

Supporting Information

Dynamics and Multi-configuration Potential Energy Surface for the Singlet O₂ Reactions with Radical Cations of Guanine, 9-Methylguanine, 2'-Deoxyguanosine and Guanosine

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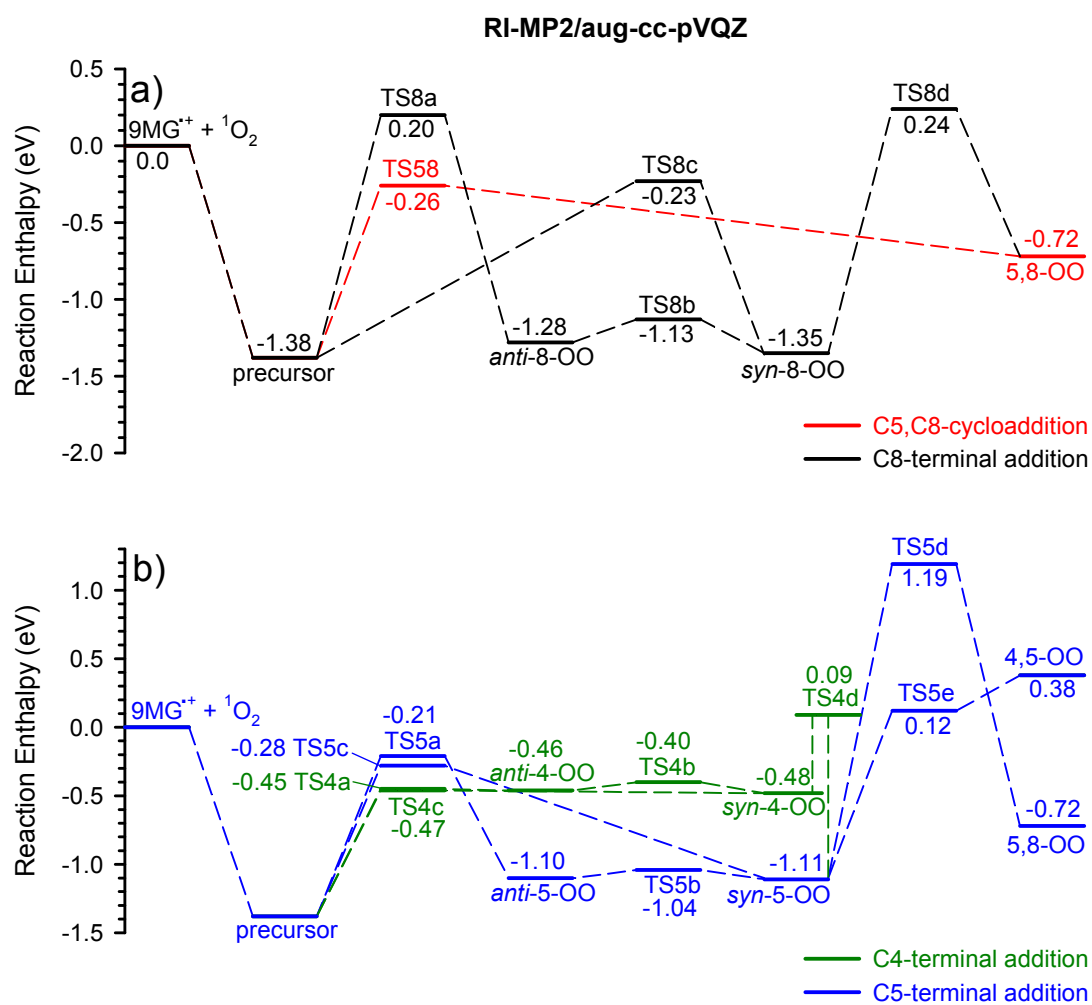


Figure S1. Reaction enthalpies for the ¹O₂ addition to 9MG⁺ calculated at RI-MP2/aug-cc-pVQZ// ω B97XD/6-31+G(d,p), including thermal corrections at 298 K. See Figure 1 for structures.

