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Supporting Information

Quantum Mechanics Study and Monte Carlo Simulation on the Hydrolytic Deamination of 5-Methylcytosine Glycol

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CONTENT

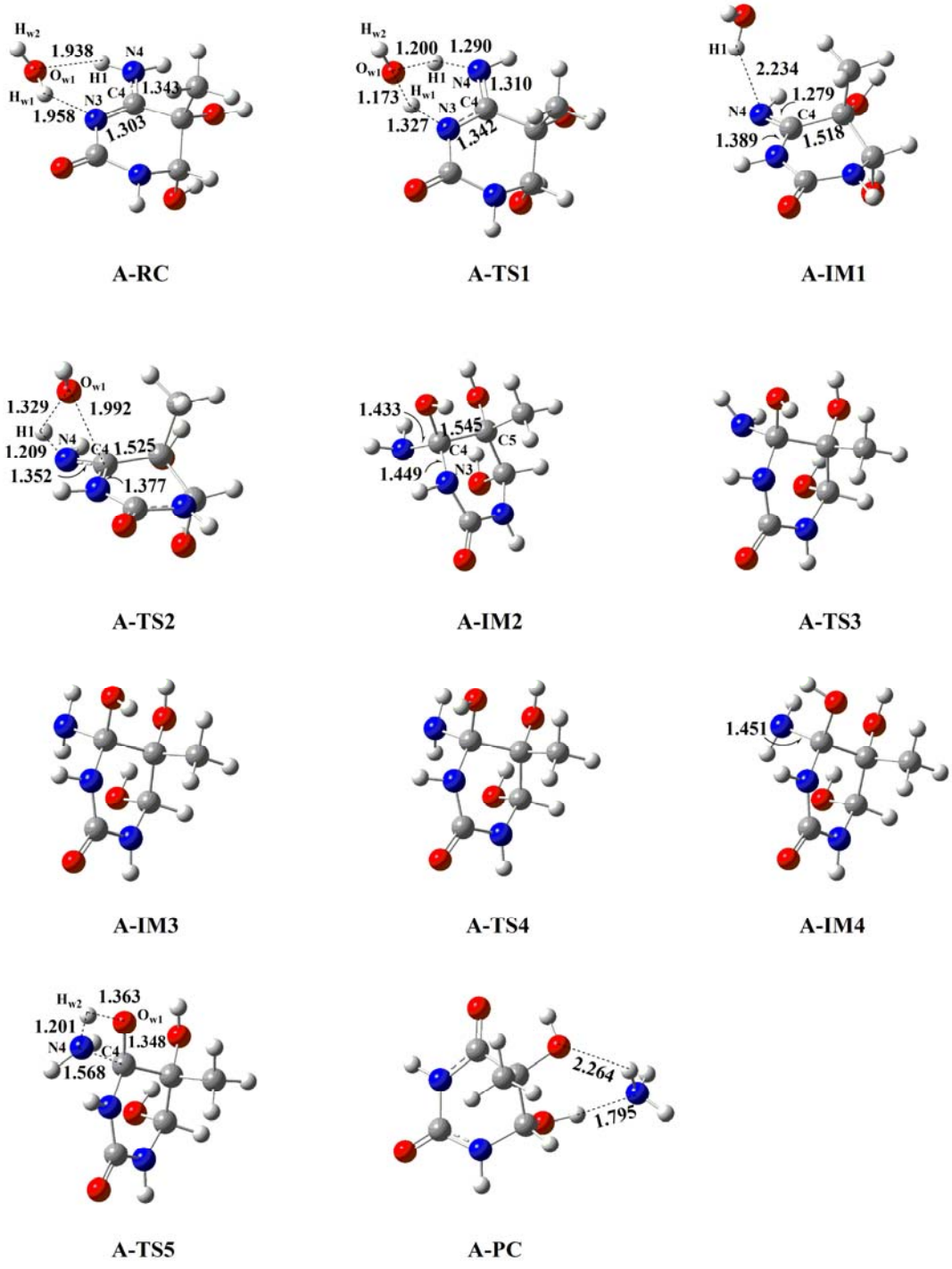

Figure S1. Selected MP2/6-311G(d,p) geometrical parameters for the direct deamination mechanism of mCg (path A). (bond length in angstroms).

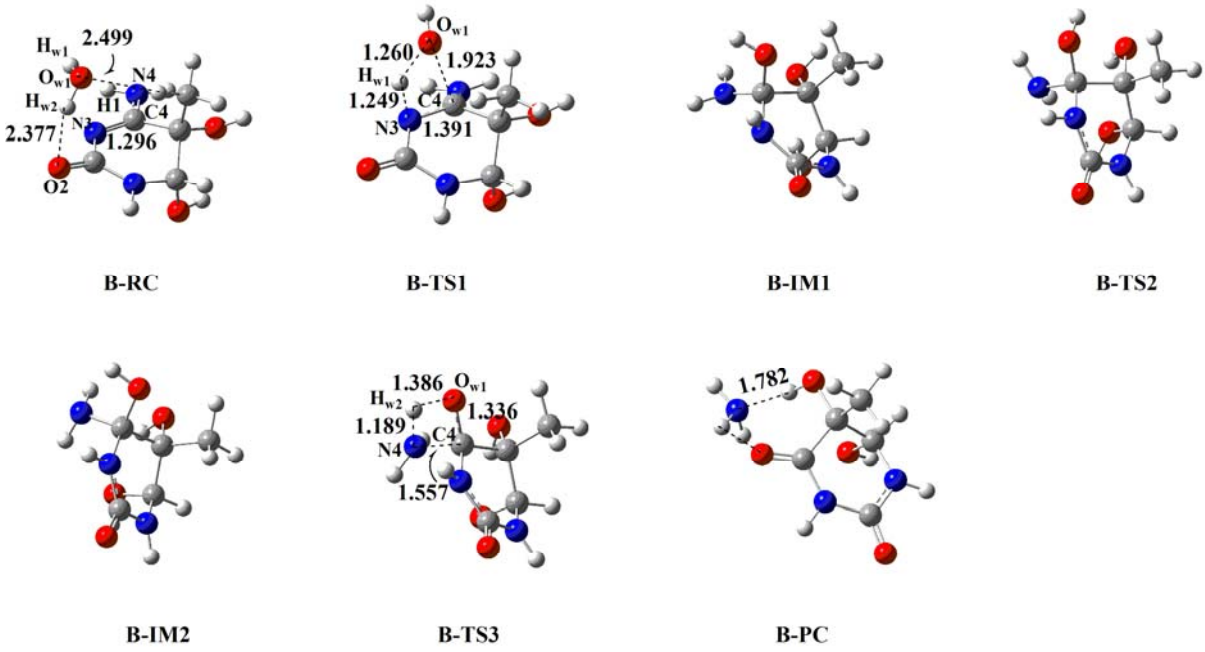

Figure S2. Selected MP2/6-311G(d,p) geometrical parameters for the direct deamination mechanism of mCg (path B). (bond length in angstroms).

