-1.842688
N25	-2.617709	-2.201322	-1.038036
H26	-2.731138	-3.075518	-0.549960
H27	-3.439440	-1.621124	-1.110448

Zero-point correction= 0.217835
Thermal correction to Energy= 0.232716
Thermal correction to Enthalpy= 0.233660
Thermal correction to Gibbs Free Energy= 0.175473
Sum of electronic and zero-point Energies= -752.215218
Sum of electronic and thermal Energies= -752.200337
Sum of electronic and thermal Enthalpies= -752.199392
Sum of electronic and thermal Free Energies= -752.257580

208 C4-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	1.447247	-0.225123	-0.495981
C2	-0.181669	0.956762	0.586874
C3	-1.511006	1.481198	0.335530
O4	-1.773304	2.667450	0.436592
N5	-2.400677	0.496226	-0.026756
H6	-3.365505	0.783543	-0.136984
C7	-1.964096	-0.753268	-0.505741
N8	-2.938011	-1.510748	-1.057782
N9	-0.756159	-1.191141	-0.422652
C10	0.220222	-0.457044	0.320780
C11	2.090949	-1.266525	-1.305024
H12	2.799409	-1.827894	-0.697916
H13	1.308182	-1.933132	-1.663155
H14	2.590958	-0.785710	-2.146146
C15	1.960883	0.996616	-0.448262
O16	2.913199	1.551423	-0.896195
N17	0.947846	1.828244	0.470102
H18	0.710033	2.734203	0.043212
H19	-3.796959	-1.109848	-1.398535
H20	1.417839	2.031741	1.360760
H21	-2.653552	-2.393903	-1.453429
C22	0.558944	-1.213812	1.632874
H23	1.303867	-0.635181	2.192402
H24	-0.366957	-1.230595	2.229737
N25	1.117907	-2.508288	1.324236
H26	1.550131	-2.929677	2.137416
H27	0.410948	-3.142280	0.969125

Zero-point correction= 0.220578
Thermal correction to Energy= 0.234971
Thermal correction to Enthalpy= 0.235915
Thermal correction to Gibbs Free Energy= 0.179253
Sum of electronic and zero-point Energies= -752.253156
Sum of electronic and thermal Energies= -752.238763
Sum of electronic and thermal Enthalpies= -752.237819
Sum of electronic and thermal Free Energies= -752.294480

209 TS_C4-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-1.485608	0.253457	-0.528757
C2	0.142594	-1.018592	0.444159
C3	1.444477	-1.562749	0.339980
O4	1.769652	-2.731065	0.473559
N5	2.383468	-0.556201	0.009432
H6	3.344269	-0.873980	-0.033249
C7	2.022476	0.652591	-0.542396
N8	3.018767	1.430754	-1.014018
N9	0.785241	1.085182	-0.610641
C10	-0.155245	0.295038	0.011978
C11	-2.150527	1.349589	-1.223743
H12	-2.946040	1.773640	-0.606541
H13	-1.395648	2.100567	-1.452410
H14	-2.586757	0.974651	-2.150648
C15	-2.095777	-0.928660	-0.347691
O16	-3.195103	-1.326510	-0.589472
N17	-1.045435	-1.841227	0.333891
H18	-0.885323	-2.680567	-0.240579
H19	3.939666	1.064679	-1.194095
H20	-1.431386	-2.179829	1.223028
H21	2.751724	2.275830	-1.494658
C22	-0.419352	1.347720	1.718989
H23	-1.192460	0.755836	2.203933
H24	0.589660	1.194354	2.091548
N25	-0.760042	2.635310	1.476686
H26	-1.723755	2.908001	1.365775
H27	-0.066953	3.286876	1.141403

Zero-point correction= 0.218610
Thermal correction to Energy= 0.233195
Thermal correction to Enthalpy= 0.234139
Thermal correction to Gibbs Free Energy= 0.176923
Sum of electronic and zero-point Energies= -752.245699
Sum of electronic and thermal Energies= -752.231115

Sum of electronic and thermal Enthalpies= -752.230170
Sum of electronic and thermal Free Energies= -752.287386

210 C5-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	1.609136	-0.966345	0.066523
C2	0.075958	0.823541	0.151565
C3	-1.017489	1.137292	-0.849943
O4	-0.964831	2.097258	-1.594193
N5	-2.045600	0.225329	-0.821609
H6	-2.826380	0.442269	-1.431246
C7	-1.900459	-1.075803	-0.320091
N8	-3.015337	-1.834426	-0.249472
N9	-0.734647	-1.541818	0.063390
C10	0.249099	-0.657284	0.174543
C11	2.144531	-2.322296	0.173068
H12	1.949789	-2.709554	1.173838
H13	1.656369	-2.957259	-0.567560
H14	3.216901	-2.279595	-0.011533
C15	2.379873	0.090158	-0.242664
O16	3.550774	0.247860	-0.414924
N17	1.400447	1.288922	-0.370158
H18	1.332182	1.598996	-1.350648
H19	-3.892257	-1.545331	-0.650640
H20	1.787564	2.080805	0.153265
H21	-2.902650	-2.808655	-0.014127
C22	-0.166020	1.480565	1.561807
H23	0.739077	1.287222	2.153208
H24	-0.247144	2.563616	1.407049
N25	-1.300719	1.021385	2.286656
H26	-1.285691	0.049589	2.562404
H27	-2.201220	1.308572	1.931901

Zero-point correction= 0.220013
Thermal correction to Energy= 0.234853
Thermal correction to Enthalpy= 0.235797
Thermal correction to Gibbs Free Energy= 0.178077
Sum of electronic and zero-point Energies= -752.277798
Sum of electronic and thermal Energies= -752.262959
Sum of electronic and thermal Enthalpies= -752.262014
Sum of electronic and thermal Free Energies= -752.319734

211 TS_C5-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-1.686179	0.925686	0.083801
C2	-0.078708	-0.649025	-0.312905
C3	1.173307	-0.977690	-0.948890
O4	1.429966	-2.000044	-1.558115
N5	2.119250	0.033716	-0.736234
H6	3.047179	-0.177703	-1.084192
C7	1.839155	1.270886	-0.196857
N8	2.865768	2.120096	-0.002495
N9	0.615440	1.641318	0.131364
C10	-0.307975	0.694692	-0.030198
C11	-2.288732	2.188912	0.502000
H12	-2.048418	2.381416	1.548319
H13	-1.894758	2.993574	-0.119477
H14	-3.367277	2.107205	0.374444
C15	-2.411581	-0.143627	-0.297768
O16	-3.579358	-0.379363	-0.356400
N17	-1.360671	-1.203388	-0.747451
H18	-1.424348	-1.326309	-1.767268
H19	3.795393	1.938024	-0.342556
H20	-1.600743	-2.105398	-0.324933
H21	2.644733	3.056045	0.300209
C22	0.142886	-1.876252	1.587982
H23	-0.793729	-1.596471	2.064832
H24	0.189381	-2.854080	1.113998
N25	1.287161	-1.454609	2.209645
H26	1.230060	-0.853650	3.015741
H27	2.122186	-2.014512	2.146413

Zero-point correction= 0.216689
Thermal correction to Energy= 0.232213
Thermal correction to Enthalpy= 0.233157
Thermal correction to Gibbs Free Energy= 0.172961
Sum of electronic and zero-point Energies= -752.248924
Sum of electronic and thermal Energies= -752.233401
Sum of electronic and thermal Enthalpies= -752.232456
Sum of electronic and thermal Free Energies= -752.292652

212 C6-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-2.098091	0.433515	0.160478
C2	-0.069412	-0.626425	0.209686
C3	1.285950	-0.706865	-0.432849
O4	0.797373	-0.873326	-1.678727
N5	1.892397	0.613761	-0.169076
H6	2.858992	0.567785	0.147466
C7	1.189696	1.747870	-0.048167
N8	1.829815	2.914714	0.040436
N9	-0.163527	1.792324	0.019741
C10	-0.716371	0.608983	0.135728
C11	-3.075572	1.520466	0.192203
H12	-3.009876	2.039607	1.149097
H13	-2.859338	2.213666	-0.620606
H14	-4.066115	1.085368	0.067904
C15	-2.444520	-0.874141	0.121630
O16	-3.485574	-1.447582	0.150051
N17	-1.104766	-1.645107	0.054122
H18	-1.024540	-2.099039	-0.868239
H19	2.817880	3.001336	-0.136402
H20	-1.123474	-2.374450	0.773646
H21	1.280157	3.750916	0.167245
C22	2.291085	-1.797300	-0.018499
H23	2.911414	-1.977178	-0.901013
H24	1.729441	-2.724211	0.165946
N25	3.146784	-1.367698	1.072095
H26	4.008444	-1.899125	1.102688
H27	2.699210	-1.443508	1.978701

Zero-point correction= 0.221028
Thermal correction to Energy= 0.235187
Thermal correction to Enthalpy= 0.236131
Thermal correction to Gibbs Free Energy= 0.179880
Sum of electronic and zero-point Energies= -752.230045
Sum of electronic and thermal Energies= -752.215886
Sum of electronic and thermal Enthalpies= -752.214942
Sum of electronic and thermal Free Energies= -752.271193

213 TS_C6-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	2.089647	0.470301	-0.174256
C2	0.087726	-0.614062	-0.074195
C3	-1.288801	-0.735713	0.493821
O4	-1.308971	-1.184188	1.746752
N5	-1.880278	0.596340	0.316319
H6	-2.885048	0.642404	0.408817
C7	-1.197927	1.745260	0.113271
N8	-1.877453	2.901067	0.106354
N9	0.119654	1.806971	-0.097018
C10	0.691633	0.608375	-0.130642
C11	3.031912	1.572368	-0.352799
H12	2.891861	2.016416	-1.339016
H13	2.853801	2.323503	0.416763
H14	4.039738	1.169362	-0.262078
C15	2.468708	-0.811881	-0.021378

O16	3.517733	-1.375954	-0.019240
N17	1.138496	-1.599465	0.157264
H18	1.114401	-1.991311	1.109246
H19	-2.852560	2.968525	0.345451
H20	1.164739	-2.389557	-0.494471
H21	-1.354381	3.749927	-0.042026
C22	-2.205366	-1.845348	-0.297086
H23	-3.019755	-2.136149	0.368856
H24	-1.535977	-2.705960	-0.411483
N25	-2.709897	-1.301325	-1.493280
H26	-3.673004	-1.497412	-1.715633
H27	-2.102417	-1.299844	-2.298156

Zero-point correction= 0.218152
Thermal correction to Energy= 0.232846
Thermal correction to Enthalpy= 0.233790
Thermal correction to Gibbs Free Energy= 0.175687
Sum of electronic and zero-point Energies= -752.222889
Sum of electronic and thermal Energies= -752.208195
Sum of electronic and thermal Enthalpies= -752.207251
Sum of electronic and thermal Free Energies= -752.265353

214 O6-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-2.201475	-0.572135	-0.094205
C2	0.087969	-0.309847	-0.034464
C3	1.220947	0.421239	0.138018
O4	2.483632	0.062074	0.320095
N5	1.048475	1.804802	0.103120
H6	1.859099	2.354140	-0.150364
C7	-0.228373	2.381077	0.028909
N8	-0.241741	3.736767	0.042589
N9	-1.322828	1.692681	-0.095665
C10	-1.155750	0.355025	-0.246722
C11	-3.614574	-0.219829	-0.219360
H12	-3.863591	0.523484	0.538330
H13	-3.791933	0.195664	-1.212245
H14	-4.205692	-1.122949	-0.075721
C15	-1.795196	-1.823903	0.108864
O16	-2.305940	-2.901122	0.210079
N17	-0.201443	-1.722019	0.162507
H18	0.153383	-2.354468	-0.561447
H19	0.469677	4.237712	0.553046
H20	0.089079	-2.096161	1.070351
H21	-1.156270	4.163776	0.022035
C22	2.930664	-1.269393	-0.173884
H23	2.464284	-1.399594	-1.156475
H24	2.565325	-2.010546	0.543626
N25	4.313043	-1.350994	-0.268935
H26	4.743867	-0.767454	-0.971822
H27	4.818895	-1.341147	0.605247

Zero-point correction= 0.220073
Thermal correction to Energy= 0.235096
Thermal correction to Enthalpy= 0.236040
Thermal correction to Gibbs Free Energy= 0.177655
Sum of electronic and zero-point Energies= -752.236989
Sum of electronic and thermal Energies= -752.221966
Sum of electronic and thermal Enthalpies= -752.221022
Sum of electronic and thermal Free Energies= -752.279407

215 TS_O6-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	2.415388	-0.239024	0.143086
C2	0.166062	-0.449965	-0.175124
C3	-1.141862	-0.034072	-0.444578
O4	-2.172532	-0.720800	-0.675452
N5	-1.246745	1.396929	-0.311663
H6	-2.059242	1.801555	-0.759102
C7	-0.163605	2.212215	-0.048071
N8	-0.391721	3.539504	-0.039755
N9	1.056521	1.774193	0.181339
C10	1.183212	0.435897	0.075300
C11	3.696988	0.408180	0.408506
H12	3.891754	1.151474	-0.365216
H13	3.659148	0.896001	1.383187
H14	4.471272	-0.357534	0.400152
C15	2.285608	-1.560340	-0.044961
O16	3.030083	-2.494830	-0.044337
N17	0.745997	-1.775578	-0.291085
H18	0.407354	-2.455427	0.397060
H19	-1.320958	3.921565	0.019068
H20	0.618317	-2.197939	-1.217202
H21	0.382835	4.138073	0.202014
C22	-3.558663	-1.045423	0.850776
H23	-3.429429	-0.075443	1.312909
H24	-3.003849	-1.886063	1.243202
N25	-4.731193	-1.303092	0.263749
H26	-5.312703	-0.550761	-0.069804
H27	-4.909078	-2.209930	-0.138738

