

## Supporting Information

### **Mass Spectrometry and Computational Study of Collision-Induced Dissociation of 9-Methylguanine–1-Methylcytosine Base-Pair Radical Cation: Intra-Base-Pair Proton Transfer and Hydrogen Transfer, Non-Statistical Dissociation, and Reaction with a Water Ligand**

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**Table S1** Relative formation enthalpies ( $\Delta H$  at 298K, eV, with respect to the global minimum) of various  $[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}$  conformers calculated at different levels of theory

Species	$\omega\text{B97XD}/$ 6-311++G(d,p)	$\omega\text{B97XD}/$ aug-cc-pVQZ	B3LYP/ aug-cc-pVQZ)	RI-MP2/ aug-cc-pVTZ	DLPNO-CCSD(T), aug-cc-pVTZ
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_1$	0.00	0.00	0.00	0.00	0.00
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_2$	0.02	0.01	0.01	0.02	0.00
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_3$	0.03	0.02	0.00	0.02	0.01
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_4$	0.06	0.05	0.05	0.02	0.05
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_5$	0.11	0.15	0.09	0.06	0.08
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_6$	0.12	0.11	0.11	0.13	0.13
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_7$	0.12	0.11	0.11	0.12	0.11
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_8$	0.15	0.13	0.11	0.13	0.13
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_9$	0.15	0.14	0.14	0.11	0.16
$[9\text{MG}\cdot 1\text{MC}]^{\bullet+}\cdot\text{H}_2\text{O}_{10}$	0.16	0.12	0.12	0.09	0.10

**Cartesian coordinates for the structures in  
Fig. 1, optimized at  $\omega$ B97XD/6-311++G(d,p).**

**[9MG-1MC]<sup>+</sup>\_1**

C1	-1.365950	1.195888	-0.005293
C2	-2.803296	0.937272	-0.005509
H3	0.419358	0.130655	-0.001767
C4	-1.157263	-1.245680	0.001186
C5	-4.905552	0.968177	-0.007972
N6	-0.628935	0.008223	-0.002505
N7	-3.839375	1.770576	-0.010401
N8	-4.606343	-0.354378	-0.003045
N9	-2.500717	-1.502297	0.003772
C10	-3.234317	-0.425620	0.000041
N11	-0.345040	-2.272025	0.002444
H12	-0.763276	-3.190207	0.005678
H13	0.697124	-2.154113	-0.001228
O14	-0.828690	2.277390	-0.006670
H15	-5.928101	1.320331	-0.011256
C16	2.865681	-0.785518	-0.002900
N17	2.177218	0.380547	0.001100
C18	2.819487	1.551205	0.006547
C19	4.910760	0.435420	0.004526
N20	4.256301	-0.753335	-0.001662
H21	5.992266	0.383412	0.005516
O22	2.305813	-1.887731	-0.007714
N23	2.091984	2.668829	0.009578
H24	1.076845	2.624089	0.004875
H25	2.538287	3.569210	0.012815
C26	4.246490	1.611508	0.009118
H27	4.776660	2.552562	0.014090
C28	4.971756	-2.029261	-0.007895
H29	4.700857	-2.610901	0.872607
H30	4.708791	-2.597928	-0.899274
H31	6.041808	-1.828740	-0.001616
C32	-5.523738	-1.487592	0.017846
H33	-5.269316	-2.173370	-0.789194
H34	-5.451279	-2.003966	0.974785
H35	-6.537017	-1.116091	-0.124083

**[9MG-1MC]<sup>+</sup>\_2**

C1	-1.304438	1.070771	-0.010918
C2	-2.758177	0.907309	-0.009447
H3	1.146649	0.183507	-0.006003
C4	-1.201824	-1.282788	-0.000185
C5	-4.858625	1.047315	-0.008110
N6	-0.586390	-0.096022	-0.006918
N7	-3.755093	1.794062	-0.015002
N8	-4.628847	-0.289752	0.000343
N9	-2.566034	-1.526305	0.006611
C10	-3.259079	-0.427856	0.001105
N11	-0.460683	-2.383928	0.000743
H12	-0.927882	-3.275632	0.005935
H13	0.555818	-2.327965	-0.006803
O14	-0.761005	2.172064	-0.014371

H15	-5.862289	1.450081	-0.010692
C16	2.931004	-0.837579	-0.006383
N17	2.196549	0.330224	-0.001636
C18	2.724454	1.577571	0.008907
C19	4.872425	0.551279	0.013834
N20	4.308552	-0.684358	0.002482
H21	5.955016	0.573633	0.019693
O22	2.408018	-1.931549	-0.017398
N23	1.912184	2.608832	0.010378
H24	0.877763	2.484414	0.000903
H25	2.295699	3.539911	0.018033
C26	4.143670	1.690448	0.017829
H27	4.621992	2.658087	0.027440
C28	5.113032	-1.910562	-0.008062
H29	4.858389	-2.524391	0.854862
H30	4.913065	-2.474778	-0.918328
H31	6.164978	-1.635315	0.032687
C32	-5.600129	-1.373344	0.028098
H33	-5.384056	-2.075285	-0.776588
H34	-5.551994	-1.891758	0.985819
H35	-6.594795	-0.953284	-0.111804

**[9MG-1MC]<sup>+</sup>\_3**

C1	-1.853630	1.348962	-0.007886
C2	-3.252808	0.921385	-0.068313
H3	0.014800	0.410990	0.156610
C4	-1.383606	-1.066836	0.142744
C5	-5.341856	0.707974	-0.185679
N6	-1.001263	0.233344	0.105047
N7	-4.374676	1.626492	-0.173788
N8	-4.896365	-0.570232	-0.093301
N9	-2.684706	-1.473001	0.086459
C10	-3.528837	-0.483314	-0.012945
N11	-0.452330	-1.989707	0.238340
H12	-0.738382	-2.955564	0.266664
H13	0.536674	-1.702207	0.273766
O14	-1.420807	2.467189	-0.045182
H15	-6.395729	0.937444	-0.264378
C16	2.850078	-0.116419	0.122164
N17	3.679158	-1.161523	0.010121
C18	4.980405	-0.958933	-0.146253
C19	4.685069	1.385274	-0.085007
N20	3.351985	1.181887	0.078111
H21	5.011356	2.417142	-0.113344
O22	1.619565	-0.256668	0.268476
N23	5.762852	-2.042851	-0.251528
H24	5.338760	-2.954210	-0.201532
H25	6.757919	-1.970161	-0.366547
C26	5.546231	0.351131	-0.203722
H27	6.605405	0.519111	-0.334276
C28	2.419671	2.299385	0.217334
H29	1.687247	2.287613	-0.589996
H30	1.897164	2.233223	1.171603
H31	2.979976	3.231789	0.177668
C32	-5.679184	-1.799629	-0.067468
H33	-5.337735	-2.465285	-0.859328

H34 -5.563130 -2.289865 0.898775  
 H35 -6.726196 -1.548939 -0.228086

**[9MG-1MC]\*\_4**

C1 3.480935 -1.914016 -0.063895  
 C2 4.024152 -0.559746 0.005215  
 H3 1.625702 -2.781687 -0.151869  
 C4 1.273319 -0.750818 -0.079735  
 C5 5.172637 1.198315 0.102487  
 N6 2.060692 -1.869329 -0.099737  
 N7 5.281329 -0.130419 0.054148  
 N8 3.895203 1.652360 0.084544  
 N9 1.799295 0.505317 -0.016555  
 C10 3.101475 0.533140 0.022159  
 N11 -0.026489 -0.857781 -0.120015  
 H12 -0.669236 -0.013336 -0.111423  
 H13 -0.490830 -1.753325 -0.156551  
 O14 4.066470 -2.956508 -0.090197  
 H15 6.015626 1.874038 0.149619  
 C16 -2.975002 0.521866 -0.053309  
 N17 -3.157031 -0.816476 0.026202  
 C18 -4.383956 -1.310509 0.106543  
 C19 -5.335710 0.852221 0.022984  
 N20 -4.084627 1.367452 -0.057080  
 H21 -6.148578 1.567415 0.015456  
 O22 -1.854103 1.043102 -0.124543  
 N23 -4.517723 -2.645422 0.187778  
 H24 -3.696343 -3.224462 0.195336  
 H25 -5.420083 -3.081055 0.255629  
 C26 -5.545248 -0.480219 0.108072  
 H27 -6.543923 -0.886526 0.174302  
 C28 -3.848590 2.806780 -0.154021  
 H29 -3.218988 3.134596 0.672343  
 H30 -3.343346 3.037762 -1.091524  
 H31 -4.807418 3.321166 -0.114945  
 C32 3.422580 3.030036 0.147539  
 H33 2.709451 3.202830 -0.657320  
 H34 2.939615 3.210943 1.107606  
 H35 4.275322 3.696668 0.032018

**[9MG-1MC]\*\_5**

C1 -2.110429 1.497216 -0.004488  
 C2 -3.359569 0.797113 -0.000090  
 C3 -1.055481 -0.551577 -0.004354  
 C4 -5.338368 0.093132 0.003432  
 N5 -1.001116 0.822244 -0.006015  
 N6 -4.627519 1.220616 0.001051  
 N7 -4.591583 -1.036644 0.003123  
 N8 -2.191463 -1.332033 -0.000564  
 C9 -3.278261 -0.619502 0.001586  
 N10 0.091933 -1.170695 -0.006677  
 H11 0.107915 -2.183105 -0.005901  
 H12 1.026890 -0.624207 -0.008189  
 O13 -2.047539 2.810747 -0.006931  
 H14 -6.419222 0.058722 0.004481  
 C15 3.376546 -0.973677 -0.005247

N16 2.474777 0.055517 -0.004839  
 C17 2.856826 1.325075 0.001287  
 C18 5.129290 0.658074 0.012768  
 N19 4.739950 -0.637726 0.007834  
 H20 6.198206 0.833491 0.019953  
 O21 3.030698 -2.140993 -0.015568  
 N22 1.898794 2.263579 -0.000428  
 H23 0.926056 1.982381 -0.005543  
 H24 2.131085 3.240459 0.003330  
 C25 4.238489 1.678674 0.009776  
 H26 4.568132 2.707112 0.015103  
 C27 5.700170 -1.739101 0.001473  
 H28 5.506517 -2.400711 0.844984  
 H29 5.601745 -2.313204 -0.919951  
 H30 6.705755 -1.328074 0.076400  
 C31 -5.049934 -2.421602 0.012183  
 H32 -4.612237 -2.951906 -0.832647  
 H33 -4.749962 -2.901943 0.943032  
 H34 -6.135055 -2.430011 -0.073420  
 H35 -2.933171 3.196000 -0.005995