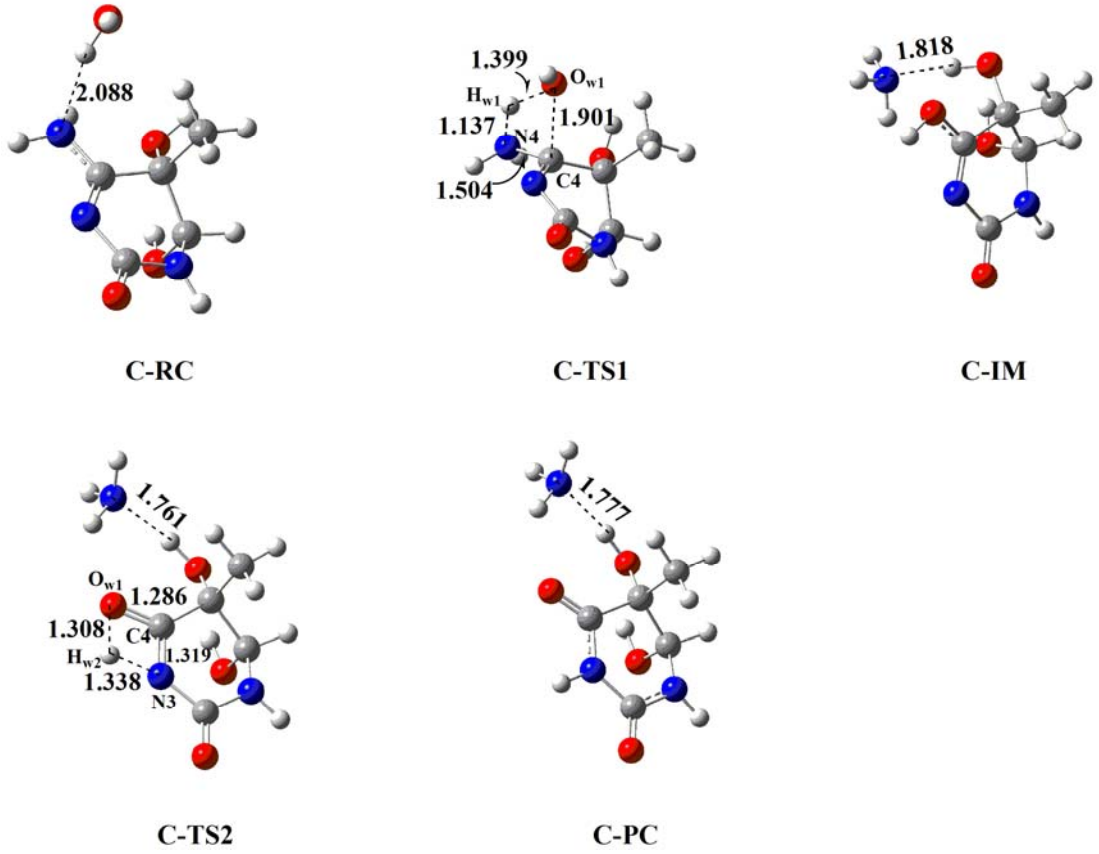

Figure S3. Selected MP2/6-311G(d,p) geometrical parameters for the direct deamination mechanism of mCg (path C). (bond length in angstroms).

I. Gas Structures of Cis-(5S,6S)-mCg

I.1 At the B3lyp/6-311g(d,p) Level

Direct Deaminaiton Mechanism

Path A

A-RE (E=-662.528191324)

Sum of electronic and zero-point Energies= -662.344279

Sum of electronic and thermal Energies= -662.331052

Sum of electronic and thermal Enthalpies= -662.330108

Sum of electronic and thermal Free Energies= -662.382922

1	7	0	-0.823207	1.721830	0.173320
2	6	0	-1.620920	0.650042	-0.334776
3	6	0	-1.102802	-0.661781	0.289153
4	6	0	0.413212	-0.689960	0.084576
5	7	0	0.965212	-1.898503	-0.075419
6	1	0	1.973366	-1.936381	-0.244563
7	1	0	0.360642	-2.677014	-0.279790
8	7	0	1.153524	0.378279	0.127013
9	6	0	0.574712	1.645779	0.225523
10	8	0	1.240201	2.648132	0.368303
11	1	0	-2.661922	0.810670	-0.019188
12	6	0	-1.436698	-0.767372	1.779749
13	1	0	-1.027616	0.077341	2.333051
14	1	0	-2.523544	-0.765420	1.918778
15	1	0	-1.029202	-1.692046	2.192742

16	8	0	-1.655727	-1.775368	-0.433096
17	1	0	-2.493379	-2.015907	-0.022400
18	8	0	-1.549597	0.591466	-1.750196
19	1	0	-1.814778	-0.302077	-2.005906
20	1	0	-1.158619	2.662953	0.024809
21	1	0	2.986491	-0.167925	-0.283487
22	8	0	3.609768	-0.914054	-0.410457
23	1	0	4.197673	-0.867105	0.349765

A-TS1 (E=-662.502210944)

Sum of electronic and zero-point Energies= -662.324703

Sum of electronic and thermal Energies= -662.312839

Sum of electronic and thermal Enthalpies= -662.311895

Sum of electronic and thermal Free Energies= -662.361657

1	7	0	-0.557941	1.789180	0.214254
2	6	0	-1.487767	0.829145	-0.301016
3	6	0	-1.143029	-0.553240	0.295378
4	6	0	0.341517	-0.800211	0.052754
5	7	0	0.810954	-1.994635	-0.188044
6	1	0	2.064244	-1.897862	-0.336626
7	1	0	0.116636	-2.720443	-0.303464
8	7	0	1.207974	0.219109	0.138130