Zero-point correction= 0.215740
Thermal correction to Energy= 0.231290
Thermal correction to Enthalpy= 0.232234
Thermal correction to Gibbs Free Energy= 0.171794
Sum of electronic and zero-point Energies= -752.229661
Sum of electronic and thermal Energies= -752.214111
Sum of electronic and thermal Enthalpies= -752.213166
Sum of electronic and thermal Free Energies= -752.273606

216 C8-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

C1	0.279649	-0.769809	-0.501496
C2	1.489379	-1.470824	-0.289731
O3	1.689605	-2.671891	-0.315813
N4	2.535841	-0.548719	-0.009054
H5	3.445943	-0.974935	0.121633
C6	2.374895	0.803899	0.086401
N7	3.455410	1.554103	0.337255
N8	1.198166	1.412181	-0.031059
C9	0.179729	0.594513	-0.318212
C10	-2.039726	-0.075797	-0.481851
O11	-3.115737	-0.076132	-1.054128
N12	-1.016616	-1.315431	-0.798243
H13	-1.153275	-1.541645	-1.789578
H14	4.387248	1.176830	0.391592
H15	-1.246668	-2.157336	-0.265359
H16	3.335015	2.554530	0.376516
C17	-2.436788	-0.409429	1.352487
H18	-2.960708	0.529499	1.515423
H19	-3.092958	-1.268976	1.234456
N20	-1.349100	-0.613188	2.143412
H21	-0.843585	0.160284	2.547997
H22	-1.015085	-1.537353	2.370516
N23	-1.109679	1.013523	-0.454830
C24	-1.576576	2.384144	-0.334220
H25	-1.786831	2.647369	0.708014
H26	-0.799030	3.046977	-0.712811
H27	-2.482541	2.491469	-0.931508

Zero-point correction= 0.218793
Thermal correction to Energy= 0.234039
Thermal correction to Enthalpy= 0.234983
Thermal correction to Gibbs Free Energy= 0.176228
Sum of electronic and zero-point Energies= -752.260578
Sum of electronic and thermal Energies= -752.245332

Sum of electronic and thermal Enthalpies= -752.244388
Sum of electronic and thermal Free Energies= -752.303143

217 TS_C8-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

C1	-0.293721	0.818569	-0.466469
C2	-1.518252	1.484804	-0.235625
O3	-1.753721	2.678857	-0.229983
N4	-2.539487	0.525161	0.021302
H5	-3.458331	0.925236	0.172577
C6	-2.349161	-0.825416	0.058457
N7	-3.407305	-1.609999	0.298037
N8	-1.162031	-1.403244	-0.112227
C9	-0.170202	-0.549137	-0.369735
C10	1.996911	0.160714	-0.633516
O11	3.108246	0.239563	-1.089544
N12	0.993732	1.393669	-0.769296
H13	1.073044	1.746319	-1.731311
H14	-4.345449	-1.256039	0.389214
H15	1.269625	2.157990	-0.148633
H16	-3.265211	-2.608310	0.289885
C17	2.413091	0.383512	1.560594
H18	3.112276	-0.442736	1.492529
H19	2.844005	1.379725	1.508618
N20	1.343079	0.217140	2.374091
H21	1.076964	-0.695315	2.709657
H22	0.824558	1.000813	2.738440
N23	1.128260	-0.935359	-0.584583
C24	1.633731	-2.298402	-0.549714
H25	2.023066	-2.548901	0.441744
H26	0.811511	-2.969970	-0.793190
H27	2.429619	-2.395600	-1.288537

Zero-point correction= 0.217668
Thermal correction to Energy= 0.232746
Thermal correction to Enthalpy= 0.233690
Thermal correction to Gibbs Free Energy= 0.174736
Sum of electronic and zero-point Energies= -752.261379
Sum of electronic and thermal Energies= -752.246302
Sum of electronic and thermal Enthalpies= -752.245358
Sum of electronic and thermal Free Energies= -752.304311

218 O8-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-0.746470	-0.916295	-0.421765
C2	0.642749	0.849530	-0.196304
C3	1.867859	1.527886	-0.001247
O4	2.098983	2.721316	-0.046465
N5	2.891518	0.577832	0.274954
H6	3.806331	0.985362	0.430241
C7	2.713164	-0.775425	0.311923
N8	3.772573	-1.547709	0.579460
N9	1.540684	-1.368109	0.094089
C10	0.541810	-0.521676	-0.154387
C11	-1.112133	-2.293386	-0.741172
H12	-0.627495	-2.614039	-1.666698
H13	-0.800150	-2.942651	0.076731
H14	-2.193454	-2.347075	-0.864825
C15	-1.519512	0.180144	-0.842166
O16	-2.793274	0.303065	-0.551883
N17	-0.644356	1.413697	-0.551201
H18	-1.057172	1.987845	0.195595
H19	4.695082	-1.181008	0.746556
H20	-0.599729	2.012092	-1.383384
H21	3.635791	-2.546558	0.598047
C22	-3.268331	-0.027366	0.881297
H23	-3.016721	-1.076977	1.032960
H24	-2.676197	0.614481	1.538756
N25	-4.619224	0.203194	1.024882
H26	-4.927871	1.163651	0.993205
H27	-5.240792	-0.426683	0.539006

Zero-point correction= 0.221016
Thermal correction to Energy= 0.235774
Thermal correction to Enthalpy= 0.236718
Thermal correction to Gibbs Free Energy= 0.178379
Sum of electronic and zero-point Energies= -752.247994
Sum of electronic and thermal Energies= -752.233235
Sum of electronic and thermal Enthalpies= -752.232291
Sum of electronic and thermal Free Energies= -752.290631

219 TS_O8-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-0.632230	-0.917637	-0.347454
C2	0.765885	0.844638	-0.173389
C3	1.988486	1.522770	0.020602
O4	2.213934	2.719448	0.012921
N5	3.025201	0.572107	0.243894
H6	3.941292	0.980493	0.386633
C7	2.850283	-0.781809	0.265666
N8	3.922135	-1.554152	0.488992
N9	1.675067	-1.374624	0.078423
C10	0.663406	-0.529839	-0.133122
C11	-1.082309	-2.286624	-0.548535
H12	-1.216122	-2.493295	-1.613421
H13	-0.324084	-2.951513	-0.137077
H14	-2.028196	-2.439360	-0.028209
C15	-1.435664	0.178315	-0.677773
O16	-2.660411	0.279854	-0.677265
N17	-0.539403	1.413649	-0.437888
H18	-0.910504	1.969891	0.346173
H19	4.848406	-1.185163	0.625870
H20	-0.558499	2.024953	-1.260752
H21	3.790820	-2.553551	0.494324
C22	-3.983224	0.189618	1.099442
H23	-3.503200	-0.692806	1.500266
H24	-3.716756	1.163178	1.487679
N25	-5.187441	0.052992	0.542830
H26	-5.693714	0.857685	0.207565
H27	-5.502117	-0.843692	0.206761

Zero-point correction= 0.216531
Thermal correction to Energy= 0.232120
Thermal correction to Enthalpy= 0.233065
Thermal correction to Gibbs Free Energy= 0.172271
Sum of electronic and zero-point Energies= -752.242348
Sum of electronic and thermal Energies= -752.226759
Sum of electronic and thermal Enthalpies= -752.225814
Sum of electronic and thermal Free Energies= -752.286608

220 N9-CH_2NH_2[9MOG + H_{N7}]$^{\bullet+}$

N1	-1.417799	0.186568	0.114879
C2	0.530799	-1.094840	-0.039277
C3	1.949485	-1.308957	-0.115432
O4	2.530108	-2.364469	-0.242871
N5	2.641869	-0.078869	-0.020975
H6	3.651938	-0.163501	-0.061594
C7	2.047249	1.142062	0.107534
N8	2.825739	2.226178	0.183987
H9	3.831712	2.186205	0.152170
H10	2.383636	3.125806	0.291805
N11	0.725997	1.295810	0.157900
C12	0.028082	0.160124	0.078693
C13	-1.928790	0.495773	1.479299
H14	-1.519927	-0.225588	2.187552
H15	-1.621918	1.505770	1.749243

H16	-3.014640	0.400856	1.457737
C17	-1.891774	-1.287001	-0.368150
O18	-2.881625	-1.754055	0.142539
N19	-0.461586	-2.121648	-0.120213
H20	-0.534946	-2.701433	0.722703
C21	-2.025746	1.177387	-0.968302
H22	-3.040376	0.797848	-1.097332
H23	-1.434486	0.960114	-1.859303
N24	-2.021567	2.527199	-0.642841
H25	-2.743013	2.875470	-0.031790
H26	-1.127422	2.982994	-0.549319
H27	-0.322810	-2.750301	-0.914552

Zero-point correction= 0.220395
Thermal correction to Energy= 0.234894
Thermal correction to Enthalpy= 0.235838
Thermal correction to Gibbs Free Energy= 0.179314
Sum of electronic and zero-point Energies= -752.233974
Sum of electronic and thermal Energies= -752.219475
Sum of electronic and thermal Enthalpies= -752.218531
Sum of electronic and thermal Free Energies= -752.275055

221 TS_N9-CH_2NH_2[9MOG + H_{N7}]$^{\cdot+}$

C1	0.665966	0.994641	0.040297
C2	2.029193	1.278368	-0.240917
O3	2.561021	2.357926	-0.416393
N4	2.777742	0.070657	-0.291955
H5	3.763667	0.198579	-0.487924
C6	2.264791	-1.170081	-0.052651
N7	3.094940	-2.222117	-0.117668
N8	0.986790	-1.388934	0.231127
C9	0.226881	-0.284658	0.275578
C10	-1.626170	-1.311931	1.515557
H11	-1.325068	-1.060097	2.536650
H12	-2.717358	-1.320522	1.471535
H13	-1.233071	-2.293888	1.250594
C14	-1.655764	1.049144	0.714695
O15	-2.730043	1.387312	0.174620
N16	-0.387445	1.949438	0.264451
H17	-0.163818	2.628825	0.995562
H18	4.083895	-2.132953	-0.282086
H19	-0.660417	2.483226	-0.567370
H20	2.720380	-3.131552	0.101925
C21	-2.435749	-0.955936	-1.506067
H22	-1.918240	-0.051382	-1.791814
H23	-2.028371	-1.929896	-1.755412
N24	-3.619083	-0.851038	-1.010990
H25	-3.894254	0.079205	-0.669915
H26	-4.181017	-1.661514	-0.780950
N27	-1.125665	-0.324752	0.558525

Zero-point correction= 0.218298
Thermal correction to Energy= 0.232971
Thermal correction to Enthalpy= 0.233915
Thermal correction to Gibbs Free Energy= 0.176394
Sum of electronic and zero-point Energies= -752.228845
Sum of electronic and thermal Energies= -752.214172
Sum of electronic and thermal Enthalpies= -752.213228
Sum of electronic and thermal Free Energies= -752.270749

222 [9MOG + H_{O8}]$^{+}\cdots{}^{\cdot}CH_2NH_2$

N1	0.247328	-1.364977	-0.002474
C2	-0.599414	0.686498	-0.004583
C3	-1.601285	1.702965	-0.002565
O4	-1.463774	2.909427	-0.004189
N5	-2.879959	1.092210	0.002009
C6	-3.127076	-0.258302	0.004895
N7	-4.409551	-0.658901	0.009792
H8	-5.187052	-0.020581	0.009780
H9	-4.594733	-1.649363	0.010361
N10	-2.169611	-1.169595	0.003133
C11	-0.939648	-0.639534	-0.001616
C12	0.379511	-2.818892	-0.002951
H13	0.981850	-3.133879	0.849486
H14	-0.624529	-3.232925	0.077683
H15	0.845012	-3.150347	-0.931764
C16	1.273966	-0.488788	-0.007183
O17	2.504741	-0.879653	-0.009870
N18	0.792665	0.761261	-0.008100
H19	1.335700	1.612634	-0.011322
H20	3.196744	-0.099233	-0.003926
H21	-3.648451	1.752748	0.003561
H22	5.960482	-0.029209	0.870980
H23	5.969762	-0.026318	-0.844500
H24	4.227265	1.614568	0.933551
H25	4.237855	1.618108	-0.920321
N26	5.574156	0.328895	0.011732
C27	4.428473	1.079945	0.006712

Zero-point correction= 0.215505
Thermal correction to Energy= 0.231758
Thermal correction to Enthalpy= 0.232702
Thermal correction to Gibbs Free Energy= 0.169492
Sum of electronic and zero-point Energies= -752.303772
Sum of electronic and thermal Energies= -752.287519
Sum of electronic and thermal Enthalpies= -752.286575
Sum of electronic and thermal Free Energies= -752.349786

223 TS_[9MOG + H_{O8}]$^{+}\cdots{}^{\cdot}CH_2NH_2$

N1	-0.423964	1.031109	-0.280917
C2	0.793734	-0.817897	-0.152473
C3	1.977943	-1.606104	-0.008249
O4	2.095017	-2.814855	-0.034447
N5	3.092027	-0.752445	0.185699
C6	3.054555	0.618630	0.227476
N7	4.213153	1.270676	0.422196
H8	5.100321	0.805746	0.515516
H9	4.187988	2.277894	0.440653
N10	1.942189	1.319362	0.090238
C11	0.853910	0.560679	-0.097258
C12	-0.817776	2.430177	-0.319139
H13	-0.690263	2.881490	0.666329
H14	-0.197813	2.961055	-1.042410
H15	-1.863012	2.476338	-0.622169
C16	-1.279220	-0.038236	-0.458266
O17	-2.507719	0.023165	-0.673672
N18	-0.521158	-1.166223	-0.367421
H19	-0.878753	-2.101890	-0.495017
H20	-3.619032	-0.045457	0.481319
H21	3.970842	-1.244214	0.296998
H22	-6.037591	0.374943	-0.412620
H23	-5.791316	-1.313622	-0.224999
H24	-4.767654	0.833836	1.556936
H25	-4.509685	-0.953059	1.764046
N26	-5.633769	-0.378951	0.126583
C27	-4.630104	-0.127955	1.058863