**[9MG-1MC]\*\_6**

C1 3.301529 -1.829420 0.072011  
 C2 3.966013 -0.559742 -0.017367  
 C3 1.287188 -0.707702 0.121949  
 C4 5.192899 1.140133 -0.153884  
 N5 2.002472 -1.875790 0.137922  
 N6 5.245934 -0.190721 -0.098559  
 N7 3.941050 1.654657 -0.113480  
 N8 1.799791 0.566116 0.043004  
 C9 3.096236 0.570905 -0.022113  
 N10 -0.014491 -0.804432 0.187361  
 H11 -0.670614 0.023937 0.175013  
 H12 -0.429928 -1.724362 0.236463  
 O13 4.022845 -2.921099 0.085000  
 H14 6.065247 1.775408 -0.225878  
 C15 -3.000306 0.533764 0.069535  
 N16 -3.154653 -0.807271 -0.020101  
 C17 -4.368080 -1.326124 -0.127766  
 C18 -5.366494 0.815871 -0.055091  
 N19 -4.128390 1.356599 0.052867  
 H20 -6.194091 1.514078 -0.061482  
 O21 -1.892611 1.076200 0.167501  
 N22 -4.470239 -2.663618 -0.217657  
 H23 -3.634570 -3.222253 -0.208936  
 H24 -5.360733 -3.119519 -0.304353  
 C25 -5.546861 -0.520285 -0.149561  
 H26 -6.535360 -0.946743 -0.237974  
 C27 -3.923788 2.799542 0.160256  
 H28 -3.445117 3.037142 1.110018  
 H29 -3.280854 3.142730 -0.649477  
 H30 -4.891252 3.295510 0.099720  
 C31 3.534562 3.053934 -0.140339  
 H32 2.800797 3.201095 -0.931918  
 H33 3.095633 3.329037 0.818431  
 H34 4.412360 3.667680 -0.334722

H35 3.438893 -3.688581 0.149809

**[9MG-1MC]\*\_7**

C1 3.260226 -1.834918 -0.072933  
 C2 3.930720 -0.568825 0.004350  
 C3 1.272654 -0.682606 -0.101069  
 C4 5.209697 1.094120 0.121424  
 N5 1.963643 -1.863076 -0.121754  
 N6 5.224382 -0.237791 0.066076  
 N7 3.970739 1.639447 0.096681  
 N8 1.796563 0.591306 -0.028505  
 C9 3.093867 0.577757 0.020763  
 N10 -0.031008 -0.762982 -0.155489  
 H11 -0.683968 0.069442 -0.143715  
 H12 -0.452342 -1.681341 -0.201371  
 O13 3.923460 -2.967902 -0.093915  
 H14 6.099037 1.706541 0.179354  
 C15 -3.013324 0.544162 -0.060086  
 N16 -3.145831 -0.799097 0.024275  
 C17 -4.351274 -1.339458 0.117650  
 C18 -5.384638 0.785989 0.039506  
 N19 -4.154709 1.347951 -0.054065  
 H20 -6.224017 1.470025 0.038738  
 O21 -1.913321 1.105504 -0.144186  
 N22 -4.430803 -2.678332 0.203062  
 H23 -3.585532 -3.222747 0.200887  
 H24 -5.314060 -3.150140 0.278255  
 C25 -5.543557 -0.553238 0.128962  
 H26 -6.525711 -0.996231 0.205946  
 C27 -3.973265 2.794344 -0.155647  
 H28 -3.348237 3.146867 0.664059  
 H29 -3.485146 3.042127 -1.097955  
 H30 -4.949708 3.273902 -0.108292  
 C31 3.602378 3.048687 0.159078  
 H32 2.950636 3.289196 -0.679912  
 H33 3.082528 3.251462 1.095118  
 H34 4.509193 3.648402 0.103521  
 H35 4.874482 -2.806376 -0.053774

**[9MG-1MC]\*\_8**

C1 -1.345460 1.149371 -0.011194  
 C2 -2.753520 0.880061 -0.007149  
 H3 0.401547 0.070178 -0.007973  
 C4 -1.179819 -1.308869 0.000625  
 C5 -4.947144 0.947630 -0.005158  
 N6 -0.631402 -0.045747 -0.007009  
 N7 -3.858335 1.703549 -0.010955  
 N8 -4.594750 -0.343544 0.001811  
 N9 -2.493243 -1.535169 0.006402  
 C10 -3.208384 -0.417336 0.001573  
 N11 -0.336226 -2.331957 0.002686  
 H12 -0.732060 -3.256836 0.007910  
 H13 0.682696 -2.203226 -0.005445  
 O14 -0.812114 2.241908 -0.017133  
 H15 -5.961401 1.312576 -0.006592  
 C16 2.948096 -0.748121 -0.007290

N17 2.246635 0.415152 -0.002278  
 C18 2.881933 1.596085 0.009852  
 C19 4.995492 0.511439 0.012621  
 N20 4.352547 -0.674771 -0.000029  
 H21 6.077629 0.471582 0.017920  
 O22 2.420245 -1.856413 -0.017985  
 N23 2.192079 2.760384 0.014452  
 H24 1.181712 2.564231 0.003178  
 C25 4.299699 1.681519 0.018488  
 H26 4.788385 2.643780 0.029105  
 C27 5.081230 -1.942589 -0.008072  
 H28 4.795946 -2.531265 0.863385  
 H29 4.823317 -2.504838 -0.905303  
 H30 6.149559 -1.735946 0.011492  
 C31 -5.484960 -1.500858 0.024392  
 H32 -5.211645 -2.170537 -0.789389  
 H33 -5.374467 -2.021155 0.975002  
 H34 -6.511600 -1.161569 -0.100455  
 H35 -3.838781 2.713800 -0.019566

**[9MG-1MC]\*\_9**

C1 1.436218 1.091794 -0.005214  
 C2 2.805151 0.902845 -0.003108  
 H3 -0.353645 0.056906 -0.006310  
 C4 1.215193 -1.315973 -0.004353  
 C5 4.905935 1.001477 -0.000550  
 N6 0.676521 -0.042033 -0.005891  
 N7 3.869366 1.778626 -0.002444  
 N8 4.602397 -0.351545 -0.002317  
 N9 2.512558 -1.540454 -0.001269  
 C10 3.250661 -0.429720 -0.001542  
 N11 0.350804 -2.335141 -0.005539  
 H12 0.741779 -3.261909 -0.003422  
 H13 -0.660899 -2.217667 -0.007707  
 O14 0.879804 2.264632 -0.006291  
 H15 5.934461 1.335129 -0.000517  
 C16 -2.978489 -0.807487 -0.003166  
 N17 -2.206762 0.311914 -0.003044  
 C18 -2.757753 1.526000 0.002423  
 C19 -4.939385 0.597293 0.008500  
 N20 -4.386443 -0.624137 0.002914  
 H21 -6.021743 0.640798 0.013033  
 O22 -2.530852 -1.939074 -0.008016  
 N23 -1.865415 2.546700 0.001848  
 H24 -0.110193 2.278489 -0.004361  
 H25 -2.323451 3.458962 0.005980  
 C26 -4.161864 1.724902 0.008474  
 H27 -4.607411 2.709198 0.013059  
 C28 -5.200395 -1.841156 0.002355  
 H29 -4.967173 -2.427178 -0.886424  
 H30 -4.955769 -2.435651 0.882365  
 H31 -6.252984 -1.565819 0.010483  
 C32 5.528539 -1.472215 0.019959  
 H33 5.502522 -1.965788 0.992046  
 H34 5.256068 -2.187131 -0.755730  
 H35 6.532775 -1.096866 -0.170524

**[9MG-1MC]\*+\_10**

C1	1.554485	1.208902	-0.035658
C2	1.950941	-0.159021	-0.030019
H3	2.451745	3.040160	0.025055
C4	3.990090	1.649964	0.019430
C5	2.098426	-2.278007	-0.024353
N6	2.676427	2.055097	-0.008886
N7	1.207229	-1.320904	-0.045684
N8	3.385166	-1.816718	0.003381
N9	4.348959	0.392923	0.021482
C10	3.303608	-0.454920	0.002655
N11	4.931938	2.617303	0.080537
H12	5.890063	2.316850	0.011536
H13	4.725585	3.574085	-0.146880
O14	0.430688	1.695281	-0.055362
H15	1.882496	-3.336632	-0.029443
C16	-4.860739	-0.583578	0.028783
N17	-3.846781	-1.461187	0.011280
C18	-2.595575	-1.055570	-0.019981
C19	-3.264744	1.289192	-0.025911
N20	-4.514526	0.889487	0.004847
H21	-3.059159	2.354213	-0.039485
O22	-6.034994	-0.811574	0.061935
N23	-1.607736	-1.935703	-0.035230
H24	-1.862274	-2.913237	-0.021236
H25	-0.607556	-1.661814	-0.049802
C26	-2.229840	0.353354	-0.040170
H27	-1.191309	0.695280	-0.062781
C28	-5.635263	1.823901	0.030410
H29	-6.305083	1.594926	-0.797705
H30	-6.186409	1.688019	0.961343
H31	-5.254925	2.840631	-0.047314
C32	4.611312	-2.597487	0.051489
H33	5.289953	-2.259122	-0.730659
H34	5.093524	-2.479120	1.022079
H35	4.366852	-3.646367	-0.109442

**[9MG-1MC]\*+\_11**

C1	-1.819400	-1.256553	-0.097166
C2	-1.879203	0.161950	-0.056248
H3	-3.116073	-2.829245	-0.057967
C4	-4.285390	-1.116984	0.004751
C5	-1.514626	2.247375	-0.000755
N6	-3.104114	-1.818207	-0.063667
N7	-0.877420	1.109717	-0.068270
N8	-2.877859	2.107747	0.053528
N9	-4.338731	0.188882	0.046502
C10	-3.124104	0.767840	0.019514
N11	-5.426024	-1.838898	0.062049
H12	-6.289240	-1.322817	0.024522
H13	-5.452210	-2.812122	-0.186733
O14	-0.843701	-1.999652	-0.150248
H15	-1.055739	3.225473	0.011788
C16	4.865854	-0.471721	0.101805
N17	4.008013	-1.499753	0.137834
C18	2.709605	-1.309791	0.041642

C19	2.988059	1.104707	-0.153730
N20	4.284239	0.919861	-0.067125
H21	2.613004	2.116398	-0.264975
O22	6.058778	-0.495300	0.185025
N23	1.878562	-2.336414	0.075676
H24	2.273332	-3.261118	0.172201
H25	0.861154	-2.212312	-0.005532
C26	2.118808	0.014766	-0.103395
H27	1.042449	0.190568	-0.158129
C28	5.238838	2.021754	-0.111980
H29	5.797962	2.042703	0.823764
H30	5.944514	1.845171	-0.923481
H31	4.702936	2.957113	-0.261922
C32	-3.879330	3.157024	0.153169
H33	-4.623312	3.030100	-0.632718
H34	-4.372015	3.114932	1.124837
H35	-3.388686	4.122036	0.034810

**[9MG-1MC]\*+\_12**

C1	-1.429485	1.055106	-0.142094
C2	-2.788321	0.882416	-0.135706
H3	0.379101	0.094521	0.026784
C4	-1.201474	-1.309038	0.149109
C5	-4.882590	1.015368	-0.158764
N6	-0.655628	-0.042903	0.002318
N7	-3.833121	1.772721	-0.252871
N8	-4.600087	-0.330329	0.019588
N9	-2.509520	-1.527225	0.170311
C10	-3.247593	-0.434390	0.032023
N11	-0.349021	-2.318216	0.278788
H12	-0.745064	-3.239962	0.358749
H13	0.661687	-2.200010	0.149310
O14	-0.791632	2.202602	-0.272209
H15	-5.905421	1.362791	-0.205609
C16	2.906372	-0.746105	-0.057050
N17	2.235034	0.422901	0.104724
C18	2.908793	1.578808	0.225267
C19	4.989429	0.457251	-0.007738
N20	4.314944	-0.700485	-0.125927
H21	6.068966	0.396127	-0.067788
O22	2.357407	-1.837864	-0.151864
N23	2.257352	2.750769	0.398040
H24	1.249709	2.571473	0.379043
C25	4.324619	1.634353	0.177927
H26	4.837894	2.578225	0.281305
C27	5.004812	-1.976059	-0.322836
H28	4.777834	-2.642928	0.508591
H29	4.650675	-2.438590	-1.243500
H30	6.075881	-1.793163	-0.380053
C31	-5.551496	-1.427526	0.125962
H32	-5.690198	-1.906692	-0.843846
H33	-5.171875	-2.156930	0.839966
H34	-6.502689	-1.035269	0.482544
H35	-1.430765	2.920780	-0.374318