9	6	0	0.821024	1.550413	0.219912
10	8	0	1.618508	2.456630	0.321585
11	1	0	-2.496701	1.118444	0.026292
12	6	0	-1.451897	-0.631161	1.793456
13	1	0	-0.900529	0.127339	2.348183
14	1	0	-2.520636	-0.461145	1.963463
15	1	0	-1.185007	-1.616843	2.179404
16	8	0	-1.858336	-1.564826	-0.426308
17	1	0	-2.711475	-1.695959	0.001170
18	8	0	-1.430920	0.783135	-1.716563
19	1	0	-1.808928	-0.065763	-1.983310
20	1	0	-0.776283	2.764597	0.067813
21	1	0	2.373911	-0.272530	-0.102563
22	8	0	3.100800	-1.216924	-0.392638
23	1	0	3.698348	-1.409211	0.337743

A-IM1 (E=-662.523404500)

Sum of electronic and zero-point Energies= -662.340088

Sum of electronic and thermal Energies= -662.326185

Sum of electronic and thermal Enthalpies= -662.325240

Sum of electronic and thermal Free Energies= -662.380349

1	7	0	1.882288	-0.078439	0.738248

2	6	0	1.223699	1.146834	0.374073
3	6	0	-0.293878	0.894809	0.248449
4	6	0	-0.529030	-0.291035	-0.692986
5	7	0	-1.494445	-0.399327	-1.514525
6	1	0	-3.136847	-1.177802	-0.387919
7	1	0	-2.019516	0.475527	-1.514976
8	7	0	0.366869	-1.331341	-0.526676
9	6	0	1.611131	-1.277668	0.105382
10	8	0	2.357565	-2.230732	0.122572
11	1	0	1.398501	1.873502	1.178710
12	6	0	-0.955554	0.611032	1.601442
13	1	0	-0.457256	-0.213735	2.111963
14	1	0	-0.879098	1.494214	2.245423
15	1	0	-2.004669	0.344726	1.454914
16	8	0	-0.875855	2.040224	-0.381232
17	1	0	-1.309901	2.572814	0.292454
18	8	0	1.745279	1.630727	-0.849567
19	1	0	1.104471	2.272748	-1.185397
20	1	0	2.843345	-0.013036	1.041784
21	1	0	0.214407	-2.157663	-1.089504
22	8	0	-3.698997	-1.109085	0.398246
23	1	0	-3.598558	-1.960462	0.834908

A-TS2 (E=-662.449451995)

Sum of electronic and zero-point Energies= -662.267672

Sum of electronic and thermal Energies= -662.255379

Sum of electronic and thermal Enthalpies= -662.254434

Sum of electronic and thermal Free Energies= -662.305047

1	7	0	1.735748	0.404468	0.623720
2	6	0	0.772670	1.416146	0.282995
3	6	0	-0.643776	0.794962	0.313926
4	6	0	-0.650044	-0.479906	-0.529535
5	7	0	-1.614755	-0.721855	-1.425664
6	1	0	-1.991698	-1.669069	-1.079570
7	1	0	-2.335864	-0.011517	-1.358721
8	7	0	0.510522	-1.177957	-0.577387
9	6	0	1.723602	-0.843650	0.039829
10	8	0	2.658389	-1.610336	0.045947
11	1	0	0.822914	2.199585	1.049477
12	6	0	-1.101998	0.490730	1.744331
13	1	0	-0.343502	-0.086936	2.271392
14	1	0	-1.251778	1.434744	2.282652
15	1	0	-2.004144	-0.119786	1.705824

16	8	0	-1.527130	1.726413	-0.324186
17	1	0	-2.111429	2.095641	0.345072
18	8	0	1.063109	1.951094	-0.993219
19	1	0	0.268705	2.420485	-1.282416
20	1	0	2.662056	0.706299	0.888693
21	1	0	0.492129	-2.091601	-1.010257
22	8	0	-1.876998	-2.054018	0.476050
23	1	0	-1.769683	-2.785352	1.097160

A-IM2 (E=-662.517259502)

Sum of electronic and zero-point Energies= -662.330717

Sum of electronic and thermal Energies= -662.318694

Sum of electronic and thermal Enthalpies= -662.317749

Sum of electronic and thermal Free Energies= -662.367243

1	7	0	1.423231	1.033720	0.405659
2	6	0	0.081966	1.500603	0.190628
3	6	0	-0.915070	0.339463	0.424566
4	6	0	-0.450419	-0.948654	-0.330324
5	7	0	-0.566446	-0.780811	-1.749140
6	1	0	-0.554251	-1.689653	-2.200680
7	1	0	-1.432380	-0.310348	-1.982941

8	7	0	0.915706	-1.234496	0.083071
9	6	0	1.893450	-0.239828	0.144449
10	8	0	3.077849	-0.496990	0.073373
11	1	0	-0.133306	2.270295	0.944945
12	6	0	-1.073574	0.087796	1.926517
13	1	0	-0.137425	-0.239712	2.380181
14	1	0	-1.394686	1.010253	2.413135
15	1	0	-1.837501	-0.671200	2.110364
16	8	0	-2.152887	0.794755	-0.127901
17	1	0	-2.813837	0.112566	0.039464
18	8	0	-0.020998	2.080198	-1.094581
19	1	0	-0.961744	2.213313	-1.264817
20	1	0	2.153352	1.729821	0.366053
21	1	0	1.299924	-2.089297	-0.300782
22	8	0	-1.260780	-2.069749	0.056514
23	1	0	-0.959165	-2.366925	0.923694

A-TS3 (E=-662.516884220)

Sum of electronic and zero-point Energies= -662.330671

Sum of electronic and thermal Energies= -662.319263

Sum of electronic and thermal Enthalpies= -662.318319

Sum of electronic and thermal Free Energies= -662.366627

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1	7	0	1.426428	1.032260	0.390249
2	6	0	0.085707	1.496446	0.194815
3	6	0	-0.907170	0.338352	0.442805
4	6	0	-0.454762	-0.942637	-0.336170
5	7	0	-0.579940	-0.797249	-1.761668
6	1	0	-0.975776	-1.640604	-2.158890
7	1	0	-1.141470	0.003784	-2.013626
8	7	0	0.914387	-1.240878	0.085211
9	6	0	1.892715	-0.246899	0.137283
10	8	0	3.077200	-0.499547	0.057416
11	1	0	-0.121789	2.278832	0.937302
12	6	0	-1.036145	0.069356	1.945166
13	1	0	-0.093059	-0.260929	2.381587
14	1	0	-1.354117	0.985618	2.445761
15	1	0	-1.796554	-0.692132	2.131844
16	8	0	-2.153335	0.801595	-0.076263
17	1	0	-2.778663	0.068949	-0.020496
18	8	0	-0.043693	2.055585	-1.104765
19	1	0	-0.960885	2.346427	-1.185823
20	1	0	2.158656	1.725869	0.348079
21	1	0	1.293713	-2.072599	-0.352599

