Supporting Information

Singlet O$_2$ Oxidation of the Radical Cation vs. the Dehydrogenated Neutral Radical of 9-Methylguanine in a Watson-Crick Base Pair. Consequences of Structural Context
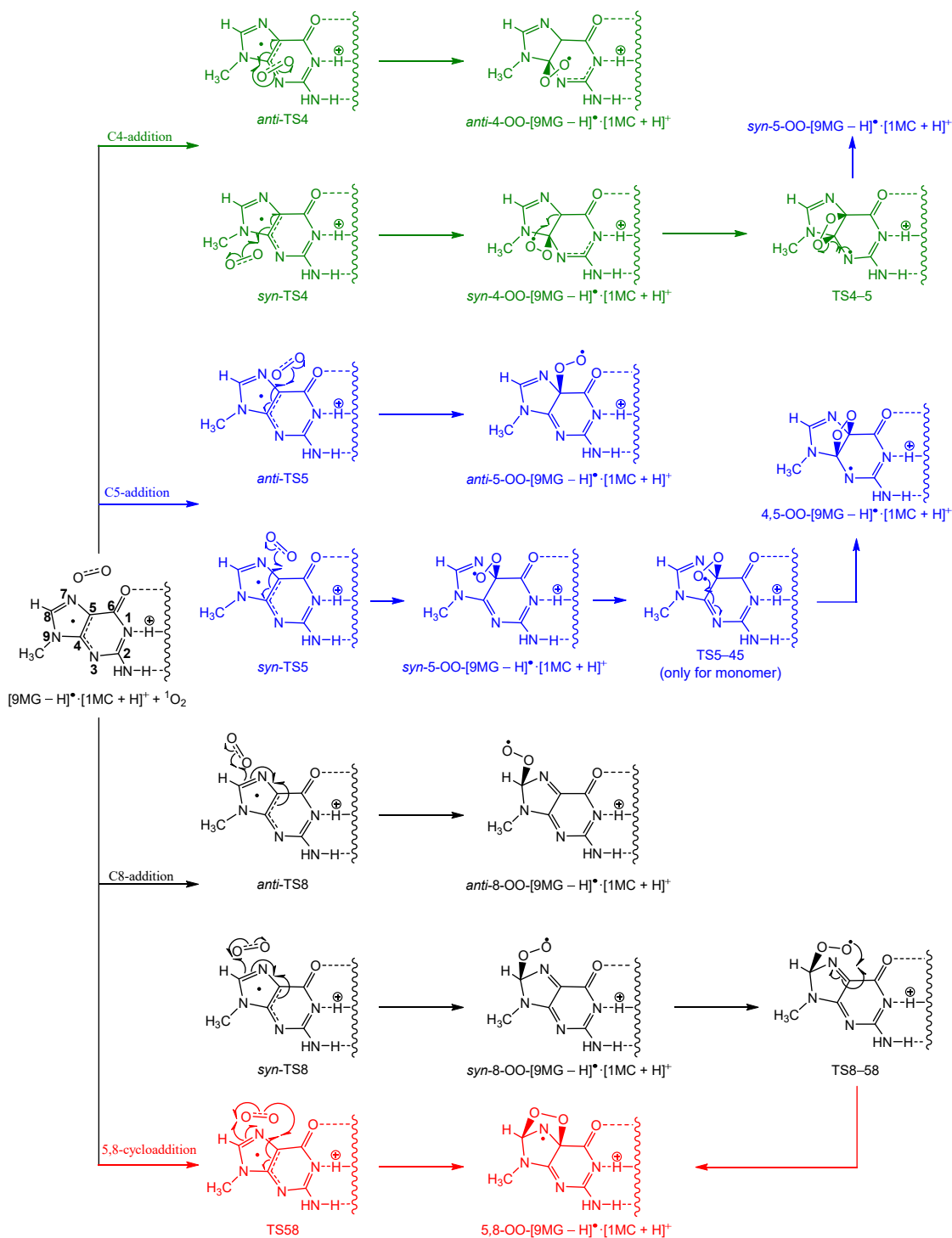
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Scheme S1 Probable pathways and products for the $^1O_2$ oxidation of [9MG – H]$^•$ and [9MG – H]$^•\cdot$[1MC + H]$^+$, in which dash lines represent intra-base pair H-bonding

Cartesian coordinates for the structures in Table 1, optimized at approximately spin-projected ωB97XD/6-31+G(d,p).

Single nucleobase reactions

9MG•+

N1	1.951120	-0.354583	-0.005039
C2	2.319075	0.954050	-0.004604
H3	3.359068	1.254439	-0.006930
N4	1.291152	1.814596	-0.002631
C5	0.216436	1.034973	-0.000529
C6	-1.205059	1.373616	0.001955
O7	-1.725525	2.455144	0.004320
N8	-1.999348	0.182762	0.001632
H9	-2.998658	0.360698	0.003190
C10	-1.529628	-1.090373	-0.000748
N11	-2.379559	-2.107286	-0.002613
H12	-3.382588	-1.994399	-0.003318
H13	-1.998201	-3.043651	-0.004190
N14	-0.209714	-1.400163	-0.001254
C15	0.580653	-0.354432	-0.001405
C16	2.813072	-1.534838	0.008346
H17	2.706734	-2.055163	0.960914
H18	2.530148	-2.196867	-0.810227
H19	3.844839	-1.211460	-0.122750

Zero-point correction= 0.146470 (Hartree/Particle)
Thermal correction to Energy= 0.156361
Thermal correction to Enthalpy= 0.157305
Thermal correction to Gibbs Free Energy= 0.110574
Sum of electronic and zero-point Energies= -581.292006
Sum of electronic and thermal Energies= -581.282115
Sum of electronic and thermal Enthalpies= -581.281170
Sum of electronic and thermal Free Energies= -581.327901

9MG•+ + ¹O₂

N1	-1.513933	0.851361	-0.708329
C2	-2.034396	-0.341784	-1.101762
H3	-3.073671	-0.446036	-1.385404
N4	-1.152731	-1.351574	-1.105354
C5	-0.021657	-0.794377	-0.690669
C6	1.299333	-1.377508	-0.468377
O7	1.660476	-2.512204	-0.619313
N8	2.211389	-0.376668	-0.006941
H9	3.147537	-0.728618	0.166071
C10	1.922451	0.933650	0.199811
N11	2.869246	1.757477	0.626540
H12	3.818190	1.467049	0.810305
H13	2.623351	2.727262	0.771506
N14	0.695686	1.470742	-0.005751
C15	-0.196422	0.606995	-0.424797
C16	-2.203815	2.131376	-0.565704
H17	-2.300354	2.380866	0.491782
H18	-1.635258	2.905992	-1.080442
H19	-3.191414	2.043088	-1.016465
O20	-2.265772	-0.993186	1.948486
O21	-1.113322	-0.714497	2.164636

Zero-point correction= 0.151393 (Hartree/Particle)
Thermal correction to Energy= 0.165226
Thermal correction to Enthalpy= 0.166170
Thermal correction to Gibbs Free Energy= 0.108225
Sum of electronic and zero-point Energies= -731.568921
Sum of electronic and thermal Energies= -731.555089
Sum of electronic and thermal Enthalpies= -731.554145
Sum of electronic and thermal Free Energies= -731.612089

syn-TS4

C1	-1.457022	1.350057	-0.089167
C2	-0.015130	1.026649	-0.306404
H3	-3.192136	0.313221	0.185631
C4	-1.693179	-1.115005	-0.121789
C5	2.003276	0.875641	-0.922751
N6	-2.200514	0.172283	0.027934
N7	0.914667	1.750793	-0.818571
N8	1.743282	-0.356453	-0.600817
N9	-0.412980	-1.404931	-0.214125
C10	0.428007	-0.356026	0.014617
N11	-2.588384	-2.100640	-0.170740
H12	-2.245690	-3.048226	-0.233016
H13	-3.583939	-1.946373	-0.190306
O14	-1.932541	2.448754	-0.028948
H15	2.967148	1.204905	-1.294108
O16	1.669335	0.488549	1.916522
O17	0.753136	-0.337479	1.573445
C18	2.635421	-1.511198	-0.577087
H19	3.542131	-1.270551	-1.130080
H20	2.877472	-1.748429	0.461198
H21	2.114837	-2.351203	-1.037744

Zero-point correction= 0.152404 (Hartree/Particle)
Thermal correction to Energy= 0.164165
Thermal correction to Enthalpy= 0.165109
Thermal correction to Gibbs Free Energy= 0.114399
Sum of electronic and zero-point Energies= -731.520449
Sum of electronic and thermal Energies= -731.508688
Sum of electronic and thermal Enthalpies= -731.507743
Sum of electronic and thermal Free Energies= -731.558453

syn-4OO-9MG•+

C1	1.499522	-1.297980	-0.039706
C2	0.047600	-1.029623	-0.285716
H3	3.185332	-0.176017	0.253662
C4	1.616174	1.153953	-0.163604
C5	-1.904735	-0.895973	-1.101847
N6	2.193609	-0.092844	0.060193
N7	-0.761888	-1.699450	-1.021512
N8	-1.794372	0.264729	-0.541660
N9	0.321998	1.371508	-0.243366
C10	-0.484864	0.313267	0.139135
N11	2.458439	2.177218	-0.300724
H12	2.067888	3.101797	-0.409410
H13	3.457609	2.065427	-0.368595
O14	2.003714	-2.379954	0.065311

H15 -2.792585 -1.219231 -1.633944
O16 -1.510260 -0.564681   2.012411
O17 -0.736242   0.400924   1.587793
C18 -2.762484   1.352917 -0.465375
H19 -3.626059   1.105892 -1.081166
H20 -3.065223   1.484079   0.575196
H21 -2.276442   2.260233 -0.827695

Zero-point correction=   0.153051 (Hartree/Particle)
Thermal correction to Energy=   0.165414
Thermal correction to Enthalpy=   0.166359
Thermal correction to Gibbs Free Energy=   0.113934
Sum of electronic and zero-point Energies=   -731.520864
Sum of electronic and thermal Energies=   -731.508501
Sum of electronic and thermal Enthalpies=   -731.507557
Sum of electronic and thermal Free Energies=   -731.559982

rot-TS4
C1   1.477916 -1.208448 -0.184835
C2   -0.004349 -1.029518 -0.292391
H3   3.109576   0.019882 -0.027484
C4   1.425825   1.242380 -0.297531
C5   -2.010508 -0.989361 -0.989731
N6   2.101744   0.038808 -0.134628
N7   -0.819298 -1.717547 -1.008556
N8   -1.942546   0.152288 -0.383556
N9   0.115805   1.374145 -0.264090
C10 -0.585685   0.271624   0.199150
N11   2.179692   2.321456 -0.501550
H12   1.719222   3.217450 -0.568002
H13   3.174200   2.278147 -0.659224
O14   2.056289 -2.256153 -0.150192
H15 -2.906812 -1.348389 -1.483527
O16 -0.118656 -0.615162   2.264441
O17 -0.807322   0.314544   1.644684
C18 -2.965552   1.181457 -0.223629
H19 -3.856278   0.888120 -0.777456
H20 -3.195697   1.288840   0.837563
H21 -2.560360   2.117268 -0.612869

Zero-point correction=   0.153091 (Hartree/Particle)
Thermal correction to Energy=   0.164574
Thermal correction to Enthalpy=   0.165518
Thermal correction to Gibbs Free Energy=   0.115354
Sum of electronic and zero-point Energies=   -731.516406
Sum of electronic and thermal Energies=   -731.504923
Sum of electronic and thermal Enthalpies=   -731.503979
Sum of electronic and thermal Free Energies=   -731.554143

anti-TS4
C1   -1.347534   1.424509   0.021053
C2   0.120216   1.169130 -0.088173
H3   -3.062919   0.326049 -0.110171
C4   -1.485501 -0.976433 -0.548545
C5   2.192769   1.180983 -0.504802
N6   -2.056383   0.239942 -0.195416
N7   1.071439   1.995219 -0.365153
N8   1.959337 -0.095166 -0.391330

N9   -0.184529 -1.206224 -0.584675
C10   0.568424 -0.239666 -0.009942
N11 -2.322281 -1.948599 -0.899420
H12 -1.932312 -2.856585 -1.106618
H13 -3.321546 -1.829545 -0.952776
O14 -1.864701   2.480283   0.255256
H15   3.175299   1.588628 -0.714193
O16 -0.253355 -1.179541   2.031373
O17   0.736835 -0.512078   1.603066
C18   2.886436 -1.218794 -0.481678
H19   3.845689 -0.858466 -0.850449
H20   3.001196 -1.661498   0.509695
H21   2.462419 -1.952466 -1.168564

Zero-point correction=   0.152193 (Hartree/Particle)
Thermal correction to Energy=   0.164129
Thermal correction to Enthalpy=   0.165074
Thermal correction to Gibbs Free Energy=   0.113854
Sum of electronic and zero-point Energies=   -731.520875
Sum of electronic and thermal Energies=   -731.508939
Sum of electronic and thermal Enthalpies=   -731.507995
Sum of electronic and thermal Free Energies=   -731.559214

anti-4OO-9MG•+
C1   -1.404068   1.366230   0.050491
C2   0.073866   1.158026 -0.064095
H3   -3.080173   0.207845 -0.108687
C4   -1.437798 -1.011859 -0.570514
C5   2.116688   1.222477 -0.621936
N6   -2.071677   0.171134 -0.204150
N7   0.956144   1.987418 -0.498424
N8   1.969679 -0.039010 -0.359599
N9   -0.133825 -1.198792 -0.555516
C10   0.590982 -0.238534   0.106387
N11 -2.228114 -2.000277 -0.982561
H12 -1.802179 -2.889268 -1.200344
H13 -3.222718 -1.898314 -1.108269
O14 -1.944881   2.401693   0.319573
H15   3.055225   1.656361 -0.948898
O16 -0.261235 -1.068394   2.094622
O17   0.799572 -0.537058   1.578199
C18   2.948380 -1.120099 -0.415062
H19   3.876016 -0.739202 -0.839721
H20   3.116891 -1.494085   0.596519
H21   2.535556 -1.914024 -1.039625

Zero-point correction=   0.152842 (Hartree/Particle)
Thermal correction to Energy=   0.165254
Thermal correction to Enthalpy=   0.166198
Thermal correction to Gibbs Free Energy=   0.113667
Sum of electronic and zero-point Energies=   -731.520755
Sum of electronic and thermal Energies=   -731.508343
Sum of electronic and thermal Enthalpies=   -731.507399
Sum of electronic and thermal Free Energies=   -731.559930

syn-TS5
C1   1.188615 -1.293258 -0.506551
C2   -0.202927 -0.822444 -0.270591

H3 3.089077 -0.552460 -0.268229
C4 1.805908 1.038069 0.065121
C5 -2.217100 -0.435189 -0.712945
N6 2.118077 -0.264250 -0.202710
N7 -1.355472 -1.397961 -0.755922
N8 -1.683308 0.836509 -0.411991
N9 0.551957 1.535948 0.030760
C10 -0.374289 0.646593 -0.214982
N11 2.781958 1.883972 0.349575
H12 2.536224 2.849234 0.523535
H13 3.751914 1.613011 0.416776
O14 1.544535 -2.381858 -0.848035
H15 -3.272815 -0.537339 -0.935855
O16 -0.306140 -1.088065 1.496429
O17 -1.480240 -1.049633 1.883319
C18 -2.416570 2.098277 -0.362198
H19 -2.904520 2.276866 -1.321427
H20 -3.157622 2.060054 0.437411
H21 -1.701801 2.895262 -0.161020

Zero-point correction=   0.152709 (Hartree/Particle)
Thermal correction to Energy=   0.164688
Thermal correction to Enthalpy=   0.165633
Thermal correction to Gibbs Free Energy=   0.114056
Sum of electronic and zero-point Energies=   -731.541943
Sum of electronic and thermal Energies=   -731.529963
Sum of electronic and thermal Enthalpies=   -731.529019
Sum of electronic and thermal Free Energies=   -731.580595

syn-5OO-9MG•+
C1 -1.098656 1.240002 -0.625759
C2 0.244476 0.871718 -0.003463
H3 -3.005584 0.467843 -0.626485
C4 -1.747555 -1.044944 0.031899
C5 2.260147 0.493451 -0.627534
N6 -2.051637 0.223041 -0.381627
N7 1.445968 1.465095 -0.495339
N8 1.723477 -0.805570 -0.382201
N9 -0.488902 -1.526357 0.081138
C10 0.443636 -0.629469 -0.084945
N11 -2.731198 -1.874792 0.326243
H12 -2.492176 -2.823780 0.582100
H13 -3.702748 -1.600566 0.341250
O14 -1.377105 2.259846 -1.175526
H15 3.296515 0.586533 -0.932987
O16 0.031792 1.233443 1.415557
O17 1.039521 0.880529 2.158515
C18 2.438694 -2.070773 -0.515337
H19 2.890587 -2.134086 -1.506435
H20 3.209420 -2.135396 0.254374
H21 1.721912 -2.880908 -0.386863

Zero-point correction=   0.153846 (Hartree/Particle)
Thermal correction to Energy=   0.165960
Thermal correction to Enthalpy=   0.166904
Thermal correction to Gibbs Free Energy=   0.114990
Sum of electronic and zero-point Energies=   -731.545158
Sum of electronic and thermal Energies=   -731.533044
Sum of electronic and thermal Enthalpies=   -731.532100

Sum of electronic and thermal Free Energies=   -731.584014

rot-TS5
C1 1.034266 -1.247841 -0.649039
C2 -0.261688 -0.920189 0.087461
H3 2.901868 -0.392482 -0.812045
C4 1.609785 1.100339 -0.178294
C5 -2.341320 -0.688883 -0.400037
N6 1.955394 -0.177746 -0.515337
N7 -1.467219 -1.607237 -0.263290
N8 -1.864944 0.645898 -0.269327
N9 0.328858 1.514322 -0.082703
C10 -0.553629 0.560016 -0.064115
N11 2.557640 2.003445 -0.015719
H12 2.278365 2.953025 0.193177
H13 3.543099 1.785957 -0.049763
O14 1.320849 -2.274354 -1.181480
H15 -3.389954 -0.856343 -0.620047
O16 0.050069 -1.281646 1.491010
O17 0.075713 -0.269998 2.308028
C18 -2.649069 1.860401 -0.473194
H19 -3.103706 1.842609 -1.465137
H20 -3.422241 1.926373 0.293632
H21 -1.978652 2.715018 -0.392333

Zero-point correction=   0.153565 (Hartree/Particle)
Thermal correction to Energy=   0.164989
Thermal correction to Enthalpy=   0.165934
Thermal correction to Gibbs Free Energy=   0.115590
Sum of electronic and zero-point Energies=   -731.542015
Sum of electronic and thermal Energies=   -731.530591
Sum of electronic and thermal Enthalpies=   -731.529646
Sum of electronic and thermal Free Energies=   -731.579990

anti-TS5
C1 1.080734 -1.256188 -0.620108
C2 -0.279372 -0.927754 -0.120623
H3 2.875678 -0.271048 -0.821134
C4 1.477513 1.162187 -0.295149
C5 -2.381692 -0.842740 -0.278084
N6 1.903474 -0.099966 -0.585691
N7 -1.411390 -1.702141 -0.271309
N8 -1.996247 0.500158 -0.215155
N9 0.170961 1.502676 -0.162217
C10 -0.649972 0.492073 -0.188417
N11 2.361635 2.138858 -0.204802
H12 2.018029 3.073941 -0.030495
H13 3.359008 1.992292 -0.258098
O14 1.502337 -2.320958 -0.964782
H15 -3.432404 -1.101873 -0.338512
O16 0.044021 -1.006093 1.683174
O17 0.811223 -0.149586 2.135175
C18 -2.857466 1.679264 -0.253060
H19 -2.552285 2.371920 0.531631
H20 -2.780770 2.165594 -1.226937
H21 -3.885411 1.364124 -0.078131

Zero-point correction=   0.152394 (Hartree/Particle)
Thermal correction to Energy=   0.164413
Thermal correction to Enthalpy=   0.165358
Thermal correction to Gibbs Free Energy=   0.113744
Sum of electronic and zero-point Energies=   -731.540024
Sum of electronic and thermal Energies=   -731.528004
Sum of electronic and thermal Enthalpies=   -731.527060
Sum of electronic and thermal Free Energies=   -731.578674

anti-**5OO-9MG•+**
C1   1.001076   -1.186574   -0.700959
C2   -0.275927   -0.912555   0.087676
H3   2.789290   -0.226671   -1.039067
C4   1.494378   1.175575   -0.225341
C5   -2.382672   -0.757620   -0.286258
N6   1.855525   -0.062034   -0.677615
N7   -1.462549   -1.641106   -0.223422
N8   -1.962943   0.589263   -0.129056
N9   0.206744   1.539781   -0.022770
C10 -0.635852   0.551333   -0.008478
N11   2.418793   2.102728   -0.076449
H12   2.122957   3.028750   0.203711
H13   3.406928   1.921168   -0.178317
O14   1.310722   -2.216154   -1.217183
H15 -3.432347   -0.967341   -0.460186
O16   0.016243   -1.237779   1.515856
O17   0.951031   -0.501154   2.030030
C18 -2.787818   1.786732   -0.263561
H19 -2.457109   2.526643   0.465288
H20 -2.696844   2.195723   -1.271957
H21 -3.824951   1.520669   -0.062375