Zero-point correction= 0.213470
Thermal correction to Energy= 0.229253
Thermal correction to Enthalpy= 0.230197
Thermal correction to Gibbs Free Energy= 0.167501
Sum of electronic and zero-point Energies= -752.298456
Sum of electronic and thermal Energies= -752.282673

Sum of electronic and thermal Enthalpies= -752.281729
Sum of electronic and thermal Free Energies= -752.344424

224 [9MOG + H_{O8}]$^{+}$

N1	1.505189	-0.776171	-0.000043
C2	0.019484	0.875782	-0.000023
C3	-1.270771	1.498059	0.000008
O4	-1.545105	2.677511	0.000032
N5	-2.267436	0.490086	0.000013
H6	-3.213844	0.853503	0.000041
C7	-2.048121	-0.865210	-0.000007
N8	-3.118519	-1.672989	0.000000
H9	-4.065992	-1.333562	0.000016
H10	-2.961700	-2.668641	-0.000007
N11	-0.837216	-1.401505	-0.000029
C12	0.137859	-0.487411	-0.000031
C13	2.098141	-2.111048	0.000057
H14	2.695297	-2.261626	0.901998
H15	1.275407	-2.825390	-0.000462
H16	2.696212	-2.261359	-0.901321
C17	2.165457	0.398399	-0.000017
O18	3.460818	0.590191	0.000007
N19	1.304658	1.409133	-0.000015
H20	1.553199	2.390574	-0.000008
H21	3.976691	-0.226416	0.000026

Zero-point correction= 0.163679
Thermal correction to Energy= 0.175441
Thermal correction to Enthalpy= 0.176385
Thermal correction to Gibbs Free Energy= 0.126213
Sum of electronic and zero-point Energies= -657.143675
Sum of electronic and thermal Energies= -657.131914
Sum of electronic and thermal Enthalpies= -657.130970
Sum of electronic and thermal Free Energies= -657.181142

225 N1-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-2.188992	0.699794	0.112863
C2	-0.551102	-0.832227	-0.124589
C3	0.698091	-1.374682	-0.363447
O4	1.125078	-2.505597	-0.551172
N5	1.791928	-0.252282	-0.305278
C6	1.327468	1.151328	-0.379327
N7	2.350252	2.057983	-0.477423
H8	3.212926	1.766769	-0.916559
H9	2.059509	3.005530	-0.673657
N10	0.090187	1.515905	-0.180228
C11	-0.795391	0.541078	-0.028020
C12	-2.885707	1.972941	0.242553
H13	-3.350936	2.061441	1.227250
H14	-2.137082	2.757369	0.134556
H15	-3.627267	2.086976	-0.551800
C16	-2.737407	-0.519046	0.098824
O17	-4.008009	-0.827786	0.222411
N18	-1.807282	-1.460154	-0.048093
H19	-1.989697	-2.453620	-0.076014
H20	-4.582117	-0.058256	0.322790
H21	2.391255	-0.452986	-1.117901
C22	2.751071	-0.517913	0.904796
H23	2.668085	-1.593921	1.058360
H24	2.305779	0.028134	1.737776
N25	4.066138	-0.110165	0.574505
H26	4.747279	-0.856177	0.557786
H27	4.407962	0.689361	1.088335

Zero-point correction= 0.220142
Thermal correction to Energy= 0.234904
Thermal correction to Enthalpy= 0.235848
Thermal correction to Gibbs Free Energy= 0.178594
Sum of electronic and zero-point Energies= -752.244118
Sum of electronic and thermal Energies= -752.229356
Sum of electronic and thermal Enthalpies= -752.228412
Sum of electronic and thermal Free Energies= -752.285666

226 TS_N1-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-2.202395	0.664142	0.156695
C2	-0.540033	-0.808003	-0.198420
C3	0.738962	-1.281369	-0.499009
O4	1.169217	-2.411256	-0.705136
N5	1.726324	-0.174690	-0.419248
C6	1.272474	1.178160	-0.487020
N7	2.293400	2.107946	-0.556226
H8	3.017690	1.927664	-1.242422
H9	1.947166	3.057312	-0.615233
N10	0.037281	1.549900	-0.210237
C11	-0.814734	0.549989	-0.056356
C12	-2.929335	1.913590	0.340082
H13	-3.390235	1.951422	1.330003
H14	-2.198793	2.718315	0.260464
H15	-3.678181	2.041681	-0.445300
C16	-2.716789	-0.572180	0.131553
O17	-3.972386	-0.918853	0.299709
N18	-1.767570	-1.478189	-0.082347
H19	-1.918742	-2.476227	-0.133481
H20	-4.561980	-0.167467	0.440030
H21	2.471583	-0.377470	-1.092465
C22	2.826296	-0.472816	1.127769
H23	2.515824	-1.498986	1.300058
H24	2.371290	0.288532	1.753978
N25	4.132359	-0.296526	0.826828
H26	4.719570	-1.077043	0.580436
H27	4.573321	0.600830	0.947502

Zero-point correction= 0.217272
Thermal correction to Energy= 0.232296
Thermal correction to Enthalpy= 0.233241
Thermal correction to Gibbs Free Energy= 0.174748
Sum of electronic and zero-point Energies= -752.242093
Sum of electronic and thermal Energies= -752.227068
Sum of electronic and thermal Enthalpies= -752.226124
Sum of electronic and thermal Free Energies= -752.284617

227 C2-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	1.737825	-0.997209	-0.151262
C2	0.701634	0.978465	0.095736
C3	-0.362909	1.978503	0.006934
O4	-0.175231	3.173244	0.141818
N5	-1.536327	1.362839	-0.317021
C6	-1.841459	-0.078566	-0.324534
N7	-2.787824	-0.282419	-1.378094
H8	-3.184724	-1.214341	-1.327944
H9	-2.370961	-0.151033	-2.293843
N10	-0.665649	-0.941801	-0.441800
C11	0.467356	-0.365715	-0.188934
C12	1.985610	-2.417253	-0.387557
H13	2.437536	-2.877427	0.493853
H14	1.015451	-2.879618	-0.569261
H15	2.612324	-2.553134	-1.271550
C16	2.642163	-0.057218	0.137020
O17	3.931198	-0.189710	0.277296
N18	2.050628	1.138522	0.289289
H19	2.525769	2.011178	0.494423
H20	4.254261	-1.091015	0.141570
H21	-2.337539	1.967689	-0.457627

C22	-2.513052	-0.444711	1.059248
H23	-1.746296	-0.286015	1.827378
H24	-3.296840	0.301070	1.214987
N25	-3.079365	-1.746545	1.176611
H26	-2.465990	-2.523020	0.977583
H27	-4.001807	-1.867328	0.785978

Zero-point correction= 0.219848
Thermal correction to Energy= 0.234272
Thermal correction to Enthalpy= 0.235216
Thermal correction to Gibbs Free Energy= 0.178662
Sum of electronic and zero-point Energies= -752.271811
Sum of electronic and thermal Energies= -752.257387
Sum of electronic and thermal Enthalpies= -752.256443
Sum of electronic and thermal Free Energies= -752.312996

228 TS_C2-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-1.727713	-0.948326	0.202487
C2	-0.671150	0.991318	-0.086735
C3	0.384471	1.961065	0.020098
O4	0.314922	3.155939	-0.194915
N5	1.551122	1.322176	0.454837
C6	1.733133	-0.067700	0.581136
N7	2.905013	-0.390715	1.289660
H8	2.938926	-1.385479	1.478395
H9	2.979225	0.118412	2.164806
N10	0.650674	-0.899967	0.675041
C11	-0.471861	-0.320012	0.280948
C12	-2.000030	-2.344052	0.524343
H13	-2.336540	-2.885513	-0.362851
H14	-1.062465	-2.776529	0.873414
H15	-2.736569	-2.414742	1.328218
C16	-2.623402	-0.020728	-0.183624
O17	-3.909866	-0.182899	-0.381904
N18	-2.026474	1.149908	-0.364714
H19	-2.485850	2.006464	-0.647515
H20	-4.218595	-1.080598	-0.205456
H21	2.372196	1.913968	0.506247
C22	2.396212	-0.525816	-1.305496
H23	1.454126	-0.390487	-1.832541
H24	3.112632	0.286511	-1.383349
N25	2.936578	-1.765285	-1.370507
H26	2.347074	-2.580359	-1.428636
H27	3.886749	-1.914956	-1.067841

Zero-point correction= 0.217826
Thermal correction to Energy= 0.232601
Thermal correction to Enthalpy= 0.233545
Thermal correction to Gibbs Free Energy= 0.176249
Sum of electronic and zero-point Energies= -752.263468
Sum of electronic and thermal Energies= -752.248693
Sum of electronic and thermal Enthalpies= -752.247748
Sum of electronic and thermal Free Energies= -752.305045

229 N2-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-1.872926	-1.062106	0.104433
C2	-0.937739	0.959650	-0.031356
C3	0.060720	1.977293	0.080670
O4	-0.066179	3.169072	-0.134673
N5	1.283350	1.413413	0.500459
C6	1.421429	0.072443	0.959867
N7	2.776145	-0.465885	0.668709
H8	3.509378	0.094238	1.110296
H9	2.821506	-1.384971	1.116177
N10	0.469160	-0.877229	0.706597
C11	-0.668798	-0.356430	0.296697
C12	-2.067379	-2.484649	0.345277
H13	-2.296707	-3.007985	-0.586126
H14	-1.128893	-2.867980	0.745858
H15	-2.852940	-2.646050	1.087864
C16	-2.801472	-0.180325	-0.315077
O17	-4.058883	-0.426350	-0.608528
N18	-2.280893	1.032146	-0.408860
H19	-2.781128	1.864708	-0.691113
H20	-4.309123	-1.348822	-0.474568
H21	1.900305	2.115704	0.893363
C22	3.151064	-0.638364	-0.816038
H23	2.408257	-1.337750	-1.203215
H24	2.992058	0.344822	-1.261382
N25	4.488391	-1.091902	-0.904445
H26	4.612607	-2.041268	-1.223510
H27	5.135635	-0.463190	-1.356522

Zero-point correction= 0.221990
Thermal correction to Energy= 0.236760
Thermal correction to Enthalpy= 0.237704
Thermal correction to Gibbs Free Energy= 0.179357
Sum of electronic and zero-point Energies= -752.248525
Sum of electronic and thermal Energies= -752.233755
Sum of electronic and thermal Enthalpies= -752.232811
Sum of electronic and thermal Free Energies= -752.291159

230 TS_N2-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	1.989019	-1.059081	-0.046671
C2	1.017720	0.949488	0.018862
C3	-0.007960	1.935937	-0.106061
O4	0.086190	3.140754	0.045100
N5	-1.227964	1.314814	-0.441060
C6	-1.365773	-0.048078	-0.765507
N7	-2.667921	-0.541237	-0.761205
H8	-3.353004	0.026306	-1.258654
H9	-2.673720	-1.483100	-1.146600
N10	-0.373969	-0.953352	-0.575362
C11	0.764133	-0.388015	-0.227182
C12	2.201330	-2.489018	-0.217489
H13	2.455711	-2.960955	0.734618
H14	1.261048	-2.905826	-0.578408
H15	2.975268	-2.676701	-0.966020
C16	2.913820	-0.139055	0.290778
O17	4.186516	-0.345848	0.547623
N18	2.372961	1.067042	0.338610
H19	2.865037	1.921039	0.565307
H20	4.442525	-1.274133	0.483358
H21	-1.942448	1.973419	-0.725705
C22	-3.629842	-0.747311	0.937637
H23	-3.192502	-1.693507	1.239057
H24	-3.220956	0.130347	1.428163
N25	-4.971282	-0.735649	0.683432
H26	-5.489037	-1.598589	0.643132
H27	-5.516041	0.091005	0.869544

Zero-point correction= 0.217727
Thermal correction to Energy= 0.232964
Thermal correction to Enthalpy= 0.233909
Thermal correction to Gibbs Free Energy= 0.173695
Sum of electronic and zero-point Energies= -752.239440
Sum of electronic and thermal Energies= -752.224202
Sum of electronic and thermal Enthalpies= -752.223258
Sum of electronic and thermal Free Energies= -752.283472

231 N3-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-1.418081	-0.981334	0.085627

C2	-0.703608	1.116991	-0.012318
C3	0.208220	2.252316	-0.101631
O4	-0.133697	3.405506	-0.271760
N5	1.513779	1.815918	0.011173
C6	1.903898	0.526558	0.474840
N7	3.266242	0.231660	0.423524
H8	3.818294	0.773086	-0.232171
H9	3.722862	0.166963	1.324424
N10	1.024951	-0.562171	0.129711
C11	-0.277898	-0.170107	0.051500
C12	-1.460160	-2.420701	0.331989
H13	-1.511748	-2.981023	-0.603444
H14	-0.554876	-2.690756	0.875732
H15	-2.314638	-2.657713	0.969089
C16	-2.490869	-0.162536	0.015447
O17	-3.760759	-0.493528	0.041362
N18	-2.090315	1.099257	-0.033016
H19	-2.694888	1.909340	-0.105199
H20	-3.933321	-1.414801	-0.189884
H21	2.199040	2.558340	0.085834
C22	1.535798	-1.623099	-0.825034
H23	0.652222	-2.043476	-1.312751
H24	2.120799	-1.106675	-1.589136
N25	2.319115	-2.658952	-0.262782
H26	1.847402	-3.216787	0.436843
H27	3.202376	-2.319508	0.095434