22	8	0	-1.267835	-2.057571	0.036981
23	1	0	-0.936938	-2.390353	0.879973

A-IM3 (E=-662.520428130)

Sum of electronic and zero-point Energies=	-662.333533
Sum of electronic and thermal Energies=	-662.321619
Sum of electronic and thermal Enthalpies=	-662.320675
Sum of electronic and thermal Free Energies=	-662.369783

1	7	0	1.443362	1.004854	0.427390
2	6	0	0.123651	1.486059	0.158009
3	6	0	-0.897605	0.370445	0.452666
4	6	0	-0.493518	-0.936473	-0.325670
5	7	0	-0.654426	-0.895424	-1.762436
6	1	0	-1.641300	-0.889717	-1.997183
7	1	0	-0.243109	-0.038370	-2.120891
8	7	0	0.885930	-1.241502	0.014609
9	6	0	1.885878	-0.281016	0.150664
10	8	0	3.065102	-0.561994	0.099889
11	1	0	-0.082491	2.331218	0.825839
12	6	0	-1.009252	0.142685	1.963700
13	1	0	-0.082549	-0.246094	2.387787

14	1	0	-1.249955	1.086377	2.457778
15	1	0	-1.816990	-0.559718	2.181585
16	8	0	-2.136753	0.860498	-0.058704
17	1	0	-2.793263	0.163364	0.056006
18	8	0	0.038887	1.941181	-1.194381
19	1	0	-0.892386	2.153817	-1.345196
20	1	0	2.193590	1.680236	0.421445
21	1	0	1.234471	-2.070286	-0.452715
22	8	0	-1.339713	-1.999386	0.088693
23	1	0	-1.025201	-2.298914	0.948425

A-TS4 (E=-662.518708387)

Sum of electronic and zero-point Energies= -662.332441

Sum of electronic and thermal Energies= -662.320947

Sum of electronic and thermal Enthalpies= -662.320003

Sum of electronic and thermal Free Energies= -662.368447

1	7	0	1.439618	1.006262	0.444128
2	6	0	0.126194	1.486193	0.141032
3	6	0	-0.901812	0.381050	0.442748
4	6	0	-0.498663	-0.938612	-0.309215
5	7	0	-0.656548	-0.935616	-1.750697

6	1	0	-1.643989	-0.889015	-1.978690
7	1	0	-0.209943	-0.108872	-2.139592
8	7	0	0.886004	-1.240826	0.012780
9	6	0	1.883450	-0.276387	0.167630
10	8	0	3.062123	-0.560268	0.118408
11	1	0	-0.089122	2.344106	0.788780
12	6	0	-1.027845	0.173959	1.953315
13	1	0	-0.096357	-0.188451	2.388979
14	1	0	-1.294019	1.120629	2.429566
15	1	0	-1.806643	-0.559358	2.163403
16	8	0	-2.132217	0.870985	-0.095096
17	1	0	-2.827302	0.249830	0.149356
18	8	0	0.069559	1.913817	-1.221940
19	1	0	-0.856157	2.133620	-1.394111
20	1	0	2.190785	1.680698	0.448818
21	1	0	1.248517	-2.028386	-0.513298
22	8	0	-1.368619	-1.952236	0.182820
23	1	0	-0.833993	-2.699142	0.466719

A-IM4 (E=-662.524597457)

Sum of electronic and zero-point Energies= -662.337410

Sum of electronic and thermal Energies= -662.325577

Sum of electronic and thermal Enthalpies= -662.324633

Sum of electronic and thermal Free Energies= -662.373652

1	7	0	1.462409	1.007142	0.376949
2	6	0	0.140830	1.484498	0.112732
3	6	0	-0.884794	0.387045	0.461794
4	6	0	-0.506300	-0.935689	-0.278729
5	7	0	-0.709385	-0.943243	-1.719646
6	1	0	-1.626912	-0.554535	-1.921670
7	1	0	-0.033588	-0.330664	-2.165684
8	7	0	0.882768	-1.230789	0.019060
9	6	0	1.892111	-0.293211	0.149854
10	8	0	3.069854	-0.591463	0.130169
11	1	0	-0.054366	2.349388	0.758217
12	6	0	-0.976021	0.197760	1.976983
13	1	0	-0.026048	-0.131416	2.397333
14	1	0	-1.260726	1.144323	2.442586
15	1	0	-1.727328	-0.556038	2.214966
16	8	0	-2.129691	0.865526	-0.055766
17	1	0	-2.812635	0.250228	0.234951
18	8	0	0.044777	1.895778	-1.252199
19	1	0	-0.882512	2.122226	-1.402493

20	1	0	2.215918	1.677536	0.347567
21	1	0	1.221083	-2.137397	-0.271801
22	8	0	-1.362396	-1.933849	0.246382
23	1	0	-1.438737	-2.595766	-0.453010

A-TS5 (E=-662.475046767)

Sum of electronic and zero-point Energies= -662.293487

Sum of electronic and thermal Energies= -662.281708

Sum of electronic and thermal Enthalpies= -662.280764

Sum of electronic and thermal Free Energies= -662.330108

1	7	0	1.432099	1.076908	0.115479
2	6	0	0.064815	1.498259	0.068625
3	6	0	-0.848854	0.354561	0.550084
4	6	0	-0.452445	-0.976781	-0.134001
5	7	0	-0.816565	-0.945349	-1.677173
6	1	0	-1.339790	-0.115317	-1.943425
7	1	0	-0.017096	-1.069787	-2.293360
8	7	0	0.952102	-1.204278	0.047375
9	6	0	1.921943	-0.220273	0.076248
10	8	0	3.112548	-0.462040	0.095028
11	1	0	-0.061763	2.358154	0.738392

12	6	0	-0.799288	0.190473	2.069570
13	1	0	0.221715	0.068811	2.433279
14	1	0	-1.242030	1.071428	2.539267
15	1	0	-1.370678	-0.695274	2.352094
16	8	0	-2.170693	0.693264	0.129550
17	1	0	-2.708753	-0.087781	0.323926
18	8	0	-0.260926	1.907836	-1.263832
19	1	0	-1.170653	2.230947	-1.228346
20	1	0	2.152709	1.778993	0.052215
21	1	0	1.270086	-2.161116	0.091960
22	8	0	-1.258000	-2.020842	0.154687
23	1	0	-1.407652	-1.893194	-1.172381