Zero-point correction=   0.154050 (Hartree/Particle)
Thermal correction to Energy=   0.166091
Thermal correction to Enthalpy=   0.167035
Thermal correction to Gibbs Free Energy=   0.115467
Sum of electronic and zero-point Energies=   -731.545195
Sum of electronic and thermal Energies=   -731.533154
Sum of electronic and thermal Enthalpies=   -731.532210
Sum of electronic and thermal Free Energies=   -731.583777

syn-**TS8**
C1   1.345153   -1.446316   -0.242157
C2   -0.003982   -0.876418   -0.446924
H3   3.218825   -0.747098   0.217510
C4   1.998236   0.923703   0.124353
C5   -2.059299   -0.451315   -0.672692
N6   2.274367   -0.413397   0.054526
N7   -1.114018   -1.464903   -0.752525
N8   -1.453718   0.803276   -0.612901
N9   0.777135   1.455968   -0.071867
C10 -0.157895   0.575437   -0.333247
N11   2.984351   1.762266   0.403763
H12   2.765699   2.747793   0.456173
H13   3.936629   1.470063   0.564856
O14   1.678647   -2.594164   -0.300081
H15 -3.047058   -0.562405   -1.101548
O16 -2.470612   -0.698605   1.114276

O17 -1.467022   -0.453987   1.784182
C18 -2.146938   2.084701   -0.521941
H19 -2.567723   2.215231   0.477804
H20 -1.424783   2.875156   -0.722488
H21 -2.938161   2.114095   -1.270659

Zero-point correction=   0.153049 (Hartree/Particle)
Thermal correction to Energy=   0.164918
Thermal correction to Enthalpy=   0.165862
Thermal correction to Gibbs Free Energy=   0.114398
Sum of electronic and zero-point Energies=   -731.546703
Sum of electronic and thermal Energies=   -731.534834
Sum of electronic and thermal Enthalpies=   -731.533890
Sum of electronic and thermal Free Energies=   -731.585354

syn-**8OO-9MG•+**
C1   -1.427688   1.501759   -0.128322
C2   -0.086052   0.882664   -0.318267
H3   -3.340125   0.871120   0.250856
C4   -2.177645   -0.845120   0.162251
C5   2.005390   0.382929   -0.621077
N6   -2.403727   0.505664   0.110401
N7   1.028740   1.452007   -0.533948
N8   1.283447   -0.874748   -0.459603
N9   -0.977956   -1.425193   -0.014583
C10   0.012938   -0.594671   -0.241440
N11 -3.205029   -1.642889   0.401560
H12 -3.031685   -2.638325   0.440384
H13 -4.145883   -1.311222   0.554693
O14 -1.700699   2.664920   -0.163919
H15   2.559169   0.429991   -1.561903
O16   3.004182   0.533450   0.403792
O17   2.470128   0.454201   1.596598
C18   1.919658   -2.185813   -0.448016
H19   2.636419   -2.235793   0.374120
H20   1.144709   -2.938622   -0.309479
H21   2.430568   -2.352096   -1.397996

Zero-point correction=   0.154845 (Hartree/Particle)
Thermal correction to Energy=   0.166856
Thermal correction to Enthalpy=   0.167800
Thermal correction to Gibbs Free Energy=   0.115759
Sum of electronic and zero-point Energies=   -731.554063
Sum of electronic and thermal Energies=   -731.542052
Sum of electronic and thermal Enthalpies=   -731.541108
Sum of electronic and thermal Free Energies=   -731.593149

rot-TS8
C1   -1.313199   1.573662   -0.157738
C2   -0.044168   0.802279   -0.286666
H3   -3.291958   1.174906   0.194491
C4   -2.327701   -0.662241   0.203389
C5   1.974205   0.067534   -0.563008
N6   -2.399040   0.702788   0.094957
N7   1.132264   1.238123   -0.489672
N8   1.121701   -1.099537   -0.318880
N9   -1.197592   -1.377832   0.082763
C10 -0.114187   -0.672330   -0.152434

N11   -3.444455   -1.329644   0.443468
H12   -3.385703   -2.335923   0.522702
H13   -4.345424   -0.889512   0.557508
O14   -1.453677   2.757239   -0.247818
H15   2.447958   0.007938   -1.549149
O16   3.019304   0.036064   0.430766
O17   3.216734   1.174089   1.046818
C18   1.603995   -2.475242   -0.282432
H19   2.354264   -2.574575   0.503722
H20   0.756457   -3.126968   -0.073921
H21   2.041697   -2.734267   -1.248596

Zero-point correction=   0.154126 (Hartree/Particle)
Thermal correction to Energy=   0.165557
Thermal correction to Enthalpy=   0.166501
Thermal correction to Gibbs Free Energy=   0.115709
Sum of electronic and zero-point Energies=   -731.545185
Sum of electronic and thermal Energies=   -731.533754
Sum of electronic and thermal Enthalpies=   -731.532810
Sum of electronic and thermal Free Energies=   -731.583602

anti-TS8

C1   1.329886   1.578650   0.165301
C2   0.089928   0.806720   0.378002
H3   3.287832   1.181493   -0.306870
C4   2.331886   -0.655142   -0.256461
C5   -1.889036   0.069694   0.664282
N6   2.405750   0.705032   -0.149668
N7   -1.102656   1.219544   0.663943
N8   -1.094723   -1.072936   0.486670
N9   1.203673   -1.366673   -0.074778
C10   0.151818   -0.645504   0.235294
N11   3.430811   -1.329976   -0.560440
H12   3.362000   -2.335333   -0.638607
H13   4.327321   -0.894256   -0.716730
O14   1.484940   2.764330   0.233465
H15   -2.766391   0.012836   1.299006
O16   -2.706872   0.215419   -0.934670
O17   -3.729878   0.902759   -0.929804
C18   -1.582318   -2.446780   0.419082
H19   -2.058728   -2.625448   -0.547076
H20   -0.732748   -3.117850   0.540249
H21   -2.297774   -2.612288   1.225013

Zero-point correction=   0.151736 (Hartree/Particle)
Thermal correction to Energy=   0.164063
Thermal correction to Enthalpy=   0.165007
Thermal correction to Gibbs Free Energy=   0.111877
Sum of electronic and zero-point Energies=   -731.537330
Sum of electronic and thermal Energies=   -731.525004
Sum of electronic and thermal Enthalpies=   -731.524060
Sum of electronic and thermal Free Energies=   -731.577189

anti-8OO-9MG•+

C1   -1.590685   1.498278   -0.034512
C2   -0.223591   0.919248   -0.165272
H3   -3.506121   0.807975   0.194081
C4   -2.295199   -0.875838   0.116176
C5   1.892419   0.488368   -0.399663

N6   -2.552965   0.470945   0.103753
N7   0.886745   1.524418   -0.291190
N8   1.199587   -0.798388   -0.269028
N9   -1.071537   -1.418871   0.002414
C10   -0.089448   -0.556649   -0.132780
N11   -3.315252   -1.707031   0.250667
H12   -3.118369   -2.698824   0.261600
H13   -4.273415   -1.405076   0.347936
O14   -1.889860   2.655498   -0.042435
H15   2.429126   0.558730   -1.350604
O16   2.816584   0.669564   0.674367
O17   3.957444   0.081300   0.398531
C18   1.859500   -2.099458   -0.284997
H19   2.435343   -2.230531   0.633238
H20   1.090354   -2.867973   -0.353405
H21   2.525711   -2.156400   -1.146583

Zero-point correction=   0.154869 (Hartree/Particle)
Thermal correction to Energy=   0.166886
Thermal correction to Enthalpy=   0.167830
Thermal correction to Gibbs Free Energy=   0.115666
Sum of electronic and zero-point Energies=   -731.551405
Sum of electronic and thermal Energies=   -731.539388
Sum of electronic and thermal Enthalpies=   -731.538444
Sum of electronic and thermal Free Energies=   -731.590607

TS4–5

C1   1.393823   -1.224087   -0.275786
C2   -0.091312   -1.024555   -0.110766
H3   3.088754   -0.096324   -0.292161
C4   1.508090   1.254190   -0.130377
C5   -2.048703   -0.818153   -0.888850
N6   2.082472   -0.005905   -0.204410
N7   -1.016503   -1.670471   -0.835693
N8   -1.889700   0.376918   -0.318791
N9   0.213240   1.488700   -0.002123
C10   -0.551695   0.398793   0.229918
N11   2.337151   2.290306   -0.209070
H12   1.942971   3.216704   -0.127172
H13   3.327661   2.201662   -0.374615
O14   1.940700   -2.275868   -0.437279
H15   -2.970417   -1.065634   -1.405748
O16   -0.336075   -1.223419   1.634627
O17   -0.721579   0.037640   1.719662
C18   -2.792280   1.525199   -0.340325
H19   -3.665690   1.267963   -0.939040
H20   -3.106295   1.767375   0.675912
H21   -2.275513   2.376262   -0.785537

Zero-point correction=   0.152575 (Hartree/Particle)
Thermal correction to Energy=   0.164114
Thermal correction to Enthalpy=   0.165058
Thermal correction to Gibbs Free Energy=   0.114652
Sum of electronic and zero-point Energies=   -731.499490
Sum of electronic and thermal Energies=   -731.487950
Sum of electronic and thermal Enthalpies=   -731.487006
Sum of electronic and thermal Free Energies=   -731.537412

4,5-OO-9MG•+
```
C1   1.326210   -1.278513   -0.254555
C2   -0.131736   -1.023889   0.078775
H3   3.064647   -0.240250   -0.399238
C4   1.581405   1.194733   -0.098809
C5   -2.069105   -0.742755   -0.886006
N6   2.074555   -0.098731   -0.232148
N7   -1.143754   -1.660460   -0.705996
N8   -1.801578   0.486737   -0.389786
N9   0.314025   1.499687   0.072662
C10  -0.512482   0.437505   0.278255
N11  2.478854   2.176467   -0.179649
H12  2.154289   3.124252   -0.055196
H13  3.461315   2.022277   -0.341590
O14  1.803222   -2.352908   -0.482726
H15  -2.999298   -0.938460   -1.408833
O16  -0.456116   -1.261816   1.468412
O17  -0.820726   0.096754   1.680605
C18  -2.655672   1.662629   -0.419800
H19  -2.031825   2.528198   -0.648587
H20  -3.424293   1.527040   -1.180039
H21  -3.122304   1.796535   0.560418
```

Zero-point correction=   0.153196 (Hartree/Particle)
Thermal correction to Energy=   0.164738
Thermal correction to Enthalpy=   0.165682
Thermal correction to Gibbs Free Energy=   0.115512
Sum of electronic and zero-point Energies=   -731.508767
Sum of electronic and thermal Energies=   -731.497224
Sum of electronic and thermal Enthalpies=   -731.496280
Sum of electronic and thermal Free Energies=   -731.546450

TS5−58
```
C1   1.198950   -1.380387   -0.284982
C2   -0.212692   -0.869729   -0.056111
H3   3.130510   -0.724089   -0.093241
C4   1.929611   0.948389   0.085382
C5   -2.207501   -0.330912   -0.430637
N6   2.174957   -0.382013   -0.065433
N7   -1.292404   -1.266321   -0.932466
N8   -1.555847   0.926336   -0.397927
N9   0.706475   1.497098   -0.031865
C10  -0.267510   0.649196   -0.197809
N11  2.938961   1.764482   0.326345
H12  2.739925   2.752388   0.413199
H13  3.890915   1.451698   0.450654
O14  1.498540   -2.496733   -0.577988
H15  -3.266346   -0.384192   -0.654933
O16  -0.652508   -1.154497   1.267439
O17  -2.049470   -0.847634   1.252713
C18  -2.206638   2.229438   -0.299949
H19  -1.456037   2.997892   -0.480031
H20  -2.988292   2.293793   -1.057068
H21  -2.633488   2.350377   0.698161
```

Zero-point correction=   0.152588 (Hartree/Particle)
Thermal correction to Energy=   0.163838
Thermal correction to Enthalpy=   0.164782

Thermal correction to Gibbs Free Energy=   0.115059
Sum of electronic and zero-point Energies=   -731.495993
Sum of electronic and thermal Energies=   -731.484743
Sum of electronic and thermal Enthalpies=   -731.483799
Sum of electronic and thermal Free Energies=   -731.533523

TS8−58
```
C1   1.241755   -1.423144   -0.239365
C2   -0.124785   -0.830796   -0.304464
H3   3.155336   -0.777014   0.103207
C4   1.970751   0.924865   0.075863
C5   -2.189957   -0.376683   -0.353332
N6   2.208965   -0.421930   0.010549
N7   -1.194870   -1.326225   -0.919778
N8   -1.519171   0.909642   -0.443238
N9   0.757844   1.490319   -0.067122
C10  -0.227612   0.653650   -0.257019
N11  2.992045   1.734904   0.293734
H12  2.806349   2.727719   0.343729
H13  3.941182   1.415199   0.419699
O14  1.531732   -2.575905   -0.358826
H15  -3.188538   -0.411340   -0.778816
O16  -0.935866   -0.867999   1.410361
O17  -2.256961   -0.809613   1.005691
C18  -2.187190   2.192240   -0.257938
H19  -1.446326   2.982543   -0.372291
H20  -2.962878   2.303964   -1.016219
H21  -2.627830   2.239290   0.741398
```

Zero-point correction=   0.152472 (Hartree/Particle)
Thermal correction to Energy=   0.163768
Thermal correction to Enthalpy=   0.164712
Thermal correction to Gibbs Free Energy=   0.114835
Sum of electronic and zero-point Energies=   -731.492655
Sum of electronic and thermal Energies=   -731.481359
Sum of electronic and thermal Enthalpies=   -731.480415
Sum of electronic and thermal Free Energies=   -731.530292

TS-58
```
C1   1.224533   -1.396029   -0.244369
C2   -0.169702   -0.842951   -0.226837
H3   3.140228   -0.720873   0.019275
C4   1.932945   0.960959   0.062114
C5   -2.158170   -0.424590   -0.418432
N6   2.185125   -0.379686   -0.025227
N7   -1.214956   -1.290482   -0.962753
N8   -1.567179   0.906128   -0.393139
N9   0.710375   1.512533   -0.067189
C10  -0.269840   0.667101   -0.229266
N11  2.945093   1.784482   0.270866
H12  2.746927   2.774893   0.321448
H13  3.899879   1.477472   0.385675
O14  1.535456   -2.538705   -0.393153
H15  -3.205158   -0.493705   -0.695488
O16  -0.774366   -1.028001   1.342980
O17  -2.066741   -0.813546   1.095343
C18  -2.267556   2.171473   -0.214103
```

H19   -1.544294   2.978371   -0.327626
H20   -3.039918   2.261534   -0.978704
H21   -2.714909   2.217707   0.781512

Zero-point correction=   0.151744 (Hartree/Particle)
Thermal correction to Energy=   0.163293
Thermal correction to Enthalpy=   0.164237
Thermal correction to Gibbs Free Energy=   0.113821
Sum of electronic and zero-point Energies=   -731.494750
Sum of electronic and thermal Energies=   -731.483200
Sum of electronic and thermal Enthalpies=   -731.482256
Sum of electronic and thermal Free Energies=   -731.532673

5,8-OO-9MG•+
C1   1.186510   -1.410084   -0.214694
C2   -0.208414   -0.830605   -0.085586
H3   3.128357   -0.790099   -0.076912
C4   1.970947   0.923345   0.075051
C5   -2.204324   -0.337638   -0.320591
N6   2.181749   -0.423806   -0.059154
N7   -1.219587   -1.111998   -1.073039
N8   -1.530978   0.974544   -0.289475
N9   0.763664   1.511182   0.014929
C10   -0.244515   0.693015   -0.132289
N11   3.019319   1.707301   0.255585
H12   2.857355   2.701990   0.340106
H13   3.966840   1.366018   0.323616
O14   1.449537   -2.559201   -0.398208
H15   -3.223540   -0.321694   -0.699283
O16   -0.776615   -1.191635   1.174622
O17   -2.189835   -0.901450   0.967629
C18   -2.180907   2.274771   -0.196971
H19   -1.420613   3.047669   -0.303391
H20   -2.913196   2.365432   -1.000528
H21   -2.674857   2.371589   0.772601

Zero-point correction=   0.155112 (Hartree/Particle)
Thermal correction to Energy=   0.166258
Thermal correction to Enthalpy=   0.167202
Thermal correction to Gibbs Free Energy=   0.117633
Sum of electronic and zero-point Energies=   -731.522554
Sum of electronic and thermal Energies=   -731.511408
Sum of electronic and thermal Enthalpies=   -731.510464
Sum of electronic and thermal Free Energies=   -731.560033

[9MG − H]•
C1   -1.265843   1.317527   0.002428
C2   0.177761   1.009818   -0.000871
C3   -1.588799   -1.004453   -0.000842
C4   2.291041   0.948733   -0.005350
N5   -2.091355   0.203874   0.001747
N6   1.269762   1.797972   -0.002813
N7   1.930685   -0.365415   -0.007508
N8   -0.242656   -1.400872   -0.001992
C9   0.550670   -0.366945   -0.002549
N10   -2.433582   -2.057859   -0.002491
H11   -2.068927   -2.994521   -0.005188
H12   -3.424911   -1.885134   -0.002796

O13   -1.694373   2.460945   0.005976
H14   3.331830   1.245898   -0.007895
C15   2.783313   -1.538083   0.010732
H16   2.685791   -2.059757   0.965180
H17   2.494292   -2.213199   -0.796498
H18   3.818072   -1.224327   -0.130502

Zero-point correction=   0.132526 (Hartree/Particle)
Thermal correction to Energy=   0.142583
Thermal correction to Enthalpy=   0.143528
Thermal correction to Gibbs Free Energy=   0.096276
Sum of electronic and zero-point Energies=   -580.919671
Sum of electronic and thermal Energies=   -580.909613
Sum of electronic and thermal Enthalpies=   -580.908669
Sum of electronic and thermal Free Energies=   -580.955921

[9MG − H]• + ¹O₂
C1   -1.181492   1.492077   -0.207420
C2   0.250430   1.136087   -0.247742
C3   -1.581480   -0.755577   -0.741651
C4   2.357837   0.986663   -0.189115
N5   -2.043187   0.440007   -0.475040
N6   1.366960   1.856865   -0.031414
N7   1.954274   -0.276495   -0.501840
N8   -0.249961   -1.194341   -0.803016
C9   0.576457   -0.219405   -0.550833
N10   -2.460953   -1.745747   -1.003632
H11   -2.128587   -2.676053   -1.189271
H12   -3.445690   -1.541371   -0.971501
O13   -1.571014   2.621627   0.044087
H14   3.406930   1.229936   -0.081289
O15   -0.552817   -1.327872   2.480750
O16   0.144645   -0.344637   2.507984
C17   2.764680   -1.457353   -0.725729
H18   3.814172   -1.196464   -0.585966
H19   2.485611   -2.236778   -0.014131
H20   2.612516   -1.829191   -1.740863

Zero-point correction=   0.137177 (Hartree/Particle)
Thermal correction to Energy=   0.151394
Thermal correction to Enthalpy=   0.152339
Thermal correction to Gibbs Free Energy=   0.092107
Sum of electronic and zero-point Energies=   -731.195690
Sum of electronic and thermal Energies=   -731.181472
Sum of electronic and thermal Enthalpies=   -731.180528
Sum of electronic and thermal Free Energies=   -731.240759

syn-TS4
C1   -1.561783   1.270046   -0.038708
C2   -0.096403   1.005733   -0.293032
C3   -1.726990   -1.057052   -0.117605
C4   1.879880   0.879913   -1.049307
N5   -2.312231   0.142868   0.002094
N6   0.783473   1.715772   -0.931956
N7   1.708752   -0.330425   -0.608376
N8   -0.407293   -1.397906   -0.176757
C9   0.406128   -0.352525   0.051750
N10   -2.570743   -2.103174   -0.190405

H11 -2.204142 -3.039586 -0.184271
H12 -3.557869 -1.929198 -0.100814
O13 -1.956534   2.416441   0.087216
H14   2.800361   1.203603 -1.521515
O15   1.743206   0.517044   1.912780
O16   0.807892 -0.319244   1.613391
C17   2.636705 -1.443441 -0.568434
H18   3.450084 -1.260897 -1.270440
H19   3.029393 -1.549672   0.445340
H20   2.086736 -2.344179 -0.845590

Zero-point correction=   0.138589 (Hartree/Particle)
Thermal correction to Energy=   0.150441
Thermal correction to Enthalpy=   0.151385
Thermal correction to Gibbs Free Energy=   0.100073
Sum of electronic and zero-point Energies=   -731.140877
Sum of electronic and thermal Energies=   -731.129025
Sum of electronic and thermal Enthalpies=   -731.128081
Sum of electronic and thermal Free Energies=   -731.179392

syn-4-OO-[9MG − H]•
C1   -1.590861   1.221719 -0.012874
C2   -0.123114   0.999007 -0.296473
C3   -1.661130 -1.091090 -0.138602
C4   1.794508   0.866549 -1.196603
N5   -2.305252   0.073686   0.027058
N6   0.658935   1.643678 -1.109590
N7   1.752957 -0.258489 -0.550930
N8   -0.327717 -1.367659 -0.185440
C9   0.459251 -0.307499   0.157407
N10 -2.452259 -2.171810 -0.275462
H11 -2.042577 -3.090036 -0.293012
H12 -3.447699 -2.047955 -0.195507
O13 -2.006218   2.356569   0.145825
H14   2.644496   1.157929 -1.803384
O15   1.594086   0.620781   1.981118
O16   0.783850 -0.341081   1.627146
C17   2.735134 -1.320827 -0.469158
H18   3.512991 -1.153507 -1.214125
H19   3.170267 -1.335567   0.532136
H20   2.219408 -2.264010 -0.660455