Zero-point correction= 0.220348
Thermal correction to Energy= 0.235156
Thermal correction to Enthalpy= 0.236101
Thermal correction to Gibbs Free Energy= 0.178160
Sum of electronic and zero-point Energies= -752.249374
Sum of electronic and thermal Energies= -752.234566
Sum of electronic and thermal Enthalpies= -752.233622
Sum of electronic and thermal Free Energies= -752.291562

232 TS_N3-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	1.514190	-0.918198	-0.286114
C2	0.646469	1.093907	0.060979
C3	-0.364538	2.126004	0.212134
O4	-0.178566	3.263042	0.607017
N5	-1.596656	1.598578	-0.139919
C6	-1.787137	0.337817	-0.727148
N7	-3.082892	0.046734	-1.128359
H8	-3.527624	0.765564	-1.688438
H9	-3.141129	-0.852785	-1.588611
N10	-0.922637	-0.694910	-0.487534
C11	0.322485	-0.184200	-0.270185
C12	1.649829	-2.319872	-0.668214
H13	1.898329	-2.936680	0.198501
H14	0.687453	-2.632724	-1.073842
H15	2.405280	-2.427081	-1.450137
C16	2.513184	-0.068327	0.022332
O17	3.797778	-0.324825	0.100114
N18	2.022837	1.147319	0.233762
H19	2.563565	1.965725	0.486140
H20	4.017241	-1.258056	-0.013310
H21	-2.378764	2.238746	-0.063397
C22	-1.382550	-1.636947	1.211622
H23	-0.590276	-2.380895	1.230783
H24	-1.251124	-0.799936	1.893998
N25	-2.645944	-2.148016	1.165977
H26	-2.817894	-2.984909	0.631523
H27	-3.427490	-1.513543	1.225937

Zero-point correction= 0.216893
Thermal correction to Energy= 0.231990
Thermal correction to Enthalpy= 0.232934
Thermal correction to Gibbs Free Energy= 0.174524
Sum of electronic and zero-point Energies= -752.239249
Sum of electronic and thermal Energies= -752.224152
Sum of electronic and thermal Enthalpies= -752.223208
Sum of electronic and thermal Free Energies= -752.281618

233 C4-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	1.534701	-0.299899	-0.374475
C2	-0.137027	1.028537	0.435999
C3	-1.482286	1.535733	0.368274
O4	-1.812277	2.690305	0.567553
N5	-2.376265	0.519877	0.020967
C6	-1.957511	-0.644370	-0.631960
N7	-2.940331	-1.333750	-1.257674
H8	-3.782978	-0.876616	-1.567586
H9	-2.661650	-2.164837	-1.756052
N10	-0.740516	-1.086253	-0.630559
C11	0.170509	-0.416832	0.242939
C12	2.250048	-1.402774	-1.002809
H13	3.010459	-1.818333	-0.336494
H14	1.509446	-2.165290	-1.242823
H15	2.704373	-1.071743	-1.940958
C16	1.949570	0.945116	-0.289780
O17	3.102536	1.440165	-0.646097
N18	1.009695	1.763972	0.224010
H19	1.086766	2.773204	0.269296
H20	3.734331	0.774820	-0.950920
H21	-3.353369	0.784102	0.011915
C22	0.266076	-1.164649	1.626617
H23	1.008062	-0.655602	2.250855
H24	-0.711641	-1.013463	2.098336
N25	0.557305	-2.563850	1.576137
H26	1.524722	-2.802707	1.415295
H27	-0.058988	-3.092535	0.972976

Zero-point correction= 0.220364
Thermal correction to Energy= 0.234717
Thermal correction to Enthalpy= 0.235661
Thermal correction to Gibbs Free Energy= 0.179807
Sum of electronic and zero-point Energies= -752.280060
Sum of electronic and thermal Energies= -752.265707
Sum of electronic and thermal Enthalpies= -752.264763
Sum of electronic and thermal Free Energies= -752.320617

234 TS_C4-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-1.481994	0.295952	-0.554885
C2	0.104804	-1.084665	0.223184
C3	1.415974	-1.618784	0.317279
O4	1.762094	-2.747948	0.612976
N5	2.360490	-0.607544	-0.007671
C6	2.049569	0.599807	-0.597107
N7	3.092706	1.350341	-1.028443
H8	3.979688	0.924475	-1.245836
H9	2.857263	2.187826	-1.538437
N10	0.828982	1.059034	-0.713750
C11	-0.118427	0.258522	-0.121462
C12	-2.147408	1.447717	-1.143170
H13	-2.870346	1.885559	-0.449087
H14	-1.373023	2.180476	-1.368793
H15	-2.637232	1.167356	-2.079276
C16	-2.035601	-0.888172	-0.271347
O17	-3.292450	-1.239411	-0.412794
N18	-1.129738	-1.732750	0.211396
H19	-1.306046	-2.697114	0.462005
H20	-3.850638	-0.535766	-0.766886
H21	3.325520	-0.907752	0.056956

C22	-0.263596	1.222529	1.768349
H23	-1.017037	0.613307	2.262708
H24	0.766701	1.001875	2.034305
N25	-0.567384	2.545462	1.653299
H26	-1.514385	2.879385	1.712687
H27	0.129049	3.204056	1.344223

Zero-point correction= 0.216824
Thermal correction to Energy= 0.231993
Thermal correction to Enthalpy= 0.232937
Thermal correction to Gibbs Free Energy= 0.174916
Sum of electronic and zero-point Energies= -752.264769
Sum of electronic and thermal Energies= -752.249601
Sum of electronic and thermal Enthalpies= -752.248657
Sum of electronic and thermal Free Energies= -752.306678

235 C5-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-1.502183	-1.103724	0.167741
C2	-0.014159	0.714961	0.152192
C3	1.139677	0.927093	-0.813759
O4	1.195231	1.836796	-1.610799
N5	2.159374	0.006278	-0.637127
C6	2.001908	-1.223282	0.005635
N7	3.105383	-1.996925	0.100195
H8	4.030103	-1.606907	0.014311
H9	3.014569	-2.868452	0.599270
N10	0.837857	-1.647418	0.432148
C11	-0.153485	-0.754945	0.410168
C12	-2.072026	-2.431173	0.369092
H13	-2.471870	-2.826862	-0.568201
H14	-1.260755	-3.081454	0.694545
H15	-2.841901	-2.405294	1.143658
C16	-2.117421	-0.043582	-0.352582
O17	-3.366382	0.032801	-0.735130
N18	-1.315316	1.013547	-0.439619
H19	-1.562199	1.879120	-0.898975
H20	-3.835829	-0.810781	-0.693758
H21	2.977741	0.159947	-1.214874
C22	0.230389	1.565681	1.456019
H23	-0.536259	1.261761	2.175924
H24	1.196716	1.248641	1.864508
N25	0.202598	2.985756	1.300895
H26	-0.713850	3.390923	1.175206
H27	0.869460	3.371479	0.645595

Zero-point correction= 0.218987
Thermal correction to Energy= 0.234039
Thermal correction to Enthalpy= 0.234984
Thermal correction to Gibbs Free Energy= 0.177340
Sum of electronic and zero-point Energies= -752.289910
Sum of electronic and thermal Energies= -752.274858
Sum of electronic and thermal Enthalpies= -752.273914
Sum of electronic and thermal Free Energies= -752.331558

236 TS_C5-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-1.269744	-1.363746	0.062638
C2	-0.059808	0.524213	-0.190119
C3	1.144504	1.117258	-0.764558
O4	1.227316	2.161580	-1.374455
N5	2.273695	0.343341	-0.452075
C6	2.248011	-0.922404	0.107523
N7	3.437828	-1.520986	0.324604
H8	4.306116	-1.012354	0.312696
H9	3.427995	-2.428971	0.761813
N10	1.130573	-1.557742	0.377845
C11	0.028075	-0.842577	0.117143
C12	-1.641243	-2.747280	0.337501
H13	-2.022110	-3.228692	-0.566348
H14	-0.735694	-3.263451	0.654801
H15	-2.376560	-2.792156	1.144021
C16	-2.066753	-0.396072	-0.411508
O17	-3.364386	-0.456061	-0.605152
N18	-1.370424	0.708530	-0.683628
H19	-1.785332	1.635777	-0.742731
H20	-3.736938	-1.331122	-0.438985
H21	3.147348	0.725740	-0.793924
C22	-0.184902	1.861797	1.517541
H23	-0.607531	1.190922	2.260377
H24	0.866487	2.103152	1.649911
N25	-1.024594	2.877079	1.077927
H26	-1.857600	3.062106	1.618864
H27	-0.578263	3.719955	0.744056

Zero-point correction= 0.216516
Thermal correction to Energy= 0.231725
Thermal correction to Enthalpy= 0.232669
Thermal correction to Gibbs Free Energy= 0.174451
Sum of electronic and zero-point Energies= -752.268782
Sum of electronic and thermal Energies= -752.253574
Sum of electronic and thermal Enthalpies= -752.252630
Sum of electronic and thermal Free Energies= -752.310848

237 C6-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	2.140129	0.390854	-0.062878
C2	0.140972	-0.607546	-0.117766
C3	-1.315041	-0.689093	0.175464
O4	-1.162154	-0.914334	1.503484
N5	-1.835568	0.653811	-0.158162
H6	-2.851466	0.664609	-0.209524
C7	-1.125230	1.792937	-0.058764
N8	-1.768527	2.968119	-0.067194
H9	-2.770929	3.037961	-0.010959
H10	-1.216918	3.810998	-0.038983
N11	0.217098	1.832636	-0.007304
C12	0.764656	0.627429	-0.061912
C13	3.169875	1.427034	-0.010417
H14	3.128254	1.922108	0.960144
H15	4.143798	0.964136	-0.157820
H16	2.972008	2.151486	-0.799962
C17	2.329551	-0.933245	-0.079290
O18	3.536532	-1.447613	-0.098822
N19	1.152483	-1.567639	-0.115307
H20	1.016262	-2.567606	-0.085855
H21	3.555772	-2.410312	-0.037264
C22	-2.187209	-1.713775	-0.558211
H23	-2.046734	-1.583675	-1.635020
H24	-1.844165	-2.718709	-0.275069
N25	-3.579266	-1.441233	-0.229096
H26	-4.212311	-1.865349	-0.895902
H27	-3.818483	-1.788342	0.693873

Zero-point correction= 0.220150
Thermal correction to Energy= 0.234739
Thermal correction to Enthalpy= 0.235683
Thermal correction to Gibbs Free Energy= 0.179087
Sum of electronic and zero-point Energies= -752.254043
Sum of electronic and thermal Energies= -752.239454
Sum of electronic and thermal Enthalpies= -752.238509
Sum of electronic and thermal Free Energies= -752.295105

238 TS_C6-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	2.146518	0.412917	-0.139571

C2	0.179160	-0.577597	0.114456
C3	-1.280052	-0.713647	0.353701
O4	-1.625098	-1.391888	1.452366
N5	-1.812300	0.644872	0.273768
H6	-2.825494	0.657925	0.222418
C7	-1.106052	1.797044	0.095753
N8	-1.816028	2.946699	0.054088
H9	-2.749646	2.996956	0.427747
H10	-1.283516	3.801993	0.018751
N11	0.202491	1.858013	-0.067350
C12	0.769344	0.634666	-0.041590
C13	3.159327	1.452770	-0.306957
H14	3.361373	1.925146	0.655120
H15	4.067419	1.002676	-0.704729
H16	2.768580	2.194040	-1.002731
C17	2.363273	-0.897763	-0.008205
O18	3.581668	-1.398910	-0.036672
N19	1.197294	-1.534503	0.143436
H20	1.080494	-2.514416	0.357953
H21	3.606987	-2.362530	-0.015827
C22	-2.045228	-1.591893	-0.798205
H23	-1.607747	-1.215843	-1.726002
H24	-1.764808	-2.639152	-0.653179
N25	-3.445952	-1.323844	-0.761168
H26	-3.864866	-1.191745	-1.670943
H27	-3.984124	-1.979237	-0.210275

Zero-point correction= 0.218344
Thermal correction to Energy= 0.232833
Thermal correction to Enthalpy= 0.233777
Thermal correction to Gibbs Free Energy= 0.177441
Sum of electronic and zero-point Energies= -752.251038
Sum of electronic and thermal Energies= -752.236549
Sum of electronic and thermal Enthalpies= -752.235605
Sum of electronic and thermal Free Energies= -752.291941

239 O6-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-2.315522	-0.164634	0.099654
C2	-0.109620	-0.431610	-0.206705
C3	1.202500	-0.021231	-0.338223
O4	2.284737	-0.771026	-0.557213
N5	1.371479	1.392217	-0.246016
C6	0.306406	2.247493	-0.029969
N7	0.595091	3.568850	-0.040212
H8	1.524841	3.892547	0.174171
H9	-0.166354	4.195329	0.171598
N10	-0.930742	1.854271	0.150627
C11	-1.100530	0.514483	0.018127
C12	-3.614165	0.453830	0.344900
H13	-4.065371	0.040525	1.249550
H14	-3.437518	1.518824	0.491466
H15	-4.270791	0.318509	-0.517391
C16	-2.071026	-1.467005	-0.072695
O17	-2.921031	-2.474397	-0.056196
N18	-0.753832	-1.666716	-0.255685
H19	-0.336446	-2.565720	-0.447032
H20	-3.842794	-2.194202	-0.001335
H21	2.180877	1.763271	-0.728524
C22	3.136729	-1.038079	0.651207
H23	2.523083	-1.641237	1.325716
H24	3.350715	-0.066679	1.104142
N25	4.314639	-1.703187	0.316310
H26	4.194745	-2.639494	-0.043807
H27	4.965808	-1.171196	-0.243870