**[9MG-1MC]\*+\_13**

C1	-1.247585	1.030379	0.099525
C2	-2.668195	0.843594	0.075058
H3	1.105403	0.171991	0.038332
C4	-1.169148	-1.335489	-0.045474
C5	-4.859782	1.011620	0.039556
N6	-0.538984	-0.133369	0.035899
N7	-3.736793	1.714092	0.107756
N8	-4.564802	-0.292352	-0.039247
N9	-2.496785	-1.556007	-0.079627
C10	-3.181059	-0.426990	-0.018473
N11	-0.389054	-2.427192	-0.108052
H12	-0.837695	-3.325979	-0.119923
H13	0.613097	-2.358386	0.000808
O14	-0.721343	2.151024	0.168563
H15	-5.856206	1.421618	0.045792
C16	2.933274	-0.792072	0.075510
N17	2.179716	0.344484	0.016479
C18	2.700020	1.610617	-0.098207
C19	4.884885	0.619283	-0.094176
N20	4.341767	-0.595284	0.019208
H21	5.966593	0.665835	-0.134409
O22	2.491891	-1.911498	0.170375
N23	1.959309	2.708935	-0.145844
H24	0.940564	2.504951	-0.024710
C25	4.102477	1.748549	-0.161228
H26	4.530379	2.735019	-0.257343
C27	5.158435	-1.810464	0.089537
H28	4.979854	-2.308970	1.041906
H29	4.869230	-2.483472	-0.716649
H30	6.206496	-1.534599	-0.003516
C31	-5.503583	-1.404170	-0.122453
H32	-5.242390	-2.022304	-0.980205
H33	-5.438387	-2.002613	0.785680
H34	-6.511968	-1.011008	-0.239919
H35	-3.668410	2.719422	0.171619

C19	5.083795	0.312261	-0.002409
N20	4.320559	-0.850133	0.000222
H21	6.153718	0.152617	0.010516
O22	2.262444	-1.801019	0.020541
N23	2.536477	2.837700	-0.062077
H24	1.520971	2.767172	-0.072095
C25	4.543831	1.534418	-0.022111
H26	5.157158	2.422794	-0.027697
C27	4.943605	-2.170742	0.046949
H28	4.774705	-2.642940	1.015890
H29	4.529562	-2.806781	-0.734188
H30	6.013017	-2.050717	-0.115650
C31	-5.612974	-1.540918	-0.048443
H32	-5.524315	-2.047301	-1.009159
H33	-5.361961	-2.230442	0.756372
H34	-6.630200	-1.177387	0.084771
H35	-1.663876	3.006300	0.065598

**[9MG-1MC]\*+\_14**

C1	-1.496841	1.121270	0.033277
C2	-2.912020	0.896551	0.022546
H3	1.394723	0.479690	-0.016933
C4	-1.215615	-1.164240	-0.005619
C5	-5.011771	0.915987	0.015213
N6	-0.691018	0.100690	0.017962
N7	-3.952664	1.729754	0.034788
N8	-4.701728	-0.400823	-0.007967
N9	-2.550272	-1.505758	-0.020085
C10	-3.324910	-0.463596	-0.005084
N11	-0.359063	-2.152908	-0.014705
H12	-0.726623	-3.094787	-0.032019
H13	0.685831	-1.979260	-0.001202
O14	-0.978116	2.325427	0.057557
H15	-6.037211	1.259771	0.018600
C16	2.960655	-0.778454	0.000167
N17	2.410975	0.466675	-0.025310
C18	3.100083	1.699066	-0.039050

**Cartesian coordinates for the structures in  
Fig. 2, optimized at  $\omega$ B97XD/6-311++G(d,p).**

**[9MG-1MC]<sup>+</sup>·H<sub>2</sub>O\_1**

C1	-1.423314	0.956761	-0.010473
C2	-2.887691	0.976361	-0.011079
H3	0.910837	-0.246105	-0.003764
C4	-1.616751	-1.391930	0.006405
C5	-4.954844	1.377191	-0.014277
N6	-0.859026	-0.292893	-0.002182
N7	-3.767622	1.980720	-0.020764
N8	-4.893093	0.021845	-0.002284
N9	-3.002249	-1.462748	0.011200
C10	-3.551147	-0.285773	0.001672
N11	-1.020198	-2.577964	0.011629
H12	-1.596330	-3.403203	0.017856
H13	-0.003930	-2.649709	0.005638
O14	-0.745064	1.978844	-0.015931
H15	-5.901659	1.899689	-0.019901
C16	2.539011	-1.497739	-0.005272
N17	1.966988	-0.243439	-0.003333
C18	2.656980	0.925054	0.001017
C19	4.649556	-0.378925	0.000675
N20	3.922299	-1.531187	-0.004337
H21	5.724788	-0.506074	0.001870
O22	1.873307	-2.513540	-0.007668
N23	2.006519	2.060465	0.002216
H24	0.971508	2.081541	-0.003299
H25	2.544065	2.926577	0.006526
C26	4.082083	0.845540	0.003921
H27	4.670624	1.751102	0.007777
C28	4.555988	-2.852447	-0.008081
H29	4.254214	-3.410801	0.877403
H30	4.254112	-3.405565	-0.896799
H31	5.635724	-2.717077	-0.007792
C32	-5.990557	-0.932615	0.026150
H33	-5.859772	-1.660896	-0.773610
H34	-6.011827	-1.448235	0.986437
H35	-6.926207	-0.395519	-0.120982
O36	3.916792	4.221266	0.021211
H37	4.074275	4.785872	-0.738805
H38	4.068094	4.773377	0.791597

**[9MG-1MC]<sup>+</sup>·H<sub>2</sub>O\_2**

C1	-1.470661	1.105521	-0.022523
C2	-2.930352	1.041765	-0.014695
H3	0.160772	-0.192843	-0.017587
C4	-1.590996	-1.340729	-0.001599
C5	-5.009463	1.355911	-0.004405
N6	-0.898731	-0.169839	-0.015580
N7	-3.845779	2.007366	-0.019201
N8	-4.890817	0.004945	0.008182
N9	-2.958336	-1.414928	0.010347
C10	-3.540452	-0.249773	0.003271
N11	-0.926618	-2.467711	0.001161

H12	-1.467944	-3.318997	0.012274
H13	0.126036	-2.495060	-0.008602
O14	-0.795974	2.106587	-0.032271
H15	-5.975727	1.841379	-0.003688
C16	2.440720	-1.459381	-0.010215
N17	1.918255	-0.211514	-0.011207
C18	2.718275	0.862726	-0.001532
C19	4.635837	-0.533714	0.012223
N20	3.819945	-1.622373	0.002625
H21	5.699188	-0.737327	0.021436
O22	1.733567	-2.476755	-0.019467
N23	2.170647	2.072750	-0.003236
H24	1.161328	2.176242	-0.014758
H25	2.767813	2.893660	0.004976
C26	4.142399	0.721259	0.010840
H27	4.785080	1.589768	0.018768
C28	4.351139	-2.984355	0.002676
H29	3.975738	-3.529130	0.868180
H30	4.040961	-3.506935	-0.901901
H31	5.437970	-2.933032	0.043602
C32	-5.951168	-0.994292	0.044875
H33	-5.799890	-1.713010	-0.759559
H34	-5.939803	-1.511078	1.004336
H35	-6.907414	-0.491986	-0.090130
O36	4.250043	4.128032	0.029797
H37	4.479243	4.668919	-0.728596
H38	4.463928	4.656015	0.801640

**[9MG-1MC]<sup>+</sup>·H<sub>2</sub>O\_3**

C1	1.206944	-1.561888	-0.005430
O2	0.609932	-2.613091	-0.007532
N3	0.390870	1.960960	0.002197
C4	3.164179	-0.053285	0.000841
H5	0.840236	2.882496	0.002740
C6	2.656163	-1.387347	-0.005609
H7	-0.508378	-0.400018	-0.001685
N8	0.541782	-0.335808	-0.001808
N9	3.643217	-2.280622	-0.011024
N10	2.498405	1.065587	0.004895
N11	4.531257	-0.204658	-0.002252
C12	4.753145	-1.542332	-0.007937
H13	5.753347	-1.953393	-0.011513
C14	1.139023	0.892797	0.001649
H15	-0.648377	1.885840	-0.000823
H16	-4.989206	-2.628460	0.011497
C17	-4.416406	-1.712663	0.007665
C18	-2.924009	0.618824	-0.001944
C19	-2.987328	-1.717726	0.004653
C20	-5.025667	-0.507351	0.005186
N21	-4.316902	0.649806	0.000378
N22	-2.291708	-0.579200	0.000360
N23	-2.312231	-2.867972	0.006166
H24	-6.103683	-0.405499	0.006936
O25	-2.314189	1.692199	-0.006002
H26	-1.295495	-2.867569	0.001826
H27	-2.799176	-3.746863	0.008615



O28 1.405171 4.618427 -0.007315  
 H29 1.394037 5.200559 -0.769008  
 H30 1.474795 5.185138 0.762840  
 C31 -4.972442 1.956468 -0.003205  
 H32 -4.675144 2.523879 0.878169  
 H33 -4.683964 2.514795 -0.893324  
 H34 -6.050659 1.805124 0.002981  
 C35 5.510874 0.873480 0.021114  
 H36 5.288794 1.580587 -0.777058  
 H37 5.475296 1.385765 0.982441  
 H38 6.500584 0.446829 -0.132128

#### [9MG-1MC]\*·H<sub>2</sub>O\_4

C1 -0.900348 1.113850 -0.003862  
 C2 -2.328019 0.811189 -0.005669  
 H3 0.915064 0.103422 -0.002591  
 C4 -0.616122 -1.320823 -0.007724  
 C5 -4.433991 0.774588 -0.006781  
 N6 -0.126847 -0.050673 -0.004345  
 N7 -3.388801 1.610871 -0.003233  
 N8 -4.088032 -0.536556 -0.011457  
 N9 -1.948084 -1.619237 -0.012519  
 C10 -2.716332 -0.565791 -0.010915  
 N11 0.230942 -2.320594 -0.006249  
 H12 -0.157549 -3.251438 -0.008944  
 H13 1.266423 -2.170109 -0.000303  
 O14 -0.393547 2.210997 -0.002363  
 H15 -5.476894 1.072142 -0.004011  
 C16 3.400051 -0.730330 0.006651  
 N17 2.672566 0.411813 -0.000317  
 C18 3.273701 1.603431 -0.004676  
 C19 5.402573 0.560806 0.004764  
 N20 4.789602 -0.649684 0.009823  
 H21 6.485271 0.546584 0.007307  
 O22 2.878881 -1.850661 0.010439  
 N23 2.507499 2.695082 -0.010833  
 H24 1.494033 2.614335 -0.009208  
 H25 2.922443 3.610249 -0.013421  
 C26 4.698058 1.713376 -0.002825  
 H27 5.195756 2.671980 -0.006876  
 C28 5.547930 -1.900206 0.019043  
 H29 5.301394 -2.477119 0.909866  
 H30 5.299143 -2.491328 -0.861706  
 H31 6.610766 -1.664033 0.015846  
 C32 -4.978337 -1.692423 -0.023840  
 H33 -4.831234 -2.255460 -0.945341  
 H34 -4.756320 -2.329262 0.831976  
 H35 -6.002935 -1.327406 0.033497  
 O36 -7.566702 0.514223 0.045651  
 H37 -8.145164 0.662887 -0.705407  
 H38 -8.106149 0.694933 0.818407