Zero-point correction=   0.139430 (Hartree/Particle)
Thermal correction to Energy=   0.151691
Thermal correction to Enthalpy=   0.152635
Thermal correction to Gibbs Free Energy=   0.100361
Sum of electronic and zero-point Energies=   -731.140776
Sum of electronic and thermal Energies=   -731.128515
Sum of electronic and thermal Enthalpies=   -731.127571
Sum of electronic and thermal Free Energies=   -731.179846

rot-TS4
C1   1.567941 -1.128123 -0.171175
C2   0.063295 -1.015735 -0.272203
C3   1.454278   1.176475 -0.336051
C4   -1.931345 -1.036105 -1.010693
N5   2.197885   0.069514 -0.230470
N6   -0.743766 -1.730078 -1.003789

N7   -1.918436   0.103071 -0.385547
N8   0.100789   1.351608 -0.261039
C9   -0.569658   0.258666   0.204156
N10   2.137849   2.315373 -0.557673
H11   1.656334   3.197881 -0.535910
H12   3.143113   2.272082 -0.576976
O13   2.082789 -2.226624 -0.071944
H14 -2.804727 -1.396304 -1.542843
O15 -0.043303 -0.462012   2.353067
O16 -0.868907   0.292269   1.673006
C17 -2.950829   1.115904 -0.274817
H18 -3.790491   0.848776 -0.916714
H19 -3.276814   1.189537   0.764064
H20 -2.514374   2.066050 -0.590323

Zero-point correction=   0.139005 (Hartree/Particle)
Thermal correction to Energy=   0.150616
Thermal correction to Enthalpy=   0.151560
Thermal correction to Gibbs Free Energy=   0.100706
Sum of electronic and zero-point Energies=   -731.135017
Sum of electronic and thermal Energies=   -731.123406
Sum of electronic and thermal Enthalpies=   -731.122462
Sum of electronic and thermal Free Energies=   -731.173316

anti-TS4
C1   -1.506408   1.294534   0.105866
C2   -0.007984   1.155493 -0.028780
C3   -1.494156 -0.921025 -0.590568
C4   2.024741   1.301447 -0.614105
N5   -2.181173   0.172236 -0.236579
N6   0.868341   2.028458 -0.440213
N7   1.920276   0.023655 -0.390460
N8   -0.149082 -1.167860 -0.576665
C9   0.551804 -0.218431   0.067986
N10 -2.233453 -1.947246 -1.048800
H11 -1.796599 -2.841418 -1.195146
H12 -3.235717 -1.864471 -1.005448
O13 -1.981509   2.352703   0.480845
H14   2.949684   1.759763 -0.945559
O15 -0.056720 -1.362608   2.060508
O16   0.826886 -0.541181   1.617260
C17   2.900036 -1.032959 -0.534622
H18   2.466320 -1.807539 -1.170219
H19   3.803586 -0.626145 -0.987936
H20   3.120916 -1.450559   0.449762

Zero-point correction=   0.138785 (Hartree/Particle)
Thermal correction to Energy=   0.150557
Thermal correction to Enthalpy=   0.151501
Thermal correction to Gibbs Free Energy=   0.100330
Sum of electronic and zero-point Energies=   -731.139917
Sum of electronic and thermal Energies=   -731.128145
Sum of electronic and thermal Enthalpies=   -731.127201
Sum of electronic and thermal Free Energies=   -731.178372

anti-4-OO-[9MG − H]•
C1   -1.769840   1.043434   0.279080
C2   -0.283015   1.151096   0.022121

C3 -1.443119 -1.111994 -0.490070
C4   1.633540   1.591686 -0.776839
N5 -2.279095 -0.172392 -0.025975
N6   0.383818   2.118030 -0.539968
N7   1.785371   0.340160 -0.458133
N8 -0.080340 -1.125897 -0.566705
C9   0.508827 -0.111814   0.129394
N10 -2.028817 -2.229220 -0.958079
H11 -1.460506 -3.019384 -1.211428
H12 -3.029566 -2.309382 -0.888005
O13 -2.370861   2.007491   0.720656
H14 2.423084   2.170974 -1.242203
O15 1.396146 -1.531097   1.748304
O16 0.803080 -0.381960   1.589952
C17 2.921595 -0.536270 -0.678468
H18 3.634744 -0.039314 -1.336620
H19 3.388574 -0.779609   0.276923
H20 2.542253 -1.450360 -1.139253

Zero-point correction=   0.139358 (Hartree/Particle)
Thermal correction to Energy=   0.151599
Thermal correction to Enthalpy=   0.152543
Thermal correction to Gibbs Free Energy=   0.100162
Sum of electronic and zero-point Energies=   -731.137008
Sum of electronic and thermal Energies=   -731.124768
Sum of electronic and thermal Enthalpies=   -731.123823
Sum of electronic and thermal Free Energies=   -731.176204

TS-4–5

C1   1.482674 -1.140925 -0.287997
C2 -0.023719 -0.983251 -0.181952
C3   1.552951   1.190427 -0.168401
C4 -2.008307 -0.828821 -0.916047
N5   2.185711   0.028323 -0.230816
N6 -0.937955 -1.638555 -0.910451
N7 -1.893603   0.342012 -0.305073
N8   0.194537   1.469491 -0.115059
C9 -0.520408   0.405158   0.172702
N10 2.317831   2.294048 -0.179074
H11 1.889829   3.200062 -0.094145
H12 3.317909   2.189508 -0.228277
O13 1.966002 -2.247902 -0.412135
H14 -2.925015 -1.093396 -1.433245
O15 -0.313070 -1.227537   1.719947
O16 -0.683138   0.023669   1.796599
C17 -2.813773   1.462042 -0.290172
H18 -3.689743   1.212263 -0.890144
H19 -3.121728   1.674832   0.735373
H20 -2.311769   2.335888 -0.710336

Zero-point correction=   0.138759 (Hartree/Particle)
Thermal correction to Energy=   0.150470
Thermal correction to Enthalpy=   0.151414
Thermal correction to Gibbs Free Energy=   0.100503
Sum of electronic and zero-point Energies=   -731.124226
Sum of electronic and thermal Energies=   -731.112515
Sum of electronic and thermal Enthalpies=   -731.111571
Sum of electronic and thermal Free Energies=   -731.162482

syn-TS_5-OO-[9MG − H]•

C1   1.290636 -1.250404 -0.484234
C2 -0.135292 -0.808809 -0.326126
C3   1.846202   0.962436   0.045004
C4 -2.171209 -0.454251 -0.719159
N5   2.216701 -0.275406 -0.177596
N6 -1.285007 -1.407709 -0.773077
N7 -1.676978   0.814037 -0.455667
N8   0.563145   1.539743 -0.035292
C9 -0.335653   0.648247 -0.258695
N10 2.787522   1.863077   0.373196
H11 2.531611   2.823983   0.523432
H12 3.745302   1.560864   0.443186
O13 1.576449 -2.381111 -0.818988
H14 -3.226927 -0.590985 -0.922100
O15 -0.313406 -1.017088   1.548621
O16 -1.509422 -1.045701   1.870178
C17 -2.414359   2.055242 -0.331153
H18 -3.381100   1.945200 -0.824127
H19 -2.566332   2.306457   0.721498
H20 -1.851165   2.854730 -0.815137

Zero-point correction=   0.138945 (Hartree/Particle)
Thermal correction to Energy=   0.151058
Thermal correction to Enthalpy=   0.152002
Thermal correction to Gibbs Free Energy=   0.099922
Sum of electronic and zero-point Energies=   -731.175046
Sum of electronic and thermal Energies=   -731.162933
Sum of electronic and thermal Enthalpies=   -731.161989
Sum of electronic and thermal Free Energies=   -731.214070

syn-5-OO-[9MG − H]•

C1   1.160464 -1.168294 -0.680700
C2 -0.191150 -0.863362   0.014490
C3   1.770521   0.973475 -0.018628
C4 -2.241734 -0.523625 -0.556428
N5   2.123136 -0.219945 -0.431683
N6 -1.410738 -1.485158 -0.424910
N7 -1.747393   0.773053 -0.338370
N8   0.478387   1.531796   0.005801
C9 -0.429790   0.629801 -0.065082
N10 2.722669   1.843351   0.344126
H11 2.472867   2.787909   0.583631
H12 3.686350   1.552959   0.310685
O13 1.328059 -2.187084 -1.307166
H14 -3.280865 -0.649046 -0.841536
O15 0.075107 -1.237433   1.414258
O16 -0.882809 -0.857229   2.212568
C17 -2.456910   2.023252 -0.523556
H18 -2.974427   2.024497 -1.485635
H19 -3.176607   2.180603   0.283468
H20 -1.721005   2.827880 -0.513211

Zero-point correction=   0.140477 (Hartree/Particle)
Thermal correction to Energy=   0.152656
Thermal correction to Enthalpy=   0.153600
Thermal correction to Gibbs Free Energy=   0.101122
Sum of electronic and zero-point Energies=   -731.183533

Sum of electronic and thermal Energies=   -731.171354
Sum of electronic and thermal Enthalpies=   -731.170409
Sum of electronic and thermal Free Energies=   -731.222888

rot-TS5

C1	1.091946	-1.189125	-0.693595
C2	-0.210046	-0.902287	0.096574
C3	1.638042	1.020911	-0.238742
C4	-2.317505	-0.701475	-0.322159
N5	2.024395	-0.184877	-0.574962
N6	-1.426593	-1.611431	-0.207677
N7	-1.882906	0.626418	-0.199557
N8	0.319333	1.511862	-0.173099
C9	-0.533154	0.566607	-0.054736
N10	2.560478	1.966165	-0.018363
H11	2.273001	2.906715	0.192857
H12	3.535362	1.719186	-0.069779
O13	1.261934	-2.237056	-1.268855
H14	-3.367225	-0.895717	-0.515595
O15	0.122312	-1.261257	1.495184
O16	0.226379	-0.248336	2.304832
C17	-2.661213	1.821491	-0.463180
H18	-3.117001	1.771342	-1.455389
H19	-3.437755	1.943878	0.295145
H20	-1.982745	2.674089	-0.425883

Zero-point correction=   0.140362 (Hartree/Particle)
Thermal correction to Energy=   0.151726
Thermal correction to Enthalpy=   0.152670
Thermal correction to Gibbs Free Energy=   0.102361
Sum of electronic and zero-point Energies=   -731.180293
Sum of electronic and thermal Energies=   -731.168929
Sum of electronic and thermal Enthalpies=   -731.167984
Sum of electronic and thermal Free Energies=   -731.218294

anti-TS5

C1	1.172349	-1.224939	-0.604940
C2	-0.228345	-0.920532	-0.156648
C3	1.541591	1.066460	-0.338707
C4	-2.341759	-0.848631	-0.284740
N5	2.013385	-0.133158	-0.572220
N6	-1.362135	-1.704437	-0.283874
N7	-1.979589	0.483771	-0.231628
N8	0.196970	1.487236	-0.228671
C9	-0.608725	0.486744	-0.225308
N10	2.401498	2.093305	-0.249325
H11	2.056114	3.022308	-0.079008
H12	3.389118	1.905853	-0.303455
O13	1.514556	-2.344719	-0.924669
H14	-3.389621	-1.122193	-0.333139
O15	0.050912	-0.961146	1.720132
O16	0.683096	-0.009308	2.198021
C17	-2.832624	1.654492	-0.286838
H18	-2.555440	2.345136	0.511430
H19	-2.725782	2.158952	-1.250170
H20	-3.868725	1.342741	-0.150423

Zero-point correction=   0.138642 (Hartree/Particle)
Thermal correction to Energy=   0.150776
Thermal correction to Enthalpy=   0.151720
Thermal correction to Gibbs Free Energy=   0.099738
Sum of electronic and zero-point Energies=   -731.172520
Sum of electronic and thermal Energies=   -731.160385
Sum of electronic and thermal Enthalpies=   -731.159441
Sum of electronic and thermal Free Energies=   -731.211423

anti-5-OO-[9MG − H]•

C1	1.058179	-1.136883	-0.742488
C2	-0.229775	-0.899371	0.087353
C3	1.556904	1.080797	-0.267648
C4	-2.351366	-0.730624	-0.261338
N5	1.952643	-0.097993	-0.682857
N6	-1.435198	-1.622222	-0.217754
N7	-1.948647	0.598683	-0.071962
N8	0.232882	1.533999	-0.090489
C9	-0.591635	0.562089	0.011013
N10	2.465489	2.044763	-0.082043
H11	2.169318	2.967097	0.189254
H12	3.440970	1.825060	-0.201786
O13	1.243703	-2.188222	-1.309063
H14	-3.401098	-0.941964	-0.436074
O15	0.071606	-1.277582	1.493273
O16	0.873250	-0.455120	2.101679
C17	-2.737607	1.794440	-0.293437
H18	-2.454223	2.550135	0.440327
H19	-2.568724	2.192747	-1.298126
H20	-3.793085	1.551016	-0.165702

Zero-point correction=   0.140637 (Hartree/Particle)
Thermal correction to Energy=   0.152687
Thermal correction to Enthalpy=   0.153631
Thermal correction to Gibbs Free Energy=   0.101877
Sum of electronic and zero-point Energies=   -731.181878
Sum of electronic and thermal Energies=   -731.169828
Sum of electronic and thermal Enthalpies=   -731.168884
Sum of electronic and thermal Free Energies=   -731.220638

syn-TS8

C1	-1.440393	1.400755	-0.208080
C2	-0.057117	0.872548	-0.433039
C3	-2.041014	-0.840550	0.128871
C4	2.003743	0.469109	-0.720367
N5	-2.372331	0.429493	0.089563
N6	1.053823	1.471456	-0.747909
N7	1.433459	-0.784266	-0.664990
N8	-0.796480	-1.452598	-0.101868
C9	0.115170	-0.578787	-0.355777
N10	-2.997927	-1.735700	0.427025
H11	-2.771001	-2.714129	0.477386
H12	-3.929115	-1.404895	0.619484
O13	-1.692957	2.586284	-0.289546
H14	2.992880	0.605564	-1.136763
O15	2.491984	0.691183	1.140756
O16	1.483288	0.403088	1.801503
C17	2.134572	-2.045801	-0.527784

H18 2.381678 -2.235310 0.520757
H19 1.485791 -2.841661 -0.894457
H20 3.047670 -2.016357 -1.123797

Zero-point correction=   0.138987 (Hartree/Particle)
Thermal correction to Energy=   0.151039
Thermal correction to Enthalpy=   0.151983
Thermal correction to Gibbs Free Energy=   0.099728
Sum of electronic and zero-point Energies=   -731.177090
Sum of electronic and thermal Energies=   -731.165039
Sum of electronic and thermal Enthalpies=   -731.164095
Sum of electronic and thermal Free Energies= -731.216350

***syn*-8-OO-[9MG − H]•**
C1   -1.525791   1.454855   -0.105104
C2   -0.144904   0.880077   -0.305599
C3   -2.207222   -0.767920   0.166802
C4   1.960842   0.408481   -0.625845
N5   -2.498554   0.515148   0.133876
N6   0.970154   1.461847   -0.519157
N7   1.274885   -0.850970   -0.511791
N8   -0.980084   -1.422419   -0.021771
C9   -0.019326   -0.595970   -0.252568
N10 -3.206591   -1.627753   0.413563
H11 -3.019454   -2.615124   0.456622
H12 -4.131218   -1.263222   0.575351
O13 -1.721515   2.650899   -0.163684
H14 2.548558   0.499235   -1.542575
O15 2.965402   0.562043   0.421015
O16 2.449107   0.395449   1.609357
C17 1.921442   -2.145028   -0.464064
H18 2.419863   -2.294296   0.498210
H19 1.155109   -2.909794   -0.595571
H20 2.654268   -2.221859   -1.270302

Zero-point correction=   0.141431 (Hartree/Particle)
Thermal correction to Energy=   0.153412
Thermal correction to Enthalpy=   0.154356
Thermal correction to Gibbs Free Energy=   0.102217
Sum of electronic and zero-point Energies=   -731.189207
Sum of electronic and thermal Energies=   -731.177227
Sum of electronic and thermal Enthalpies=   -731.176283
Sum of electronic and thermal Free Energies= -731.228421

***rot*-TS8**
C1   -1.398003   1.542126   -0.155540
C2   -0.091934   0.794496   -0.277345
C3   -2.354855   -0.562879   0.211331
C4   1.935888   0.059415   -0.563476
N5   -2.484788   0.742432   0.099178
N6   1.088062   1.225623   -0.501299
N7   1.112303   -1.102288   -0.309095
N8   -1.213086   -1.369588   0.107840
C9   -0.149244   -0.680303   -0.129220
N10 -3.461252   -1.278293   0.463804
H11 -3.400787   -2.277600   0.560989
H12 -4.339358   -0.795908   0.564791
O13 -1.443818   2.747602   -0.284961

H14 2.440002   -0.000716   -1.534036
O15 3.002003   0.056608   0.434636
O16 3.170208   1.187604   1.066302
C17 1.579034   -2.473056   -0.316614
H18 2.302175   -2.635424   0.485828
H19 0.714202   -3.119646   -0.164402
H20 2.042626   -2.709215   -1.278793

Zero-point correction=   0.140542 (Hartree/Particle)
Thermal correction to Energy=   0.152067
Thermal correction to Enthalpy=   0.153012
Thermal correction to Gibbs Free Energy=   0.101599
Sum of electronic and zero-point Energies=   -731.180919
Sum of electronic and thermal Energies=   -731.169394
Sum of electronic and thermal Enthalpies=   -731.168450
Sum of electronic and thermal Free Energies= -731.219862

***anti*-TS8**
C1   -1.486639   1.525187   -0.127880
C2   -0.186325   0.827232   -0.370055
C3   -2.351017   -0.615569   0.274472
C4   1.817726   0.169316   -0.702264
N5   -2.527999   0.682435   0.201090
N6   0.993686   1.284655   -0.671103
N7   1.093339   -1.001426   -0.561475
N8   -1.188990   -1.376974   0.055066
C9   -0.185383   -0.629870   -0.259771
N10 -3.404598   -1.382473   0.603965
H11 -3.298044   -2.379973   0.674158
H12 -4.289383   -0.938426   0.787457
O13 -1.593072   2.732248   -0.221256
H14 2.744124   0.174731   -1.263759
O15 2.666964   0.320494   0.997977
O16 3.841293   0.716399   0.952951
C17 1.636189   -2.343702   -0.484149
H18 2.077493   -2.524835   0.499363
H19 0.823312   -3.050626   -0.652264
H20 2.395646   -2.473101   -1.257246

Zero-point correction=   0.137888 (Hartree/Particle)
Thermal correction to Energy=   0.150369
Thermal correction to Enthalpy=   0.151313
Thermal correction to Gibbs Free Energy=   0.097145
Sum of electronic and zero-point Energies=   -731.168530
Sum of electronic and thermal Energies=   -731.156049
Sum of electronic and thermal Enthalpies=   -731.155105
Sum of electronic and thermal Free Energies= -731.209273

***anti*-8-OO-[9MG − H]•**
C1   1.666628   1.459794   0.032438
C2   0.269771   0.901701   0.160004
C3   2.343175   -0.775104   -0.127853
C4   -1.853506   0.461725   0.405185
N5   2.644496   0.506575   -0.106874
N6   -0.847872   1.498878   0.310025
N7   -1.184640   -0.811120   0.255124
N8   1.098517   -1.413203   -0.027064
C9   0.129668   -0.573931   0.111505

N10   3.351271 -1.648833 -0.265463
H11   3.159722 -2.635968 -0.292136
H12   4.290353 -1.296058 -0.353604
O13   1.866705   2.656222   0.062705
H14 -2.425058   0.530356   1.334974
O15 -2.784231   0.670905 -0.683590
O16 -3.941112   0.120565 -0.412436
C17 -1.829130 -2.106805   0.320111
H18 -2.549645 -2.216678 -0.493722
H19 -1.053173 -2.867293   0.226160
H20 -2.345136 -2.226262   1.276303

Zero-point correction=   0.141202 (Hartree/Particle)
Thermal correction to Energy=   0.153365
Thermal correction to Enthalpy=   0.154309
Thermal correction to Gibbs Free Energy=   0.101457
Sum of electronic and zero-point Energies=   -731.188888
Sum of electronic and thermal Energies=   -731.176725
Sum of electronic and thermal Enthalpies=   -731.175781
Sum of electronic and thermal Free Energies=   -731.228632

TS-8–58
C1   1.343968 -1.380735 -0.211716
C2   -0.061535 -0.830837 -0.304063
C3   2.001442   0.847778   0.067454
C4   -2.149237 -0.403253 -0.364444
N5   2.304901 -0.431395   0.028118
N6   -1.131425 -1.352983 -0.889147
N7   -1.513056   0.881833 -0.523740
N8   0.765123   1.484433 -0.124773
C9   -0.194744   0.652857 -0.298141
N10   2.988878   1.718765   0.318895
H11   2.789702   2.703697   0.363936
H12   3.918589   1.365751   0.477149
O13   1.555140 -2.567382 -0.340425
H14 -3.139788 -0.479645 -0.805056
O15 -2.251661 -0.778168   1.004392
O16 -0.929399 -0.804087   1.442936
C17 -2.179380   2.136787 -0.232062
H18 -2.396259   2.222806   0.837813
H19 -1.520951   2.951482 -0.534004
H20 -3.107952   2.192862 -0.802700