A-PC (E=-662.556914126)

Sum of electronic and zero-point Energies= -662.372214

Sum of electronic and thermal Energies= -662.358906

Sum of electronic and thermal Enthalpies= -662.357961

Sum of electronic and thermal Free Energies= -662.411375

1	7	0	-1.061378	-1.235674	0.731861
2	6	0	0.332631	-0.852348	0.576833
3	6	0	0.386499	0.694518	0.524400

4	6	0	-0.541947	1.170819	-0.597915
5	7	0	3.618038	-1.130159	-0.476244
6	1	0	3.523974	-0.197837	-0.080673
7	1	0	4.267128	-1.664933	0.091457
8	7	0	-1.726021	0.491564	-0.703868
9	6	0	-2.044075	-0.741588	-0.092565
10	8	0	-3.117280	-1.266228	-0.280596
11	1	0	0.866700	-1.184216	1.477332
12	6	0	-0.039936	1.335121	1.855327
13	1	0	-1.043556	1.036056	2.159174
14	1	0	0.667134	1.036155	2.632903
15	1	0	-0.002621	2.422646	1.762234
16	8	0	1.702564	1.111434	0.202915
17	1	0	1.589089	1.808591	-0.464199
18	8	0	0.846137	-1.449328	-0.575578
19	1	0	1.834885	-1.417783	-0.550460
20	1	0	-1.234338	-2.197170	0.990159
21	1	0	-2.392965	0.810126	-1.395210
22	8	0	-0.240519	2.111974	-1.306689
23	1	0	4.023863	-1.033695	-1.401857

Path B

B-RE (E=-662.521306410)

Sum of electronic and zero-point Energies= -662.338437

Sum of electronic and thermal Energies= -662.324508

Sum of electronic and thermal Enthalpies= -662.323564

Sum of electronic and thermal Free Energies= -662.378777

1	7	0	-0.521575	1.475802	-0.426227
2	6	0	0.857375	1.187992	-0.651341
3	6	0	1.063916	-0.332107	-0.468125
4	6	0	0.410037	-0.696768	0.863854
5	7	0	1.044108	-1.632439	1.593804
6	1	0	0.680561	-1.843015	2.510371
7	1	0	1.996156	-1.862606	1.360429
8	7	0	-0.719062	-0.203212	1.250711
9	6	0	-1.309134	0.816622	0.504801
10	8	0	-2.480364	1.129141	0.646470
11	1	0	1.107159	1.457476	-1.687438
12	6	0	0.439670	-1.157705	-1.596656
13	1	0	-0.649157	-1.072573	-1.607057
14	1	0	0.827538	-0.823732	-2.565341
15	1	0	0.694883	-2.211496	-1.459638
16	8	0	2.476071	-0.589944	-0.358442
17	1	0	2.808965	-0.813236	-1.234254
18	8	0	1.675527	1.915592	0.250186

19	1	0	2.538387	1.480206	0.247712
20	1	0	-0.929432	2.310522	-0.817926
21	1	0	-2.758711	-1.783774	-0.100282
22	8	0	-2.986669	-1.305267	-0.904600
23	1	0	-3.188353	-0.423209	-0.558697

B-TS1 (E=-662.448115754)

Sum of electronic and zero-point Energies= -662.269107

Sum of electronic and thermal Energies= -662.256504

Sum of electronic and thermal Enthalpies= -662.255560

Sum of electronic and thermal Free Energies= -662.306463

1	7	0	-1.191443	-1.314089	0.413473
2	6	0	0.208967	-1.551411	0.285601
3	6	0	0.972840	-0.201359	0.449183
4	6	0	0.314486	0.733081	-0.555568
5	7	0	1.021156	1.068523	-1.627804
6	1	0	0.555992	1.561489	-2.374388
7	1	0	2.027600	1.037769	-1.578290
8	7	0	-1.061717	0.802549	-0.638028
9	6	0	-1.858960	-0.184070	-0.055332
10	8	0	-3.061148	-0.076911	0.042385
11	1	0	0.527756	-2.214054	1.101754

12	6	0	0.924900	0.301132	1.887241
13	1	0	-0.098155	0.479114	2.210529
14	1	0	1.375749	-0.451077	2.544793
15	1	0	1.446920	1.253107	1.962219
16	8	0	2.330341	-0.422620	0.025337
17	1	0	2.892937	-0.400506	0.805204
18	8	0	0.504088	-2.148177	-0.966439
19	1	0	1.464731	-2.116213	-1.066099
20	1	0	-1.798136	-2.089005	0.632884
21	1	0	-1.086871	1.866661	-0.187647
22	8	0	-0.068174	2.551735	0.491110
23	1	0	0.301260	3.357386	0.109662

B-IM1 (E=-662.530769246)

Sum of electronic and zero-point Energies= -662.343023

Sum of electronic and thermal Energies= -662.331481

Sum of electronic and thermal Enthalpies= -662.330537

Sum of electronic and thermal Free Energies= -662.379028

1	7	0	1.388589	1.089440	0.315800
2	6	0	0.008058	1.485779	0.196054
3	6	0	-0.917332	0.279290	0.510593

4	6	0	-0.416903	-0.944878	-0.314933
5	7	0	-0.582303	-0.632001	-1.746107
6	1	0	-0.168437	-1.378065	-2.297445
7	1	0	-1.572836	-0.589633	-1.970403
8	7	0	0.968245	-1.177668	-0.015786
9	6	0	1.911865	-0.177110	0.118739
10	8	0	3.106930	-0.397825	0.116331
11	1	0	-0.194941	2.280346	0.917100
12	6	0	-0.963150	-0.017844	2.005343
13	1	0	0.021783	-0.275515	2.394228
14	1	0	-1.338901	0.862348	2.530517
15	1	0	-1.637390	-0.850885	2.202617
16	8	0	-2.242654	0.582902	0.076669
17	1	0	-2.154069	1.317057	-0.550936
18	8	0	-0.317735	2.057152	-1.065711
19	1	0	-0.183508	1.337408	-1.713057
20	1	0	2.089950	1.814464	0.319538
21	1	0	1.338033	-2.102434	-0.178626
22	8	0	-1.086988	-2.137528	0.048081
23	1	0	-2.033060	-1.962510	-0.028631