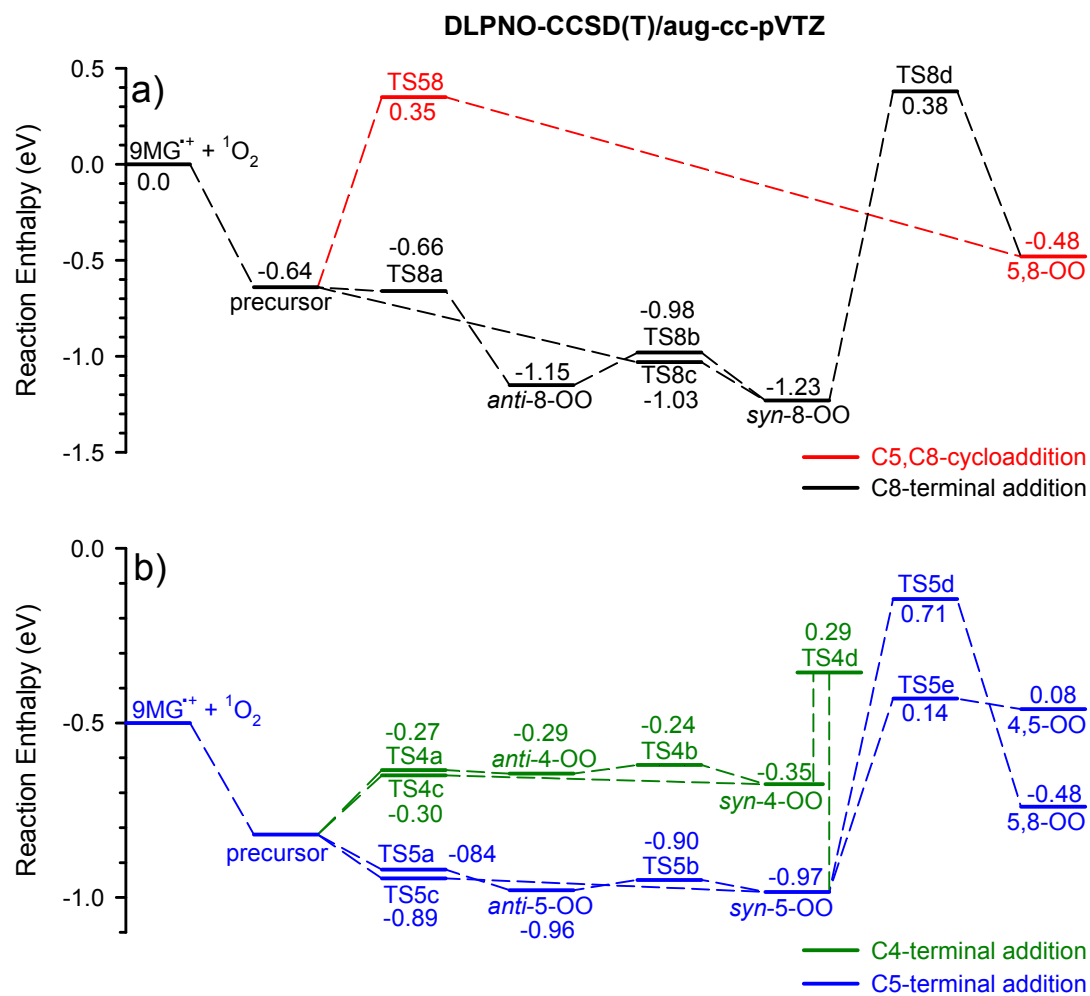


Figure S2. Reaction enthalpies for the ${}^1\text{O}_2$ addition to $9\text{MG}^{\bullet+}$ calculated at DLPNO-CCSD(T)/aug-cc-pVTZ// $\omega\text{B97XD}/6\text{-}31\text{+G(d,p)}$, including thermal corrections at 298 K. See Figure 1 for structures.