Zero-point correction=   0.139125 (Hartree/Particle)
Thermal correction to Energy=   0.150393
Thermal correction to Enthalpy=   0.151338
Thermal correction to Gibbs Free Energy=   0.101322
Sum of electronic and zero-point Energies=   -731.129732
Sum of electronic and thermal Energies=   -731.118464
Sum of electronic and thermal Enthalpies=   -731.117520
Sum of electronic and thermal Free Energies=   -731.167536

TS-5–45
C1   1.185297 -1.320541 -0.408949
C2   -0.168505 -0.984156   0.224828
C3   1.685423   0.973290 -0.206814
C4   -2.203325 -0.807382 -0.464445
N5   2.081876 -0.274844 -0.393269

N6   -1.346934 -1.714545 -0.160912
N7   -1.795973   0.522425 -0.393673
N8   0.395038   1.462871 -0.154996
C9   -0.506733   0.504258   0.107376
N10   2.634442   1.923835 -0.135457
H11   2.368447   2.888878 -0.038887
H12   3.599527   1.658532 -0.241387
O13   1.434763 -2.423757 -0.836957
H14 -3.212679 -1.025807 -0.799065
O15 -0.003851 -0.894130   1.652276
O16 -0.515340   0.394534   1.773535
C17 -2.581460   1.703423 -0.690695
H18 -1.908904   2.483009 -1.051669
H19 -3.302427   1.467188 -1.475227
H20 -3.111853   2.063484   0.195754

Zero-point correction=   0.138206 (Hartree/Particle)
Thermal correction to Energy=   0.149799
Thermal correction to Enthalpy=   0.150743
Thermal correction to Gibbs Free Energy=   0.099857
Sum of electronic and zero-point Energies=   -731.137755
Sum of electronic and thermal Energies=   -731.126162
Sum of electronic and thermal Enthalpies=   -731.125218
Sum of electronic and thermal Free Energies=   -731.176104

4,5-OO-[9MG − H]•
C1   1.257910 -1.293636 -0.301713
C2   -0.152289 -1.010041   0.200743
C3   1.677489   1.041728 -0.210353
C4   -2.108300 -0.835185 -0.687296
N5   2.111853 -0.195306 -0.363009
N6   -1.230302 -1.734234 -0.408995
N7   -1.787284   0.484995 -0.441605
N8   0.367494   1.470485 -0.184673
C9   -0.531112   0.469951   0.216400
N10   2.587042   2.034641 -0.175170
H11   2.283273   2.992865 -0.141186
H12   3.561783   1.806068 -0.281501
O13   1.628120 -2.406146 -0.593139
H14 -3.066435 -1.063026 -1.144904
O15 -0.188609 -0.993084   1.647409
O16 -0.579313   0.417834   1.662867
C17 -2.686787   1.619561 -0.487469
H18 -2.118758   2.512517 -0.755492
H19 -3.441266   1.444498 -1.256775
H20 -3.183275   1.779903   0.475049

Zero-point correction=   0.139342 (Hartree/Particle)
Thermal correction to Energy=   0.151126
Thermal correction to Enthalpy=   0.152070
Thermal correction to Gibbs Free Energy=   0.100483
Sum of electronic and zero-point Energies=   -731.144135
Sum of electronic and thermal Energies=   -731.132350
Sum of electronic and thermal Enthalpies=   -731.131406
Sum of electronic and thermal Free Energies=   -731.182993

TS-58
C1   1.332508 -1.347733 -0.226757

C2 -0.103153 -0.852764 -0.245912
C3   1.945143   0.897532   0.042896
C4 -2.118480 -0.484301 -0.386452
N5   2.272519 -0.372621   0.008539
N6 -1.162719 -1.362339 -0.900756
N7 -1.578885   0.849443 -0.499630
N8   0.697874   1.506016 -0.185261
C9 -0.249958   0.654859 -0.309156
N10 2.906983   1.793949   0.307744
H11 2.689313   2.775867   0.317393
H12 3.844616   1.465477   0.471684
O13 1.583816 -2.520501 -0.390614
H14 -3.166412 -0.605475 -0.642764
O15 -0.706742 -0.894375   1.392250
O16 -2.015901 -0.763727   1.134128
C17 -2.280503   2.082274 -0.198753
H18 -1.691465   2.914293 -0.585879
H19 -3.251840   2.068665 -0.695874
H20 -2.417334   2.209657   0.879662

Zero-point correction=   0.138399 (Hartree/Particle)
Thermal correction to Energy=   0.149894
Thermal correction to Enthalpy=   0.150838
Thermal correction to Gibbs Free Energy=   0.100405
Sum of electronic and zero-point Energies=   -731.131624
Sum of electronic and thermal Energies=   -731.120130
Sum of electronic and thermal Enthalpies=   -731.119186
Sum of electronic and thermal Free Energies=   -731.169619

5,8-OO-[9MG – H]•
C1   1.285279 -1.359133 -0.212864
C2 -0.148880 -0.822607 -0.085924
C3   1.992022   0.854046   0.061774
C4 -2.166739 -0.369652 -0.307237
N5   2.271844 -0.427310 -0.035673
N6 -1.179006 -1.155689 -1.039438
N7 -1.538914   0.944688 -0.350967
N8   0.760657   1.513144 -0.061307
C9 -0.220675   0.696094 -0.177163
N10 3.006358   1.701177   0.287276
H11 2.829850   2.689480   0.349151
H12 3.938367   1.330319   0.374830
O13 1.469032 -2.535750 -0.430093
H14 -3.191658 -0.399963 -0.669878
O15 -0.706319 -1.150201   1.197619
O16 -2.133120 -0.889445   1.005759
C17 -2.203252   2.220132 -0.180278
H18 -1.466446   3.007915 -0.339695
H19 -3.002171   2.319099 -0.918214
H20 -2.617808   2.310965   0.828433

Zero-point correction=   0.141446 (Hartree/Particle)
Thermal correction to Energy=   0.152620
Thermal correction to Enthalpy=   0.153564
Thermal correction to Gibbs Free Energy=   0.103693
Sum of electronic and zero-point Energies=   -731.159440
Sum of electronic and thermal Energies=   -731.148266
Sum of electronic and thermal Enthalpies=   -731.147322
Sum of electronic and thermal Free Energies=   -731.197192

Base-pair reactions

9MG•+·1MC
```
C1  -1.370863  1.199721  -0.004826
C2  -2.808239  0.937588  -0.005955
H3  0.421997  0.141223  -0.000071
C4  -1.151816  -1.242470  0.002837
C5  -4.913851  0.961273  -0.009560
N6  -0.627718  0.016178  -0.000791
N7  -3.848633  1.770359  -0.011955
N8  -4.609506  -0.362113  -0.003367
N9  -2.496630  -1.505787  0.005113
C10  -3.235872  -0.428210  0.000149
N11  -0.332697  -2.265895  0.004352
H12  -0.747275  -3.187473  0.007555
H13  0.712753  -2.143923  0.000333
O14  -0.834544  2.289937  -0.006422
C15  2.869679  -0.786814  -0.002824
N16  2.175795  0.377749  0.001858
C17  2.816386  1.553335  0.007130
C18  4.914363  0.439378  0.003438
N19  4.261073  -0.752744  -0.002692
H20  5.997101  0.390028  0.003621
O21  2.310941  -1.896908  -0.007391
N22  2.083191  2.669083  0.010714
H23  1.066473  2.620623  0.006218
H24  2.525791  3.572978  0.013897
C25  4.245222  1.616870  0.008913
H26  4.774158  2.560233  0.013839
C27  4.977885  -2.029000  -0.010092
H28  4.706172  -2.611663  0.870871
H29  4.714052  -2.597107  -0.902948
H30  6.048772  -1.827925  -0.003669
C31  -5.522490  -1.499530  0.016516
H32  -5.270479  -2.179686  -0.797536
H33  -5.439901  -2.021690  0.970716
H34  -6.539030  -1.130761  -0.115672
H35  -5.938305  1.310239  -0.013626
```

Zero-point correction=　　　　　　0.277088 (Hartree/Particle)
Thermal correction to Energy=　　　　　　0.295954
Thermal correction to Enthalpy=　　　　　　0.296898
Thermal correction to Gibbs Free Energy=　　　　0.228058
Sum of electronic and zero-point Energies=　　　　-1015.368420
Sum of electronic and thermal Energies=　　　　-1015.349554
Sum of electronic and thermal Enthalpies=　　　　-1015.348610
Sum of electronic and thermal Free Energies=　　-1015.417449

9MG•+·1MC + $^1O_2$
```
C1  0.997910  1.083280  -0.488396
C2  2.423138  0.778988  -0.595222
H3  -0.808959  0.082953  -0.233756
C4  0.726614  -1.342845  -0.255431
C5  4.520987  0.740045  -0.765530
N6  0.232750  -0.073058  -0.319034
N7  3.477596  1.577326  -0.754221
N8  4.187539  -0.569315  -0.626607
```

```
N9  2.058667  -1.645695  -0.352936
C10  2.818224  -0.594775  -0.509742
N11  -0.112823  -2.336427  -0.092222
H12  0.278890  -3.266854  -0.048682
H13  -1.150493  -2.182906  -0.010139
O14  0.488683  2.185536  -0.534133
C15  -3.267779  -0.765626  0.070145
N16  -2.551106  0.373260  -0.093904
C17  -3.162065  1.563753  -0.134654
C18  -5.274972  0.518103  0.157472
N19  -4.651683  -0.689129  0.198429
H20  -6.353375  0.502523  0.264890
O21  -2.737057  -1.888489  0.112279
N22  -2.407063  2.652812  -0.297791
H23  -1.396308  2.573232  -0.388130
H24  -2.827260  3.566548  -0.335165
C25  -4.582454  1.670565  -0.006659
H26  -5.087760  2.626256  -0.037899
C27  -5.392060  -1.939279  0.375773
H28  -5.228827  -2.591774  -0.482737
H29  -5.045288  -2.449234  1.275157
H30  -6.452736  -1.707812  0.468432
C31  5.071831  -1.727487  -0.575271
H32  4.984636  -2.210864  0.398751
H33  4.796153  -2.432165  -1.360469
H34  6.096191  -1.389764  -0.728048
H35  5.549794  1.056242  -0.877422
O36  3.171801  0.435593  2.394900
O37  4.293069  0.878219  2.380495
```

Zero-point correction=　　　　　　0.281686 (Hartree/Particle)
Thermal correction to Energy=　　　　　　0.304674
Thermal correction to Enthalpy=　　　　　　0.305618
Thermal correction to Gibbs Free Energy=　　　　0.224119
Sum of electronic and zero-point Energies=　　　　-1165.645211
Sum of electronic and thermal Energies=　　　　-1165.622223
Sum of electronic and thermal Enthalpies=　　　　-1165.621279
Sum of electronic and thermal Free Energies=　　-1165.702778

syn-**TS4**
```
C1  0.956230  1.169972  -0.268785
C2  2.423264  0.915716  -0.380554
H3  -0.795013  0.104344  -0.105038
C4  0.832408  -1.271946  -0.179271
C5  4.471691  0.825329  -0.902514
N6  0.255183  0.000827  -0.146636
N7  3.337655  1.643378  -0.919606
N8  4.264335  -0.384089  -0.479695
N9  2.142257  -1.507069  -0.167463
C10  2.911894  -0.415286  0.062457
N11  -0.016511  -2.276795  -0.226114
H12  0.373607  -3.207472  -0.206845
H13  -1.049528  -2.140204  -0.229574
O14  0.460048  2.276749  -0.292672
H15  5.432009  1.172536  -1.266009
O16  3.996501  0.610582  1.976873
O17  3.148954  -0.292147  1.632881
```

C18 5.205118 -1.485792 -0.327083
H19 6.125325 -1.246633 -0.858116
H20 5.408019 -1.632489 0.735855
H21 4.741685 -2.382226 -0.740650
C22 -3.249609 -0.786527 -0.063903
N23 -2.553914 0.379546 -0.052916
C24 -3.190338 1.550638 0.053355
C25 -5.285373 0.437813 0.164785
N26 -4.638850 -0.751109 0.047377
H27 -6.364706 0.387965 0.250687
O28 -2.696848 -1.891025 -0.169321
N29 -2.457871 2.669080 0.045225
H30 -1.449038 2.623850 -0.068832
H31 -2.898402 3.570912 0.116387
C32 -4.613891 1.614335 0.173369
H33 -5.136995 2.556328 0.266369
C34 -5.357281 -2.025779 0.027301
H35 -5.188742 -2.531468 -0.924389
H36 -4.997096 -2.666203 0.832992
H37 -6.421031 -1.829734 0.158928

Zero-point correction=   0.283473 (Hartree/Particle)
Thermal correction to Energy=   0.304072
Thermal correction to Enthalpy=   0.305016
Thermal correction to Gibbs Free Energy=   0.232920
Sum of electronic and zero-point Energies=   -1165.590404
Sum of electronic and thermal Energies=   -1165.569805
Sum of electronic and thermal Enthalpies=   -1165.568861
Sum of electronic and thermal Free Energies=   -1165.640957

syn-4-OO-9MG•+·1MC
C1 0.957448 1.182608 -0.258037
C2 2.423483 0.917824 -0.391603
H3 -0.795391 0.115596 -0.067199
C4 0.853060 -1.242097 -0.173194
C5 4.414122 0.728909 -1.094295
N6 0.256409 0.019068 -0.109999
N7 3.268139 1.522002 -1.150527
N8 4.285347 -0.368921 -0.421524
N9 2.165533 -1.457285 -0.151243
C10 2.937663 -0.370039 0.183717
N11 0.021048 -2.258497 -0.262262
H12 0.422874 -3.184331 -0.256551
H13 -1.012843 -2.134356 -0.268637
O14 0.470659 2.293308 -0.277703
H15 5.323901 1.000902 -1.617323
O16 3.854326 0.700883 2.023355
O17 3.117406 -0.315111 1.655206
C18 5.249057 -1.435384 -0.189206
H19 6.131236 -1.262932 -0.804020
H20 5.520373 -1.442676 0.868262
H21 4.770494 -2.379901 -0.453871
C22 -3.229992 -0.794699 -0.074377
N23 -2.543078 0.376189 -0.042107
C24 -3.186925 1.541811 0.074962
C25 -5.274726 0.413486 0.160463
N26 -4.619985 -0.769714 0.030683

H27 -6.354146 0.355364 0.239909
O28 -2.668417 -1.893093 -0.193726
N29 -2.460569 2.664479 0.084663
H30 -1.451669 2.627411 -0.031532
H31 -2.906659 3.563073 0.162093
C32 -4.611440 1.594528 0.187844
H33 -5.141544 2.531698 0.289602
C34 -5.329996 -2.048581 -0.009980
H35 -5.154794 -2.540156 -0.967862
H36 -4.968610 -2.697816 0.788092
H37 -6.395445 -1.861199 0.120425

Zero-point correction=   0.283788 (Hartree/Particle)
Thermal correction to Energy=   0.305081
Thermal correction to Enthalpy=   0.306025
Thermal correction to Gibbs Free Energy=   0.231802
Sum of electronic and zero-point Energies=   -1165.591005
Sum of electronic and thermal Energies=   -1165.569711
Sum of electronic and thermal Enthalpies=   -1165.568767
Sum of electronic and thermal Free Energies=   -1165.642990

rot-TS4
C1 1.010317 1.196560 -0.248895
C2 2.479273 0.937122 -0.358310
C3 0.917520 -1.224900 -0.163798
C4 4.462056 0.732382 -1.089980
N5 0.311684 0.029014 -0.111436
N6 3.317411 1.521632 -1.143691
N7 4.348497 -0.349893 -0.387229
N8 2.234384 -1.431598 -0.138043
C9 2.999041 -0.347021 0.223225
N10 0.097156 -2.250120 -0.251945
H11 0.508417 -3.171795 -0.241349
H12 -0.938352 -2.135738 -0.269998
O13 0.517535 2.302861 -0.288523
H14 5.362413 0.991410 -1.635758
O15 2.605880 0.710724 2.232639
O16 3.265220 -0.274844 1.674081
C17 5.310075 -1.423604 -0.171169
H18 6.188491 -1.248319 -0.790810
H19 5.587260 -1.444828 0.884041
H20 4.825389 -2.362672 -0.444875
H21 -0.740748 0.118649 -0.080416
C22 -3.165998 -0.813404 -0.107853
N23 -2.488257 0.362388 -0.075534
C24 -3.140928 1.524190 0.029193
C25 -5.221390 0.381281 0.100247
N26 -4.556976 -0.798083 -0.016019
H27 -6.301098 0.315769 0.169373
O28 -2.595169 -1.908491 -0.215827
N29 -2.422064 2.651471 0.040169
H30 -1.411299 2.620494 -0.062385
H31 -2.874368 3.547457 0.111518
C32 -4.566986 1.567256 0.127276
H33 -5.104866 2.501099 0.218334
C34 -5.257522 -2.082132 -0.055747
H35 -5.072569 -2.576833 -1.010196

H36   -4.896905   -2.725067   0.747737
H37   -6.325101   -1.901696   0.066804

Zero-point correction=   0.283582 (Hartree/Particle)
Thermal correction to Energy=   0.304127
Thermal correction to Enthalpy=   0.305071
Thermal correction to Gibbs Free Energy=   0.232598
Sum of electronic and zero-point Energies=   -1165.586881
Sum of electronic and thermal Energies=   -1165.566337
Sum of electronic and thermal Enthalpies=   -1165.565392
Sum of electronic and thermal Free Energies=   -1165.637865

anti-TS-4

C1   1.016016   1.278087   -0.169765
C2   2.488880   1.054257   -0.285982
H3   -0.719472   0.171308   -0.119414
C4   0.940380   -1.154926   -0.305968
C5   4.529708   1.030541   -0.840964
N6   0.333010   0.093974   -0.166055
N7   3.383549   1.818765   -0.818116
N8   4.365585   -0.186357   -0.415092
N9   2.259801   -1.356332   -0.314475
C10   2.995963   -0.291620   0.075245
N11   0.122000   -2.171667   -0.460684
H12   0.537177   -3.089832   -0.519018
H13   -0.914718   -2.062902   -0.450898
O14   0.505110   2.376003   -0.093462
H15   5.475100   1.404242   -1.217609
O16   2.275665   -0.830348   2.264733
O17   3.250402   -0.263087   1.660138
C18   5.328406   -1.274727   -0.308998
H19   6.246405   -0.993854   -0.823267
H20   5.525603   -1.466344   0.747542
H21   4.883850   -2.159552   -0.767070
C22   -3.145757   -0.779351   -0.180475
N23   -2.478070   0.396775   -0.061566
C24   -3.141697   1.539905   0.138296
C25   -5.211315   0.375127   0.128901
N26   -4.536382   -0.784750   -0.082397
H27   -6.289941   0.293918   0.198030
O28   -2.566355   -1.857997   -0.373934
N29   -2.434330   2.670283   0.236007
H30   -1.423191   2.656663   0.134351
H31   -2.895360   3.553018   0.379742
C32   -4.567545   1.561384   0.246007
H33   -5.113229   2.480234   0.412233
C34   -5.224628   -2.069169   -0.215309
H35   -5.026540   -2.497411   -1.198711
H36   -4.866044   -2.762030   0.546641
H37   -6.294827   -1.905918   -0.091616

Zero-point correction=   0.283325 (Hartree/Particle)
Thermal correction to Energy=   0.303962
Thermal correction to Enthalpy=   0.304906
Thermal correction to Gibbs Free Energy=   0.232687
Sum of electronic and zero-point Energies=   -1165.590952
Sum of electronic and thermal Energies=   -1165.570314
Sum of electronic and thermal Enthalpies=   -1165.569370
Sum of electronic and thermal Free Energies=   -1165.641590

anti-4-OO-9MG•+·1MC

C1   1.012527   1.276433   -0.170792
C2   2.485542   1.048383   -0.292021
H3   -0.723836   0.169741   -0.111965
C4   0.944832   -1.151182   -0.290476
C5   4.508448   0.993537   -0.913946
N6   0.329054   0.094651   -0.158710
N7   3.357480   1.775712   -0.904965
N8   4.368459   -0.191606   -0.404103
N9   2.263204   -1.348002   -0.283280
C10   3.005015   -0.284466   0.129516
N11   0.131414   -2.171625   -0.452255
H12   0.549462   -3.088917   -0.502149
H13   -0.904970   -2.065592   -0.453930
O14   0.506772   2.376960   -0.097007
H15   5.436600   1.345529   -1.349791
O16   2.259229   -0.730524   2.295661
O17   3.274133   -0.259520   1.652884
C18   5.337662   -1.271591   -0.275009
H19   6.248285   -1.003564   -0.808982
H20   5.548394   -1.429232   0.784366
H21   4.891007   -2.172277   -0.699588
C22   -3.143585   -0.783065   -0.185243
N23   -2.478199   0.393851   -0.060789
C24   -3.143326   1.535236   0.142823
C25   -5.211036   0.367253   0.127782
N26   -4.534377   -0.790777   -0.088019
H27   -6.289580   0.284179   0.196038
O28   -2.562030   -1.859590   -0.382867
N29   -2.437233   2.666169   0.244899
H30   -1.426359   2.654620   0.140584
H31   -2.899387   3.548020   0.390433
C32   -4.569224   1.554131   0.249995
H33   -5.116521   2.471421   0.419501
C34   -5.220629   -2.075659   -0.226368
H35   -5.020005   -2.500475   -1.210729
H36   -4.862609   -2.770493   0.534070
H37   -6.291290   -1.914240   -0.104255