Zero-point correction= 0.218452
Thermal correction to Energy= 0.234108
Thermal correction to Enthalpy= 0.235053
Thermal correction to Gibbs Free Energy= 0.175043
Sum of electronic and zero-point Energies= -752.269091
Sum of electronic and thermal Energies= -752.253435
Sum of electronic and thermal Enthalpies= -752.252490
Sum of electronic and thermal Free Energies= -752.312500

240 TS_O6-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-2.320523	-0.273490	0.148441
C2	-0.134224	-0.400125	-0.279071
C3	1.177067	0.070738	-0.521795
O4	2.235840	-0.578335	-0.723982
N5	1.224094	1.498161	-0.347305
C6	0.143880	2.284174	-0.035211
N7	0.346657	3.619037	0.017421
H8	1.269730	4.012897	0.091196
H9	-0.430440	4.186836	0.316357
N10	-1.064962	1.814607	0.193828
C11	-1.147033	0.473713	0.035999
C12	-3.633699	0.262327	0.488037
H13	-4.004484	-0.192433	1.409329
H14	-3.506656	1.332967	0.645689
H15	-4.335760	0.107102	-0.334360
C16	-2.014452	-1.555583	-0.096074
O17	-2.811301	-2.605956	-0.069619
N18	-0.707422	-1.667565	-0.355251
H19	-0.241328	-2.528272	-0.604195
H20	-3.741979	-2.373276	0.034014
H21	2.067711	1.934484	-0.694522
C22	3.436518	-1.089602	0.874338
H23	2.743499	-1.817376	1.275732
H24	3.459936	-0.105033	1.323888
N25	4.590057	-1.558105	0.363023
H26	4.610652	-2.477002	-0.050784
H27	5.269155	-0.908935	-0.001974

Zero-point correction= 0.215196
Thermal correction to Energy= 0.231081
Thermal correction to Enthalpy= 0.232025
Thermal correction to Gibbs Free Energy= 0.171106
Sum of electronic and zero-point Energies= -752.256394
Sum of electronic and thermal Energies= -752.240510
Sum of electronic and thermal Enthalpies= -752.239565
Sum of electronic and thermal Free Energies= -752.300484

241 N7-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-0.463748	1.782791	-0.031887
C2	-0.030169	-0.413131	0.164967
C3	0.771262	-1.578580	0.192543
O4	0.447072	-2.754833	0.271083
N5	2.142807	-1.221991	0.103800
C6	2.618816	0.050676	-0.027845
N7	3.942605	0.230899	-0.106614
H8	4.607595	-0.522899	-0.053260
H9	4.285256	1.174437	-0.201726
N10	1.829221	1.117641	-0.089844
C11	0.530640	0.838221	0.010939
C12	-0.272692	3.210496	-0.236462
H13	-0.933296	3.761833	0.433954
H14	0.765161	3.444252	-0.003502
H15	-0.481450	3.479246	-1.275211
C16	-1.705853	1.157940	-0.077283
O17	-2.734090	1.699919	0.609430
N18	-1.473632	-0.282114	0.225662
H19	-1.830005	-0.479440	1.172181
H20	-3.449195	1.978870	0.026386
H21	2.774948	-2.013960	0.119193

C22	-2.293135	-1.283688	-0.742724
H23	-3.241457	-0.767586	-0.896042
H24	-1.685142	-1.266960	-1.648333
N25	-2.461596	-2.546234	-0.214087
H26	-3.211770	-2.702610	0.440434
H27	-1.627301	-3.104421	-0.072204

Zero-point correction= 0.220712
Thermal correction to Energy= 0.235406
Thermal correction to Enthalpy= 0.236350
Thermal correction to Gibbs Free Energy= 0.179387
Sum of electronic and zero-point Energies= -752.266899
Sum of electronic and thermal Energies= -752.252206
Sum of electronic and thermal Enthalpies= -752.251261
Sum of electronic and thermal Free Energies= -752.308224

242 TS_N7-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	0.040277	1.933942	0.057527
C2	0.116328	-0.268411	-0.261059
C3	-0.403247	-1.580039	-0.304761
O4	0.186552	-2.655593	-0.432061
N5	-1.809887	-1.564403	-0.175408
C6	-2.567261	-0.446390	0.056835
N7	-3.894097	-0.604963	0.193354
H8	-4.358605	-1.489403	0.074927
H9	-4.452723	0.220518	0.342417
N10	-2.052497	0.765415	0.163025
C11	-0.724495	0.808216	-0.011628
C12	-0.427916	3.279018	0.344782
H13	0.053011	3.981432	-0.337909
H14	-1.505639	3.299281	0.188123
H15	-0.207890	3.550107	1.380597
C16	1.375736	1.566177	-0.069482
O17	2.296844	2.372917	-0.629155
N18	1.446961	0.201463	-0.286856
H19	2.071144	-0.115058	-1.027481
H20	2.775999	2.886644	0.030607
H21	-2.238600	-2.481413	-0.209436
C22	2.691231	-1.435780	1.053576
H23	3.521956	-0.840976	1.412828
H24	1.759873	-1.453072	1.602584
N25	2.903900	-2.365607	0.143178
H26	3.809524	-2.499179	-0.281958
H27	2.099928	-2.895164	-0.198894

Zero-point correction= 0.216035
Thermal correction to Energy= 0.231385
Thermal correction to Enthalpy= 0.232329
Thermal correction to Gibbs Free Energy= 0.173624
Sum of electronic and zero-point Energies= -752.262664
Sum of electronic and thermal Energies= -752.247314
Sum of electronic and thermal Enthalpies= -752.246369
Sum of electronic and thermal Free Energies= -752.305074

243 C8-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	0.766902	1.148311	-0.066763
C2	-0.355282	-0.782069	-0.114214
C3	-1.532568	-1.603975	-0.099235
O4	-1.589238	-2.811777	-0.196823
N5	-2.693754	-0.807036	0.050644
C6	-2.700396	0.555864	0.158660
N7	-3.874572	1.173246	0.295306
H8	-4.757733	0.688886	0.314875
H9	-3.871697	2.179596	0.370751
N10	-1.598574	1.306701	0.135966
C11	-0.462595	0.634649	-0.001449
C12	1.100792	2.561322	-0.090195
H13	1.693056	2.779691	-0.981844
H14	0.171342	3.128415	-0.129036
H15	1.654797	2.843500	0.808444
C16	1.781230	0.088742	-0.255726
O17	2.367052	0.176594	-1.507578
N18	0.939125	-1.105996	-0.230105
H19	1.286980	-2.012427	-0.513392
H20	3.268464	0.512114	-1.451076
H21	-3.560243	-1.332377	0.072888
C22	2.809448	0.090718	0.907453
H23	3.379938	1.026209	0.835497
H24	2.242321	0.137336	1.841747
N25	3.711954	-1.017439	0.957148
H26	4.352136	-1.128195	0.184477
H27	3.316770	-1.897299	1.254739

Zero-point correction= 0.219508
Thermal correction to Energy= 0.234475
Thermal correction to Enthalpy= 0.235419
Thermal correction to Gibbs Free Energy= 0.177524
Sum of electronic and zero-point Energies= -752.315598
Sum of electronic and thermal Energies= -752.300631
Sum of electronic and thermal Enthalpies= -752.299687
Sum of electronic and thermal Free Energies= -752.357583

244 TS_C8-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	0.807454	-1.227696	0.349184
C2	-0.324201	0.677605	0.471438
C3	-1.450621	1.548298	0.360277
O4	-1.508712	2.746534	0.552614
N5	-2.586770	0.799258	-0.038585
C6	-2.609091	-0.547089	-0.302298
N7	-3.778138	-1.091337	-0.682138
H8	-4.644836	-0.580292	-0.689648
H9	-3.804459	-2.086884	-0.836105
N10	-1.539863	-1.318824	-0.217122
C11	-0.438588	-0.660841	0.173187
C12	1.154820	-2.622272	0.143507
H13	1.668577	-3.013999	1.024070
H14	0.225862	-3.172073	-0.003507
H15	1.779162	-2.740223	-0.747035
C16	1.702203	-0.210244	0.617633
O17	2.853953	-0.379046	1.278422
N18	0.990329	0.918048	0.835169
H19	1.391542	1.805802	1.099897
H20	3.425963	-1.024898	0.848665
H21	-3.428565	1.354261	-0.138899
C22	2.480453	0.212743	-1.467890
H23	3.180221	-0.611814	-1.580057
H24	1.508811	0.103080	-1.940871
N25	3.018257	1.458009	-1.477105
H26	4.003600	1.610254	-1.333876
H27	2.463455	2.265479	-1.711869

Zero-point correction= 0.216132
Thermal correction to Energy= 0.231754
Thermal correction to Enthalpy= 0.232698
Thermal correction to Gibbs Free Energy= 0.173324
Sum of electronic and zero-point Energies= -752.282331
Sum of electronic and thermal Energies= -752.266710
Sum of electronic and thermal Enthalpies= -752.265765
Sum of electronic and thermal Free Energies= -752.325139

245 N9-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	-1.353799	-0.485180	-0.310176

C2	0.314447	1.043408	0.041119
C3	1.670219	1.508291	0.189959
O4	2.054278	2.634493	0.415604
N5	2.569700	0.425759	0.032204
C6	2.226712	-0.879065	-0.211886
N7	3.213153	-1.785677	-0.320682
H8	4.188897	-1.540042	-0.300706
H9	2.961051	-2.736102	-0.541114
N10	0.968419	-1.269400	-0.327445
C11	0.091144	-0.267880	-0.190983
C12	-1.716642	-0.834938	-1.726479
H13	-1.443891	-0.003296	-2.375793
H14	-1.159608	-1.731485	-1.998034
H15	-2.790335	-1.008415	-1.780710
C16	-1.935894	0.846838	0.135004
O17	-3.089986	1.198867	-0.470233
N18	-0.881286	1.742180	0.083350
H19	-0.964405	2.707964	0.367493
H20	-3.839560	1.119741	0.130049
H21	3.544292	0.689838	0.124144
C22	-1.837030	-1.643287	0.659000
H23	-2.923211	-1.619826	0.549867
H24	-1.426015	-2.545315	0.204842
N25	-1.434767	-1.508402	1.979872
H26	-1.838322	-0.763370	2.526900
H27	-0.470903	-1.711734	2.195833

Zero-point correction= 0.219719
Thermal correction to Energy= 0.234444
Thermal correction to Enthalpy= 0.235388
Thermal correction to Gibbs Free Energy= 0.178814
Sum of electronic and zero-point Energies= -752.252335
Sum of electronic and thermal Energies= -752.237611
Sum of electronic and thermal Enthalpies= -752.236666
Sum of electronic and thermal Free Energies= -752.293241

246 TS_N9-CH_2NH_2[9MOG + H_{O8}]$^{\bullet+}$

N1	1.327111	0.442500	-0.429780
C2	-0.325140	-1.048984	-0.056397
C3	-1.672647	-1.485858	0.182248
O4	-2.066747	-2.596738	0.470501
N5	-2.563234	-0.393556	0.037901
C6	-2.210688	0.897210	-0.263017
N7	-3.195568	1.816296	-0.343389
H8	-4.167657	1.557508	-0.382725
H9	-2.941955	2.735266	-0.670724
N10	-0.957957	1.271276	-0.435607
C11	-0.076134	0.260178	-0.324110
C12	1.838224	1.266326	-1.545122
H13	1.664591	0.759790	-2.496964
H14	1.306317	2.217180	-1.529709
H15	2.907314	1.423706	-1.411474
C16	1.895263	-0.834690	-0.191768
O17	3.057124	-1.081183	-0.839049
N18	0.861152	-1.764970	-0.104196
H19	0.963035	-2.675940	0.319564
H20	3.626461	-1.672939	-0.336690
H21	-3.535803	-0.636864	0.186873
C22	1.731634	1.661769	1.267497
H23	2.769028	1.805363	0.988265
H24	0.997968	2.408047	0.983735
N25	1.481060	0.918481	2.335333
H26	2.181858	0.308770	2.728047
H27	0.554818	0.867593	2.732366

Zero-point correction= 0.216942
Thermal correction to Energy= 0.232145
Thermal correction to Enthalpy= 0.233089
Thermal correction to Gibbs Free Energy= 0.174572
Sum of electronic and zero-point Energies= -752.245585
Sum of electronic and thermal Energies= -752.230382
Sum of electronic and thermal Enthalpies= -752.229437
Sum of electronic and thermal Free Energies= -752.287955

247 [9MOG + H_{N9}]$^{+}$···$^{\bullet}CH_2NH_2$

N1	0.337403	2.001566	0.315661
C2	-0.028515	-0.201413	-0.073225
C3	0.314466	-1.585305	-0.258997
O4	-0.425340	-2.517051	-0.505698
N5	1.709531	-1.761681	-0.114439
H6	2.014917	-2.721215	-0.235654
C7	2.623297	-0.775947	0.158733
N8	3.916372	-1.115997	0.263397
H9	4.248577	-2.061519	0.169910
H10	4.582767	-0.389193	0.473201
N11	2.269344	0.490674	0.318599
C12	0.956213	0.683699	0.189801
C13	-1.219474	1.714117	0.098102
O14	-1.992086	2.617931	0.153972
N15	-1.290458	0.400329	-0.131027
H16	-2.191533	-0.155579	-0.298769
C17	-3.910869	-1.562480	0.839100
H18	-3.318482	-2.158495	1.519320
H19	-4.694357	-0.907168	1.193233
N20	-3.386669	-1.329962	-0.450934
H21	-4.100584	-1.079564	-1.128457
H22	-2.850046	-2.121857	-0.799319
C23	0.841370	3.033927	-0.646610
H24	0.444487	2.361622	1.270344
H25	0.248361	3.937002	-0.505720
H26	1.895716	3.209873	-0.438090
H27	0.712003	2.644970	-1.656413