**Cartesian coordinates for radical cations in
Scheme 1, optimized at ω B97XD/6-31+G(d,p)**

9HG^{•+}

C1	-0.246525	1.479497	0.000004
C2	0.854816	0.518755	0.000002
H3	-2.305573	1.419067	0.000005
C4	-1.679426	-0.548633	0.000006
C5	2.692392	-0.514115	-0.000013
N6	-1.503772	0.796299	0.000005
N7	2.171493	0.715558	-0.000015
N8	1.751847	-1.500377	0.000006
N9	-0.652665	-1.437674	0.000017
C10	0.531203	-0.880468	0.000012
N11	-2.901167	-1.058213	-0.000036
H12	-2.995044	-2.065277	0.000073
H13	-3.739392	-0.495433	-0.000028
O14	-0.200466	2.678487	0.000007
H15	3.753107	-0.726499	-0.000026
H16	1.915718	-2.499117	0.000006

9MG^{•+}

C1	-1.205070	1.373596	0.001909
C2	0.216428	1.034962	-0.000522
H3	-2.998666	0.360694	0.003252
C4	-1.529625	-1.090377	-0.000782
C5	2.319045	0.954060	-0.004547
N6	-1.999354	0.182769	0.001621
N7	1.291141	1.814595	-0.002535
N8	1.951099	-0.354609	-0.005088
N9	-0.209725	-1.400171	-0.001351
C10	0.580661	-0.354448	-0.001494
N11	-2.379566	-2.107281	-0.002544
H12	-1.998213	-3.043648	-0.003980
H13	-3.382593	-1.994381	-0.003027
O14	-1.725507	2.455145	0.004289
H15	3.359046	1.254418	-0.006786
C16	2.813108	-1.534800	0.008352
H17	2.706734	-2.055129	0.960908
H18	2.530419	-2.196847	-0.810291
H19	3.844872	-1.211340	-0.122617

dGuo^{•+}

O1	3.140448	-1.988426	0.263691
C2	3.792203	-1.268264	-0.779029
H3	3.565923	-1.712828	-1.754991
H4	4.879527	-1.272390	-0.633525
C5	3.313546	0.171276	-0.771517
H6	3.861401	0.727109	-1.537403
O7	1.916106	0.228549	-1.108670
C8	1.157033	0.709596	-0.039624
H9	0.741628	1.696114	-0.266117
N10	-0.008668	-0.182237	0.102732
C11	0.036825	-1.540927	0.198333
H12	0.991096	-2.058686	0.233253

N13	-1.172865	-2.121615	0.220904
C14	-2.024340	-1.107168	0.119355
C15	-3.483676	-1.094136	0.081465
O16	-4.251920	-2.015476	0.150819
N17	-3.966405	0.243899	-0.063457
H18	-4.978053	0.310048	-0.103108
C19	-3.200679	1.362457	-0.148610
N20	-3.783266	2.546383	-0.292686
H21	-4.782583	2.670308	-0.353659
H22	-3.188400	3.360622	-0.358663
N23	-1.850649	1.350316	-0.092301
C24	-1.331123	0.151151	0.030131
C25	3.446887	0.899850	0.572656
H26	4.235349	0.458602	1.191450
C27	2.061183	0.714596	1.195547
H28	2.013497	-0.249782	1.707256
H29	1.802167	1.509435	1.897171
O30	3.716715	2.255894	0.276660
H31	3.557908	-2.848164	0.366957
H32	3.995565	2.717480	1.072780