Zero-point correction=   0.283746 (Hartree/Particle)
Thermal correction to Energy=   0.304996
Thermal correction to Enthalpy=   0.305940
Thermal correction to Gibbs Free Energy=   0.232069
Sum of electronic and zero-point Energies=   -1165.590581
Sum of electronic and thermal Energies=   -1165.569332
Sum of electronic and thermal Enthalpies=   -1165.568388
Sum of electronic and thermal Free Energies=   -1165.642259

TS-4–5

C1   1.035270   1.161975   -0.097119
C2   2.524204   0.943235   -0.085272
C3   0.884065   -1.284468   -0.009372
C4   4.410367   0.728393   -1.019337
N5   3.387539   1.587931   -0.879601
N6   4.292712   -0.463440   -0.443338
N7   2.202017   -1.542396   -0.024085
C8   2.986332   -0.485388   0.185828

N9   0.036022   -2.284077   -0.020512
H10   0.428098   -3.214708   -0.002059
H11   -1.001901   -2.147225   -0.035521
O12   0.524502   2.257354   -0.165958
H13   5.286213   0.973463   -1.611494
O14   2.920849   1.119664   1.678291
O15   3.286001   -0.141780   1.718304
C16   5.171983   -1.621715   -0.548491
H17   5.948762   -1.407413   -1.282194
H18   5.628896   -1.830153   0.420090
H19   4.581626   -2.479221   -0.874848
C20   -3.183656   -0.806002   -0.042529
N21   -2.491031   0.360765   -0.062029
C22   -3.135452   1.533120   -0.075599
C23   -5.231629   0.416861   -0.041147
N24   -4.576202   -0.773304   -0.032205
H25   -6.314277   0.365928   -0.030633
O26   -2.623568   -1.913396   -0.033379
N27   -2.406405   2.652739   -0.100982
H28   -1.391444   2.606976   -0.126788
H29   -2.852158   3.554812   -0.116851
C30   -4.564121   1.595264   -0.062929
H31   -5.094207   2.537944   -0.071436
C32   -5.289736   -2.051049   -0.009876
H33   -5.020672   -2.640630   -0.887051
H34   -5.019733   -2.610989   0.886313
H35   -6.361195   -1.852781   -0.012567
N36   0.326424   -0.011059   -0.005707
H37   -0.723594   0.097789   -0.018751

Zero-point correction=   0.283028 (Hartree/Particle)
Thermal correction to Energy=   0.303658
Thermal correction to Enthalpy=   0.304602
Thermal correction to Gibbs Free Energy=   0.231710
Sum of electronic and zero-point Energies=   -1165.572299
Sum of electronic and thermal Energies=   -1165.551669
Sum of electronic and thermal Enthalpies=   -1165.550725
Sum of electronic and thermal Free Energies=   -1165.623617

syn-TS-5
C1   -1.056779   -1.060955   -0.267029
C2   -2.507440   -0.773485   -0.119320
H3   0.759114   -0.060745   -0.180515
C4   -0.786547   1.368839   -0.149447
C5   -4.555589   -0.766116   -0.569980
N6   -0.289268   0.091368   -0.186950
N7   -3.557042   -1.588659   -0.464389
N8   -4.225581   0.592862   -0.517316
N9   -2.115421   1.676270   -0.261763
C10   -2.891885   0.639658   -0.317173
N11   0.062695   2.354087   -0.030501
H12   -0.317669   3.290446   -0.027980
H13   1.099420   2.193073   0.049489
O14   -0.571703   -2.163002   -0.388633
C15   3.214655   0.772873   0.050933
N16   2.493578   -0.360972   -0.132559
C17   3.104419   -1.547689   -0.237335

C18   5.224731   -0.508235   0.019784
N19   4.601740   0.694693   0.129762
H20   6.306143   -0.494241   0.091027
O21   2.683890   1.891539   0.153556
N22   2.346399   -2.633291   -0.411698
H23   1.332695   -2.557855   -0.438829
H24   2.766313   -3.544960   -0.485296
C25   4.528312   -1.655210   -0.165496
H26   5.033151   -2.607749   -0.251563
C27   5.346228   1.938503   0.334053
H28   5.140805   2.631325   -0.482661
H29   5.041081   2.402552   1.272629
H30   6.410690   1.707990   0.364979
C31   -5.134719   1.725973   -0.635341
H32   -5.611497   1.927440   0.325769
H33   -4.557300   2.596379   -0.946506
H34   -5.890550   1.504693   -1.389350
H35   -5.582293   -1.064916   -0.746257
O36   -2.599157   -0.717552   1.695799
O37   -3.770796   -0.825093   2.078161

Zero-point correction=   0.282873 (Hartree/Particle)
Thermal correction to Energy=   0.303966
Thermal correction to Enthalpy=   0.304910
Thermal correction to Gibbs Free Energy=   0.230516
Sum of electronic and zero-point Energies=   -1165.619223
Sum of electronic and thermal Energies=   -1165.598130
Sum of electronic and thermal Enthalpies=   -1165.597185
Sum of electronic and thermal Free Energies=   -1165.671579

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C1   1.081833   1.055653   -0.117783
C2   2.530415   0.761309   0.256423
H3   -0.743792   0.065252   -0.169224
C4   0.813312   -1.364071   -0.103112
C5   4.499744   0.873841   -0.582151
N6   0.307332   -0.088612   -0.133289
N7   3.579474   1.644041   -0.143872
N8   4.181850   -0.502945   -0.657163
N9   2.137856   -1.649224   -0.294323
C10   2.914640   -0.616293   -0.245016
N11   -0.025528   -2.354205   0.023221
H12   0.355308   -3.289972   -0.013855
H13   -1.061307   -2.194354   0.120357
O14   0.633523   2.161836   -0.293239
C15   -3.175514   -0.762601   0.047806
N16   -2.452900   0.366316   -0.161338
C17   -3.062007   1.547798   -0.320065
C18   -5.185521   0.512065   -0.077842
N19   -4.563778   -0.684819   0.090103
H20   -6.268312   0.498085   -0.032169
O21   -2.644020   -1.874525   0.204226
N22   -2.301249   2.628893   -0.512533
H23   -1.287724   2.559386   -0.493248
H24   -2.720256   3.538009   -0.617109
C25   -4.486966   1.653849   -0.287038
H26   -4.991411   2.601530   -0.417570

C27 -5.312043 -1.922019 0.320995
H28 -5.073809 -2.648053 -0.456816
H29 -5.042569 -2.344011 1.289879
H30 -6.377455 -1.694924 0.300269
C31 5.031801 -1.575605 -1.156210
H32 5.548090 -2.061597 -0.326027
H33 4.408264 -2.302863 -1.677143
H34 5.760104 -1.158389 -1.851784
H35 5.473711 1.209589 -0.921078
O36 2.446500 0.707266 1.737144
O37 3.574197 0.345755 2.273597

Zero-point correction=   0.284138 (Hartree/Particle)
Thermal correction to Energy=   0.305322
Thermal correction to Enthalpy=   0.306266
Thermal correction to Gibbs Free Energy=   0.231988
Sum of electronic and zero-point Energies=   -1165.623152
Sum of electronic and thermal Energies=   -1165.601967
Sum of electronic and thermal Enthalpies=   -1165.601023
Sum of electronic and thermal Free Energies=   -1165.675301

rot-TS5
C1 1.115155 1.094295 -0.079786
C2 2.554480 0.795932 0.326926
C3 0.863949 -1.323074 -0.174852
C4 4.536374 0.965478 -0.485539
N5 0.346174 -0.054574 -0.134922
N6 3.604491 1.706914 -0.021030
N7 4.241209 -0.411091 -0.601290
N8 2.192361 -1.577071 -0.384466
C9 2.961959 -0.554910 -0.224291
N10 0.038418 -2.329312 -0.104781
H11 0.430912 -3.257151 -0.188087
H12 -0.998369 -2.186371 0.004235
O13 0.661055 2.201947 -0.229515
H14 5.508515 1.326994 -0.802855
O15 2.477837 0.781252 1.810717
O16 2.721281 -0.379209 2.345428
C17 5.088327 -1.428712 -1.210305
H18 5.189477 -1.247826 -2.282593
H19 6.069084 -1.414730 -0.733522
H20 4.620778 -2.399265 -1.048291
H21 -0.706419 0.092843 -0.173408
C22 -3.125549 -0.765494 -0.006197
N23 -2.412504 0.376716 -0.172033
C24 -3.031190 1.557618 -0.293080
C25 -5.146210 0.495368 -0.096727
N26 -4.514650 -0.701058 0.033422
H27 -6.229023 0.470211 -0.056670
O28 -2.584539 -1.877339 0.112706
N29 -2.278898 2.651277 -0.443416
H30 -1.264852 2.589657 -0.423626
H31 -2.705201 3.559805 -0.520035
C32 -4.457174 1.649795 -0.264006
H33 -4.969508 2.596785 -0.365557
C34 -5.252992 -1.951545 0.220518
H35 -4.997042 -2.653483 -0.573515

H36 -4.992083 -2.397285 1.181145
H37 -6.320307 -1.734513 0.191731

Zero-point correction=   0.283976 (Hartree/Particle)
Thermal correction to Energy=   0.304399
Thermal correction to Enthalpy=   0.305343
Thermal correction to Gibbs Free Energy=   0.233039
Sum of electronic and zero-point Energies=   -1165.620016
Sum of electronic and thermal Energies=   -1165.599593
Sum of electronic and thermal Enthalpies=   -1165.598649
Sum of electronic and thermal Free Energies=   -1165.670953

anti-TS5
C1 1.134357 1.147061 -0.145487
C2 2.577247 0.859481 0.048482
H3 -0.669204 0.115165 -0.187229
C4 0.905886 -1.282865 -0.195206
C5 4.627702 0.954733 -0.438835
N6 0.383070 -0.017656 -0.184175
N7 3.627806 1.731529 -0.145831
N8 4.330480 -0.398870 -0.539730
N9 2.246625 -1.552318 -0.335925
C10 2.997020 -0.499122 -0.309743
N11 0.083059 -2.294190 -0.141048
H12 0.486131 -3.219720 -0.189691
H13 -0.957082 -2.160918 -0.055085
O14 0.638261 2.250123 -0.210960
C15 -3.100271 -0.775202 -0.043085
N16 -2.396764 0.378932 -0.153581
C17 -3.026396 1.557816 -0.232371
C18 -5.133080 0.468827 -0.099527
N19 -4.490680 -0.726077 -0.014908
H20 -6.215920 0.431398 -0.071155
O21 -2.550309 -1.886537 0.034632
N22 -2.283712 2.663112 -0.332085
H23 -1.268009 2.607891 -0.319084
H24 -2.718494 3.569378 -0.383195
C25 -4.453943 1.635491 -0.210895
H26 -4.974476 2.581147 -0.277305
C27 -5.218363 -1.989997 0.111772
H28 -4.941747 -2.658578 -0.703833
H29 -4.969160 -2.469598 1.059209
H30 -6.287346 -1.782792 0.072745
C31 5.227398 -1.492764 -0.891992
H32 5.242327 -2.230133 -0.088339
H33 4.889543 -1.963959 -1.816379
H34 6.228689 -1.087178 -1.033378
H35 5.639378 1.302692 -0.612466
O36 2.566132 0.623029 1.881878
O37 1.944772 -0.364964 2.291635

Zero-point correction=   0.282935 (Hartree/Particle)
Thermal correction to Energy=   0.303923
Thermal correction to Enthalpy=   0.304867
Thermal correction to Gibbs Free Energy=   0.231481
Sum of electronic and zero-point Energies=   -1165.617453
Sum of electronic and thermal Energies=   -1165.596465
Sum of electronic and thermal Enthalpies=   -1165.595521
Sum of electronic and thermal Free Energies=   -1165.668907

***anti*-5-OO-9MG•+·1MC**

C1	1.149517	1.084386	-0.064506
C2	2.595827	0.789749	0.313792
H3	-0.667212	0.086603	-0.180848
C4	0.897538	-1.332341	-0.103950
C5	4.564986	0.931774	-0.525772
N6	0.384767	-0.061071	-0.146721
N7	3.634937	1.687997	-0.077138
N8	4.275886	-0.446262	-0.586081
N9	2.229921	-1.606788	-0.285838
C10	2.996323	-0.574029	-0.194171
N11	0.067196	-2.329596	0.001319
H12	0.456951	-3.261949	-0.029671
H13	-0.971891	-2.179128	0.081562
O14	0.695657	2.195669	-0.197276
C15	-3.094787	-0.763320	-0.021079
N16	-2.375954	0.376671	-0.174378
C17	-2.989431	1.558040	-0.316196
C18	-5.110598	0.499386	-0.172893
N19	-4.484378	-0.697467	-0.021828
H20	-6.194151	0.475581	-0.163461
O21	-2.558930	-1.875273	0.120048
N22	-2.231730	2.649659	-0.452055
H23	-1.218208	2.585867	-0.408238
H24	-2.654548	3.558275	-0.544877
C25	-4.415692	1.652428	-0.324150
H26	-4.923808	2.599807	-0.442055
C27	-5.229405	-1.946426	0.147378
H28	-4.944952	-2.653703	-0.632024
H29	-5.004059	-2.385862	1.119892
H30	-6.294853	-1.729599	0.077593
C31	5.104571	-1.501323	-1.155664
H32	5.218872	-2.306498	-0.428759
H33	4.641842	-1.890786	-2.064687
H34	6.083510	-1.084414	-1.389782
H35	5.531557	1.286350	-0.866983
O36	2.650058	0.772642	1.809172
O37	1.916132	-0.155849	2.339888

Zero-point correction= 0.284373 (Hartree/Particle)
Thermal correction to Energy= 0.305434
Thermal correction to Enthalpy= 0.306378
Thermal correction to Gibbs Free Energy= 0.232868
Sum of electronic and zero-point Energies= -1165.623159
Sum of electronic and thermal Energies= -1165.602098
Sum of electronic and thermal Enthalpies= -1165.601154
Sum of electronic and thermal Free Energies= -1165.674664

***syn*-TS-8**

C1	0.951913	1.073882	-0.389205
C2	2.398931	0.771546	-0.447582
H3	-0.853055	0.074787	-0.196980
C4	0.687786	-1.359727	-0.218996
C5	4.509393	0.724920	-0.426448
N6	0.190933	-0.079580	-0.265101
N7	3.413676	1.563617	-0.579275
N8	4.142958	-0.611591	-0.506446

N9	2.013932	-1.671605	-0.289996
C10	2.794272	-0.636140	-0.387455
N11	-0.169116	-2.340201	-0.098465
H12	0.208849	-3.276633	-0.062219
H13	-1.205522	-2.177210	-0.035785
O14	0.461509	2.180666	-0.437848
C15	-3.319725	-0.754966	0.059782
N16	-2.595708	0.384510	-0.070013
C17	-3.200987	1.578403	-0.076974
C18	-5.319966	0.536770	0.182512
N19	-4.703385	-0.674269	0.188679
H20	-6.398560	0.524265	0.288420
O21	-2.795387	-1.880966	0.069557
N22	-2.441147	2.668971	-0.208356
H23	-1.431694	2.587805	-0.300837
H24	-2.857219	3.585294	-0.218462
C25	-4.620630	1.689571	0.052681
H26	-5.120457	2.648633	0.049333
C27	-5.451034	-1.925283	0.326040
H28	-5.294932	-2.548480	-0.555240
H29	-5.104350	-2.467807	1.206157
H30	-6.509853	-1.690462	0.430671
C31	5.031380	-1.756587	-0.354100
H32	5.217848	-1.952565	0.704649
H33	4.553126	-2.624297	-0.807431
H34	5.970056	-1.548986	-0.867398
H35	5.507198	1.037619	-0.705637
O36	3.629777	0.461394	1.937353
O37	4.652298	0.925750	1.424941

Zero-point correction= 0.283523 (Hartree/Particle)
Thermal correction to Energy= 0.304350
Thermal correction to Enthalpy= 0.305294
Thermal correction to Gibbs Free Energy= 0.231994
Sum of electronic and zero-point Energies= -1165.622202
Sum of electronic and thermal Energies= -1165.601375
Sum of electronic and thermal Enthalpies= -1165.600431
Sum of electronic and thermal Free Energies= -1165.673731

***syn*-8-OO-9MG•+·1MC**

C1	0.874606	1.039760	-0.315321
C2	2.329914	0.721185	-0.365205
H3	-0.945018	0.067808	-0.153908
C4	0.585607	-1.387762	-0.158777
C5	4.500608	0.666105	-0.420141
N6	0.099517	-0.099432	-0.209494
N7	3.320888	1.513439	-0.437282
N8	4.043796	-0.710280	-0.400617
N9	1.905363	-1.718920	-0.214490
C10	2.718356	-0.707102	-0.311850
N11	-0.287047	-2.353118	-0.049352
H12	0.076047	-3.295587	-0.010435
H13	-1.322321	-2.174134	0.006064
O14	0.410382	2.156253	-0.361705
C15	-3.415279	-0.726710	0.079922
N16	-2.677029	0.404453	-0.044703
C17	-3.269390	1.604998	-0.060059

C18 -5.402117 0.586696 0.177780
N19 -4.798733 -0.630891 0.193826
H20 -6.481849 0.586389 0.272050
O21 -2.902877 -1.858246 0.097846
N22 -2.496849 2.687630 -0.183782
H23 -1.487298 2.596986 -0.257777
H24 -2.903018 3.608412 -0.196275
C25 -4.688841 1.731543 0.052881
H26 -5.178317 2.695850 0.041603
C27 -5.561384 -1.873444 0.327778
H28 -5.396084 -2.504878 -0.545851
H29 -5.235759 -2.412539 1.218046
H30 -6.619396 -1.627171 0.411942
C31 4.924287 -1.865592 -0.321834
H32 5.400318 -1.908370 0.660595
H33 4.323487 -2.761358 -0.476628
H34 5.686409 -1.797040 -1.099731
H35 5.164712 0.885222 -1.259015
O36 4.641818 0.694177 1.849970
O37 5.296996 0.964338 0.751329

Zero-point correction=   0.284990 (Hartree/Particle)
Thermal correction to Energy=   0.306147
Thermal correction to Enthalpy=   0.307091
Thermal correction to Gibbs Free Energy=   0.232342
Sum of electronic and zero-point Energies=   -1165.631056
Sum of electronic and thermal Energies=   -1165.609900
Sum of electronic and thermal Enthalpies=   -1165.608956
Sum of electronic and thermal Free Energies=   -1165.683704

rot-TS8
C1   -0.875887 -0.950211 -0.245272
C2   -2.320990 -0.584723 -0.294768
C3   -0.511323 1.463505 -0.029218
C4   -4.479973 -0.464865 -0.439697
N5   -0.066033 0.161408 -0.111683
N6   -3.333756 -1.345689 -0.402079
N7   -3.987780 0.899369 -0.286286
N8   -1.818928 1.836435 -0.075066
C9   -2.664353 0.852874 -0.202691
N10 0.392247 2.397856 0.100488
H11 0.059994 3.350535 0.159252
H12 1.421792 2.185298 0.139881
O13 -0.447009 -2.079318 -0.316824
H14 -5.018996 -0.592282 -1.384737
O15 -5.426324 -0.699521 0.629102
O16 -5.240550 -1.816001 1.285019
C17 -4.831940 2.085230 -0.267470
H18 -5.328421 2.204561 -1.233253
H19 -5.576861 1.992392 0.524405
H20 -4.195001 2.948194 -0.075281
H21 0.973251 -0.039139 -0.072017
C22 3.472537 0.677722 0.108313
N23 2.698413 -0.429155 -0.016968
C24 3.255812 -1.644166 -0.091527
C25 5.424355 -0.690237 0.079648
N26 4.856615 0.542326 0.153394

H27 6.506790 -0.721843 0.125125
O28 2.992876 1.821066 0.184889
N29 2.448459 -2.701334 -0.213060
H30 1.440032 -2.580540 -0.249009
H31 2.827546 -3.631884 -0.270377
C32 4.674623 -1.811893 -0.042307
H33 5.136557 -2.787950 -0.101677
C34 5.660053 1.758804 0.287903
H35 5.423987 2.447501 -0.523560
H36 5.440716 2.247127 1.238341
H37 6.714527 1.487480 0.246753