B-TS2 (E=-662.514505893)

Sum of electronic and zero-point Energies= -662.329095

Sum of electronic and thermal Energies= -662.317313

Sum of electronic and thermal Enthalpies= -662.316369

Sum of electronic and thermal Free Energies= -662.365514

1	7	0	1.416717	1.049927	0.242924
2	6	0	0.053160	1.480590	0.232369
3	6	0	-0.893184	0.294335	0.509960
4	6	0	-0.447187	-0.938464	-0.354548
5	7	0	-0.595815	-0.736078	-1.792707
6	1	0	-1.309216	-1.341824	-2.173316
7	1	0	-0.756999	0.228599	-2.047132
8	7	0	0.933498	-1.228724	0.000141
9	6	0	1.898067	-0.256355	0.098441
10	8	0	3.091234	-0.483946	0.110343
11	1	0	-0.096547	2.248121	0.997322
12	6	0	-0.901761	-0.031286	2.002297
13	1	0	0.092724	-0.287711	2.364841
14	1	0	-1.277539	0.834883	2.550598
15	1	0	-1.560628	-0.876192	2.196756
16	8	0	-2.229772	0.632918	0.163327
17	1	0	-2.194532	1.149107	-0.651928

18	8	0	-0.332568	2.076906	-1.032322
19	1	0	0.477260	2.235551	-1.528979
20	1	0	2.142241	1.709489	0.479376
21	1	0	1.289733	-2.113869	-0.334986
22	8	0	-1.182671	-2.083095	0.016842
23	1	0	-2.111645	-1.817209	-0.001695

B-IM2 (E=-662.521650903)

Sum of electronic and zero-point Energies= -662.334864

Sum of electronic and thermal Energies= -662.322846

Sum of electronic and thermal Enthalpies= -662.321902

Sum of electronic and thermal Free Energies= -662.371584

1	7	0	1.485747	0.974082	0.423945
2	6	0	0.183377	1.468633	0.119936
3	6	0	-0.895491	0.419618	0.459760
4	6	0	-0.552214	-0.943384	-0.259432
5	7	0	-0.961149	-1.031062	-1.651978
6	1	0	-1.934344	-0.745697	-1.721427
7	1	0	-0.406500	-0.399066	-2.219824
8	7	0	0.883352	-1.186053	-0.188256
9	6	0	1.900952	-0.315752	0.109456

10	8	0	3.073871	-0.636505	0.124476
11	1	0	-0.001100	2.365254	0.719110
12	6	0	-1.013795	0.244889	1.971440
13	1	0	-0.117720	-0.207214	2.396499
14	1	0	-1.183167	1.217406	2.439592
15	1	0	-1.863012	-0.401136	2.183599
16	8	0	-2.149951	0.895725	-0.007521
17	1	0	-1.966078	1.396252	-0.813457
18	8	0	-0.006374	1.798366	-1.276704
19	1	0	0.526155	2.571790	-1.487476
20	1	0	2.249583	1.617627	0.562800
21	1	0	1.195566	-2.109707	-0.450028
22	8	0	-1.251047	-1.958483	0.426198
23	1	0	-1.424000	-2.641131	-0.233931

B-TS3 (E=-662.467203350)

Sum of electronic and zero-point Energies= -662.285941

Sum of electronic and thermal Energies= -662.274048

Sum of electronic and thermal Enthalpies= -662.273104

Sum of electronic and thermal Free Energies= -662.322654

1	7	0	1.501298	1.042707	0.169145

2	6	0	0.152859	1.487176	0.049204
3	6	0	-0.846980	0.416709	0.534354
4	6	0	-0.516890	-0.978869	-0.101663
5	7	0	-1.147336	-1.094004	-1.543088
6	1	0	-1.883129	-0.407122	-1.685544
7	1	0	-0.489054	-1.108824	-2.317900
8	7	0	0.922371	-1.180662	-0.196782
9	6	0	1.931224	-0.269174	0.020249
10	8	0	3.106245	-0.570594	0.092372
11	1	0	0.030243	2.391451	0.654857
12	6	0	-0.831680	0.277161	2.052219
13	1	0	0.153612	-0.011227	2.422041
14	1	0	-1.127696	1.222850	2.511395
15	1	0	-1.543116	-0.500587	2.325757
16	8	0	-2.161665	0.818166	0.145616
17	1	0	-2.050428	1.475212	-0.554211
18	8	0	-0.236176	1.788136	-1.312618
19	1	0	0.306881	2.515698	-1.632168
20	1	0	2.246492	1.703783	0.320474
21	1	0	1.199388	-2.145955	-0.079256
22	8	0	-1.157436	-2.041727	0.401597
23	1	0	-1.516470	-2.061433	-0.912285

B-PC (E=-662.549015894)

Sum of electronic and zero-point Energies= -662.365512

Sum of electronic and thermal Energies= -662.351588

Sum of electronic and thermal Enthalpies= -662.350644

Sum of electronic and thermal Free Energies= -662.405616

1	7	0	-1.727474	-0.812767	-0.513565
2	6	0	-0.338616	-1.219504	-0.617903
3	6	0	0.456113	-0.693240	0.600274
4	6	0	0.226595	0.834594	0.679392
5	7	0	3.232765	0.820500	-0.996514
6	1	0	2.979417	1.588033	-0.379945
7	1	0	4.244750	0.761919	-1.036177
8	7	0	-1.063361	1.239440	0.364533
9	6	0	-2.086061	0.484445	-0.227772
10	8	0	-3.182070	0.954290	-0.440673
11	1	0	-0.302095	-2.312463	-0.613078
12	6	0	-0.060264	-1.324561	1.904773
13	1	0	-1.126186	-1.163175	2.064437
14	1	0	0.139529	-2.397956	1.870830
15	1	0	0.502664	-0.902544	2.738088
16	8	0	1.801340	-1.031562	0.503945

17	1	0	2.277310	-0.445979	-0.137130
18	8	0	0.296517	-0.697987	-1.778600
19	1	0	-0.028592	-1.171513	-2.550156
20	1	0	-2.432160	-1.317103	-1.031371
21	1	0	-1.274651	2.221408	0.487385
22	8	0	1.065446	1.635401	1.027780
23	1	0	2.890025	1.037611	-1.926263

Path C

C-RE (E=-662.516475883)