#### [9MG-1MC]\*·H<sub>2</sub>O\_5

C1 1.343784 0.799291 -0.018666  
 O2 0.805110 1.905300 -0.025208  
 N3 0.482466 -2.647140 -0.005533

C4 3.291149 -0.707138 0.002009  
 H5 0.945902 -3.540998 0.002546  
 C6 2.795948 0.629372 -0.012118  
 H7 -1.163186 -0.129033 -0.012383  
 N8 0.619211 -0.360129 -0.015412  
 N9 3.796220 1.512864 -0.015015  
 N10 2.592777 -1.801857 0.006500  
 N11 4.661921 -0.573968 0.006223  
 C12 4.897099 0.761532 -0.003051  
 H13 5.902384 1.160192 -0.002228  
 C14 1.229087 -1.550369 -0.005275  
 H15 -0.535262 -2.590810 -0.016095  
 H16 -4.640916 2.321321 0.039432  
 C17 -4.159551 1.355457 0.026151  
 C18 -2.932930 -1.170852 -0.007981  
 C19 -2.738415 1.250212 0.010583  
 C20 -4.879709 0.212077 0.024167  
 N21 -4.309605 -1.023925 0.009355  
 N22 -2.207805 -0.000099 -0.003368  
 N23 -1.920466 2.267851 0.009084  
 H24 -5.962333 0.227159 0.034960  
 O25 -2.399940 -2.261516 -0.025461  
 H26 -0.896174 2.130554 -0.005183  
 H27 -2.232406 3.228361 0.018158  
 O28 -0.362074 4.549000 0.001509  
 H29 0.444069 4.021346 -0.011124  
 H30 -0.083102 5.464750 0.000240  
 C31 -5.110630 -2.251771 -0.006406  
 H32 -4.947936 -2.788910 -0.940479  
 H33 -4.820391 -2.890196 0.826679  
 H34 -6.160703 -1.981845 0.086114  
 C35 5.628958 -1.661478 0.039555  
 H36 5.574423 -2.178136 0.997851  
 H37 5.413218 -2.363600 -0.765029  
 H38 6.625859 -1.245607 -0.096829

#### [9MG-1MC]\*·H<sub>2</sub>O\_6

C1 -1.813363 1.075421 -0.006021  
 C2 -3.267142 0.906603 -0.005795  
 H3 0.651823 0.191392 -0.003618  
 C4 -1.702629 -1.277806 0.001522  
 C5 -5.368350 1.039159 -0.006957  
 N6 -1.092320 -0.089511 -0.002999  
 N7 -4.267905 1.789729 -0.011048  
 N8 -5.133635 -0.297206 -0.000729  
 N9 -3.066891 -1.526752 0.006062  
 C10 -3.763186 -0.430379 0.001657  
 N11 -0.957057 -2.376005 0.002157  
 H12 -1.420642 -3.269476 0.005686  
 H13 0.060089 -2.315074 -0.003277  
 O14 -1.273432 2.177940 -0.007995  
 H15 -6.373578 1.437987 -0.010108  
 C16 2.432066 -0.834158 -0.006962  
 N17 1.698979 0.334739 -0.002295  
 C18 2.229724 1.581091 0.005268  
 C19 4.378355 0.551027 0.003807

N20	3.807285	-0.681756	-0.004442
H21	5.464721	0.560905	0.005874
O22	1.903804	-1.927213	-0.012923
N23	1.415213	2.613536	0.008597
H24	0.383103	2.490721	0.002897
H25	1.799258	3.544012	0.014015
C26	3.645923	1.690894	0.009065
H27	4.125282	2.658113	0.015639
C28	4.617093	-1.905736	-0.011219
H29	4.382315	-2.503322	0.869075
H30	4.390571	-2.488029	-0.903898
H31	5.666995	-1.618758	-0.003996
C32	-6.100582	-1.384289	0.023275
H33	-5.880671	-2.083846	-0.782490
H34	-6.052051	-1.904843	0.979858
H35	-7.096719	-0.967832	-0.117230
O36	7.514198	-0.024703	0.008260
H37	8.096863	0.014698	-0.752933
H38	8.092932	0.006795	0.772809

**[9MG-1MC]<sup>+</sup>·H<sub>2</sub>O<sub>7</sub>**

C1	-1.888203	1.196718	-0.005434
C2	-3.321043	0.911905	-0.005961
H3	-0.080380	0.163616	-0.001235
C4	-1.635058	-1.239840	0.001681
C5	-5.423694	0.904984	-0.008799
N6	-1.129364	0.023551	-0.002216
N7	-4.372693	1.726406	-0.011263
N8	-5.100479	-0.412041	-0.003483
N9	-2.974500	-1.521198	0.004096
C10	-3.727161	-0.458037	-0.000115
N11	-0.804774	-2.250749	0.003314
H12	-1.207886	-3.175645	0.006678
H13	0.239033	-2.113941	-0.000428
O14	-1.372782	2.288868	-0.006880
H15	-6.452641	1.237909	-0.012356
C16	2.370287	-0.726666	-0.002677
N17	1.662771	0.428365	0.001731
C18	2.290304	1.608174	0.007332
C19	4.399982	0.522044	0.004210
N20	3.757332	-0.673634	-0.002140
H21	5.484291	0.474982	0.004575
O22	1.824182	-1.838052	-0.007320
N23	1.545062	2.716150	0.010925
H24	0.531177	2.658124	0.005913
H25	1.979675	3.621964	0.013984
C26	3.713471	1.687748	0.009463
H27	4.229248	2.636904	0.014517
C28	4.498360	-1.936377	-0.008482
H29	4.235877	-2.521334	0.872770
H30	4.238651	-2.510761	-0.897506
H31	5.563128	-1.708841	-0.005573
C32	-5.996163	-1.561994	0.017806
H33	-5.729103	-2.243225	-0.789049
H34	-5.913731	-2.077033	0.974698
H35	-7.016515	-1.210212	-0.123939

O36	7.535520	-0.256450	-0.000869
H37	8.115793	-0.245068	-0.764462
H38	8.118047	-0.252259	0.761079

**[9MG-1MC]<sup>+</sup>·H<sub>2</sub>O<sub>8</sub>**

C1	1.129609	-1.454254	-0.014939
O2	0.523467	-2.524908	-0.018716
N3	0.502831	2.044478	-0.004931
C4	3.172000	-0.081894	0.000427
H5	1.001956	2.933758	-0.000140
C6	2.590469	-1.381754	-0.012288
H7	-1.254559	-0.419814	-0.009703
N8	0.485492	-0.249505	-0.011231
N9	3.531296	-2.330298	-0.016810
N10	2.551653	1.058701	0.005713
N11	4.531674	-0.305422	0.002015
C12	4.678025	-1.654341	-0.007134
H13	5.655098	-2.117729	-0.008225
C14	1.171852	0.905475	-0.003876
H15	-0.514118	2.033332	-0.013688
H16	-4.855230	-2.713425	0.038154
C17	-4.329756	-1.770591	0.024708
C18	-2.988602	0.691801	-0.009618
C19	-2.905647	-1.729917	0.011908
C20	-4.999847	-0.596740	0.019263
N21	-4.373489	0.608173	0.002830
N22	-2.313615	-0.511674	-0.003558
N23	-2.149639	-2.802271	0.014304
H24	-6.082130	-0.563173	0.028037
O25	-2.413131	1.758179	-0.024586
H26	-1.106834	-2.732355	0.001306
H27	-2.583170	-3.711030	0.025780
O28	1.559034	4.724406	0.006241
H29	1.785444	5.254937	-0.759095
H30	1.821819	5.234479	0.773853
C31	-5.113817	1.873288	-0.007851
H32	-4.831581	2.472491	0.856903
H33	-4.882404	2.428914	-0.915996
H34	-6.178651	1.652049	0.028672
C35	5.566767	0.715277	0.034656
H36	5.392395	1.435217	-0.764359
H37	5.552950	1.230285	0.995483
H38	6.534307	0.237282	-0.110344

**[9MG-1MC]<sup>+</sup>·H<sub>2</sub>O<sub>9</sub>**

C1	-0.840045	0.974016	0.002691
C2	-2.285127	0.753328	-0.003455
H3	1.638159	0.177295	0.006018
C4	-0.643358	-1.373809	-0.008355
C5	-4.393185	0.806993	-0.011745
N6	-0.074620	-0.162540	0.001234
N7	-3.316108	1.598462	-0.000148
N8	-4.104365	-0.518191	-0.022600
N9	-1.993851	-1.671421	-0.021527
C10	-2.731993	-0.601893	-0.017586
N11	0.143329	-2.444182	-0.005611

H12	-0.288497	-3.353332	-0.012260	O28	-0.508972	4.670607	0.008996
H13	1.156103	-2.348018	0.009108	H29	0.359767	4.260545	-0.001576
O14	-0.339393	2.096854	0.007837	H30	-0.353381	5.615502	0.014907
H15	-5.421723	1.148578	-0.009765	C31	-4.923786	-2.408690	-0.007920
C16	3.467598	-0.766750	0.015314	H32	-4.653392	-2.977629	-0.896951
N17	2.683587	0.368018	0.003460	H33	-4.650983	-2.985987	0.874931
C18	3.158001	1.636686	-0.010710	H34	-5.995758	-2.218330	-0.005578
C19	5.348519	0.703586	-0.008349	C35	5.554483	-1.753341	0.017773
N20	4.837892	-0.555006	0.006408	H36	5.480761	-2.270679	0.974078
H21	6.429134	0.772587	-0.012379	H37	5.302823	-2.438778	-0.790428
O22	2.993181	-1.882506	0.031941	H38	6.567413	-1.379965	-0.121663
N23	2.302761	2.632009	-0.017249				
H24	1.272252	2.463279	-0.007795				
H25	2.647110	3.578192	-0.027378				
C26	4.571630	1.810169	-0.017828				
H27	5.008554	2.797175	-0.030676				
C28	5.694265	-1.745053	0.028789				
H29	5.544687	-2.290939	0.959885				
H30	5.442067	-2.393803	-0.808652				
H31	6.731726	-1.426602	-0.050931				
C32	-5.038968	-1.635023	-0.048705				
H33	-4.925975	-2.185937	-0.982724				
H34	-4.833382	-2.299983	0.789951				
H35	-6.048201	-1.232760	0.028660				
O36	-7.567286	0.640614	0.066435				
H37	-8.151090	0.809124	-0.675936				
H38	-8.087351	0.841903	0.847048				

**[9MG-1MC]<sup>+</sup>·H<sub>2</sub>O\_10**

C1	1.392379	0.921793	-0.006777
O2	0.858933	2.007386	-0.009519
N3	0.375543	-2.542792	0.006577
C4	3.262579	-0.695766	0.000095
H5	0.799765	-3.458582	0.011086
C6	2.829147	0.664817	-0.007281
H7	-0.400460	-0.149475	-0.001045
N8	0.653857	-0.261067	-0.001973
N9	3.863519	1.501220	-0.014088
N10	2.529693	-1.772213	0.005866
N11	4.635013	-0.621696	-0.003852
C12	4.931479	0.700954	-0.011078
H13	5.953316	1.055073	-0.015576
C14	1.184813	-1.516164	0.003452
H15	-0.674505	-2.435318	0.002711
H16	-4.777000	2.176037	0.008243
C17	-4.239012	1.239582	0.005204
C18	-2.831821	-1.141966	-0.002125
C19	-2.809724	1.196905	0.004758
C20	-4.889536	0.057334	0.001076
N21	-4.221414	-1.126009	-0.002781
N22	-2.154663	0.027773	0.001353
N23	-2.093088	2.312162	0.007713
H24	-5.970311	-0.007499	0.000577
O25	-2.260933	-2.241444	-0.004836
H26	-1.080499	2.278186	0.004709
H27	-2.505000	3.230112	0.009691