Zero-point correction= 0.216030
Thermal correction to Energy= 0.231921
Thermal correction to Enthalpy= 0.232865
Thermal correction to Gibbs Free Energy= 0.171428
Sum of electronic and zero-point Energies= -752.263680
Sum of electronic and thermal Energies= -752.247790
Sum of electronic and thermal Enthalpies= -752.246846
Sum of electronic and thermal Free Energies= -752.308283

248 TS_[9MOG + H_{N9}]$^{+}$···$^{\bullet}CH_2NH_2$

C1	-0.526494	1.082677	0.179271
C2	-0.119134	-0.076819	-0.389094
C3	-2.119018	-1.042873	-0.382772
C4	-1.904489	1.253958	0.539931
C5	1.674497	1.428456	-0.245304
N6	-0.837885	-1.166362	-0.689619
O7	-2.438498	2.214143	1.051483
N8	1.297304	0.020474	-0.621003
N9	-2.957048	-2.066712	-0.629794
H10	-3.955854	-1.985373	-0.533757
H11	-2.591815	-2.856970	-1.137399
N12	1.847010	-2.408833	1.728879
H13	1.709442	-3.303835	1.284488
C14	2.658016	-1.456732	1.178894
H15	2.959248	-0.660987	1.859232
H16	3.443495	-1.835922	0.525771
H17	1.885394	-0.666341	0.209881
C18	1.819171	-0.433283	-1.935354
H19	1.598847	-1.495092	-2.038205
H20	1.333875	0.128054	-2.734385
H21	2.893383	-0.250702	-1.946595

O22	2.785896	1.851487	-0.391042
N23	0.551837	1.969759	0.288580
H24	0.498693	2.924171	0.616345
N25	-2.632166	0.083461	0.203215
H26	-3.618405	0.138482	0.431668
H27	1.285863	-2.215328	2.544181

Zero-point correction= 0.212625
Thermal correction to Energy= 0.227943
Thermal correction to Enthalpy= 0.228887
Thermal correction to Gibbs Free Energy= 0.168158
Sum of electronic and zero-point Energies= -752.272202
Sum of electronic and thermal Energies= -752.256884
Sum of electronic and thermal Enthalpies= -752.255940
Sum of electronic and thermal Free Energies= -752.316669

249 [9MOG + H_{N9}]$^{+}$

N1	1.507433	-0.937661	-0.283705
C2	0.098932	0.827886	-0.020177
C3	-1.161818	1.508190	0.123272
O4	-1.357907	2.692649	0.269250
N5	-2.219106	0.565334	0.070719
H6	-3.139213	0.981629	0.166246
C7	-2.087691	-0.788551	-0.092475
N8	-3.196047	-1.538797	-0.125334
H9	-4.123995	-1.155592	-0.048632
H10	-3.094317	-2.533838	-0.253165
N11	-0.902725	-1.375461	-0.216948
C12	0.108513	-0.511717	-0.171567
C13	1.954229	-1.926778	0.756063
H14	1.769026	-1.491166	1.737529
H15	1.372546	-2.837782	0.624275
H16	3.018823	-2.104204	0.607703
C17	2.332554	0.399519	-0.195856
O18	3.518640	0.384121	-0.263047
N19	1.399839	1.355122	-0.034384
H20	1.632717	2.335567	0.060306
H21	1.684472	-1.339814	-1.211884

Zero-point correction= 0.164586
Thermal correction to Energy= 0.175775
Thermal correction to Enthalpy= 0.176719
Thermal correction to Gibbs Free Energy= 0.127959
Sum of electronic and zero-point Energies= -657.108815
Sum of electronic and thermal Energies= -657.097627
Sum of electronic and thermal Enthalpies= -657.096683
Sum of electronic and thermal Free Energies= -657.145442

250 N1-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-2.117390	0.821664	0.487073
C2	-0.579586	-0.801897	-0.104618
C3	0.607287	-1.350191	-0.554845
O4	0.949708	-2.430813	-1.007626
N5	1.771928	-0.308742	-0.352038
H6	2.372173	-0.450093	-1.173111
C7	1.388493	1.123515	-0.302878
N8	2.361503	1.956875	-0.763549
H9	3.315403	1.734195	-0.499077
H10	2.120840	2.938366	-0.766353
N11	0.210292	1.501448	0.080973
C12	-0.700252	0.535910	0.257341
C13	-2.826242	-0.558343	0.300684
O14	-3.999210	-0.663552	0.488003
N15	-1.854537	-1.405027	-0.068605
H16	-2.039032	-2.384509	-0.238594
C17	2.607120	-0.746167	0.873796
H18	2.715706	-1.824334	0.741294
H19	1.969224	-0.538305	1.734632
N20	3.840747	-0.039767	0.909023
H21	4.652251	-0.612627	0.718766
H22	3.986243	0.503475	1.748860
C23	-2.718663	1.854448	-0.423230
H24	-3.783353	1.921640	-0.201055
H25	-2.210317	2.799481	-0.239545
H26	-2.556071	1.531741	-1.451218
H27	-2.303789	1.107075	1.454749

Zero-point correction= 0.221359
Thermal correction to Energy= 0.235549
Thermal correction to Enthalpy= 0.236494
Thermal correction to Gibbs Free Energy= 0.180212
Sum of electronic and zero-point Energies= -752.225579
Sum of electronic and thermal Energies= -752.211388
Sum of electronic and thermal Enthalpies= -752.210444
Sum of electronic and thermal Free Energies= -752.266726

251 TS_N1-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-2.271144	0.589348	0.475247
C2	-0.466655	-0.692929	-0.188313
C3	0.828608	-0.978413	-0.609992
O4	1.356316	-2.027489	-0.979559
N5	1.713162	0.199172	-0.433584
H6	2.416595	0.174907	-1.174379
C7	1.153582	1.494308	-0.213426
N8	2.080782	2.516781	-0.188804
H9	2.746362	2.548912	-0.951871
H10	1.662117	3.421865	-0.015950
N11	-0.085968	1.683201	0.159495
C12	-0.834276	0.585296	0.200224
C13	-2.708681	-0.898483	0.250352
O14	-3.841374	-1.225456	0.433490
N15	-1.596644	-1.535083	-0.141901
H16	-1.595201	-2.521721	-0.362026
C17	2.944249	-0.393290	1.040996
H18	2.131723	-0.869338	1.579531
H19	3.244245	0.599627	1.361765
N20	3.893479	-1.193007	0.558296
H21	3.661901	-2.140650	0.291399
H22	4.774755	-0.825892	0.233416
C23	-3.087605	1.521028	-0.372376
H24	-2.769636	2.538939	-0.152319
H25	-2.893218	1.282143	-1.417569
H26	-4.138536	1.366655	-0.128863
H27	-2.471645	0.800128	1.459392

Zero-point correction= 0.218769
Thermal correction to Energy= 0.233023
Thermal correction to Enthalpy= 0.233967
Thermal correction to Gibbs Free Energy= 0.177301
Sum of electronic and zero-point Energies= -752.220003
Sum of electronic and thermal Energies= -752.205749
Sum of electronic and thermal Enthalpies= -752.204805
Sum of electronic and thermal Free Energies= -752.261471

252 C2-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.966184	-0.995279	-0.427550
C2	-0.699893	0.878740	0.052152
C3	0.500931	1.726171	0.119382
O4	0.439036	2.937034	0.217114
N5	1.611854	0.960526	-0.058722
H6	2.521927	1.414948	-0.090198
C7	1.681935	-0.492016	0.101733
N8	1.803673	-0.784118	1.521560
H9	2.543844	-0.224137	1.934086

H10	2.002965	-1.767241	1.682934
N11	0.458480	-1.209276	-0.309692
C12	-0.584603	-0.482097	-0.239136
C13	-2.874771	0.245813	-0.211017
O14	-4.055947	0.173441	-0.287683
N15	-2.016138	1.266457	0.058471
H16	-2.331111	2.217772	0.223023
C17	2.848349	-0.988786	-0.779142
H18	2.586542	-0.815095	-1.826545
H19	2.936792	-2.072670	-0.632963
N20	4.046445	-0.238073	-0.444708
H21	4.626124	-0.057562	-1.254065
H22	4.619489	-0.702724	0.249084
H23	-2.103757	-1.303844	-1.397346
C24	-2.336848	-2.128018	0.491173
H25	-3.386758	-2.364607	0.322457
H26	-1.689067	-2.969592	0.251075
H27	-2.169202	-1.799542	1.516628

Zero-point correction= 0.220827
Thermal correction to Energy= 0.234920
Thermal correction to Enthalpy= 0.235864
Thermal correction to Gibbs Free Energy= 0.179719
Sum of electronic and zero-point Energies= -752.249673
Sum of electronic and thermal Energies= -752.235581
Sum of electronic and thermal Enthalpies= -752.234636
Sum of electronic and thermal Free Energies= -752.290782

253 TS_C2-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	1.906398	-0.992179	0.303881
C2	0.615299	0.859960	-0.054417
C3	-0.521948	1.613036	-0.532460
O4	-0.564124	2.814290	-0.719853
N5	-1.571396	0.743333	-0.819395
H6	-2.367697	1.158134	-1.287372
C7	-1.631031	-0.629227	-0.467489
N8	-2.605934	-1.331420	-1.178181
H9	-3.558629	-1.033682	-1.004107
H10	-2.496550	-2.334469	-1.107363
N11	-0.457449	-1.306293	-0.235833
C12	0.552911	-0.501323	-0.013598
C13	2.771432	0.306953	0.464069
O14	3.927322	0.234989	0.738842
N15	1.913683	1.312475	0.223032
H16	2.196604	2.284299	0.230628
C17	-2.302862	-0.537808	1.382504
H18	-1.500430	0.072536	1.797317
H19	-2.272200	-1.592450	1.641145
N20	-3.540693	0.029151	1.411726
H21	-3.653898	1.025955	1.509313
H22	-4.370500	-0.531954	1.517686
C23	2.489033	-1.913041	-0.729415
H24	3.513858	-2.139046	-0.436691
H25	1.871522	-2.809234	-0.764481
H26	2.465935	-1.398577	-1.689708
H27	1.917144	-1.472513	1.209949

Zero-point correction= 0.217945
Thermal correction to Energy= 0.232330
Thermal correction to Enthalpy= 0.233274
Thermal correction to Gibbs Free Energy= 0.176728
Sum of electronic and zero-point Energies= -752.235217
Sum of electronic and thermal Energies= -752.220832
Sum of electronic and thermal Enthalpies= -752.219887
Sum of electronic and thermal Free Energies= -752.276433

254 N2-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	1.860164	-1.111181	0.147893
C2	0.760770	0.900839	-0.029626
C3	-0.307905	1.802437	-0.305099
O4	-0.288652	3.018721	-0.261388
N5	-1.491084	1.094314	-0.663420
H6	-2.112086	1.680232	-1.211494
C7	-1.506600	-0.301438	-0.897381
N8	-2.838095	-0.915057	-0.697707
H9	-3.440704	-0.750381	-1.509032
H10	-2.653898	-1.921990	-0.652932
N11	-0.494946	-1.111641	-0.520018
C12	0.578833	-0.457923	-0.165880
C13	2.822101	0.070900	0.532200
O14	3.949125	-0.155645	0.855601
N15	2.081229	1.173786	0.380601
H16	2.454347	2.099660	0.543087
C17	-3.609830	-0.493749	0.589383
H18	-3.808607	0.569546	0.448505
H19	-4.546430	-1.053756	0.548829
N20	-2.839060	-0.782549	1.726406
H21	-2.420804	0.011921	2.186268
H22	-3.231384	-1.445783	2.376264
C23	2.438451	-1.934217	-0.962483
H24	1.743040	-2.744733	-1.175041
H25	2.548167	-1.291484	-1.835605
H26	3.407879	-2.309751	-0.636149
H27	1.774336	-1.702893	0.980619

Zero-point correction= 0.222037
Thermal correction to Energy= 0.236422
Thermal correction to Enthalpy= 0.237366
Thermal correction to Gibbs Free Energy= 0.179708
Sum of electronic and zero-point Energies= -752.218022
Sum of electronic and thermal Energies= -752.203637
Sum of electronic and thermal Enthalpies= -752.202693
Sum of electronic and thermal Free Energies= -752.260351

255 TS_N2-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	1.872499	-1.129303	0.190207
C2	0.783130	0.897470	0.031063
C3	-0.252429	1.804613	-0.313971
O4	-0.217649	3.022045	-0.345320
N5	-1.452251	1.098194	-0.639329
H6	-2.119502	1.676759	-1.136039
C7	-1.508442	-0.297900	-0.763237
N8	-2.776775	-0.849196	-0.961192
H9	-3.319452	-0.409383	-1.702066
H10	-2.686287	-1.843513	-1.158156
N11	-0.499552	-1.109339	-0.444009
C12	0.590249	-0.468120	-0.085921
C13	2.860153	0.052498	0.512542
O14	3.995911	-0.182375	0.800902
N15	2.125631	1.159819	0.370880
H16	2.514480	2.082712	0.511210
C17	-3.868540	-0.670460	0.744170
H18	-4.403107	0.226048	0.452667
H19	-4.403815	-1.609682	0.665986
N20	-2.988736	-0.548101	1.742877
H21	-2.596654	0.349906	1.980693
H22	-2.605320	-1.356017	2.205994
C23	2.402699	-1.981136	-0.922840
H24	3.381762	-2.356709	-0.626169
H25	1.694822	-2.791463	-1.090379
H26	2.482160	-1.358974	-1.813887
H27	1.828185	-1.703354	1.038618

Zero-point correction= 0.217966
Thermal correction to Energy= 0.232671
Thermal correction to Enthalpy= 0.233615
Thermal correction to Gibbs Free Energy= 0.175205
Sum of electronic and zero-point Energies= -752.215237
Sum of electronic and thermal Energies= -752.200532
Sum of electronic and thermal Enthalpies= -752.199588
Sum of electronic and thermal Free Energies= -752.257998