Sum of electronic and zero-point Energies= -662.333248

Sum of electronic and thermal Energies= -662.319490

Sum of electronic and thermal Enthalpies= -662.318546

Sum of electronic and thermal Free Energies= -662.373222

1	7	0	1.922110	-0.012945	0.716318
2	6	0	1.196844	1.175881	0.393807
3	6	0	-0.293404	0.801442	0.252106
4	6	0	-0.352427	-0.421233	-0.666496
5	7	0	-1.477189	-0.514409	-1.447486
6	1	0	-1.408522	-1.202612	-2.186173
7	1	0	-1.891869	0.373867	-1.698301
8	7	0	0.526445	-1.353534	-0.693339
9	6	0	1.694160	-1.236861	0.084684

10	8	0	2.470507	-2.155288	0.213061
11	1	0	1.306965	1.888829	1.222740
12	6	0	-0.948223	0.496514	1.601911
13	1	0	-0.401908	-0.288664	2.125180
14	1	0	-0.925421	1.393344	2.231396
15	1	0	-1.983019	0.177366	1.461331
16	8	0	-0.971090	1.883014	-0.414038
17	1	0	-1.475942	2.376825	0.240281
18	8	0	1.686024	1.749672	-0.807908
19	1	0	1.017071	2.382592	-1.101102
20	1	0	2.861994	0.087357	1.071469
21	1	0	-3.123975	-1.023376	-0.208538
22	8	0	-3.795373	-0.987652	0.489475
23	1	0	-3.677173	-1.811730	0.972480

C-TS1 (E=-662.437175831)

Sum of electronic and zero-point Energies= -662.255659

Sum of electronic and thermal Energies= -662.243575

Sum of electronic and thermal Enthalpies= -662.242631

Sum of electronic and thermal Free Energies= -662.292714

1	7	0	1.740430	0.669097	0.331313
2	6	0	0.579278	1.464577	0.115737

3	6	0	-0.650740	0.599307	0.473072
4	6	0	-0.468061	-0.687820	-0.345644
5	7	0	-1.405356	-0.829325	-1.520875
6	1	0	-0.877729	-1.184947	-2.314836
7	1	0	-1.867629	0.059504	-1.712247
8	7	0	0.672821	-1.254831	-0.535485
9	6	0	1.826017	-0.695616	0.012206
10	8	0	2.868867	-1.294498	0.153223
11	1	0	0.606351	2.331917	0.786135
12	6	0	-0.728809	0.355945	1.977324
13	1	0	0.157318	-0.166957	2.336705
14	1	0	-0.799146	1.315886	2.496362
15	1	0	-1.596881	-0.265762	2.192159
16	8	0	-1.806287	1.320538	0.014366
17	1	0	-2.554302	1.027681	0.547498
18	8	0	0.507806	1.911774	-1.241559
19	1	0	-0.257809	2.496711	-1.297109
20	1	0	2.629549	1.121362	0.476859
21	1	0	-2.025964	-1.556889	-0.967382
22	8	0	-1.871499	-1.800060	0.493113
23	1	0	-1.406223	-2.593477	0.781871

C-IM1 (E=-662.521857672)

Sum of electronic and zero-point Energies= -662.337780

Sum of electronic and thermal Energies= -662.324203

Sum of electronic and thermal Enthalpies= -662.323259

Sum of electronic and thermal Free Energies= -662.377559

1	7	0	1.684354	0.325488	-0.881638
2	6	0	0.347364	0.701358	-1.221729
3	6	0	-0.485983	0.951609	0.064505
4	6	0	-0.095755	-0.118434	1.076231
5	7	0	-2.604225	-1.775696	-0.462826
6	1	0	-1.770623	-2.200989	-0.860172
7	1	0	-3.388782	-2.020285	-1.059362
8	7	0	0.992788	-0.781604	1.119496
9	6	0	1.985991	-0.572460	0.135987
10	8	0	3.061797	-1.119485	0.199424
11	1	0	0.380038	1.635054	-1.795566
12	6	0	-0.172866	2.331192	0.657504
13	1	0	0.897827	2.462479	0.822724
14	1	0	-0.525164	3.093854	-0.040462
15	1	0	-0.706232	2.455515	1.600321
16	8	0	-1.860429	0.929252	-0.255064

17	1	0	-2.190161	-0.002727	-0.263994
18	8	0	-0.246907	-0.320444	-2.022037
19	1	0	-1.155225	-0.029670	-2.177906
20	1	0	2.363908	0.314984	-1.629453
21	1	0	-2.766955	-2.200863	0.444673
22	8	0	-1.017300	-0.324112	2.030049
23	1	0	-0.618851	-0.965931	2.640006

C-TS2 (E=-662.478090500)

Sum of electronic and zero-point Energies= -662.298831

Sum of electronic and thermal Energies= -662.285703

Sum of electronic and thermal Enthalpies= -662.284759

Sum of electronic and thermal Free Energies= -662.337955

1	7	0	-1.946328	-0.706250	0.336235
2	6	0	-0.735999	-1.396019	-0.038495
3	6	0	0.512862	-0.569771	0.382042
4	6	0	0.219532	0.851885	-0.045624
5	7	0	3.788003	0.525478	-0.284055
6	1	0	4.325429	0.439083	-1.141178
7	1	0	4.446790	0.594774	0.484859
8	7	0	-0.985433	1.364509	-0.157493

9	6	0	-2.172166	0.633380	0.022100
10	8	0	-3.272162	1.124525	-0.037769
11	1	0	-0.712239	-2.349413	0.503170
12	6	0	0.730452	-0.599717	1.903606
13	1	0	-0.152979	-0.255543	2.444421
14	1	0	0.953969	-1.626853	2.198591
15	1	0	1.579125	0.031035	2.175696
16	8	0	1.590823	-1.140459	-0.319615
17	1	0	2.416105	-0.588994	-0.234658
18	8	0	-0.718810	-1.617936	-1.433792
19	1	0	0.211134	-1.769228	-1.660215
20	1	0	-2.796208	-1.252047	0.301433
21	1	0	3.257346	1.392489	-0.333943
22	8	0	1.057636	1.786921	-0.319458
23	1	0	-0.110154	2.355586	-0.457690

C-PC (E=-662.558184078)