**Cartesian coordinates for the structures in  
Fig. 5, optimized at  $\omega$ B97XD/6-311++G(d,p).**

**9MG<sup>+</sup>**

N1	1.947625	-0.353540	-0.005643
C2	2.315095	0.953144	-0.004812
H3	3.354398	1.253134	-0.007230
N4	1.288855	1.810559	-0.002588
C5	0.215752	1.034053	-0.000509
C6	-1.204737	1.375218	0.002035
O7	-1.721565	2.449543	0.004616
N8	-1.997021	0.181551	0.001626
H9	-2.995489	0.355940	0.003518
C10	-1.527133	-1.088852	-0.000929
N11	-2.375063	-2.104886	-0.002525
H12	-3.376555	-1.991117	-0.002734
H13	-1.993311	-3.039347	-0.003959
N14	-0.209624	-1.396550	-0.001778
C15	0.578553	-0.353825	-0.001595
C16	2.810103	-1.532777	0.009063
H17	2.713488	-2.046256	0.965146
H18	2.521148	-2.200388	-0.801328
H19	3.839639	-1.210018	-0.133490

**1MC**

C1	-0.620815	0.898800	-0.000284
N2	0.733672	1.069034	0.001571
C3	1.536978	0.033497	-0.002247
C4	-0.265977	-1.493960	0.000477
N5	-1.110750	-0.440485	0.000406
H6	-0.723003	-2.476723	0.000468
O7	-1.430826	1.802101	0.000462
N8	2.870694	0.282571	-0.028837
H9	3.164662	1.239768	0.069692
H10	3.538735	-0.449954	0.125487
C11	1.076251	-1.322992	-0.001065
H12	1.751205	-2.166727	-0.008629
C13	-2.555971	-0.612486	0.001694
H14	-2.987769	-0.140920	0.885032
H15	-2.989253	-0.139038	-0.879874
H16	-2.786087	-1.678199	0.000701

**9MG<sup>+</sup>·1MC**

C1	-1.365950	1.195888	-0.005293
C2	-2.803296	0.937272	-0.005509
H3	0.419358	0.130655	-0.001767
C4	-1.157263	-1.245680	0.001186
C5	-4.905552	0.968177	-0.007972
N6	-0.628935	0.008223	-0.002505
N7	-3.839375	1.770576	-0.010401
N8	-4.606343	-0.354378	-0.003045
N9	-2.500717	-1.502297	0.003772
C10	-3.234317	-0.425620	0.000041
N11	-0.345040	-2.272025	0.002444
H12	-0.763276	-3.190207	0.005678

H13	0.697124	-2.154113	-0.001228
O14	-0.828690	2.277390	-0.006670
H15	-5.928101	1.320331	-0.011256
C16	2.865681	-0.785518	-0.002900
N17	2.177218	0.380547	0.001100
C18	2.819487	1.551205	0.006547
C19	4.910760	0.435420	0.004526
N20	4.256301	-0.753335	-0.001662
H21	5.992266	0.383412	0.005516
O22	2.305813	-1.887731	-0.007714
N23	2.091984	2.668829	0.009578
H24	1.076845	2.624089	0.004875
H25	2.538287	3.569210	0.012815
C26	4.246490	1.611508	0.009118
H27	4.776660	2.552562	0.014090
C28	4.971756	-2.029261	-0.007895
H29	4.700857	-2.610901	0.872607
H30	4.708791	-2.597928	-0.899274
H31	6.041808	-1.828740	-0.001616
C32	-5.523738	-1.487592	0.017846
H33	-5.269316	-2.173370	-0.789194
H34	-5.451279	-2.003966	0.974785
H35	-6.537017	-1.116091	-0.124083

**TS\_PT1**

C1	1.274444	1.124458	0.105398
C2	2.718432	0.907786	0.080327
H3	-0.790663	0.150998	0.039822
C4	1.101144	-1.254124	-0.030494
C5	4.819156	0.993833	0.046636
N6	0.517120	-0.034486	0.044904
N7	3.736115	1.767401	0.120973
N8	4.552007	-0.333738	-0.042364
N9	2.455042	-1.509653	-0.083454
C10	3.180762	-0.433762	-0.023592
N11	0.345024	-2.331247	-0.059103
H12	0.810780	-3.223212	-0.113580
H13	-0.680688	-2.266877	0.019682
O14	0.769352	2.231416	0.167478
H15	5.833302	1.369391	0.055509
C16	-2.824610	-0.807130	0.068469
N17	-2.078042	0.341020	0.014265
C18	-2.664206	1.553520	-0.086823
C19	-4.803261	0.513551	-0.100923
N20	-4.207240	-0.699248	0.012978
H21	-5.885110	0.511456	-0.143243
O22	-2.318702	-1.917896	0.161956
N23	-1.909154	2.636589	-0.120424
H24	-0.888389	2.574551	-0.017357
H25	-2.342425	3.541978	-0.186678
C26	-4.085740	1.654483	-0.156312
H27	-4.570120	2.615504	-0.244334
C28	-4.982063	-1.940620	0.079957
H29	-4.685724	-2.605679	-0.730005
H30	-4.801091	-2.440122	1.031128
H31	-6.038244	-1.694786	-0.012840

C32	5.493781	-1.439548	-0.152056
H33	5.298609	-2.164167	0.637747
H34	5.387771	-1.921116	-1.124007
H35	6.503654	-1.047243	-0.045257

**[9MG – H<sub>N1</sub>]<sup>+</sup>[1MC + H<sub>N3</sub>]<sup>+</sup>**

C1	-1.304438	1.070771	-0.010918
C2	-2.758177	0.907309	-0.009447
H3	1.146649	0.183507	-0.006003
C4	-1.201824	-1.282788	-0.000185
C5	-4.858625	1.047315	-0.008110
N6	-0.586390	-0.096022	-0.006918
N7	-3.755093	1.794062	-0.015002
N8	-4.628847	-0.289752	0.000343
N9	-2.566034	-1.526305	0.006611
C10	-3.259079	-0.427856	0.001105
N11	-0.460683	-2.383928	0.000743
H12	-0.927882	-3.275632	0.005935
H13	0.555818	-2.327965	-0.006803
O14	-0.761005	2.172064	-0.014371
H15	-5.862289	1.450081	-0.010692
C16	2.931004	-0.837579	-0.006383
N17	2.196549	0.330224	-0.001636
C18	2.724454	1.577571	0.008907
C19	4.872425	0.551279	0.013834
N20	4.308552	-0.684358	0.002482
H21	5.955016	0.573633	0.019693
O22	2.408018	-1.931549	-0.017398
N23	1.912184	2.608832	0.010378
H24	0.877763	2.484414	0.000903
H25	2.295699	3.539911	0.018033
C26	4.143670	1.690448	0.017829
H27	4.621992	2.658087	0.027440
C28	5.113032	-1.910562	-0.008062
H29	4.858389	-2.524391	0.854862
H30	4.913065	-2.474778	-0.918328
H31	6.164978	-1.635315	0.032687
C32	-5.600129	-1.373344	0.028098
H33	-5.384056	-2.075285	-0.776588
H34	-5.551994	-1.891758	0.985819
H35	-6.594795	-0.953284	-0.111804

**[9MG – H<sub>N1</sub>]<sup>\*</sup>**

N1	1.928242	-0.363151	-0.007921
C2	2.286445	0.949585	-0.005452
H3	3.326154	1.247685	-0.008150
N4	1.265940	1.794537	-0.002739
C5	0.176100	1.007984	-0.000813
C6	-1.267246	1.316908	0.002496
O7	-1.692959	2.453394	0.006123
N8	-2.088910	0.201723	0.001746
C9	-1.586604	-1.001875	-0.000957
N10	-2.427655	-2.056675	-0.002576
H11	-3.417949	-1.886764	-0.001956
H12	-2.059107	-2.990156	-0.004450
N13	-0.241291	-1.397178	-0.002337

C14	0.549283	-0.366739	-0.002590
C15	2.782395	-1.533943	0.011145
H16	2.693279	-2.050928	0.967760
H17	2.489873	-2.213272	-0.789731
H18	3.814902	-1.220028	-0.138651

**[1MC + H<sub>N3</sub>]<sup>+</sup>**

C1	-0.694782	0.868720	-0.000005
N2	0.705654	0.985457	0.000015
C3	1.586930	-0.038147	-0.000005
C4	-0.294512	-1.489483	-0.000012
N5	-1.151596	-0.448891	0.000014
H6	-0.748727	-2.472873	-0.000022
O7	-1.407146	1.826580	-0.000026
N8	2.887604	0.220777	0.000002
H9	3.256595	1.158974	0.000050
H10	3.553684	-0.535240	0.000081
C11	1.059573	-1.346091	-0.000025
H12	1.708959	-2.208199	-0.000044
C13	-2.611530	-0.627263	0.000021
H14	-3.034802	-0.159323	0.887745
H15	-3.034785	-0.159664	-0.887893
H16	-2.828919	-1.693152	0.000226
H17	1.019447	1.949015	0.000003

**[9MG + H<sub>O6</sub>]<sup>+</sup>[1MC – H<sub>N4</sub>]<sup>\*</sup>**

C1	1.436218	1.091794	-0.005214
C2	2.805151	0.902845	-0.003108
H3	-0.353645	0.056906	-0.006310
C4	1.215193	-1.315973	-0.004353
C5	4.905935	1.001477	-0.000550
N6	0.676521	-0.042033	-0.005891
N7	3.869366	1.778626	-0.002444
N8	4.602397	-0.351545	-0.002317
N9	2.512558	-1.540454	-0.001269
C10	3.250661	-0.429720	-0.001542
N11	0.350804	-2.335141	-0.005539
H12	0.741779	-3.261909	-0.003422
H13	-0.660899	-2.217667	-0.007707
O14	0.879804	2.264632	-0.006291
H15	5.934461	1.335129	-0.000517
C16	-2.978489	-0.807487	-0.003166
N17	-2.206762	0.311914	-0.003044
C18	-2.757753	1.526000	0.002423
C19	-4.939385	0.597293	0.008500
N20	-4.386443	-0.624137	0.002914
H21	-6.021743	0.640798	0.013033
O22	-2.530852	-1.939074	-0.008016
N23	-1.865415	2.546700	0.001848
H24	-0.110193	2.278489	-0.004361
H25	-2.323451	3.458962	0.005980
C26	-4.161864	1.724902	0.008474
H27	-4.607411	2.709198	0.013059
C28	-5.200395	-1.841156	0.002355
H29	-4.967173	-2.427178	-0.886424
H30	-4.955769	-2.435651	0.882365

H31	-6.252984	-1.565819	0.010483
C32	5.528539	-1.472215	0.019959
H33	5.502522	-1.965788	0.992046
H34	5.256068	-2.187131	-0.755730
H35	6.532775	-1.096866	-0.170524