Zero-point correction=   0.284716 (Hartree/Particle)
Thermal correction to Energy=   0.305116
Thermal correction to Enthalpy=   0.306060
Thermal correction to Gibbs Free Energy=   0.233572
Sum of electronic and zero-point Energies=   -1165.621889
Sum of electronic and thermal Energies=   -1165.601489
Sum of electronic and thermal Enthalpies=   -1165.600545
Sum of electronic and thermal Free Energies=   -1165.673033

anti-TS8
C1   0.872813 0.954834 -0.377380
C2   2.301483 0.586379 -0.440061
H3   -0.975416 0.041893 -0.156108
C4   0.501951 -1.456555 -0.120253
C5   4.427882 0.451718 -0.475146
N6   0.060779 -0.160111 -0.216413
N7   3.352265 1.333531 -0.560600
N8   3.984535 -0.870698 -0.435974
N9   1.814484 -1.825083 -0.173996
C10 2.638902 -0.829979 -0.334230
N11 -0.394247 -2.396765 0.035555
H12 -0.054795 -3.345777 0.107369
H13 -1.422712 -2.188165 0.095954
O14 0.428718 2.080144 -0.455387
C15 -3.474166 -0.674896 0.135582
N16 -2.704487 0.426990 -0.045054
C17 -3.260652 1.642858 -0.110357
C18 -5.420596 0.700797 0.188745
N19 -4.853477 -0.532425 0.256204
H20 -6.498955 0.737738 0.291144
O21 -2.995972 -1.819523 0.200194
N22 -2.455923 2.694068 -0.287094
H23 -1.449476 2.568057 -0.361536
H24 -2.833609 3.625480 -0.338577
C25 -4.675019 1.816984 0.006206
H26 -5.136484 2.793644 -0.046682
C27 -5.651344 -1.743020 0.457340
H28 -5.513877 -2.422686 -0.384397
H29 -5.333830 -2.247168 1.370744
H30 -6.700778 -1.461038 0.537370
C31 4.824620 -2.055254 -0.317196
H32 5.045116 -2.257925 0.733048
H33 4.292853 -2.902109 -0.750469
H34 5.752195 -1.888470 -0.864955
H35 5.366933 0.687701 -0.962246

O36   5.778343   1.649442   1.389216
O37   4.953920   0.741072   1.246161

Zero-point correction=   0.282202 (Hartree/Particle)
Thermal correction to Energy=   0.303584
Thermal correction to Enthalpy=   0.304528
Thermal correction to Gibbs Free Energy=   0.229076
Sum of electronic and zero-point Energies=   -1165.612823
Sum of electronic and thermal Energies=   -1165.591441
Sum of electronic and thermal Enthalpies=   -1165.590497
Sum of electronic and thermal Free Energies=   -1165.665949

anti-8-OO-9MG•+·1MC

C1   0.794414   1.038148   -0.179082
C2   2.248892   0.711115   -0.220710
H3   -1.033813   0.075739   -0.072511
C4   0.488627   -1.390300   -0.074415
C5   4.419619   0.650036   -0.314121
N6   0.011033   -0.097320   -0.107873
N7   3.244493   1.499394   -0.278458
N8   3.954822   -0.730936   -0.238625
N9   1.806442   -1.727911   -0.107463
C10   2.628937   -0.719921   -0.179637
N11   -0.392651   -2.351543   -0.004039
H12   -0.036981   -3.297304   0.022014
H13   -1.427983   -2.166550   0.027996
O14   0.339547   2.159089   -0.207758
C15   -3.513426   -0.708248   0.064023
N16   -2.765563   0.421431   -0.006710
C17   -3.351456   1.625311   -0.015051
C18   -5.496226   0.613514   0.118682
N19   -4.899748   -0.607542   0.125429
H20   -6.578744   0.617105   0.172242
O21   -3.007145   -1.842593   0.076583
N22   -2.569925   2.706350   -0.085270
H23   -1.559181   2.611916   -0.131398
H24   -2.971288   3.629305   -0.093006
C25   -4.773317   1.757096   0.050217
H26   -5.257554   2.724093   0.045329
C27   -5.673604   -1.848289   0.199803
H28   -5.450247   -2.474397   -0.664510
H29   -5.412849   -2.394575   1.107138
H30   -6.734135   -1.598582   0.211372
C31   4.823806   -1.899262   -0.221100
H32   5.361821   -1.951123   0.727715
H33   4.199456   -2.784710   -0.338781
H34   5.538946   -1.836022   -1.042577
H35   5.015412   0.832671   -1.212930
O36   6.459796   0.612796   0.646001
O37   5.213704   0.977430   0.834088

Zero-point correction=   0.284703 (Hartree/Particle)
Thermal correction to Energy=   0.306066
Thermal correction to Enthalpy=   0.307011
Thermal correction to Gibbs Free Energy=   0.231294
Sum of electronic and zero-point Energies=   -1165.628995
Sum of electronic and thermal Energies=   -1165.607631
Sum of electronic and thermal Enthalpies=   -1165.606687
Sum of electronic and thermal Free Energies=   -1165.682404

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C1   -0.992300   -1.039646   -0.299655
C2   -2.452915   -0.738812   -0.274649
C3   -0.714587   1.390070   -0.191152
C4   -4.565238   -0.699107   -0.147944
N5   -0.223624   0.104217   -0.204799
N6   -3.449003   -1.476679   -0.752913
N7   -4.181494   0.676104   -0.385897
N8   -2.038551   1.709530   -0.260585
C9   -2.844003   0.696331   -0.305560
N10   0.149789   2.364063   -0.106647
H11   -0.219625   3.304877   -0.095904
H12   1.186422   2.192622   -0.040596
O13   -0.523956   -2.152203   -0.373722
H14   -5.567789   -0.963068   -0.471676
O15   -4.436600   -1.039584   1.233973
O16   -3.102209   -0.804827   1.517044
C17   -5.062208   1.815638   -0.172803
H18   -5.263368   1.944605   0.894359
H19   -4.571624   2.706140   -0.564466
H20   -5.995846   1.649575   -0.710958
H21   0.824028   -0.056542   -0.168243
C22   3.283774   0.756998   0.047865
N23   2.553398   -0.378411   -0.084231
C24   3.154220   -1.574837   -0.108103
C25   5.279572   -0.542903   0.137628
N26   4.667484   0.670201   0.162885
H27   6.359216   -0.535477   0.232518
O28   2.763548   1.884998   0.071911
N29   2.389784   -2.662130   -0.239102
H30   1.379367   -2.579265   -0.309121
H31   2.802684   -3.579847   -0.256806
C32   4.574605   -1.691759   0.003265
H33   5.070876   -2.652467   -0.015523
C34   5.421029   1.917149   0.307692
H35   5.254806   2.553187   -0.562430
H36   5.088075   2.447999   1.200165
H37   6.480343   1.677581   0.394556

Zero-point correction=   0.282802 (Hartree/Particle)
Thermal correction to Energy=   0.303170
Thermal correction to Enthalpy=   0.304114
Thermal correction to Gibbs Free Energy=   0.231842
Sum of electronic and zero-point Energies=   -1165.570206
Sum of electronic and thermal Energies=   -1165.549837
Sum of electronic and thermal Enthalpies=   -1165.548893
Sum of electronic and thermal Free Energies=   -1165.621166

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C1   -1.013005   -1.050758   -0.203367
C2   -2.485729   -0.767941   -0.153076
H3   0.803805   -0.062316   -0.116306
C4   -0.730407   1.381722   -0.166773
C5   -4.523882   -0.732884   -0.248195
N6   -0.244459   0.096969   -0.143823
N7   -3.465994   -1.475827   -0.762016
N8   -4.196379   0.667571   -0.407812

N9   -2.052820   1.699662   -0.292692
C10 -2.860477   0.690226   -0.303397
N11   0.130181   2.358725   -0.082793
H12 -0.238889   3.299162   -0.115897
H13   1.165661   2.189825   0.011844
O14 -0.537461 -2.160032   -0.260579
H15 -5.552361 -1.022596   -0.437072
O16 -2.962962 -0.869774   1.466252
O17 -4.285193 -0.927919   1.295274
C18 -5.096211   1.801078   -0.253968
H19 -4.617580   2.677902   -0.689773
H20 -6.023067   1.591689   -0.788674
H21 -5.305951   1.986495   0.802538
C22   3.264750   0.762867   0.069780
N23   2.536231 -0.373024   -0.067355
C24   3.141846 -1.565023   -0.142607
C25   5.269125 -0.526669   0.054705
N26   4.652042   0.681722   0.133669
H27   6.351398 -0.514991   0.111680
O28   2.739589   1.886718   0.141988
N29   2.378806 -2.653173   -0.272766
H30   1.365577 -2.575546   -0.294288
H31   2.795513 -3.567687   -0.327476
C32   4.566001 -1.675897   -0.085121
H33   5.066211 -2.632692   -0.147658
C34   5.404599   1.928049   0.288289
H35   5.167505   2.606457   -0.531650
H36   5.138209   2.408833   1.230398
H37   6.469268   1.696521   0.280336

Zero-point correction=   0.282269 (Hartree/Particle)
Thermal correction to Energy=   0.302805
Thermal correction to Enthalpy=   0.303749
Thermal correction to Gibbs Free Energy=   0.231246
Sum of electronic and zero-point Energies=   -1165.572453
Sum of electronic and thermal Energies=   -1165.551917
Sum of electronic and thermal Enthalpies=   -1165.550973
Sum of electronic and thermal Free Energies=   -1165.623477

5,8-OO-9MG•+·1MC
C1   -1.014089 -1.017760   -0.090695
C2   -2.501054 -0.736002   0.000834
H3   0.808373 -0.048283   -0.049390
C4   -0.716816   1.411735   -0.041053
C5   -4.555149 -0.686582   -0.251054
N6   -0.238716   0.120028   -0.055082
N7   -3.428326 -1.314061   -0.938171
N8   -4.172296   0.724750   -0.357070
N9   -2.033551   1.741922   -0.143321
C10 -2.846743   0.734668   -0.189884
N11   0.157769   2.375645   0.051182
H12 -0.200429   3.320817   0.043756
H13   1.192886   2.194404   0.114062
O14 -0.555551 -2.133094   -0.161057
H15 -5.553154 -0.920896   -0.613429
O16 -2.991311 -1.087976   1.298536
O17 -4.433443 -1.118968   1.085678

C18 -5.072176   1.867081   -0.353133
H19 -4.490902   2.761684   -0.575153
H20 -5.833919   1.727883   -1.121900
H21 -5.544698   1.969564   0.626911
C22   3.283235   0.752863   0.071859
N23   2.540753 -0.376792   -0.042654
C24   3.133957 -1.572643   -0.147337
C25   5.275495 -0.551361   -0.032920
N26   4.671415   0.661087   0.076239
H27   6.359293 -0.548047   -0.022053
O28   2.770419   1.879814   0.173679
N29   2.358227 -2.654802   -0.252288
H30   1.345769 -2.569560   -0.236233
H31   2.765777 -3.572012   -0.326569
C32   4.558301 -1.694726   -0.147555
H33   5.048254 -2.654897   -0.234614
C34   5.439196   1.901085   0.204501
H35   5.161553   2.590488   -0.593106
H36   5.228118   2.372239   1.165393
H37   6.500288   1.663830   0.134414

Zero-point correction=   0.285604 (Hartree/Particle)
Thermal correction to Energy=   0.305692
Thermal correction to Enthalpy=   0.306636
Thermal correction to Gibbs Free Energy=   0.235444
Sum of electronic and zero-point Energies=   -1165.599913
Sum of electronic and thermal Energies=   -1165.579825
Sum of electronic and thermal Enthalpies=   -1165.578881
Sum of electronic and thermal Free Energies=   -1165.650073

[9MG – H]•·[1MC + H]+
C1   -1.308266   1.074931   -0.013489
C2   -2.762462   0.908049   -0.011530
H3   1.144512   0.177906   -0.007529
C4   -1.197517 -1.281834   0.000144
C5   -4.866556   1.041862   -0.008839
N6   -0.584459 -0.089703   -0.008308
N7   -3.763114   1.794771   -0.017890
N8   -4.632210 -0.296318   0.002017
N9   -2.562807 -1.530275   0.008687
C10 -3.260704 -0.429972   0.001626
N11 -0.450564 -2.380771   0.001192
H12 -0.913604 -3.276357   0.007787
H13   0.567522 -2.320512   -0.008099
O14 -0.766716   2.184387   -0.018216
C15   2.936387 -0.837388   -0.007867
N16   2.195961   0.327081   -0.002234
C17   2.720799   1.578572   0.010630
C18   4.876653   0.556638   0.017344
N19   4.314456 -0.682419   0.003386
H20   5.960236   0.582447   0.024760
O21   2.414303 -1.939875   -0.021670
N22   1.901877   2.607382   0.011942
H23   0.865191   2.478805   0.000238
H24   2.281477   3.541700   0.021437
C25   4.141944   1.696116   0.021967
H26   4.618043   2.666388   0.033816

C27 5.120182 -1.908730 -0.009897
H28 4.855701 -2.530587 0.845628
H29 4.928773 -2.465123 -0.928140
H30 6.172486 -1.633590 0.044472
C31 -5.599938 -1.383812 0.032055
H32 -5.386074 -2.082720 -0.777368
H33 -5.542410 -1.905466 0.988718
H34 -6.597649 -0.966014 -0.099727
H35 -5.872017 1.442203 -0.011337

Zero-point correction=   0.277193 (Hartree/Particle)
Thermal correction to Energy=   0.296132
Thermal correction to Enthalpy=   0.297077
Thermal correction to Gibbs Free Energy=   0.227183
Sum of electronic and zero-point Energies=   -1015.366680
Sum of electronic and thermal Energies=   -1015.347741
Sum of electronic and thermal Enthalpies=   -1015.346797
Sum of electronic and thermal Free Energies=   -1015.416690

[9MG – H]•·[1MC + H]+ + ¹O₂

C1 -0.929935 -0.957608 -0.459687
C2 -2.372900 -0.745852 -0.585532
H3 1.531071 -0.141668 -0.154547
C4 -0.767094 1.385821 -0.238368
C5 -4.469854 -0.814138 -0.784052
N6 -0.184116 0.178900 -0.285508
N7 -3.387937 -1.597839 -0.756450
N8 -4.205713 0.511512 -0.645898
N9 -2.118892 1.676446 -0.348396
C10 -2.838024 0.602931 -0.511122
N11 0.002347 2.455513 -0.067899
H12 -0.436956 3.362296 -0.033233
H13 1.013776 2.362338 0.022783
O14 -0.417441 -2.079946 -0.507077
C15 3.339562 0.812686 0.090331
N16 2.574815 -0.323352 -0.079289
C17 3.067975 -1.585806 -0.150048
C18 5.239244 -0.635990 0.123490
N19 4.708834 0.615464 0.188374
H20 6.317653 -0.696328 0.213715
O21 2.845198 1.926288 0.150799
N22 2.227774 -2.584054 -0.312584
H23 1.198058 -2.423078 -0.388834
H24 2.583703 -3.526110 -0.366629
C25 4.480605 -1.747427 -0.041434
H26 4.932362 -2.728100 -0.090994
C27 5.540910 1.809922 0.371523
H28 5.357617 2.512321 -0.441753
H29 5.295372 2.290915 1.319079
H30 6.587153 1.507551 0.370061
C31 -5.145878 1.622108 -0.607498
H32 -5.090076 2.117038 0.363301
H33 -4.902604 2.336464 -1.395037
H34 -6.151474 1.232544 -0.763268
H35 -5.480180 -1.181702 -0.907133
O36 -3.220347 -0.435313 2.401800
O37 -4.325275 -0.915092 2.349527

Zero-point correction=   0.281867 (Hartree/Particle)
Thermal correction to Energy=   0.304838
Thermal correction to Enthalpy=   0.305783
Thermal correction to Gibbs Free Energy=   0.224514
Sum of electronic and zero-point Energies=   -1165.643165
Sum of electronic and thermal Energies=   -1165.620194
Sum of electronic and thermal Enthalpies=   -1165.619250
Sum of electronic and thermal Free Energies=   -1165.700519

syn-TS4

C1 0.899379 1.052761 -0.277829
C2 2.380424 0.878541 -0.394667
H3 -1.517359 0.166168 -0.118926
C4 0.867802 -1.304702 -0.181237
C5 4.427418 0.853701 -0.933573
N6 0.208174 -0.092545 -0.181464
N7 3.265960 1.624861 -0.964558
N8 4.275224 -0.349896 -0.471146
N9 2.189137 -1.534456 -0.130014
C10 2.924701 -0.419667 0.074870
N11 0.079552 -2.374596 -0.233116
H12 0.509202 -3.285271 -0.191487
H13 -0.933503 -2.283256 -0.252461
O14 0.405204 2.184539 -0.288578
H15 5.371103 1.225374 -1.315956
O16 3.988709 0.684149 1.967033
O17 3.169077 -0.253968 1.647279
C18 5.258893 -1.406646 -0.293478
H19 6.166813 -1.147629 -0.836599
H20 5.473518 -1.516401 0.771580
H21 4.829253 -2.332361 -0.678480
C22 -3.315281 -0.838351 -0.062418
N23 -2.567033 0.322302 -0.056567
C24 -3.081211 1.572850 0.048911
C25 -5.237990 0.560618 0.175668
N26 -4.688321 -0.677818 0.060418
H27 -6.317444 0.590973 0.269021
O28 -2.804556 -1.939790 -0.168589
N29 -2.259756 2.600858 0.029342
H30 -1.230830 2.477081 -0.087244
H31 -2.634772 3.533584 0.108183
C32 -4.496020 1.695801 0.174919
H33 -4.962489 2.666427 0.267113
C34 -5.501072 -1.899304 0.050752
H35 -5.385363 -2.410836 -0.905461
H36 -5.174352 -2.563616 0.851022
H37 -6.544061 -1.624246 0.200747

Zero-point correction=   0.283503 (Hartree/Particle)
Thermal correction to Energy=   0.304025
Thermal correction to Enthalpy=   0.304969
Thermal correction to Gibbs Free Energy=   0.233187
Sum of electronic and zero-point Energies=   -1165.588140
Sum of electronic and thermal Energies=   -1165.567618
Sum of electronic and thermal Enthalpies=   -1165.566674
Sum of electronic and thermal Free Energies=   -1165.638456

syn-4OO-[9MG − H]•·[1MC + H]⁺

C1	0.898872	1.066923	-0.260769
C2	2.376839	0.876430	-0.414159
H3	-1.501761	0.166566	-0.087282
C4	0.886916	-1.273152	-0.152084
C5	4.358943	0.728586	-1.153944
N6	0.206611	-0.072928	-0.134342
N7	3.187392	1.474347	-1.220837
N8	4.290802	-0.337851	-0.422714
N9	2.209937	-1.480921	-0.087315
C10	2.951986	-0.363709	0.201512
N11	0.118182	-2.355305	-0.236668
H12	0.560433	-3.260118	-0.200386
H13	-0.895884	-2.278327	-0.264672
O14	0.416784	2.203033	-0.263403
H15	5.246102	1.004469	-1.712681
O16	3.871079	0.793060	1.991872
O17	3.154462	-0.252701	1.670687
C18	5.298112	-1.354356	-0.163740
H19	6.132013	-1.217802	-0.851096
H20	5.640372	-1.263451	0.868944
H21	4.831033	-2.329222	-0.314926
C22	-3.296490	-0.847579	-0.070957
N23	-2.555324	0.316850	-0.040726
C24	-3.077223	1.562670	0.073480
C25	-5.229650	0.537964	0.161018
N26	-4.672052	-0.696006	0.036543
H27	-6.310363	0.561347	0.241030
O28	-2.777767	-1.944609	-0.184925
N29	-2.260837	2.595701	0.075691
H30	-1.231667	2.481416	-0.039269
H31	-2.641908	3.525449	0.160031
C32	-4.493947	1.677131	0.184025
H33	-4.966833	2.644064	0.282166
C34	-5.477958	-1.921454	0.001648
H35	-5.349733	-2.419488	-0.960121
H36	-5.155719	-2.594909	0.796058
H37	-6.523943	-1.654198	0.144745

Zero-point correction=   0.284025 (Hartree/Particle)
Thermal correction to Energy=   0.305116
Thermal correction to Enthalpy=   0.306060
Thermal correction to Gibbs Free Energy=   0.232697
Sum of electronic and zero-point Energies=   -1165.588506
Sum of electronic and thermal Energies=   -1165.567415
Sum of electronic and thermal Enthalpies=   -1165.566471
Sum of electronic and thermal Free Energies=   -1165.639835

rot-TS4

C1	0.950079	1.084259	-0.267093
C2	2.432598	0.902249	-0.384072
C3	0.952192	-1.251478	-0.153325
C4	4.412662	0.744213	-1.138444
N5	0.261419	-0.060790	-0.152559
N6	3.241811	1.484600	-1.207621
N7	4.355813	-0.307975	-0.383284
N8	2.280154	-1.448172	-0.080898

C9	3.012238	-0.332592	0.239101
N10	0.198555	-2.343799	-0.235960
H11	0.651761	-3.242757	-0.190740
H12	-0.816097	-2.279113	-0.280471
O13	0.460176	2.214739	-0.297139
H14	5.293493	1.008946	-1.712677
O15	2.584426	0.742938	2.238118
O16	3.298785	-0.207053	1.687729
C17	5.359843	-1.333267	-0.138938
H18	6.194072	-1.189746	-0.824702
H19	5.700999	-1.261948	0.895108
H20	4.887979	-2.303332	-0.306917
H21	-1.439969	0.161253	-0.120360
C22	-3.227906	-0.867308	-0.112754
N23	-2.496540	0.302758	-0.079215
C24	-3.028980	1.543856	0.035785
C25	-5.173219	0.501845	0.116039
N26	-4.605054	-0.727355	-0.009149
H27	-6.254302	0.515932	0.193177
O28	-2.700077	-1.960306	-0.226265
N29	-2.221245	2.583658	0.041609
H30	-1.191119	2.478529	-0.073118
H31	-2.610086	3.509941	0.128186
C32	-4.446997	1.646841	0.142945
H33	-4.927762	2.609857	0.241360
C34	-5.400735	-1.959222	-0.047506
H35	-5.265864	-2.455361	-1.009355
H36	-5.075360	-2.630897	0.747153
H37	-6.449284	-1.700713	0.092936