256 N3-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	1.270324	-1.292916	0.069976
C2	0.848151	0.891148	-0.487562
C3	0.224582	2.081226	-0.081054
O4	0.680713	3.203946	0.046036
N5	-1.178051	1.853949	0.205149
H6	-1.708149	2.699052	0.379766
C7	-1.791181	0.662157	0.256743
N8	-3.097605	0.584556	0.551291
H9	-3.611260	1.441227	0.696381
H10	-3.595927	-0.189573	0.107418
N11	-1.098892	-0.469826	0.006968
C12	0.229114	-0.379660	-0.515239
C13	1.230088	-1.534147	1.553850
H14	1.190435	-0.565098	2.052305
H15	0.344954	-2.120381	1.798146
H16	2.133787	-2.075084	1.835817
C17	2.606602	-0.557521	-0.274718
O18	3.640666	-1.153696	-0.259992
N19	2.241378	0.708242	-0.498748
H20	2.914948	1.432637	-0.711041
H21	1.325876	-2.189997	-0.415400
C22	-1.793995	-1.769840	-0.052462
H23	-1.028088	-2.500318	-0.333006
H24	-2.154342	-2.016583	0.951213
N25	-2.928225	-1.733607	-0.948479
H26	-2.648180	-1.680340	-1.923000
H27	-3.517757	-2.550514	-0.827404

Zero-point correction= 0.222303
Thermal correction to Energy= 0.236156
Thermal correction to Enthalpy= 0.237101
Thermal correction to Gibbs Free Energy= 0.181755
Sum of electronic and zero-point Energies= -752.238669
Sum of electronic and thermal Energies= -752.224815
Sum of electronic and thermal Enthalpies= -752.223871
Sum of electronic and thermal Free Energies= -752.279216

257 TS_N3-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	1.455447	-1.257683	0.195004
C2	0.806421	0.876897	-0.397657
C3	0.061918	2.045257	-0.188732
O4	0.341251	3.222695	-0.361244
N5	-1.248262	1.698293	0.348280
H6	-1.796778	2.511320	0.603112
C7	-1.667757	0.456744	0.667805
N8	-2.901489	0.300015	1.194400
H9	-3.443428	1.095068	1.495029
H10	-3.103974	-0.584698	1.632144
N11	-0.944199	-0.643516	0.421634
C12	0.301200	-0.384523	-0.080937
C13	1.688576	-1.590190	1.643985
H14	1.777196	-0.650795	2.189783
H15	0.830134	-2.155929	2.002846
H16	2.609017	-2.169323	1.719880
C17	2.671998	-0.449887	-0.364412
O18	3.745186	-0.968376	-0.455533
N19	2.189449	0.772218	-0.621829
H20	2.776693	1.517164	-0.972396
H21	1.437486	-2.133433	-0.333004
C22	-2.047943	-1.542115	-1.204005
H23	-1.624567	-0.779691	-1.848821
H24	-1.483813	-2.450276	-1.043216
N25	-3.373756	-1.637596	-1.136647
H26	-3.971038	-0.879543	-1.428988
H27	-3.825227	-2.449623	-0.744346

Zero-point correction= 0.217435
Thermal correction to Energy= 0.232302
Thermal correction to Enthalpy= 0.233246
Thermal correction to Gibbs Free Energy= 0.174678
Sum of electronic and zero-point Energies= -752.214155
Sum of electronic and thermal Energies= -752.199288
Sum of electronic and thermal Enthalpies= -752.198344
Sum of electronic and thermal Free Energies= -752.256912

258 C4-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.550735	-0.960915	-0.242577
C2	-0.202590	0.889718	0.136706
C3	0.965791	1.657743	-0.194435
O4	1.001152	2.871203	-0.283929
N5	2.063939	0.833272	-0.435509
H6	2.945856	1.304911	-0.587751
C7	1.957663	-0.543882	-0.577517
N8	3.067807	-1.166224	-1.024248
H9	3.820931	-0.668325	-1.469808
H10	3.022323	-2.165510	-1.147682
N11	0.896368	-1.244615	-0.301480
C12	-0.161698	-0.582883	0.354212
C13	-1.533641	-1.421926	-1.669229
H14	-1.093211	-0.636231	-2.282936
H15	-0.919016	-2.317754	-1.723160
H16	-2.563365	-1.615309	-1.968837
C17	-2.395743	0.304377	-0.116230
O18	-3.583752	0.286306	-0.189673
N19	-1.501739	1.318437	0.039345
H20	-1.785695	2.292269	0.012076
H21	-1.998737	-1.687097	0.324020
C22	-0.223640	-0.960873	1.860351
H23	-1.094871	-0.482596	2.324005
H24	-0.361439	-2.051843	1.914847
N25	0.982260	-0.485710	2.492184
H26	0.830040	-0.162901	3.438322
H27	1.715835	-1.183042	2.498571

Zero-point correction= 0.221132
Thermal correction to Energy= 0.235458
Thermal correction to Enthalpy= 0.236402
Thermal correction to Gibbs Free Energy= 0.180278
Sum of electronic and zero-point Energies= -752.278430
Sum of electronic and thermal Energies= -752.264105
Sum of electronic and thermal Enthalpies= -752.263161
Sum of electronic and thermal Free Energies= -752.319284

259 TS_C4-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.576816	0.949478	0.199044
C2	-0.210493	-0.880308	0.206488
C3	0.989627	-1.611262	0.433304
O4	1.138130	-2.816826	0.507985
N5	2.078848	-0.714571	0.589951
H6	2.968981	-1.168585	0.755971
C7	1.985150	0.655199	0.582767
N8	3.123226	1.356506	0.788661
H9	3.931295	0.930994	1.214293

H10	3.027105	2.355752	0.886217
N11	0.859092	1.298672	0.364212
C12	-0.177173	0.486851	0.051427
C13	-1.868521	1.595896	1.525746
H14	-1.592047	0.893284	2.311580
H15	-1.265117	2.499295	1.596581
H16	-2.934737	1.818175	1.561676
C17	-2.423565	-0.349570	0.034141
O18	-3.608144	-0.292531	-0.093437
N19	-1.527083	-1.349149	0.100066
H20	-1.798297	-2.323195	0.063480
H21	-1.861286	1.593314	-0.543047
C22	-0.123296	0.721322	-2.274426
H23	-0.981782	0.122359	-2.567223
H24	-0.228359	1.802632	-2.263408
N25	1.092360	0.245026	-2.627545
H26	1.216166	-0.704878	-2.938443
H27	1.900429	0.845210	-2.651479

Zero-point correction= 0.217065
Thermal correction to Energy= 0.232086
Thermal correction to Enthalpy= 0.233031
Thermal correction to Gibbs Free Energy= 0.174944
Sum of electronic and zero-point Energies= -752.246581
Sum of electronic and thermal Energies= -752.231559
Sum of electronic and thermal Enthalpies= -752.230615
Sum of electronic and thermal Free Energies= -752.288702

260 C5-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.673147	0.874599	0.572733
C2	-0.080815	-0.867138	0.069707
C3	1.017705	-0.923196	-0.985584
O4	1.087607	-1.801773	-1.810756
N5	1.969218	0.079805	-0.878048
H6	2.741493	0.006856	-1.530791
C7	1.788493	1.242495	-0.141895
N8	2.805432	2.117972	-0.112117
H9	3.703116	1.932700	-0.528686
H10	2.680981	2.975945	0.403057
N11	0.661055	1.515099	0.476243
C12	-0.241934	0.539086	0.556751
C13	-2.356052	-0.267172	-0.235051
O14	-3.520666	-0.215925	-0.480886
N15	-1.386412	-1.146112	-0.508982
H16	-1.592584	-1.994500	-1.021973
C17	0.244683	-1.902837	1.209145
H18	-0.599301	-1.865302	1.908398
H19	0.247243	-2.897304	0.751100
N20	1.468340	-1.705027	1.916835
H21	1.558806	-0.832244	2.417221
H22	2.313678	-1.962255	1.428774
H23	-2.059906	0.809830	1.521858
C24	-2.047258	2.220250	0.028403
H25	-3.134707	2.284664	0.029072
H26	-1.598451	2.980247	0.664477
H27	-1.656231	2.299677	-0.984868

Zero-point correction= 0.220203
Thermal correction to Energy= 0.234841
Thermal correction to Enthalpy= 0.235785
Thermal correction to Gibbs Free Energy= 0.178328
Sum of electronic and zero-point Energies= -752.273977
Sum of electronic and thermal Energies= -752.259339
Sum of electronic and thermal Enthalpies= -752.258395
Sum of electronic and thermal Free Energies= -752.315852

261 TS_C5-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-1.199460	-1.551697	-0.400082
C2	-0.153528	0.424374	0.177089
C3	0.972300	1.078811	0.824004
O4	0.938010	2.063682	1.531841
N5	2.182161	0.451130	0.478839
H6	3.003775	0.886076	0.882191
C7	2.296136	-0.754964	-0.188226
N8	3.539172	-1.228215	-0.406881
H9	4.365099	-0.671084	-0.265198
H10	3.629164	-2.091466	-0.919096
N11	1.247107	-1.447658	-0.570866
C12	0.078577	-0.847953	-0.303175
C13	-2.230822	-0.546467	0.203294
O14	-3.392285	-0.814428	0.226553
N15	-1.501841	0.508974	0.597498
H16	-1.935601	1.388496	0.854131
C17	-0.307311	2.165552	-1.371548
H18	0.753169	2.387405	-1.430308
H19	-0.740456	1.609666	-2.196831
N20	-1.115722	3.088836	-0.768293
H21	-0.695678	3.835201	-0.234562
H22	-2.031190	3.282772	-1.144608
C23	-1.244368	-2.877871	0.302429
H24	-2.253716	-3.276238	0.204141
H25	-0.507703	-3.528643	-0.165885
H26	-0.993546	-2.711933	1.349603
H27	-1.484941	-1.702767	-1.375442

Zero-point correction= 0.216854
Thermal correction to Energy= 0.231976
Thermal correction to Enthalpy= 0.232920
Thermal correction to Gibbs Free Energy= 0.174443
Sum of electronic and zero-point Energies= -752.244650
Sum of electronic and thermal Energies= -752.229529
Sum of electronic and thermal Enthalpies= -752.228585
Sum of electronic and thermal Free Energies= -752.287062

262 C6-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-2.192142	0.561447	-0.286042
C2	-0.206062	-0.584911	-0.189855
C3	1.222694	-0.709739	0.197093
O4	0.909121	-0.785051	1.508745
N5	1.856264	0.568377	-0.206034
H6	2.873175	0.505871	-0.193626
C7	1.219798	1.748380	-0.202922
N8	1.916516	2.889384	-0.237606
H9	2.919991	2.912709	-0.157006
H10	1.411367	3.759627	-0.297418
N11	-0.128344	1.852986	-0.222023
C12	-0.727810	0.680027	-0.251094
C13	-2.458521	-0.968330	-0.310394
O14	-3.564394	-1.402217	-0.373021
N15	-1.233345	-1.531706	-0.253779
H16	-1.120774	-2.534337	-0.196476
C17	2.088508	-1.844694	-0.358062
H18	1.676631	-2.793263	0.011239
H19	2.027692	-1.834389	-1.450353
N20	3.467908	-1.594748	0.037951
H21	3.627472	-1.853704	1.006154
H22	4.120038	-2.116924	-0.534538
C23	-2.879716	1.213526	0.884722
H24	-2.675993	2.281654	0.831443
H25	-3.945107	1.000152	0.807188
H26	-2.457686	0.789529	1.795756
H27	-2.575959	0.955499	-1.152336

Zero-point correction= 0.220930
Thermal correction to Energy= 0.235008
Thermal correction to Enthalpy= 0.235952
Thermal correction to Gibbs Free Energy= 0.180277
Sum of electronic and zero-point Energies= -752.225705
Sum of electronic and thermal Energies= -752.211628
Sum of electronic and thermal Enthalpies= -752.210683
Sum of electronic and thermal Free Energies= -752.266358

263 TS_C6-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	2.187405	0.487727	-0.424644
C2	0.228883	-0.547128	0.069483
C3	-1.211903	-0.687686	0.414943
O4	-1.471396	-1.270343	1.575804
N5	-1.796455	0.641994	0.233837
H6	-2.809760	0.628693	0.276805
C7	-1.136982	1.799046	-0.042205
N8	-1.866754	2.931828	-0.105067
H9	-2.794740	2.985696	0.281360
H10	-1.365361	3.794622	-0.246818
N11	0.162664	1.865194	-0.285014
C12	0.740806	0.652926	-0.216611
C13	2.447319	-1.029967	-0.196602
O14	3.545438	-1.486586	-0.270889
N15	1.231709	-1.541879	0.071882
H16	1.122536	-2.491314	0.400291
C17	-2.010802	-1.704318	-0.628924
H18	-1.599554	-1.423364	-1.601215
H19	-1.709739	-2.721731	-0.371028
N20	-3.404645	-1.452594	-0.573458
H21	-3.849610	-1.313283	-1.468870
H22	-3.934646	-2.082723	0.012389
C23	3.045714	1.332646	0.471261
H24	4.087694	1.089470	0.267106
H25	2.822753	2.376165	0.254856
H26	2.788543	1.097254	1.503639
H27	2.433885	0.696940	-1.398671

Zero-point correction= 0.218963
Thermal correction to Energy= 0.233008
Thermal correction to Enthalpy= 0.233952
Thermal correction to Gibbs Free Energy= 0.178397
Sum of electronic and zero-point Energies= -752.221490
Sum of electronic and thermal Energies= -752.207445
Sum of electronic and thermal Enthalpies= -752.206501
Sum of electronic and thermal Free Energies= -752.262056