**[9MG + H<sub>06</sub>]<sup>+</sup>**

C1	-1.132797	1.236816	0.001562
C2	0.216956	0.986315	-0.000624
H3	-2.952143	0.274305	0.007439
C4	-1.470364	-1.166797	-0.001471
C5	2.316375	0.986652	-0.004163
N6	-1.950557	0.135155	0.001448
N7	1.318355	1.811323	-0.001588
N8	1.950942	-0.354727	-0.007562
N9	-0.191055	-1.442631	-0.003224
C10	0.603723	-0.370957	-0.002892
N11	-2.376137	-2.154762	-0.000261
H12	-2.030469	-3.100934	-0.003072
H13	-3.370312	-2.008751	-0.008254
O14	-1.630223	2.445895	0.004286
H15	3.359510	1.271882	-0.006559
H16	-2.591098	2.497862	0.004765
C17	2.832689	-1.515455	0.010512
H18	2.815142	-1.985592	0.993872
H19	2.506420	-2.230523	-0.743411
H20	3.844406	-1.185361	-0.218297

**[1MC - H<sub>N4</sub>]<sup>+</sup>**

C1	0.607178	-0.891980	0.000002
N2	-0.755139	-1.113000	0.000003
C3	-1.598986	-0.092366	0.000000
C4	0.175898	1.492574	0.000000
N5	1.047851	0.455797	0.000009
H6	0.611152	2.484636	-0.000010
O7	1.431838	-1.777814	-0.000005
N8	-2.916813	-0.434326	-0.000002
H9	-3.474606	0.424404	0.000010
C10	-1.159071	1.277682	-0.000003
H11	-1.858272	2.101754	-0.000008
C12	2.488881	0.666298	0.000000
H13	2.929928	0.201190	0.882309
H14	2.929900	0.201349	-0.882409
H15	2.692508	1.736637	0.000088

**Cartesian coordinates for the structures in  
Fig. 8, optimized at  $\omega$ B97XD/6-311++G(d,p).**

**9MG<sup>+</sup>**

N1	1.947625	-0.353540	-0.005643
C2	2.315095	0.953144	-0.004812
H3	3.354398	1.253134	-0.007230
N4	1.288855	1.810559	-0.002588
C5	0.215752	1.034053	-0.000509
C6	-1.204737	1.375218	0.002035
O7	-1.721565	2.449543	0.004616
N8	-1.997021	0.181551	0.001626
H9	-2.995489	0.355940	0.003518
C10	-1.527133	-1.088852	-0.000929
N11	-2.375063	-2.104886	-0.002525
H12	-3.376555	-1.991117	-0.002734
H13	-1.993311	-3.039347	-0.003959
N14	-0.209624	-1.396550	-0.001778
C15	0.578553	-0.353825	-0.001595
C16	2.810103	-1.532777	0.009063
H17	2.713488	-2.046256	0.965146
H18	2.521148	-2.200388	-0.801328
H19	3.839639	-1.210018	-0.133490

**1MC**

C1	-0.620815	0.898800	-0.000284
N2	0.733672	1.069034	0.001571
C3	1.536978	0.033497	-0.002247
C4	-0.265977	-1.493960	0.000477
N5	-1.110750	-0.440485	0.000406
H6	-0.723003	-2.476723	0.000468
O7	-1.430826	1.802101	0.000462
N8	2.870694	0.282571	-0.028837
H9	3.164662	1.239768	0.069692
H10	3.538735	-0.449954	0.125487
C11	1.076251	-1.322992	-0.001065
H12	1.751205	-2.166727	-0.008629
C13	-2.555971	-0.612486	0.001694
H14	-2.987769	-0.140920	0.885032
H15	-2.989253	-0.139038	-0.879874
H16	-2.786087	-1.678199	0.000701

**H<sub>2</sub>O**

O1	0.000000	0.000000	0.116335
H2	0.000000	0.760673	-0.465340
H3	0.000000	-0.760673	-0.465340

**9MG<sup>+</sup>·1MC**

C1	-1.365950	1.195888	-0.005293
C2	-2.803296	0.937272	-0.005509
H3	0.419358	0.130655	-0.001767
C4	-1.157263	-1.245680	0.001186
C5	-4.905552	0.968177	-0.007972
N6	-0.628935	0.008223	-0.002505
N7	-3.839375	1.770576	-0.010401

N8	-4.606343	-0.354378	-0.003045
N9	-2.500717	-1.502297	0.003772
C10	-3.234317	-0.425620	0.000041
N11	-0.345040	-2.272025	0.002444
H12	-0.763276	-3.190207	0.005678
H13	0.697124	-2.154113	-0.001228
O14	-0.828690	2.277390	-0.006670
H15	-5.928101	1.320331	-0.011256
C16	2.865681	-0.785518	-0.002900
N17	2.177218	0.380547	0.001100
C18	2.819487	1.551205	0.006547
C19	4.910760	0.435420	0.004526
N20	4.256301	-0.753335	-0.001662
H21	5.992266	0.383412	0.005516
O22	2.305813	-1.887731	-0.007714
N23	2.091984	2.668829	0.009578
H24	1.076845	2.624089	0.004875
H25	2.538287	3.569210	0.012815
C26	4.246490	1.611508	0.009118
H27	4.776660	2.552562	0.014090
C28	4.971756	-2.029261	-0.007895
H29	4.700857	-2.610901	0.872607
H30	4.708791	-2.597928	-0.899274
H31	6.041808	-1.828740	-0.001616
C32	-5.523738	-1.487592	0.017846
H33	-5.269316	-2.173370	-0.789194
H34	-5.451279	-2.003966	0.974785
H35	-6.537017	-1.116091	-0.124083

**9MG<sup>+</sup>·1MC·H<sub>2</sub>O**

C1	-1.470661	1.105521	-0.022523
C2	-2.930352	1.041765	-0.014695
H3	0.160772	-0.192843	-0.017587
C4	-1.590996	-1.340729	-0.001599
C5	-5.009463	1.355911	-0.004405
N6	-0.898731	-0.169839	-0.015580
N7	-3.845779	2.007366	-0.019201
N8	-4.890817	0.004945	0.008182
N9	-2.958336	-1.414928	0.010347
C10	-3.540452	-0.249773	0.003271
N11	-0.926618	-2.467711	0.001161
H12	-1.467944	-3.318997	0.012274
H13	0.126036	-2.495060	-0.008602
O14	-0.795974	2.106587	-0.032271
H15	-5.975727	1.841379	-0.003688
C16	2.440720	-1.459381	-0.010215
N17	1.918255	-0.211514	-0.011207
C18	2.718275	0.862726	-0.001532
C19	4.635837	-0.533714	0.012223
N20	3.819945	-1.622373	0.002625
H21	5.699188	-0.737327	0.021436
O22	1.733567	-2.476755	-0.019467
N23	2.170647	2.072750	-0.003236
H24	1.161328	2.176242	-0.014758
H25	2.767813	2.893660	0.004976
C26	4.142399	0.721259	0.010840

H27	4.785080	1.589768	0.018768
C28	4.351139	-2.984355	0.002676
H29	3.975738	-3.529130	0.868180
H30	4.040961	-3.506935	-0.901901
H31	5.437970	-2.933032	0.043602
C32	-5.951168	-0.994292	0.044875
H33	-5.799890	-1.713010	-0.759559
H34	-5.939803	-1.511078	1.004336
H35	-6.907414	-0.491986	-0.090130
O36	4.250043	4.128032	0.029797
H37	4.479243	4.668919	-0.728596
H38	4.463928	4.656015	0.801640

**TS\_PT1-H<sub>2</sub>O**

C1	-1.379703	1.021827	-0.120745
C2	-2.841152	0.999984	-0.103408
H3	0.514365	-0.234278	-0.028479
C4	-1.528687	-1.357804	0.076764
C5	-4.912337	1.366058	-0.090185
N6	-0.787427	-0.229256	-0.025662
N7	-3.735956	1.986248	-0.175295
N8	-4.824553	0.017668	0.035858
N9	-2.905662	-1.426229	0.126037
C10	-3.478732	-0.264244	0.031223
N11	-0.924812	-2.524690	0.139920
H12	-1.508634	-3.342887	0.211736
H13	0.103608	-2.601780	0.062502
O14	-0.729587	2.046939	-0.203593
H15	-5.868049	1.871255	-0.118294
C16	2.410775	-1.475581	-0.058899
N17	1.834815	-0.234850	-0.021308
C18	2.592501	0.884966	0.033864
C19	4.562863	-0.448573	0.019356
N20	3.793449	-1.568155	-0.048100
H21	5.633545	-0.608390	0.031372
O22	1.749872	-2.509028	-0.101287
N23	2.017759	2.069700	0.057589
H24	1.001532	2.158383	-0.021493
H25	2.606257	2.898301	0.091847
C26	4.018803	0.782071	0.066230
H27	4.623040	1.676294	0.114818
C28	4.381255	-2.907732	-0.097899
H29	4.076523	-3.482922	0.775992
H30	4.046622	-3.426418	-0.995333
H31	5.465026	-2.807543	-0.113524
C32	-5.903764	-0.951693	0.161844
H33	-5.820707	-1.696504	-0.629065
H34	-5.847161	-1.442919	1.133027
H35	-6.854416	-0.428982	0.071175
O36	4.047605	4.154548	0.167951
H37	4.260907	4.721600	-0.576139
H38	4.220188	4.678376	0.953135

**[9MG - H<sub>N1</sub>]<sup>+</sup>·[1MC + H<sub>N3</sub>]<sup>+</sup>·H<sub>2</sub>O**

C1	-1.423314	0.956761	-0.010473
C2	-2.887691	0.976361	-0.011079

H3	0.910837	-0.246105	-0.003764
C4	-1.616751	-1.391930	0.006405
C5	-4.954844	1.377191	-0.014277
N6	-0.859026	-0.292893	-0.002182
N7	-3.767622	1.980720	-0.020764
N8	-4.893093	0.021845	-0.002284
N9	-3.002249	-1.462748	0.011200
C10	-3.551147	-0.285773	0.001672
N11	-1.020198	-2.577964	0.011629
H12	-1.596330	-3.403203	0.017856
H13	-0.003930	-2.649709	0.005638
O14	-0.745064	1.978844	-0.015931
H15	-5.901659	1.899689	-0.019901
C16	2.539011	-1.497739	-0.005272
N17	1.966988	-0.243439	-0.003333
C18	2.656980	0.925054	0.001017
C19	4.649556	-0.378925	0.000675
N20	3.922299	-1.531187	-0.004337
H21	5.724788	-0.506074	0.001870
O22	1.873307	-2.513540	-0.007668
N23	2.006519	2.060465	0.002216
H24	0.971508	2.081541	-0.003299
H25	2.544065	2.926577	0.006526
C26	4.082083	0.845540	0.003921
H27	4.670624	1.751102	0.007777
C28	4.555988	-2.852447	-0.008081
H29	4.254214	-3.410801	0.877403
H30	4.254112	-3.405565	-0.896799
H31	5.635724	-2.717077	-0.007792
C32	-5.990557	-0.932615	0.026150
H33	-5.859772	-1.660896	-0.773610
H34	-6.011827	-1.448235	0.986437
H35	-6.926207	-0.395519	-0.120982
O36	3.916792	4.221266	0.021211
H37	4.074275	4.785872	-0.738805
H38	4.068094	4.773377	0.791597