Guo^{•+}

O1	3.035367	-2.087249	0.455746
C2	3.771234	-1.527828	-0.625177
H3	3.625974	-2.114054	-1.540080
H4	4.844101	-1.493551	-0.396376
C5	3.280964	-0.112421	-0.870549
H6	3.862178	0.319883	-1.691202
O7	1.902681	-0.147250	-1.290259
C8	1.083186	0.503531	-0.370392
H9	0.707929	1.459488	-0.751534
N10	-0.099329	-0.336755	-0.150275
C11	-0.093406	-1.675056	0.102790
H12	0.842703	-2.221480	0.155946
N13	-1.317723	-2.197586	0.271120
C14	-2.138089	-1.163295	0.122412
C15	-3.594007	-1.089201	0.198700
O16	-4.386935	-1.964838	0.419441
N17	-4.037573	0.249447	-0.034484
H18	-5.045156	0.358632	0.011727
C19	-3.241839	1.317879	-0.299125
N20	-3.789975	2.508997	-0.504901
H21	-4.784420	2.675994	-0.476892
H22	-3.171514	3.286358	-0.690657
N23	-1.894354	1.247793	-0.366988
C24	-1.410575	0.047497	-0.153053
C25	3.325483	0.818746	0.351503
H26	4.083438	0.516342	1.080141
C27	1.906940	0.703549	0.921930
H28	1.841415	-0.200383	1.533251
O29	3.471896	2.176602	-0.022246
H30	3.439289	-2.916119	0.728029
H31	4.399013	2.422626	-0.076735
O32	1.483740	1.784078	1.685992
H33	1.934363	2.571840	1.349442

**Cartesian coordinates for monohydrated
9MG^{•+} and its peroxides in Scheme 2 and
Table 2, optimized at ω B97XD/6-31+G(d,p)**

9MG^{•+}·H₂O

C1	0.610261	1.452293	-0.001944
C2	-0.791531	1.031967	0.000496
H3	2.474569	0.514452	-0.002625
C4	1.075676	-0.978664	0.001088
C5	-2.886951	0.829043	0.004646
N6	1.468848	0.319876	-0.001498
N7	-1.912343	1.747426	0.002493
N8	-2.443349	-0.455688	0.005471
N9	-0.225728	-1.373871	0.001615
C10	-1.074036	-0.375744	0.001682
N11	1.999374	-1.924952	0.003088
H12	1.696579	-2.888361	0.004708
H13	2.989292	-1.687822	0.003142
O14	1.056348	2.569552	-0.004402
H15	-3.942924	1.066665	0.006917
O16	4.311613	-0.182968	-0.000489
H17	4.861473	0.002521	-0.769997
H18	4.860897	0.007710	0.768152
C19	-3.233315	-1.683505	-0.009088
H20	-3.100469	-2.194789	-0.963341
H21	-2.909024	-2.331340	0.805606
H22	-4.282315	-1.423591	0.127096

anti-[8-OO-9MG]^{•+}·H₂O

C1	1.148165	-1.418372	-0.107257
C2	-0.243028	-0.884919	-0.195239
H3	3.063528	-0.636310	0.069410
C4	1.773999	0.967114	0.039877
C5	-2.378217	-0.522079	-0.375039
N6	2.075179	-0.369616	0.008394
N7	-1.335970	-1.524954	-0.302293
N8	-1.728554	0.783918	-0.243536
N9	0.527893	1.478737	-0.032440
C10	-0.425532	0.586410	-0.145209
N11	2.781764	1.811595	0.149722
H12	2.574211	2.799845	0.174939
H13	3.741990	1.479553	0.209279
O14	1.473859	-2.571076	-0.132649
H15	-2.937887	-0.601200	-1.311779
O16	-3.270732	-0.748522	0.718885
O17	-4.445191	-0.218377	0.468524
C18	-2.429561	2.061875	-0.252347
H19	-3.116505	2.110056	0.594406
H20	-1.685139	2.853318	-0.172943
H21	-2.988175	2.167008	-1.184011
O22	4.930346	-0.140419	0.227306
H23	5.521390	-0.338094	-0.508016
H24	5.403205	-0.404955	1.024544