Zero-point correction=   0.283795 (Hartree/Particle)
Thermal correction to Energy=   0.304141
Thermal correction to Enthalpy=   0.305085
Thermal correction to Gibbs Free Energy=   0.233448
Sum of electronic and zero-point Energies=   -1165.584048
Sum of electronic and thermal Energies=   -1165.563702
Sum of electronic and thermal Enthalpies=   -1165.562758
Sum of electronic and thermal Free Energies=   -1165.634395

anti-TS4

C1	0.957756	1.170307	-0.199671
C2	2.444121	1.024453	-0.305957
H3	-1.432802	0.213703	-0.142019
C4	0.974612	-1.175317	-0.332298
C5	4.483470	1.056461	-0.874351
N6	0.283617	0.012632	-0.226276
N7	3.310311	1.797679	-0.880008
N8	4.374304	-0.144387	-0.389366
N9	2.304461	-1.373469	-0.286457
C10	3.005502	-0.286310	0.103839
N11	0.222452	-2.254337	-0.515246
H12	0.678119	-3.152891	-0.544297
H13	-0.793267	-2.192131	-0.524826
O14	0.450026	2.291841	-0.103571
H15	5.411081	1.447103	-1.277142
O16	2.290401	-0.806135	2.293213
O17	3.254223	-0.226986	1.673825

C18	5.376429	-1.189940	-0.250551
H19	6.285359	-0.890091	-0.770597
H20	5.578258	-1.346310	0.810767
H21	4.966881	-2.103656	-0.684475
C22	-3.208507	-0.833670	-0.189654
N23	-2.488072	0.337845	-0.069615
C24	-3.031649	1.560331	0.149337
C25	-5.164607	0.492280	0.165920
N26	-4.585557	-0.716999	-0.060611
H27	-6.244876	0.488346	0.254701
O28	-2.672006	-1.908397	-0.396348
N29	-2.234171	2.604432	0.232673
H30	-1.202355	2.517854	0.112769
H31	-2.631528	3.516663	0.395934
C32	-4.449585	1.639335	0.276103
H33	-4.938715	2.586768	0.453138
C34	-5.368340	-1.951910	-0.180695
H35	-5.220867	-2.387881	-1.169382
H36	-5.042586	-2.667591	0.574555
H37	-6.420484	-1.712375	-0.033872

anti-4OO-[9MG – H]•·[1MC + H]+

C1	0.956498	1.170708	-0.197586
C2	2.442807	1.023223	-0.306861
H3	-1.432015	0.212921	-0.140045
C4	0.975859	-1.173045	-0.327968
C5	4.476119	1.044000	-0.899042
N6	0.282092	0.013674	-0.222468
N7	3.301661	1.783104	-0.908223
N8	4.374811	-0.145236	-0.386131
N9	2.305036	-1.369404	-0.277008
C10	3.008090	-0.282824	0.122222
N11	0.225485	-2.252820	-0.515075
H12	0.681950	-3.150997	-0.542723
H13	-0.790213	-2.191543	-0.527426
O14	0.450639	2.293001	-0.100724
H15	5.398028	1.426569	-1.322180
O16	2.286411	-0.780104	2.302651
O17	3.261974	-0.226539	1.671203
C18	5.378669	-1.188239	-0.241201
H19	6.284614	-0.893415	-0.769308
H20	5.586309	-1.333078	0.820577
H21	4.967392	-2.106918	-0.663115
C22	-3.207526	-0.834967	-0.190811
N23	-2.487736	0.336712	-0.068958
C24	-3.031968	1.558706	0.150565
C25	-5.164470	0.489784	0.164673
N26	-4.584747	-0.719051	-0.062423
H27	-6.244800	0.485306	0.252700
O28	-2.670373	-1.909191	-0.398434
N29	-2.234973	2.603144	0.235449
H30	-1.203112	2.517412	0.116090
H31	-2.632888	3.515063	0.399059
C32	-4.450036	1.637090	0.276244
H33	-4.939711	2.584181	0.453610

C34	-5.366885	-1.954218	-0.183865
H35	-5.218695	-2.389407	-1.172789
H36	-5.041187	-2.670306	0.571027
H37	-6.419218	-1.715294	-0.037391

Zero-point correction=	0.283763 (Hartree/Particle)
Thermal correction to Energy=	0.305012
Thermal correction to Enthalpy=	0.305956
Thermal correction to Gibbs Free Energy=	0.232007
Sum of electronic and zero-point Energies=	-1165.588077
Sum of electronic and thermal Energies=	-1165.566829
Sum of electronic and thermal Enthalpies=	-1165.565885
Sum of electronic and thermal Free Energies=	-1165.639834

TS4–5

C1	0.973760	1.045487	-0.083030
C2	2.475517	0.914797	-0.096057
C3	0.926547	-1.313290	-0.019380
C4	4.368656	0.785554	-1.035899
N5	3.304155	1.594070	-0.900816
N6	4.315850	-0.402309	-0.444994
N7	2.262794	-1.558702	-0.035631
C8	3.007142	-0.481456	0.179882
N9	0.148013	-2.385819	-0.025033
H10	0.587729	-3.292923	-0.004545
H11	-0.867374	-2.302131	-0.033725
O12	0.461745	2.164385	-0.123639
H13	5.227608	1.066446	-1.636890
O14	2.887632	1.121980	1.692606
O15	3.300483	-0.123174	1.729680
C16	5.245430	-1.517614	-0.546534
H17	6.018373	-1.267885	-1.273305
H18	5.703994	-1.709094	0.424973
H19	4.696829	-2.400707	-0.878292
C20	-3.246880	-0.860332	-0.036991
N21	-2.507356	0.305518	-0.054723
C22	-3.034902	1.555304	-0.074191
C23	-5.189353	0.530750	-0.055298
N24	-4.625510	-0.706919	-0.038812
H25	-6.273004	0.555396	-0.053589
O26	-2.723274	-1.961292	-0.021138
N27	-2.219843	2.587928	-0.092651
H28	-1.185024	2.465334	-0.101320
H29	-2.603280	3.520547	-0.107152
C30	-4.455834	1.671081	-0.073825
H31	-4.933074	2.640737	-0.089005
C32	-5.429052	-1.934517	-0.011746
H33	-5.163836	-2.564647	-0.860896
H34	-5.235763	-2.481047	0.912045
H35	-6.481893	-1.661863	-0.068196
N36	0.279916	-0.107134	-0.020014
H37	-1.456299	0.155640	-0.043043

Zero-point correction=	0.283091 (Hartree/Particle)
Thermal correction to Energy=	0.303770
Thermal correction to Enthalpy=	0.304714
Thermal correction to Gibbs Free Energy=	0.231412
Sum of electronic and zero-point Energies=	-1165.570237

Sum of electronic and thermal Energies=   -1165.549558
Sum of electronic and thermal Enthalpies=   -1165.548614
Sum of electronic and thermal Free Energies=   -1165.621916

syn-TS5
C1   -0.997314   -0.941274   -0.269473
C2   -2.466890   -0.747140   -0.139246
H3   1.474025   -0.131084   -0.145421
C4   -0.837920   1.406964   -0.145321
C5   -4.518778   -0.836963   -0.570251
N6   -0.251524   0.194679   -0.187480
N7   -3.477939   -1.611545   -0.475779
N8   -4.259552   0.531744   -0.516961
N9   -2.187250   1.701935   -0.269145
C10   -2.922542   0.641912   -0.321754
N11   -0.059485   2.467574   -0.004725
H12   -0.489233   3.379890   0.005383
H13   0.951728   2.366281   0.082399
O14   -0.504164   -2.061128   -0.388386
C15   3.283390   0.822723   0.065495
N16   2.517711   -0.312262   -0.110661
C17   3.012149   -1.569717   -0.233874
C18   5.187493   -0.617709   -0.007655
N19   4.655481   0.628687   0.112822
H20   6.268569   -0.675931   0.044353
O21   2.785877   1.931169   0.172571
N22   2.170229   -2.567893   -0.394451
H23   1.140584   -2.413382   -0.413216
H24   2.526425   -3.507276   -0.482625
C25   4.427703   -1.727667   -0.180329
H26   4.881299   -2.704285   -0.273690
C27   5.489057   1.821338   0.303273
H28   5.278560   2.544430   -0.484863
H29   5.270658   2.275393   1.270513
H30   6.535694   1.523428   0.261476
C31   -5.220208   1.620006   -0.620318
H32   -5.672366   1.822169   0.352797
H33   -4.694272   2.508783   -0.969172
H34   -5.992828   1.352287   -1.341750
H35   -5.529738   -1.189215   -0.738686
O36   -2.577985   -0.693695   1.701989
O37   -3.743683   -0.878440   2.073060

Zero-point correction=   0.283300 (Hartree/Particle)
Thermal correction to Energy=   0.304369
Thermal correction to Enthalpy=   0.305313
Thermal correction to Gibbs Free Energy=   0.231443
Sum of electronic and zero-point Energies=   -1165.618606
Sum of electronic and thermal Energies=   -1165.597537
Sum of electronic and thermal Enthalpies=   -1165.596593
Sum of electronic and thermal Free Energies=   -1165.670462

syn-5OO-[9MG – H]•·[1MC + H]+
C1   -1.026730   -0.940228   -0.132595
C2   -2.488367   -0.735020   0.270658
H3   1.432167   -0.134153   -0.170115

C4   -0.871013   1.399754   -0.134325
C5   -4.466227   -0.959576   -0.533909
N6   -0.276865   0.190127   -0.169240
N7   -3.503389   -1.676327   -0.094378
N8   -4.222523   0.426222   -0.637356
N9   -2.216066   1.663159   -0.339846
C10   -2.951362   0.609541   -0.245193
N11   -0.107028   2.466401   0.008569
H12   -0.540172   3.377018   -0.023510
H13   0.902624   2.371499   0.122507
O14   -0.572897   -2.063810   -0.306922
C15   3.241226   0.813323   0.055963
N16   2.476263   -0.317141   -0.150202
C17   2.970168   -1.567988   -0.322121
C18   5.145950   -0.619702   -0.091543
N19   4.613960   0.620142   0.082083
H20   6.227682   -0.677865   -0.054928
O21   2.741552   1.915920   0.204993
N22   2.126901   -2.563399   -0.502164
H23   1.099885   -2.417423   -0.476820
H24   2.482426   -3.499510   -0.622101
C25   4.385967   -1.724791   -0.295777
H26   4.840409   -2.696448   -0.428506
C27   5.447948   1.806799   0.306691
H28   5.244614   2.548904   -0.465629
H29   5.222590   2.237538   1.282831
H30   6.494400   1.508174   0.266063
C31   -5.120820   1.445524   -1.156652
H32   -5.604283   1.977636   -0.334753
H33   -4.544882   2.149051   -1.759521
H34   -5.877161   0.968467   -1.780280
H35   -5.426476   -1.350736   -0.852036
O36   -2.380492   -0.660676   1.747218
O37   -3.512294   -0.340467   2.303130

Zero-point correction=   0.284714 (Hartree/Particle)
Thermal correction to Energy=   0.305889
Thermal correction to Enthalpy=   0.306834
Thermal correction to Gibbs Free Energy=   0.232510
Sum of electronic and zero-point Energies=   -1165.623785
Sum of electronic and thermal Energies=   -1165.602609
Sum of electronic and thermal Enthalpies=   -1165.601665
Sum of electronic and thermal Free Energies=   -1165.675989

rot-TS5
C1   1.059333   0.985165   -0.116376
C2   2.505517   0.771707   0.335952
C3   0.922716   -1.351353   -0.233682
C4   4.507679   1.051154   -0.400531
N5   0.316911   -0.149362   -0.208813
N6   3.525249   1.739724   0.043697
N7   4.288412   -0.332145   -0.549269
N8   2.273929   -1.580960   -0.442515
C9   2.998266   -0.543128   -0.223350
N10   0.173650   -2.434852   -0.157977
H11   0.620872   -3.336417   -0.227498
H12   -0.836963   -2.360427   -0.037241

O13   0.600397   2.110554   -0.260846
H14   5.471719   1.466158   -0.674072
O15   2.382719   0.731556   1.816513
O16   2.663376   -0.422858   2.346178
C17   5.192591   -1.293071   -1.163241
H18   5.260139   -1.125422   -2.240808
H19   6.179879   -1.202422   -0.708591
H20   4.800236   -2.292540   -0.977799
H21   -1.390182   0.154219   -0.202802
C22   -3.189867   -0.818528   -0.006385
N23   -2.436419   0.326191   -0.172001
C24   -2.942290   1.578181   -0.290454
C25   -5.107917   0.602257   -0.081603
N26   -4.563976   -0.638608   0.039162
H27   -6.189771   0.649247   -0.033998
O28   -2.679443   -1.921750   0.093129
N29   -2.108886   2.587776   -0.435702
H30   -1.080708   2.451224   -0.421184
H31   -2.473334   3.524747   -0.515144
C32   -4.359111   1.721270   -0.248413
H33   -4.822839   2.693223   -0.340529
C34   -5.385656   -1.840266   0.226308
H35   -5.167676   -2.559059   -0.563688
H36   -5.162141   -2.294221   1.192419
H37   -6.435288   -1.553017   0.185720

Zero-point correction=   0.284629 (Hartree/Particle)
Thermal correction to Energy=   0.305036
Thermal correction to Enthalpy=   0.305981
Thermal correction to Gibbs Free Energy=   0.233658
Sum of electronic and zero-point Energies=   -1165.620664
Sum of electronic and thermal Energies=   -1165.600256
Sum of electronic and thermal Enthalpies=   -1165.599312
Sum of electronic and thermal Free Energies=   -1165.671635

anti-TS5

C1   1.073243   1.039108   -0.139275
C2   2.534211   0.843312   0.049042
H3   -1.375345   0.173466   -0.156554
C4   0.956040   -1.308284   -0.221970
C5   4.586177   1.047261   -0.407771
N6   0.345180   -0.109816   -0.193943
N7   3.544594   1.769469   -0.113310
N8   4.360286   -0.314011   -0.537172
N9   2.317279   -1.558268   -0.379164
C10   3.025181   -0.482712   -0.323917
N11   0.206629   -2.395958   -0.174457
H12   0.660133   -3.295168   -0.227575
H13   -0.805904   -2.327021   -0.070423
O14   0.567528   2.159673   -0.186085
C15   -3.169834   -0.824423   -0.036967
N16   -2.423908   0.332539   -0.135280
C17   -2.940447   1.584073   -0.218927
C18   -5.101108   0.579524   -0.109114
N19   -4.546657   -0.660076   -0.024486
H20   -6.184367   0.613313   -0.091787
O21   -2.651868   -1.926538   0.033970

N22   -2.114821   2.605018   -0.304140
H23   -1.081395   2.473409   -0.282398
H24   -2.488078   3.540108   -0.362208
C25   -4.360223   1.711158   -0.207733
H26   -4.831234   2.681734   -0.273743
C27   -5.359949   -1.876337   0.088417
H28   -5.101924   -2.564770   -0.716333
H29   -5.169257   -2.361078   1.046666
H30   -6.410675   -1.599642   0.015310
C31   5.311411   -1.355996   -0.894320
H32   5.355791   -2.103899   -0.101181
H33   5.006830   -1.832451   -1.827823
H34   6.293854   -0.901757   -1.021112
H35   5.580797   1.449609   -0.561566
O36   2.534134   0.564981   1.895410
O37   1.975515   -0.469145   2.281657

Zero-point correction=   0.283363 (Hartree/Particle)
Thermal correction to Energy=   0.304327
Thermal correction to Enthalpy=   0.305271
Thermal correction to Gibbs Free Energy=   0.232009
Sum of electronic and zero-point Energies=   -1165.617165
Sum of electronic and thermal Energies=   -1165.596201
Sum of electronic and thermal Enthalpies=   -1165.595256
Sum of electronic and thermal Free Energies=   -1165.668518

anti-5OO-[9MG – H]•·[1MC + H]+

C1   1.091233   0.974214   -0.092863
C2   2.543091   0.764642   0.336775
H3   -1.353672   0.152330   -0.203592
C4   0.954539   -1.361622   -0.178919
C5   4.535526   1.029048   -0.422734
N6   0.352757   -0.156044   -0.208896
N7   3.552679   1.726029   0.011012
N8   4.324416   -0.357399   -0.525704
N9   2.309924   -1.607588   -0.357959
C10   3.032241   -0.558599   -0.191612
N11   0.199071   -2.437700   -0.090282
H12   0.642871   -3.343153   -0.122107
H13   -0.813229   -2.354985   0.011300
O14   0.633081   2.103798   -0.221891
C15   -3.159068   -0.813905   -0.026584
N16   -2.399725   0.327953   -0.182741
C17   -2.900193   1.580927   -0.315428
C18   -5.072016   0.610948   -0.144443
N19   -4.533359   -0.630807   -0.008733
H20   -6.154494   0.660518   -0.118545
O21   -2.653731   -1.918191   0.087734
N22   -2.061677   2.587437   -0.449201
H23   -1.033246   2.447518   -0.412813
H24   -2.422492   3.524794   -0.539892
C25   -4.317441   1.727482   -0.300271
H26   -4.776936   2.700255   -0.404273
C27   -5.361395   -1.829915   0.165628
H28   -5.130173   -2.551166   -0.618329
H29   -5.157475   -2.282092   1.136903
H30   -6.409325   -1.540199   0.104081

C31   5.212995   -1.338523   -1.130185
H32   5.073124   -2.295793   -0.627714
H33   4.995400   -1.453512   -2.194879
H34   6.243893   -1.010952   -0.995325
H35   5.494600   1.441857   -0.716336
O36   2.544116   0.721691   1.832851
O37   1.880969   -0.278145   2.325413

Zero-point correction=   0.285043 (Hartree/Particle)
Thermal correction to Energy=   0.306021
Thermal correction to Enthalpy=   0.306965
Thermal correction to Gibbs Free Energy=   0.233753
Sum of electronic and zero-point Energies=   -1165.623499
Sum of electronic and thermal Energies=   -1165.602522
Sum of electronic and thermal Enthalpies=   -1165.601578
Sum of electronic and thermal Free Energies=   -1165.674789

syn-TS8
C1   0.893082   0.949030   -0.381788
C2   2.359463   0.738623   -0.442283
H3   -1.575234   0.146467   -0.148044
C4   0.734563   -1.402044   -0.225913
C5   4.472162   0.790862   -0.429028
N6   0.150118   -0.184977   -0.261959
N7   3.338982   1.578128   -0.571139
N8   4.173414   -0.558306   -0.512818
N9   2.080963   -1.704060   -0.300036
C10   2.821972   -0.646238   -0.391876
N11 -0.055678   -2.457750   -0.105023
H12   0.369167   -3.371722   -0.071901
H13 -1.067479   -2.351341   -0.035986
O14   0.398365   2.075216   -0.434696
C15 -3.386040   -0.804130   0.075954
N16 -2.615958   0.332496   -0.068106
C17 -3.102632   1.598704   -0.103611
C18 -5.276380   0.653621   0.165378
N19 -4.752497   -0.601536   0.196952
H20 -6.353555   0.717851   0.266872
O21 -2.897339   -1.921316   0.097132
N22 -2.258529   2.597283   -0.247227
H23 -1.232031   2.434921   -0.328863
H24 -2.609380   3.542450   -0.272792
C25 -4.513084   1.764837   0.018966
H26 -4.960139   2.748671   -0.002567
C27 -5.589634   -1.796639   0.353347
H28 -5.485056   -2.437888   -0.522439
H29 -5.277342   -2.349724   1.239534
H30 -6.626635   -1.481947   0.460661
C31   5.111675   -1.658836   -0.352188
H32   5.306522   -1.841421   0.707728
H33   4.672933   -2.550296   -0.799784
H34   6.041451   -1.414310   -0.865971
H35   5.455201   1.154307   -0.698281
O36   3.608078   0.471664   1.947352
O37   4.611520   0.989222   1.444659

Zero-point correction=   0.283606 (Hartree/Particle)
Thermal correction to Energy=   0.304501