**[9MG - H<sub>N1</sub>]<sup>+</sup>·[1MC + H<sub>N3</sub>]<sup>+</sup>**

C1	-1.304438	1.070771	-0.010918
C2	-2.758177	0.907309	-0.009447
H3	1.146649	0.183507	-0.006003
C4	-1.201824	-1.282788	-0.000185
C5	-4.858625	1.047315	-0.008110
N6	-0.586390	-0.096022	-0.006918
N7	-3.755093	1.794062	-0.015002
N8	-4.628847	-0.289752	0.000343
N9	-2.566034	-1.526305	0.006611
C10	-3.259079	-0.427856	0.001105
N11	-0.460683	-2.383928	0.000743
H12	-0.927882	-3.275632	0.005935
H13	0.555818	-2.327965	-0.006803
O14	-0.761005	2.172064	-0.014371
H15	-5.862289	1.450081	-0.010692
C16	2.931004	-0.837579	-0.006383
N17	2.196549	0.330224	-0.001636
C18	2.724454	1.577571	0.008907



C19	4.872425	0.551279	0.013834
N20	4.308552	-0.684358	0.002482
H21	5.955016	0.573633	0.019693
O22	2.408018	-1.931549	-0.017398
N23	1.912184	2.608832	0.010378
H24	0.877763	2.484414	0.000903
H25	2.295699	3.539911	0.018033
C26	4.143670	1.690448	0.017829
H27	4.621992	2.658087	0.027440
C28	5.113032	-1.910562	-0.008062
H29	4.858389	-2.524391	0.854862
H30	4.913065	-2.474778	-0.918328
H31	6.164978	-1.635315	0.032687
C32	-5.600129	-1.373344	0.028098
H33	-5.384056	-2.075285	-0.776588
H34	-5.551994	-1.891758	0.985819
H35	-6.594795	-0.953284	-0.111804

**[9MG - H<sub>Ni</sub>]<sup>\*</sup>**

N1	1.928242	-0.363151	-0.007921
C2	2.286445	0.949585	-0.005452
H3	3.326154	1.247685	-0.008150
N4	1.265940	1.794537	-0.002739
C5	0.176100	1.007984	-0.000813
C6	-1.267246	1.316908	0.002496
O7	-1.692959	2.453394	0.006123
N8	-2.088910	0.201723	0.001746
C9	-1.586604	-1.001875	-0.000957
N10	-2.427655	-2.056675	-0.002576
H11	-3.417949	-1.886764	-0.001956
H12	-2.059107	-2.990156	-0.004450
N13	-0.241291	-1.397178	-0.002337
C14	0.549283	-0.366739	-0.002590
C15	2.782395	-1.533943	0.011145
H16	2.693279	-2.050928	0.967760
H17	2.489873	-2.213272	-0.789731
H18	3.814902	-1.220028	-0.138651

**[1MC + H<sub>N3</sub>]<sup>+</sup>**

C1	-0.694782	0.868720	-0.000005
N2	0.705654	0.985457	0.000015
C3	1.586930	-0.038147	-0.000005
C4	-0.294512	-1.489483	-0.000012
N5	-1.151596	-0.448891	0.000014
H6	-0.748727	-2.472873	-0.000022
O7	-1.407146	1.826580	-0.000026
N8	2.887604	0.220777	0.000002
H9	3.256595	1.158974	0.000050
H10	3.553684	-0.535240	0.000081
C11	1.059573	-1.346091	-0.000025
H12	1.708959	-2.208199	-0.000044
C13	-2.611530	-0.627263	0.000021
H14	-3.034802	-0.159323	0.887745
H15	-3.034785	-0.159664	-0.887893
H16	-2.828919	-1.693152	0.000226
H17	1.019447	1.949015	0.000003

**TS\_HT4'·H<sub>2</sub>O**

C1	-1.444717	0.912361	-0.009672
C2	-2.847970	0.927483	-0.004417
H3	0.118005	-0.421143	-0.013186
C4	-1.641575	-1.521314	-0.006326
C5	-4.909456	1.356729	0.001526
N6	-0.910806	-0.360456	-0.010768
N7	-3.756492	1.956981	-0.003068
N8	-4.825609	-0.022112	0.000904
N9	-2.958292	-1.538419	-0.000241
C10	-3.499644	-0.315136	-0.000468
N11	-0.945544	-2.669133	-0.007947
H12	-1.468840	-3.527534	-0.003594
H13	0.068692	-2.699445	-0.011352
O14	-0.681949	1.915928	-0.012887
H15	-5.870363	1.852119	0.002765
C16	2.619268	-1.452855	-0.005097
N17	1.935061	-0.294206	-0.009276
C18	2.556587	0.885562	-0.002998
C19	4.686986	-0.179303	0.012882
N20	4.060607	-1.356635	0.007232
H21	5.770366	-0.199964	0.021890
O22	2.120026	-2.559186	-0.010378
N23	1.783402	1.976120	-0.006591
H24	0.574453	1.887933	-0.011132
H25	2.275705	2.878456	-0.001944
C26	3.977173	1.001412	0.007857
H27	4.465800	1.966413	0.012572
C28	4.791746	-2.622245	0.011657
H29	4.491881	-3.202757	0.884226
H30	4.528063	-3.188657	-0.881818
H31	5.860491	-2.419420	0.035067
C32	-5.916026	-0.981325	0.027196
H33	-5.760804	-1.733936	-0.745430
H34	-5.969295	-1.470495	1.000609
H35	-6.849560	-0.454382	-0.165059
O36	3.520888	4.281285	0.007631
H37	3.597080	4.858120	-0.756367
H38	3.586075	4.857294	0.773261

**[9MG + H<sub>O6</sub>]<sup>+</sup>·[1MC - H<sub>N4</sub>]<sup>\*</sup>·H<sub>2</sub>O**

C1	-1.533772	0.978090	-0.005313
C2	-2.917466	0.959335	-0.001595
H3	0.114055	-0.274375	-0.009463
C4	-1.614810	-1.438802	-0.007673
C5	-4.990259	1.317957	0.003290
N6	-0.922911	-0.242212	-0.008354
N7	-3.865029	1.960502	0.001343
N8	-4.856578	-0.061683	-0.000764
N9	-2.930481	-1.501301	-0.003355
C10	-3.524071	-0.306716	-0.001342
N11	-0.882829	-2.557126	-0.011218
H12	-1.384952	-3.428552	-0.009105
H13	0.136427	-2.566080	-0.012403
O14	-0.835876	2.069658	-0.005727
H15	-5.969307	1.776659	0.004845

C16	2.597988	-1.464452	-0.003618
N17	1.955679	-0.267215	-0.005759
C18	2.638744	0.879385	-0.001714
C19	4.702411	-0.285557	0.010115
N20	4.015686	-1.439613	0.006338
H21	5.782549	-0.367103	0.017060
O22	2.025911	-2.540527	-0.009052
N23	1.879969	2.001054	-0.004231
H24	0.156560	1.963206	-0.006347
H25	2.461682	2.850516	-0.002149
C26	4.057449	0.920931	0.005698
H27	4.591670	1.860857	0.008544
C28	4.689586	-2.738631	0.010609
H29	4.372292	-3.305118	0.885789
H30	4.404990	-3.294958	-0.882332
H31	5.765845	-2.579908	0.031509
C32	-5.913645	-1.058884	0.021723
H33	-5.726823	-1.807148	-0.747979
H34	-5.955783	-1.546255	0.996479
H35	-6.863197	-0.564656	-0.178093
O36	3.842950	4.209392	0.002345
H37	3.975177	4.774669	-0.762251
H38	3.967466	4.777293	0.766289

**[9MG + H<sub>06</sub>]<sup>+</sup>**

C1	-1.132797	1.236816	0.001562
C2	0.216956	0.986315	-0.000624
H3	-2.952143	0.274305	0.007439
C4	-1.470364	-1.166797	-0.001471
C5	2.316375	0.986652	-0.004163
N6	-1.950557	0.135155	0.001448
N7	1.318355	1.811323	-0.001588
N8	1.950942	-0.354727	-0.007562
N9	-0.191055	-1.442631	-0.003224
C10	0.603723	-0.370957	-0.002892
N11	-2.376137	-2.154762	-0.000261
H12	-2.030469	-3.100934	-0.003072
H13	-3.370312	-2.008751	-0.008254
O14	-1.630223	2.445895	0.004286
H15	3.359510	1.271882	-0.006559
H16	-2.591098	2.497862	0.004765
C17	2.832689	-1.515455	0.010512
H18	2.815142	-1.985592	0.993872
H19	2.506420	-2.230523	-0.743411
H20	3.844406	-1.185361	-0.218297

**[1MC - H<sub>N4</sub>]<sup>+</sup>**

C1	0.607178	-0.891980	0.000002
N2	-0.755139	-1.113000	0.000003
C3	-1.598986	-0.092366	0.000000
C4	0.175898	1.492574	0.000000
N5	1.047851	0.455797	0.000009
H6	0.611152	2.484636	-0.000010
O7	1.431838	-1.777814	-0.000005
N8	-2.916813	-0.434326	-0.000002
H9	-3.474606	0.424404	0.000010

C10	-1.159071	1.277682	-0.000003
H11	-1.858272	2.101754	-0.000008
C12	2.488881	0.666298	0.000000
H13	2.929928	0.201190	0.882309
H14	2.929900	0.201349	-0.882409
H15	2.692508	1.736637	0.000088

**TS1-H<sub>2</sub>O**

C1	1.849225	1.234493	-0.032289
C2	3.246250	0.806135	0.000283
H3	-0.061509	0.383307	-0.058610
C4	1.349772	-1.162092	-0.033233
C5	5.336772	0.585793	0.055535
N6	0.975249	0.145344	-0.048437
N7	4.375613	1.509613	0.026104
N8	4.881314	-0.691751	0.051617
N9	2.654493	-1.578801	-0.000997
C10	3.510998	-0.597620	0.014355
N11	0.421229	-2.082732	-0.050066
H12	0.735337	-3.041315	-0.034667
H13	-0.613946	-1.841281	-0.077299
O14	1.448959	2.373897	-0.043735
H15	6.394109	0.811152	0.083010
C16	-2.597493	-0.308334	-0.033126
N17	-1.759969	0.762496	-0.036012
C18	-2.274030	1.998133	0.009172
C19	-4.460042	1.095667	0.068669
N20	-3.954786	-0.155139	0.052468
H21	-5.542400	1.173099	0.117318
O22	-2.136925	-1.476664	-0.113896
N23	-1.426633	3.033511	0.007286
H24	-0.422890	2.886388	-0.023493
H25	-1.776797	3.974441	0.040435
C26	-3.680150	2.209539	0.051574
H27	-4.105064	3.202789	0.085407
C28	-4.908263	-1.921238	-1.140788
H29	-5.203101	-1.030907	-1.675102
H30	-3.862327	-2.209826	-1.148090
H31	-5.666033	-2.678249	-1.018076
C32	5.654938	-1.926593	0.060402
H33	5.309257	-2.565414	0.872213
H34	5.534060	-2.445116	-0.890518
H35	6.704104	-1.679700	0.213058
O36	-5.428025	-2.077581	1.012933
H37	-4.793270	-1.337771	1.085851
H38	-5.035029	-2.839893	1.449071

**9MG<sup>+</sup>-1HC**

C1	-0.996997	1.147759	-0.003300
C2	-2.449815	1.003807	-0.004239
H3	0.696006	-0.052837	-0.000822
C4	-0.982709	-1.303114	0.000259
C5	-4.542772	1.201854	-0.007030
N6	-0.357346	-0.094811	-0.001632
N7	-3.416047	1.916867	-0.008296
N8	-4.349941	-0.140413	-0.003716