syn-[8-OO-9MG]^{•+}·H₂O

C1	1.020769	-1.396258	-0.246094
C2	-0.361615	-0.848267	-0.367111
H3	2.930945	-0.638324	0.054023
C4	1.654720	0.975095	0.035508
C5	-2.489280	-0.457095	-0.566426
N6	1.948698	-0.360638	-0.043152
N7	-1.454286	-1.473246	-0.539839
N8	-1.830905	0.833739	-0.421072
N9	0.416424	1.500672	-0.075245
C10	-0.535265	0.621524	-0.265130
N11	2.660201	1.805973	0.233506
H12	2.456469	2.793407	0.294949
H13	3.614179	1.464064	0.327806
O14	1.341939	-2.548766	-0.309246
H15	-3.086275	-0.524088	-1.479127
O16	-3.431000	-0.675551	0.502008
O17	-2.848694	-0.579594	1.670379
C18	-2.532644	2.108310	-0.359974
H19	-3.208751	2.114324	0.497497
H20	-1.789936	2.897540	-0.249810
H21	-3.098122	2.260494	-1.281079
O22	4.790711	-0.162728	0.336518
H23	5.422507	-0.330285	-0.371839
H24	5.214299	-0.469360	1.146289

anti-[4-OO-9MG]^{•+}·H₂O

C1	-0.844840	1.489864	0.143870
C2	0.606608	1.166386	-0.041975
H3	-2.630874	0.455843	0.005065
C4	-1.098171	-0.868301	-0.469744
C5	2.617798	1.074371	-0.701334
N6	-1.614079	0.358698	-0.070679
N7	1.533237	1.928520	-0.511011
N8	2.382773	-0.174764	-0.442203
N9	0.189264	-1.164854	-0.528481
C10	1.017652	-0.267439	0.089200
N11	-1.997020	-1.775018	-0.834265
H12	-1.670834	-2.699366	-1.072307
H13	-2.990786	-1.570142	-0.807014
O14	-1.281042	2.572888	0.427541
H15	3.570533	1.434449	-1.073658
O16	0.222962	-1.069306	2.121817
O17	1.281978	-0.585986	1.560969
C18	3.264928	-1.330623	-0.552955
H19	4.190882	-1.029075	-1.040423
H20	3.468348	-1.715090	0.448265
H21	2.748129	-2.090123	-1.141955
O22	-4.420427	-0.220301	-0.244040
H23	-4.991879	0.226448	-0.878196
H24	-4.964360	-0.384934	0.534019

syn-[4-OO-9MG]^{•+}·H₂O

C1	-0.941183	1.427447	-0.053335
C2	0.493081	1.052992	-0.273414
H3	-2.735580	0.412655	0.126614

C4 -1.241201 -0.997255 -0.210787
 C5 2.441580 0.781626 -1.064780
 N6 -1.724553 0.286071 0.019931
 N7 1.366012 1.669971 -0.985193
 N8 2.234027 -0.376184 -0.525971
 N9 0.036595 -1.320251 -0.276546
 C10 0.913298 -0.334282 0.132460
 N11 -2.168232 -1.935820 -0.374085
 H12 -1.865220 -2.891919 -0.481268
 H13 -3.156853 -1.708551 -0.343698
 O14 -1.356471 2.550334 0.042551
 H15 3.359328 1.041007 -1.580685
 O16 1.980437 0.434061 2.036834
 O17 1.139506 -0.461248 1.587608
 C18 3.111829 -1.537419 -0.454618
 H19 4.006195 -1.346925 -1.045981
 H20 3.379515 -1.712820 0.589032
 H21 2.564940 -2.396911 -0.845737
 O22 -4.542733 -0.253272 0.064414
 H23 -5.133629 0.101333 -0.608978
 H24 -5.055975 -0.282036 0.879341