Thermal correction to Enthalpy=   0.305445
Thermal correction to Gibbs Free Energy=   0.231617
Sum of electronic and zero-point Energies=   -1165.621146
Sum of electronic and thermal Energies=   -1165.600251
Sum of electronic and thermal Enthalpies=   -1165.599307
Sum of electronic and thermal Free Energies=   -1165.673135

syn-8OO-[9MG – H]•·[1MC + H]+
C1   -0.819358   -0.909277   -0.311231
C2   -2.294842   -0.679433   -0.363683
H3   1.664124   -0.153566   -0.104801
C4   -0.633843   1.436636   -0.154053
C5   -4.468342   -0.719888   -0.422537
N6   -0.061598   0.209708   -0.202535
N7   -3.252406   -1.514626   -0.437148
N8   -4.077229   0.672760   -0.404525
N9   -1.972656   1.761118   -0.209883
C10 -2.748374   0.727171   -0.310408
N11   0.176501   2.474799   -0.038509
H12 -0.230894   3.396594   0.003704
H13   1.186988   2.348969   0.021312
O14 -0.351213   -2.044936   -0.365570
C15   3.487680   0.772671   0.096023
N16   2.701520   -0.354454   -0.038450
C17   3.170779   -1.626852   -0.079345
C18   5.360025   -0.708866   0.153698
N19   4.853389   0.553142   0.189665
H20   6.437725   -0.787015   0.238518
O21   3.011557   1.894876   0.130551
N22   2.311510   -2.614935   -0.209065
H23   1.288080   -2.439956   -0.276126
H24   2.648791   -3.564970   -0.237356
C25   4.580264   -1.810808   0.022480
H26   5.014769   -2.800142   -0.004291
C27   5.708344   1.736650   0.340042
H28   5.522395   2.428679   -0.481315
H29   5.486528   2.235919   1.284040
H30   6.749144   1.416553   0.325706
C31 -5.005132   1.786810   -0.317917
H32 -5.480114   1.809382   0.665996
H33 -4.443236   2.707882   -0.472004
H34 -5.767691   1.691205   -1.093060
H35 -5.124662   -0.971885   -1.258310
O36 -4.620699   -0.751873   1.850735
O37 -5.255692   -1.055460   0.749625

Zero-point correction=   0.285642 (Hartree/Particle)
Thermal correction to Energy=   0.306721
Thermal correction to Enthalpy=   0.307665
Thermal correction to Gibbs Free Energy=   0.233251
Sum of electronic and zero-point Energies=   -1165.630650
Sum of electronic and thermal Energies=   -1165.609572
Sum of electronic and thermal Enthalpies=   -1165.608627
Sum of electronic and thermal Free Energies=   -1165.683041

rot-TS8
C1   0.819877   0.817036   -0.250556

C2   2.288192   0.540718   -0.295397
C3   0.562516   -1.518020   -0.032638
C4   4.453241   0.518776   -0.432097
N5   0.028385   -0.275179   -0.117034
N6   3.268091   1.346421   -0.403181
N7   4.027701   -0.864164   -0.277978
N8   1.889667   -1.884155   -0.071232
C9   2.698517   -0.876660   -0.197998
N10   -0.282091   -2.526509   0.102973
H11   0.094501   -3.459931   0.168078
H12   -1.288712   -2.367378   0.144774
O13   0.387396   1.964836   -0.335499
H14   4.997584   0.671380   -1.370134
O15   5.383859   0.801307   0.644125
O16   5.141552   1.905886   1.300227
C17   4.921066   -2.010471   -0.261624
H18   5.423578   -2.110015   -1.226981
H19   5.662231   -1.891494   0.530593
H20   4.321094   -2.900340   -0.071687
H21   -1.688760   0.142542   -0.061139
C22   -3.544165   -0.723357   0.113818
N23   -2.720593   0.376100   -0.027115
C24   -3.149663   1.660348   -0.114643
C25   -5.371661   0.813751   0.076686
N26   -4.904780   -0.461361   0.159934
H27   -6.448574   0.925653   0.126466
O28   -3.103108   -1.857582   0.192714
N29   -2.258066   2.619135   -0.245356
H30   -1.239055   2.412325   -0.282511
H31   -2.565899   3.577522   -0.307613
C32   -4.555313   1.888237   -0.058598
H33   -4.958975   2.888820   -0.124085
C34   -5.799746   -1.614526   0.313630
H35   -5.615952   -2.329894   -0.488056
H36   -5.616956   -2.099560   1.273234
H37   -6.829053   -1.262224   0.265949

Zero-point correction=   0.285185 (Hartree/Particle)
Thermal correction to Energy=   0.305571
Thermal correction to Enthalpy=   0.306516
Thermal correction to Gibbs Free Energy=   0.234013
Sum of electronic and zero-point Energies=   -1165.621760
Sum of electronic and thermal Energies=   -1165.601374
Sum of electronic and thermal Enthalpies=   -1165.600429
Sum of electronic and thermal Free Energies=   -1165.672933

anti-TS8

C1   0.811457   0.822926   -0.343978
C2   2.261897   0.539393   -0.426036
H3   -1.693026   0.143081   -0.080964
C4   0.544306   -1.507738   -0.081477
C5   4.392215   0.497624   -0.500213
N6   0.016072   -0.269036   -0.170482
N7   3.279048   1.331471   -0.568921
N8   4.013908   -0.840311   -0.447513
N9   1.875625   -1.872267   -0.146839
C10   2.664497   -0.857793   -0.321480

N11   -0.291398   -2.521139   0.091309
H12   0.092312   -3.450945   0.162411
H13   -1.297328   -2.366782   0.156286
O14   0.367949   1.968824   -0.431542
C15   -3.547615   -0.715628   0.155682
N16   -2.725394   0.378178   -0.027208
C17   -3.154265   1.661447   -0.131003
C18   -5.372974   0.824874   0.131981
N19   -4.906303   -0.449277   0.231504
H20   -6.448070   0.940278   0.206142
O21   -3.108420   -1.849899   0.245544
N22   -2.264133   2.614673   -0.301819
H23   -1.244409   2.404016   -0.356068
H24   -2.572270   3.571957   -0.377743
C25   -4.558183   1.893902   -0.046537
H26   -4.961199   2.893923   -0.123596
C27   -5.799347   -1.596700   0.430041
H28   -5.653156   -2.319294   -0.373094
H29   -5.579574   -2.075872   1.384734
H30   -6.828045   -1.239375   0.423327
C31   4.910363   -1.982125   -0.351963
H32   5.348594   -2.040416   0.646824
H33   4.331422   -2.884340   -0.548474
H34   5.699260   -1.887415   -1.099454
H35   5.319227   0.777714   -0.986428
O36   5.752680   1.740963   1.358673
O37   4.936563   0.820902   1.234296

Zero-point correction=   0.282365 (Hartree/Particle)
Thermal correction to Energy=   0.303756
Thermal correction to Enthalpy=   0.304700
Thermal correction to Gibbs Free Energy=   0.229211
Sum of electronic and zero-point Energies=   -1165.611746
Sum of electronic and thermal Energies=   -1165.590356
Sum of electronic and thermal Enthalpies=   -1165.589411
Sum of electronic and thermal Free Energies=   -1165.664900

anti-8OO-[9MG − H]•·[1MC + H]+

C1   -0.742065   -0.902374   -0.178090
C2   -2.216786   -0.660959   -0.219447
H3   1.753198   -0.166481   -0.047574
C4   -0.535262   1.445197   -0.077671
C5   -4.390848   -0.690415   -0.310330
N6   0.026095   0.211812   -0.107857
N7   -3.181261   -1.490161   -0.274974
N8   -3.988672   0.706204   -0.245042
N9   -1.871268   1.779284   -0.112370
C10   -2.658916   0.750100   -0.182782
N11   0.287001   2.477864   -0.003868
H12   -0.110536   3.404557   0.023287
H13   1.297429   2.343577   0.035399
O14   -0.285530   -2.043585   -0.211675
C15   3.587965   0.749381   0.077066
N16   2.790019   -0.374418   -0.008309
C17   3.248561   -1.651014   -0.036971
C18   5.450578   -0.745015   0.105537
N19   4.954404   0.521386   0.130175

H20	6.529934	-0.829697	0.156797
O21	3.120567	1.875416	0.104035
N22	2.378540	-2.635021	-0.117868
H23	1.355237	-2.453509	-0.157072
H24	2.707838	-3.588082	-0.137482
C25	4.659161	-1.843544	0.023852
H26	5.085779	-2.836501	0.004742
C27	5.822202	1.701194	0.229132
H28	5.603563	2.384546	-0.591293
H29	5.644929	2.212237	1.176290
H30	6.859396	1.374352	0.171877
C31	-4.903049	1.836493	-0.233461
H32	-5.429645	1.887982	0.722070
H33	-4.317099	2.744314	-0.377772
H34	-5.628647	1.731346	-1.041733
H35	-4.989752	-0.906856	-1.199262
O36	-6.426697	-0.737870	0.667107
O37	-5.165200	-1.045796	0.848222

Zero-point correction=   0.285353 (Hartree/Particle)
Thermal correction to Energy=   0.306653
Thermal correction to Enthalpy=   0.307597
Thermal correction to Gibbs Free Energy=   0.232252
Sum of electronic and zero-point Energies=   -1165.628933
Sum of electronic and thermal Energies=   -1165.607633
Sum of electronic and thermal Enthalpies=   -1165.606688
Sum of electronic and thermal Free Energies=   -1165.682034

4,5-OO-[9MG − H]•·[1MC + H]⁺

C1	1.020680	1.041213	0.027497
C2	2.510690	0.914675	0.281337
H3	-1.455430	0.181541	-0.083083
C4	0.894744	-1.314048	-0.157486
C5	4.379328	1.025275	-0.772434
N6	0.300186	-0.117513	-0.082787
N7	3.385484	1.778102	-0.425298
N8	4.277358	-0.320636	-0.520520
N9	2.245557	-1.537920	-0.362775
C10	3.046902	-0.527096	0.158162
N11	0.147093	-2.407027	-0.140087
H12	0.592070	-3.304863	-0.255769
H13	-0.864902	-2.339608	-0.020892
O14	0.484861	2.141180	-0.016559
C15	-3.233873	-0.837019	-0.000675
N16	-2.499054	0.329595	-0.078012
C17	-3.026277	1.577422	-0.157291
C18	-5.176800	0.548257	-0.094558
N19	-4.611369	-0.686419	-0.009956
H20	-6.260493	0.570640	-0.096346
O21	-2.703753	-1.933186	0.070163
N22	-2.208763	2.606809	-0.216439
H23	-1.178886	2.482314	-0.170348
H24	-2.587018	3.540177	-0.271236
C25	-4.446523	1.688889	-0.170785
H26	-4.926800	2.654924	-0.236365
C27	-5.414349	-1.912059	0.080818
H28	-5.137980	-2.590799	-0.726056

H29	-5.232457	-2.402421	1.037867
H30	-6.466516	-1.645018	-0.005153
C31	5.282440	-1.342525	-0.754729
H32	5.817764	-1.581025	0.167896
H33	4.795527	-2.240715	-1.140000
H34	5.991171	-0.977639	-1.498951
H35	5.255881	1.401863	-1.289789
O36	2.763846	0.824919	1.704258
O37	3.127655	-0.588189	1.592165

Zero-point correction=   0.284425 (Hartree/Particle)
Thermal correction to Energy=   0.304997
Thermal correction to Enthalpy=   0.305941
Thermal correction to Gibbs Free Energy=   0.233385
Sum of electronic and zero-point Energies=   -1165.579373
Sum of electronic and thermal Energies=   -1165.558801
Sum of electronic and thermal Enthalpies=   -1165.557857
Sum of electronic and thermal Free Energies=   -1165.630413

TS-8−58

C1	-0.935777	-0.918703	-0.299663
C2	-2.416448	-0.711615	-0.276370
C3	-0.770276	1.431039	-0.201948
C4	-4.532827	-0.772295	-0.140465
N5	-0.189285	0.209586	-0.218533
N6	-3.379392	-1.499503	-0.740156
N7	-4.219639	0.615265	-0.395756
N8	-2.114093	1.737382	-0.278547
C9	-2.879474	0.699709	-0.314223
N10	0.026863	2.480637	-0.106360
H11	-0.390212	3.398925	-0.089924
H12	1.037903	2.366379	-0.032982
O13	-0.459377	-2.048939	-0.369526
H14	-5.520218	-1.089810	-0.463314
O15	-4.395109	-1.092935	1.244011
O16	-3.071885	-0.793468	1.530184
C17	-5.147117	1.710697	-0.163013
H18	-5.343673	1.824515	0.907072
H19	-4.700169	2.625284	-0.551951
H20	-6.078938	1.510002	-0.693008
H21	1.542579	-0.138382	-0.137979
C22	3.354285	0.807496	0.066408
N23	2.581331	-0.327920	-0.075316
C24	3.064837	-1.594591	-0.124791
C25	5.243111	-0.653212	0.116362
N26	4.722019	0.602602	0.162114
H27	6.321552	-0.719622	0.201907
O28	2.865195	1.923944	0.105154
N29	2.216869	-2.591675	-0.260712
H30	1.191672	-2.429168	-0.318810
H31	2.564677	-3.537742	-0.294270
C32	4.476280	-1.763033	-0.024873
H33	4.922044	-2.747089	-0.059187
C34	5.563019	1.794731	0.322857
H35	5.375940	2.487672	-0.497513
H36	5.328507	2.288216	1.266803
H37	6.607336	1.486071	0.315746

Zero-point correction=   0.283417 (Hartree/Particle)
Thermal correction to Energy=   0.303737
Thermal correction to Enthalpy=   0.304682
Thermal correction to Gibbs Free Energy=   0.232585
Sum of electronic and zero-point Energies=   -1165.570683
Sum of electronic and thermal Energies=   -1165.550363
Sum of electronic and thermal Enthalpies=   -1165.549419
Sum of electronic and thermal Free Energies=   -1165.621515

TS-58

C1	-0.955893	-0.930201	-0.200584
C2	-2.446928	-0.743675	-0.154205
H3	1.522928	-0.139705	-0.090356
C4	-0.788721	1.421979	-0.172571
C5	-4.488133	-0.811269	-0.238230
N6	-0.211204	0.202860	-0.148629
N7	-3.395639	-1.507805	-0.743732
N8	-4.235804	0.598676	-0.424095
N9	-2.130645	1.723521	-0.319942
C10	-2.897337	0.689158	-0.318232
N11	0.000981	2.476926	-0.071569
H12	-0.416845	3.394339	-0.104760
H13	1.009758	2.367294	0.033370
O14	-0.470440	-2.056165	-0.252931
H15	-5.500599	-1.157951	-0.417632
O16	-2.922131	-0.835901	1.476428
O17	-4.239785	-0.969592	1.309953
C18	-5.184661	1.686161	-0.250020
H19	-4.753728	2.586541	-0.687989
H20	-6.109311	1.438185	-0.772435
H21	-5.388527	1.859417	0.810056
C22	3.333967	0.813155	0.084526
N23	2.563814	-0.324141	-0.056574
C24	3.053295	-1.585894	-0.153552
C25	5.232765	-0.634716	0.032109
N26	4.705453	0.615768	0.128051
H27	6.314054	-0.695062	0.076849
O28	2.839520	1.925028	0.165664
N29	2.207097	-2.585306	-0.281480
H30	1.179001	-2.428387	-0.289433
H31	2.559206	-3.527740	-0.351952
C32	4.468597	-1.746321	-0.108841
H33	4.919010	-2.726016	-0.183483
C34	5.544090	1.809864	0.286075
H35	5.323958	2.519352	-0.511620
H36	5.339733	2.280900	1.248305
H37	6.589424	1.508917	0.235115

Zero-point correction=   0.282857 (Hartree/Particle)
Thermal correction to Energy=   0.303349
Thermal correction to Enthalpy=   0.304293
Thermal correction to Gibbs Free Energy=   0.232080
Sum of electronic and zero-point Energies=   -1165.572998
Sum of electronic and thermal Energies=   -1165.552507
Sum of electronic and thermal Enthalpies=   -1165.551562
Sum of electronic and thermal Free Energies=   -1165.623775

5,8-OO-[9MG – H]$^\bullet$·[1MC + H]$^+$

C1	-0.957315	-0.896264	-0.095059
C2	-2.462017	-0.709651	0.006540
H3	1.526930	-0.131446	-0.047928
C4	-0.774768	1.453199	-0.060136
C5	-4.521022	-0.765890	-0.224636
N6	-0.204880	0.225885	-0.066775
N7	-3.371128	-1.350746	-0.909627
N8	-4.213301	0.657498	-0.365937
N9	-2.110896	1.767955	-0.182132
C10	-2.883902	0.735169	-0.205858
N11	0.031173	2.494977	0.044705
H12	-0.375889	3.417825	0.035688
H13	1.040587	2.371909	0.123920
O14	-0.491534	-2.029437	-0.169255
H15	-5.509237	-1.059176	-0.570721
O16	-2.925435	-1.061573	1.316931
O17	-4.367709	-1.164204	1.121019
C18	-5.166598	1.753089	-0.353253
H19	-4.631993	2.673214	-0.588560
H20	-5.932983	1.575657	-1.109737
H21	-5.630204	1.841826	0.632742
C22	3.351332	0.803845	0.081585
N23	2.566736	-0.325716	-0.042521
C24	3.041727	-1.590931	-0.161727
C25	5.234484	-0.660053	-0.039561
N26	4.721743	0.594289	0.079897
H27	6.316084	-0.730168	-0.030772
O28	2.869887	1.919362	0.185710
N29	2.183344	-2.582518	-0.269932
H30	1.157159	-2.417425	-0.248435
H31	2.525293	-3.527422	-0.355543
C32	4.456151	-1.764124	-0.161750
H33	4.895433	-2.747217	-0.255725
C34	5.575328	1.780461	0.216802
H35	5.340717	2.492988	-0.574054
H36	5.400434	2.251955	1.184571
H37	6.616062	1.469837	0.137882

Zero-point correction=   0.286098 (Hartree/Particle)
Thermal correction to Energy=   0.306175
Thermal correction to Enthalpy=   0.307119
Thermal correction to Gibbs Free Energy=   0.235887
Sum of electronic and zero-point Energies=   -1165.600525
Sum of electronic and thermal Energies=   -1165.580448
Sum of electronic and thermal Enthalpies=   -1165.579504
Sum of electronic and thermal Free Energies=   -1165.650736

TS-5–45

C1	0.990817	1.024692	0.042228
C2	2.498783	0.915963	0.179588
H3	-1.456438	0.151911	-0.015489
C4	0.923765	-1.347331	0.065190
C5	4.310650	0.887409	-1.008419
N6	0.297273	-0.128699	0.045162
N7	3.351897	1.698781	-0.662333
N8	4.209935	-0.408702	-0.589241

N9   2.248697   -1.607967   0.028753
C10   3.021076   -0.515312   0.200420
N11   0.123603   -2.408332   0.077401
H12   0.546378   -3.323049   0.096182
H13   -0.889271   -2.307824   0.071944
O14   0.474151   2.141363   -0.032887
C15   -3.255886   -0.846920   -0.024406
N16   -2.503148   0.311087   -0.049144
C17   -3.016498   1.565994   -0.110714
C18   -5.181728   0.563541   -0.133457
N19   -4.632135   -0.679042   -0.072087
H20   -6.264583   0.599400   -0.165627
O21   -2.745597   -1.952095   0.034578
N22   -2.190252   2.589043   -0.127216
H23   -1.155782   2.454492   -0.095469
H24   -2.563458   3.524896   -0.170792
C25   -4.435653   1.695574   -0.154764
H26   -4.901812   2.669376   -0.205714
C27   -5.449530   -1.897324   -0.039826
H28   -5.155913   -2.556735   -0.856650
H29   -5.300952   -2.416297   0.907872
H30   -6.496004   -1.616509   -0.149359
C31   5.132365   -1.499327   -0.854823
H32   5.881386   -1.563404   -0.061436
H33   4.556391   -2.424624   -0.894912
H34   5.625312   -1.326432   -1.812064
H35   5.150241   1.191872   -1.624532
O36   2.937587   1.067513   1.555078
O37   3.440666   -0.244532   1.624591

Zero-point correction=   0.282593 (Hartree/Particle)
Thermal correction to Energy=   0.302852
Thermal correction to Enthalpy=   0.303796
Thermal correction to Gibbs Free Energy=   0.231964
Sum of electronic and zero-point Energies=   -1165.578283
Sum of electronic and thermal Energies=   -1165.558024
Sum of electronic and thermal Enthalpies=   -1165.557080
Sum of electronic and thermal Free Energies=   -1165.628913

Cartesian coordinates for the structures in Scheme 4, optimized at ωB97XD/ 6-311++G(d,p).

9MG•+·1MC·H₂O_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

Zero-point correction=	0.300874 (Hartree/Particle)
Thermal correction to Energy=	0.323462
Thermal correction to Enthalpy=	0.324406
Thermal correction to Gibbs Free Energy=	0.246137
Sum of electronic and zero-point Energies=	-1092.007930
Sum of electronic and thermal Energies=	-1091.985343
Sum of electronic and thermal Enthalpies=	-1091.984399
Sum of electronic and thermal Free Energies=	-1092.062667

9MG•+·1MC·H₂O_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

Zero-point correction=	0.300300 (Hartree/Particle)
Thermal correction to Energy=	0.322880
Thermal correction to Enthalpy=	0.323824
Thermal correction to Gibbs Free Energy=	0.245255
Sum of electronic and zero-point Energies=	-1092.007078
Sum of electronic and thermal Energies=	-1091.984499
Sum of electronic and thermal Enthalpies=	-1091.983555
Sum of electronic and thermal Free Energies=	-1092.062124

9MG•+·1MC·H₂O_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

Zero-point correction=   0.299970 (Hartree/Particle)
Thermal correction to Energy=   0.323000
Thermal correction to Enthalpy=   0.323944
Thermal correction to Gibbs Free Energy=   0.244014
Sum of electronic and zero-point Energies=   -1092.007181
Sum of electronic and thermal Energies=   -1091.984151
Sum of electronic and thermal Enthalpies=   -1091.983207
Sum of electronic and thermal Free Energies=   -1092.063138