N9	-2.342092	-1.452263	0.002101
C10	-2.987942	-0.320650	-0.000475
N11	-0.254380	-2.390995	0.000453
H12	-0.742865	-3.273874	0.002293
H13	0.791928	-2.357289	-0.002245
O14	-0.374162	2.182544	-0.003291
H15	-5.533799	1.634668	-0.010022
C16	3.060681	-1.145668	-0.003510
N17	2.466634	0.071293	0.000970
C18	3.204702	1.185602	0.005207
C19	5.214305	-0.078251	0.000641
N20	4.445133	-1.196889	-0.004006
H21	6.286227	-0.227736	0.000035
O22	2.430440	-2.205551	-0.007137
N23	2.569033	2.355439	0.009148
H24	1.552760	2.388408	0.006314
H25	3.083380	3.219037	0.011686
C26	4.638356	1.141168	0.005630
H27	5.231952	2.043508	0.009349
C28	-5.355011	-1.196742	0.015909
H29	-5.156936	-1.899434	-0.792406
H30	-5.323858	-1.718873	0.971958
H31	-6.335345	-0.745084	-0.124633
H32	4.856565	-2.118631	-0.007783

**CH<sub>3</sub>OH**

C1	0.661363	-0.020245	0.000001
H2	1.082520	0.985326	0.000098
H3	1.024454	-0.544778	0.892371
H4	1.024458	-0.544594	-0.892477
O5	-0.744663	0.121755	0.000002
H6	-1.142307	-0.748524	-0.000012

**TS1\_PT1**

C1	-0.910456	1.078904	-0.042843
C2	-2.367084	0.978391	-0.036153
H3	1.079070	-0.050379	-0.015751
C4	-0.927890	-1.307991	0.010911
C5	-4.454593	1.230380	-0.023304
N6	-0.248007	-0.136989	-0.018238
N7	-3.312546	1.917495	-0.054958
N8	-4.294962	-0.116624	0.015250
N9	-2.298540	-1.456644	0.034527
C10	-2.935805	-0.324877	0.008868
N11	-0.261308	-2.443262	0.019505
H12	-0.798087	-3.295936	0.040598
H13	0.767376	-2.462952	-0.015347
O14	-0.317952	2.144165	-0.064168
H15	-5.435494	1.685623	-0.028481
C16	3.020753	-1.167722	-0.038608
N17	2.367626	0.037035	-0.006931
C18	3.053987	1.201925	0.038796
C19	5.118468	0.013367	0.029039
N20	4.402915	-1.138345	-0.022245
H21	6.196091	-0.086331	0.040643
O22	2.445220	-2.243569	-0.078994

N23	2.387697	2.338745	0.061806
H24	1.358623	2.351728	0.020049
H25	2.889990	3.210144	0.091908
C26	4.487182	1.202122	0.062304
H27	5.036260	2.131019	0.102036
C28	-5.322626	-1.147337	0.073905
H29	-5.161854	-1.867309	-0.727755
H30	-5.281770	-1.656966	1.036447
H31	-6.295865	-0.675623	-0.050105
H32	4.855766	-2.040621	-0.047441

**[9MG - H<sub>N1</sub>]<sup>+</sup>·[1HC + H<sub>N3</sub>]<sup>+</sup>**

C1	-0.937569	1.025275	-0.006536
C2	-2.399204	0.972550	-0.006500
H3	1.425525	-0.041819	-0.003668
C4	-1.012983	-1.329871	-0.000991
C5	-4.482906	1.270454	-0.006738
N6	-0.309737	-0.192008	-0.004324
N7	-3.326066	1.932166	-0.010583
N8	-4.354683	-0.079910	-0.001875
N9	-2.391265	-1.468707	0.003254
C10	-2.999321	-0.321036	-0.000099
N11	-0.357887	-2.483866	-0.001291
H12	-0.891892	-3.337382	0.001411
H13	0.659451	-2.508051	-0.005793
O14	-0.311717	2.082527	-0.007539
H15	-5.453606	1.747094	-0.009028
C16	3.133605	-1.194066	-0.005509
N17	2.486168	0.024881	-0.001643
C18	3.109423	1.229275	0.006176
C19	5.189543	0.066403	0.006555
N20	4.513188	-1.113024	-0.001719
H21	6.269697	-0.004292	0.009413
O22	2.547113	-2.251881	-0.011634
N23	2.377547	2.316293	0.008962
H24	1.334508	2.268244	0.003112
H25	2.828275	3.217170	0.014794
C26	4.539522	1.248417	0.010902
H27	5.075820	2.185244	0.017453
C28	-5.404977	-1.087266	0.022317
H29	-5.241948	-1.801569	-0.784007
H30	-5.397083	-1.610227	0.978726
H31	-6.365467	-0.593959	-0.117179
H32	5.001898	-1.997211	-0.004785

**TS2-H<sub>2</sub>O**

C1	-0.858247	1.440514	-0.035188
C2	-2.309303	1.314173	-0.044672
H3	0.814119	0.211104	-0.013411
C4	-0.878433	-1.011984	-0.025831
C5	-4.399268	1.496016	-0.075287
N6	-0.235560	0.188542	-0.022393
N7	-3.262157	2.232295	-0.076876
N8	-4.240088	0.159424	-0.031014
N9	-2.231213	-1.146527	-0.028303
C10	-2.881983	-0.003705	-0.025051

N11	-0.147362	-2.105091	-0.025790
H12	-0.635129	-2.986420	-0.016984
H13	0.895429	-2.075861	-0.023860
O14	-0.213787	2.464577	-0.036196
H15	-5.377106	1.958968	-0.097258
C16	3.201531	-0.909813	0.005771
N17	2.610749	0.308400	0.008822
C18	3.344094	1.422867	0.033903
C19	5.339712	0.143116	0.056924
N20	4.591983	-0.989243	0.030347
H21	6.413432	0.004443	0.075802
O22	2.555483	-1.962441	-0.017604
N23	2.708014	2.594737	0.034236
H24	1.691267	2.629331	0.010254
H25	3.224402	3.456489	0.051334
C26	4.771984	1.368517	0.060364
H27	5.376051	2.263778	0.081867
C28	5.202791	-2.317456	0.023033
H29	4.858198	-2.889059	0.884057
H30	4.924494	-2.850502	-0.885738
H31	6.284671	-2.202901	0.066411
C32	-5.313770	-1.655249	-1.019780
H33	-6.210679	-2.238162	-0.890191
H34	-5.351227	-0.856318	-1.743762
H35	-4.353476	-2.109558	-0.806773
O36	-6.183344	-1.265366	0.989411
H37	-6.247614	-1.952719	1.660207
H38	-5.448861	-0.676522	1.214839

**9HG<sup>+</sup>·1MC**

C1	1.748533	0.987701	0.000093
C2	3.165909	0.630983	0.000006
H3	-0.107059	0.049354	0.000135
C4	1.372910	-1.432383	0.000049
C5	5.269720	0.537174	-0.000128
N6	0.931595	-0.145568	0.000107
N7	4.256858	1.397760	-0.000042
N8	4.874744	-0.764068	-0.000137
N9	2.697315	-1.780095	-0.000034
C10	3.502400	-0.758135	-0.000052
N11	0.495914	-2.402134	0.000071
H12	0.853340	-3.346014	0.000022
H13	-0.537513	-2.214342	0.000134
O14	1.289564	2.104163	0.000147
H15	6.312340	0.821923	-0.000189
C16	-2.601782	-0.703038	0.000058
N17	-1.838899	0.415838	0.000082
C18	-2.404019	1.625925	0.000014
C19	-4.562973	0.647274	-0.000174
N20	-3.986802	-0.581283	-0.000118
H21	-5.645558	0.666277	-0.000278
O22	-2.114395	-1.839447	0.000177
N23	-1.605487	2.694048	0.000062
H24	-0.595668	2.584012	0.000136
H25	-1.992715	3.621417	0.000015
C26	-3.823748	1.778092	-0.000110

H27	-4.292819	2.751016	-0.000167
C28	-4.782923	-1.808859	-0.000074
H29	-4.552205	-2.399987	-0.885656
H30	-4.553445	-2.399166	0.886386
H31	-5.837987	-1.540434	-0.000942
H32	5.467115	-1.581688	-0.000195

**TS2\_PT1**

C1	1.654737	0.925450	0.077220
C2	3.081232	0.608051	0.050229
H3	-0.467311	0.095728	0.025914
C4	1.315769	-1.435299	-0.051906
C5	5.186702	0.566595	0.015888
N6	0.818506	-0.177719	0.021613
N7	4.156280	1.401310	0.085456
N8	4.822327	-0.741938	-0.065634
N9	2.650047	-1.784023	-0.101431
C10	3.448784	-0.762992	-0.045910
N11	0.489583	-2.457757	-0.081722
H12	0.895052	-3.379118	-0.135070
H13	-0.531128	-2.323373	-0.010173
O14	1.230431	2.065021	0.137847
H15	6.222626	0.874607	0.022092
C16	-2.565577	-0.723277	0.056723
N17	-1.745463	0.373761	0.013619
C18	-2.252451	1.623280	-0.060287
C19	-4.455012	0.725682	-0.065437
N20	-3.938384	-0.525320	0.018857
H21	-5.535008	0.795860	-0.094276
O22	-2.132751	-1.866708	0.125451
N23	-1.428450	2.655589	-0.087035
H24	-0.413061	2.526131	-0.007316
H25	-1.802398	3.588247	-0.133769
C26	-3.664691	1.818210	-0.109060
H27	-4.087187	2.809824	-0.174189
C28	-4.791973	-1.714929	0.072957
H29	-4.548747	-2.382066	-0.752779
H30	-4.632771	-2.242552	1.012715
H31	-5.830679	-1.398653	-0.001881
H32	5.432917	-1.543101	-0.126204

**[9HG - H<sub>N1</sub>]<sup>+</sup>·[1MC + H<sub>N3</sub>]<sup>+</sup>**

C1	1.682225	0.879128	-0.006059
C2	3.123794	0.623470	-0.001584
H3	-0.824409	0.153218	-0.005519
C4	1.430500	-1.461951	-0.001218
C5	5.232101	0.649529	0.005029
N6	0.891821	-0.239135	-0.005715
N7	4.174413	1.451779	-0.000538
N8	4.913063	-0.672660	0.007789
N9	2.777957	-1.791441	0.004150
C10	3.539088	-0.740957	0.003571
N11	0.623605	-2.514569	-0.001618
H12	1.034997	-3.433636	0.001801
H13	-0.387695	-2.395235	-0.006332
O14	1.211874	2.012861	-0.009518

H15	6.256963	0.992505	0.007296
C16	-2.666148	-0.756064	-0.002090
N17	-1.861711	0.365013	-0.001609
C18	-2.311107	1.642629	0.000562
C19	-4.517717	0.749652	0.009739
N20	-4.031476	-0.518577	0.007789
H21	-5.596810	0.839280	0.014441
O22	-2.209891	-1.879463	-0.009908
N23	-1.436110	2.621599	-0.002721
H24	-0.412589	2.433511	-0.006566
H25	-1.760334	3.574978	-0.001248
C26	-3.720389	1.842209	0.006647
H27	-4.139589	2.836981	0.009462
C28	-4.911096	-1.692441	-0.000768
H29	-4.776850	-2.248227	-0.928287
H30	-4.666999	-2.338640	0.840974
H31	-5.941549	-1.352843	0.081698
H32	5.550565	-1.454360	0.012024