264 O6-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	2.413539	-0.175238	-0.353682
C2	0.135562	-0.435661	-0.014156
C3	-1.125657	0.000362	0.239527
O4	-2.174288	-0.735970	0.599353
N5	-1.307582	1.404201	0.123785
H6	-2.099327	1.772226	0.636749
C7	-0.231835	2.259214	-0.089063
N8	-0.495267	3.583735	0.011551
H9	-1.428560	3.931488	-0.143495
H10	0.260257	4.206389	-0.232294
N11	0.980549	1.842984	-0.345010
C12	1.117153	0.495899	-0.366340
C13	2.059459	-1.671360	-0.148106
O14	2.903464	-2.511567	-0.177056
N15	0.726086	-1.706129	0.056430
H16	0.249020	-2.572110	0.263321
C17	-3.231998	-0.935271	-0.464004
H18	-2.723512	-1.429874	-1.295567
H19	-3.565079	0.061957	-0.760749
N20	-4.293085	-1.695781	0.006592
H21	-4.088233	-2.661847	0.216980
H22	-4.868976	-1.264040	0.714874
C23	3.378711	0.295958	0.702927
H24	3.582239	1.348662	0.513381
H25	2.899753	0.172932	1.673994
H26	4.282523	-0.308727	0.633575
H27	2.888432	-0.108014	-1.261521

Zero-point correction= 0.220041
Thermal correction to Energy= 0.234915
Thermal correction to Enthalpy= 0.235859
Thermal correction to Gibbs Free Energy= 0.177088
Sum of electronic and zero-point Energies= -752.247638
Sum of electronic and thermal Energies= -752.232763
Sum of electronic and thermal Enthalpies= -752.231819
Sum of electronic and thermal Free Energies= -752.290590

265 TS_O6-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-2.419502	-0.340538	0.407785
C2	-0.196786	-0.398771	-0.139771
C3	1.080180	0.115022	-0.452854
O4	2.113007	-0.494281	-0.771577
N5	1.092102	1.541752	-0.289790
H6	1.925362	1.994010	-0.642050
C7	0.006197	2.302344	0.075262
N8	0.171505	3.641390	0.120962
H9	1.083998	4.065757	0.128082
H10	-0.604240	4.189731	0.457865
N11	-1.171165	1.785960	0.358564
C12	-1.200533	0.444639	0.222636
C13	-1.974262	-1.810158	0.132039
O14	-2.751426	-2.710149	0.213749
N15	-0.668930	-1.722982	-0.180102
H16	-0.126698	-2.528806	-0.457881
C17	3.750464	-1.022255	0.776655
H18	3.104683	-1.788712	1.179152
H19	3.772086	-0.041065	1.229369
N20	4.794706	-1.399593	0.027120
H21	4.805365	-2.305985	-0.412941
H22	5.425133	-0.713918	-0.356471
C23	-3.573655	0.052501	-0.471408
H24	-4.399098	-0.629936	-0.271331
H25	-3.832767	1.083068	-0.233478
H26	-3.247538	-0.026465	-1.508104
H27	-2.739574	-0.304092	1.383286

Zero-point correction= 0.214641
Thermal correction to Energy= 0.230507
Thermal correction to Enthalpy= 0.231451
Thermal correction to Gibbs Free Energy= 0.169713
Sum of electronic and zero-point Energies= -752.231592
Sum of electronic and thermal Energies= -752.215726
Sum of electronic and thermal Enthalpies= -752.214782
Sum of electronic and thermal Free Energies= -752.276521

266 N7-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-0.358351	1.896149	-0.218898
C2	-0.069644	-0.364482	0.213923
C3	0.687620	-1.580703	0.331718
O4	0.267326	-2.697253	0.563355
N5	2.063845	-1.337980	0.129661
H6	2.648178	-2.163596	0.207756
C7	2.608509	-0.122509	-0.174677
N8	3.929836	-0.035760	-0.351462
H9	4.553269	-0.822140	-0.265407

H10	4.319246	0.866736	-0.578767
N11	1.869339	0.975146	-0.305831
C12	0.567338	0.789775	-0.107099
C13	0.043242	3.136867	0.500408
H14	0.177506	2.891777	1.553436
H15	0.969966	3.517826	0.072725
H16	-0.766508	3.857140	0.386768
C17	-1.794495	1.325852	0.379527
O18	-2.791445	1.724432	-0.183277
N19	-1.491982	-0.260120	0.350176
H20	-0.517008	2.123413	-1.207211
H21	-1.796727	-0.617888	1.259982
C22	-2.334065	-1.075447	-0.722496
H23	-3.172336	-0.413001	-0.942259
H24	-1.659011	-1.139424	-1.578533
N25	-2.750991	-2.320066	-0.272042
H26	-3.597404	-2.378536	0.271227
H27	-2.049115	-3.017448	-0.069389

Zero-point correction= 0.220774
Thermal correction to Energy= 0.235301
Thermal correction to Enthalpy= 0.236245
Thermal correction to Gibbs Free Energy= 0.179207
Sum of electronic and zero-point Energies= -752.236265
Sum of electronic and thermal Energies= -752.221738
Sum of electronic and thermal Enthalpies= -752.220794
Sum of electronic and thermal Free Energies= -752.277832

267 TS_N7-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	0.111040	1.966067	0.288410
C2	0.094185	-0.248406	-0.277063
C3	-0.472729	-1.556553	-0.419159
O4	0.107089	-2.600169	-0.674565
N5	-1.864353	-1.523139	-0.199080
H6	-2.321769	-2.422486	-0.300602
C7	-2.582452	-0.416149	0.172694
N8	-3.903092	-0.548289	0.363006
H9	-4.399498	-1.411121	0.213979
H10	-4.426671	0.271072	0.629532
N11	-2.014040	0.765489	0.358689
C12	-0.701296	0.772320	0.123285
C13	-0.406500	3.201407	-0.368498
H14	-0.557674	2.984766	-1.425407
H15	-1.344488	3.489221	0.104799
H16	0.354393	3.972452	-0.249176
C17	1.537954	1.535726	-0.312676
O18	2.513727	2.209912	-0.033178
N19	1.453854	0.115219	-0.371668
H20	0.239842	2.167000	1.289085
H21	1.966239	-0.284214	-1.155573
C22	2.599340	-1.295752	1.004089
H23	3.299908	-0.542707	1.342242
H24	1.705497	-1.489824	1.582073
N25	3.037544	-2.256701	0.194303
H26	3.955754	-2.216960	-0.221241
H27	2.404256	-2.981229	-0.119445

Zero-point correction= 0.216960
Thermal correction to Energy= 0.231941
Thermal correction to Enthalpy= 0.232885
Thermal correction to Gibbs Free Energy= 0.174553
Sum of electronic and zero-point Energies= -752.223842
Sum of electronic and thermal Energies= -752.208862
Sum of electronic and thermal Enthalpies= -752.207917
Sum of electronic and thermal Free Energies= -752.266249

268 C8-$\dot{C}H_2NH_2$···[9MOG + H_{N9}]$^+$

N1	-0.806516	1.397645	-0.024702
C2	0.243935	-0.570531	0.486853
C3	1.361119	-1.481066	0.563267
O4	1.366790	-2.617761	0.983803
N5	2.536460	-0.861846	0.075867
H6	3.356578	-1.456853	0.112593
C7	2.619530	0.401720	-0.447028
N8	3.810427	0.827349	-0.899587
H9	4.651454	0.278274	-0.838667
H10	3.870758	1.764999	-1.264033
N11	1.570454	1.202645	-0.525003
C12	0.447397	0.659873	-0.037766
C13	-0.840441	2.521401	0.957178
H14	-0.598348	2.120405	1.940965
H15	-0.105876	3.268429	0.656812
H16	-1.850121	2.930824	0.964250
C17	-1.921356	0.220907	0.390296
O18	-2.960891	0.589117	0.895714
N19	-1.087659	-0.828331	0.808965
H20	-1.016248	1.767599	-0.953719
H21	-1.343487	-1.325041	1.652970
C22	-2.402459	-0.340488	-1.482850
H23	-2.927018	0.564154	-1.781151
H24	-1.407212	-0.500800	-1.897425
N25	-3.170082	-1.443407	-1.403714
H26	-4.148477	-1.362768	-1.166818
H27	-2.747124	-2.349345	-1.264391

Zero-point correction= 0.218167
Thermal correction to Energy= 0.233581
Thermal correction to Enthalpy= 0.234525
Thermal correction to Gibbs Free Energy= 0.175822
Sum of electronic and zero-point Energies= -752.249750
Sum of electronic and thermal Energies= -752.234336
Sum of electronic and thermal Enthalpies= -752.233392
Sum of electronic and thermal Free Energies= -752.292095

269 TS_C8-$\dot{C}H_2NH_2$···[9MOG + H_{N9}]$^{\bullet+}$

N1	0.819310	1.401320	0.019076
C2	-0.241656	-0.542426	-0.535503
C3	-1.351314	-1.458588	-0.619295
O4	-1.353111	-2.584373	-1.069426
N5	-2.520042	-0.860993	-0.092550
H6	-3.337410	-1.459686	-0.131717
C7	-2.602007	0.386835	0.469806
N8	-3.788680	0.790364	0.953259
H9	-4.628459	0.240554	0.882054
H10	-3.849919	1.716637	1.345633
N11	-1.556176	1.190972	0.556470
C12	-0.440132	0.666593	0.036320
C13	0.831998	2.559372	-0.928589
H14	0.570644	2.188814	-1.919430
H15	0.100866	3.291815	-0.587497
H16	1.840620	2.971266	-0.938830
C17	1.907217	0.269984	-0.441586
O18	2.986799	0.626433	-0.848374
N19	1.084909	-0.753515	-0.891828
H20	1.054617	1.740525	0.953856
H21	1.391594	-1.394565	-1.609106
C22	2.352604	-0.428372	1.571671
H23	2.886207	0.467307	1.878054
H24	1.353118	-0.591965	1.970010
N25	3.109422	-1.531482	1.417332
H26	4.083728	-1.448589	1.167068
H27	2.683434	-2.435643	1.283045

Zero-point correction= 0.217133
Thermal correction to Energy= 0.232280
Thermal correction to Enthalpy= 0.233224
Thermal correction to Gibbs Free Energy= 0.174867
Sum of electronic and zero-point Energies= -752.250641
Sum of electronic and thermal Energies= -752.235494
Sum of electronic and thermal Enthalpies= -752.234549
Sum of electronic and thermal Free Energies= -752.292907

N20	5.198403	0.551968	0.520525
H21	5.831710	-0.191748	0.272633
H22	5.351576	1.438967	0.067459
C23	0.556973	-2.458039	-0.932073
H24	1.586873	-2.810082	-0.980688
H25	-0.104974	-3.206914	-0.498608
H26	0.208474	-2.165269	-1.921730
H27	0.843602	-1.530979	0.882765

270 O8-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	-0.577426	-1.260874	-0.010511
C2	0.515922	0.738000	0.131084
C3	1.659706	1.617681	0.156975
O4	1.675388	2.812529	0.354043
N5	2.845981	0.880735	-0.077371
H6	3.685380	1.449272	-0.072215
C7	2.927983	-0.471284	-0.290786
N8	4.139648	-1.009678	-0.505960
H9	4.984551	-0.464938	-0.549100
H10	4.195526	-2.001912	-0.672675
N11	1.860128	-1.251131	-0.283805
C12	0.728053	-0.579264	-0.057611
C13	-1.538248	-0.173853	0.392602
O14	-2.716545	-0.398050	-0.185834
N15	-0.841124	1.050466	0.253299
H16	-1.090007	1.815793	0.870293
C17	-3.755903	0.684778	-0.042046
H18	-3.888413	0.821677	1.033516
H19	-3.316763	1.571343	-0.505186
N20	-4.945587	0.333636	-0.657886
H21	-4.942505	0.299002	-1.666305
H22	-5.472750	-0.415202	-0.234158
C23	-0.617782	-2.457859	0.892468
H24	-0.375072	-2.124118	1.900121
H25	-1.625186	-2.870107	0.854547
H26	0.119653	-3.175155	0.534055
H27	-0.834880	-1.572757	-0.959044

Zero-point correction= 0.215510
Thermal correction to Energy= 0.231162
Thermal correction to Enthalpy= 0.232107
Thermal correction to Gibbs Free Energy= 0.171169
Sum of electronic and zero-point Energies= -752.231336
Sum of electronic and thermal Energies= -752.215684
Sum of electronic and thermal Enthalpies= -752.214740
Sum of electronic and thermal Free Energies= -752.275677

Zero-point correction= 0.221180
Thermal correction to Energy= 0.235774
Thermal correction to Enthalpy= 0.236719
Thermal correction to Gibbs Free Energy= 0.178898
Sum of electronic and zero-point Energies= -752.239352
Sum of electronic and thermal Energies= -752.224757
Sum of electronic and thermal Enthalpies= -752.223813
Sum of electronic and thermal Free Energies= -752.281634

271 TS_O8-CH_2NH_2[9MOG + H_{N9}]$^{\bullet+}$

N1	0.533078	-1.243275	-0.057729
C2	-0.580853	0.741005	-0.218566
C3	-1.726313	1.615651	-0.198156
O4	-1.758471	2.806151	-0.424810
N5	-2.892048	0.883810	0.128855
H6	-3.733126	1.448939	0.155709
C7	-2.952663	-0.460863	0.395302
N8	-4.149228	-0.993655	0.700565
H9	-4.995259	-0.452275	0.756444
H10	-4.192309	-1.980657	0.897907
N11	-1.884120	-1.235387	0.357228
C12	-0.766538	-0.571880	0.036852
C13	1.488004	-0.131948	-0.564144
O14	2.699809	-0.316145	-0.576655
N15	0.758786	1.049477	-0.444710
H16	1.022281	1.854927	-0.997158
C17	4.038399	0.287117	1.128734
H18	3.412665	1.120376	1.419443
H19	3.941621	-0.662162	1.636701