N8 -2.163800 0.806480 -0.419341
 N9 0.028393 1.532613 0.122175
 C10 -0.890088 0.633196 -0.080330
 N11 2.274407 1.863630 0.440076
 H12 2.042744 2.813580 0.694643
 H13 3.243406 1.551971 0.412907
 O14 0.983994 -2.258770 -1.101183
 H15 -3.704493 -0.582499 -1.050992
 O16 -0.537364 -1.247520 1.412145
 O17 -1.577588 -0.908608 2.115388
 C18 -2.878034 2.070548 -0.556603
 H19 -3.333890 2.129258 -1.546120
 H20 -3.645856 2.143591 0.215468
 H21 -2.159156 2.880353 -0.436951
 O22 4.466328 0.056342 -0.134781
 H23 4.956107 -0.454127 0.520145
 H24 5.055570 0.148212 -0.892059

anti-[5-OO-9MG]⁺·H₂O

C1 0.571048 -1.238091 -0.581793
 C2 -0.769051 -0.905343 0.069642
 H3 2.462182 -0.367835 -0.639049
 C4 1.141383 1.074484 -0.004568
 C5 -2.815237 -0.610864 -0.506133
 N6 1.474685 -0.172914 -0.447583
 N7 -1.957615 -1.550526 -0.388008
 N8 -2.340638 0.700087 -0.255255
 N9 -0.140789 1.517148 0.082631
 C10 -1.032054 0.580520 -0.010685
 N11 2.109389 1.927084 0.247877
 H12 1.861082 2.866910 0.523896
 H13 3.085235 1.646464 0.166832
 O14 0.870880 -2.286121 -1.072207
 H15 -3.852248 -0.753590 -0.789504
 O16 -0.657205 -1.289287 1.509113
 O17 0.260250 -0.632323 2.148170
 C18 -3.076515 1.946682 -0.438483
 H19 -2.715841 2.676521 0.286111
 H20 -2.928992 2.329818 -1.450575
 H21 -4.135071 1.757326 -0.262625
 O22 4.321509 0.186860 -0.422440
 H23 4.881340 0.286702 -1.200674
 H24 4.846175 -0.305831 0.218978

syn-[5-OO-9MG]⁺·H₂O

C1 0.684717 -1.230101 -0.573536
 C2 -0.688195 -0.868664 -0.012045
 H3 2.607645 -0.437967 -0.428837
 C4 1.293238 1.047537 0.115272
 C5 -2.681318 -0.488231 -0.704229
 N6 1.616368 -0.216134 -0.291897
 N7 -1.867790 -1.459396 -0.558431

**Cartesian coordinates for the structures
in Table 1 and Figure 2, optimized at
 ω B97XD/6-31+G(d,p)**

$^1\text{O}_2$

O1	0.000000	0.000000	0.602307
O2	0.000000	0.000000	-0.602307

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

precursor

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

TS58

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

[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

TS8a

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

anti-[8-OO-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

TS8b

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

TS8c

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

syn-[8-OO-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

TS8d

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

TS4a

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

anti-[4-OO-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

TS4b

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

TS4c

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

syn-[4-OO-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

TS4d

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

TS5a

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

anti-[5-OO-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

TS5b

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

TS5c

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

syn-[5-OO-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

TS5d

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

TS5e

C1 1.302343 -1.287944 -0.290635
 C2 -0.149049 -1.015799 0.061652
 H3 3.061711 -0.275024 -0.419095
 C4 1.602257 1.175057 -0.102951
 C5 -2.106719 -0.761033 -0.801069
 N6 2.075222 -0.119289 -0.241674
 N7 -1.191087 -1.673489 -0.644025
 N8 -1.811793 0.504154 -0.363453
 N9 0.326207 1.500724 0.029099
 C10 -0.515038 0.468930 0.188627
 N11 2.504932 2.149029 -0.140083
 H12 2.178677 3.098704 -0.029470
 H13 3.492083 1.991637 -0.271467
 O14 1.763956 -2.361237 -0.546181
 H15 -3.063998 -0.958784 -1.271722
 O16 -0.404473 -1.212982 1.489132
 O17 -0.782831 0.072079 1.737666
 C18 -2.644667 1.697630 -0.463963
 H19 -2.009667 2.539648 -0.741352
 H20 -3.399023 1.534343 -1.233373
 H21 -3.132130 1.897663 0.492534

[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