Sum of electronic and zero-point Energies= -662.373505

Sum of electronic and thermal Energies= -662.360208

Sum of electronic and thermal Enthalpies= -662.359264

Sum of electronic and thermal Free Energies= -662.412690

1	7	0	1.946908	0.740244	0.348101

2	6	0	0.708889	1.384119	-0.014887
3	6	0	-0.493692	0.499802	0.381192
4	6	0	-0.266454	-0.935086	-0.145845
5	7	0	-3.874959	-0.463358	-0.223820
6	1	0	-3.336188	-1.316508	-0.355935
7	1	0	-4.496658	-0.590397	0.567975
8	7	0	1.047598	-1.342586	-0.196514
9	6	0	2.202848	-0.571533	0.027791
10	8	0	3.305257	-1.066508	-0.025222
11	1	0	0.645257	2.324379	0.545647
12	6	0	-0.679464	0.436318	1.905377
13	1	0	0.206084	0.045225	2.410293
14	1	0	-0.886089	1.441921	2.277924
15	1	0	-1.531093	-0.202776	2.147416
16	8	0	-1.592772	1.106272	-0.254186
17	1	0	-2.422301	0.564812	-0.167051
18	8	0	0.690228	1.633294	-1.406099
19	1	0	-0.246291	1.752930	-1.626548
20	1	0	2.780435	1.310523	0.344291
21	1	0	-4.450500	-0.322423	-1.048010
22	8	0	-1.171959	-1.689375	-0.443700
23	1	0	1.221722	-2.298966	-0.478483

Water-Mediated Deamination Mechanism

Path A

wA-RC (E=-738.999681352)

Sum of electronic and zero-point Energies=	-738.790638
Sum of electronic and thermal Energies=	-738.774733
Sum of electronic and thermal Enthalpies=	-738.773788
Sum of electronic and thermal Free Energies=	-738.833102

1	7	0	-1.434066	1.616231	0.221638
2	6	0	-2.073538	0.473305	-0.353262
3	6	0	-1.415813	-0.786520	0.244220
4	6	0	0.101912	-0.628825	0.095684
5	7	0	0.791984	-1.754418	-0.074483
6	1	0	1.822846	-1.747413	-0.129058
7	1	0	0.275218	-2.595008	-0.277221
8	7	0	0.694630	0.527597	0.199162
9	6	0	-0.042246	1.705882	0.314689
10	8	0	0.497976	2.776582	0.506041
11	1	0	-3.136151	0.491293	-0.071112
12	6	0	-1.779838	-0.985480	1.718305
13	1	0	-1.489982	-0.119813	2.313076
14	1	0	-2.862863	-1.116061	1.821108

15	1	0	-1.278086	-1.870681	2.113496
16	8	0	-1.807506	-1.930266	-0.532633
17	1	0	-2.625965	-2.281076	-0.164755
18	8	0	-1.948846	0.480883	-1.765400
19	1	0	-2.082100	-0.429234	-2.062325
20	1	0	-1.877315	2.514116	0.088231
21	1	0	2.445966	0.963700	-0.229124
22	8	0	3.407508	1.011358	-0.436102
23	1	0	3.742928	1.720391	0.119852
24	8	0	3.631630	-1.648474	-0.095338
25	1	0	3.966040	-1.761973	0.799581
26	1	0	3.742670	-0.684952	-0.276325

wA-TS1 (E=-738.973897974)

Sum of electronic and zero-point Energies= -738.773202

Sum of electronic and thermal Energies= -738.759262

Sum of electronic and thermal Enthalpies= -738.758318

Sum of electronic and thermal Free Energies= -738.813215

1	7	0	-1.462044	1.576643	0.197851
2	6	0	-2.041052	0.385635	-0.343374
3	6	0	-1.311804	-0.824390	0.273129

4	6	0	0.198692	-0.629106	0.078063
5	7	0	0.957919	-1.672602	-0.109339
6	1	0	2.254077	-1.632142	-0.154900
7	1	0	0.426547	-2.528045	-0.221125
8	7	0	0.706304	0.605598	0.173198
9	6	0	-0.078924	1.748708	0.258109
10	8	0	0.412521	2.850425	0.404041
11	1	0	-3.100159	0.353325	-0.049446
12	6	0	-1.626502	-0.989789	1.763004
13	1	0	-1.335568	-0.104272	2.327106
14	1	0	-2.702459	-1.139448	1.905705
15	1	0	-1.093296	-1.854683	2.162291
16	8	0	-1.683316	-2.003172	-0.455803
17	1	0	-2.474653	-2.373559	-0.050248
18	8	0	-1.930566	0.366727	-1.756488
19	1	0	-2.017399	-0.556611	-2.029432
20	1	0	-1.955008	2.445295	0.047382
21	1	0	1.993038	0.840944	-0.074434
22	8	0	3.129071	0.909299	-0.336420
23	1	0	3.561955	1.490929	0.295751
24	8	0	3.439020	-1.457968	-0.177636
25	1	0	3.812337	-1.748815	0.660251

26	1	0	3.439043	-0.229225	-0.246006

wA-IM1 (E=-738.995538276)

Sum of electronic and zero-point Energies= -738.785872

Sum of electronic and thermal Energies= -738.769869

Sum of electronic and thermal Enthalpies= -738.768924

Sum of electronic and thermal Free Energies= -738.827917

1	7	0	-0.870678	1.733456	0.211956
2	6	0	-1.878107	0.715966	0.135368
3	6	0	-1.228343	-0.653767	0.431520
4	6	0	-0.021916	-0.851378	-0.486296
5	7	0	0.408940	-1.982220	-0.893267
6	1	0	2.941670	-0.231941	0.938006
7	1	0	-0.229221	-2.720966	-0.605824
8	7	0	0.675418	0.298940	-0.778279
9	6	0	0.377823	1.586138	-0.345823
10	8	0	1.183338	2.491355	-0.441680
11	1	0	-2.626665	0.925917	0.911450
12	6	0	-0.754921	-0.775830	1.885552
13	1	0	0.126747	-0.160963	2.075019
14	1	0	-1.553525	-0.482316	2.574835

15	1	0	-0.477079	-1.813908	2.082404
16	8	0	-2.175236	-1.676392	0.099605
17	1	0	-2.669276	-1.898737	0.895814
18	8	0	-2.485041	0.712805	-1.143042
19	1	0	-2.904407	-0.153035	-1.242439
20	1	0	-1.146170	2.691616	0.363265
21	1	0	1.616898	0.172645	-1.141942
22	8	0	2.606657	0.358282	1.631290
23	1	0	2.607000	1.226125	1.210723
24	1	0	2.309003	-1.801903	-0.939280
25	8	0	3.089449	-1.221593	-0.802554
26	1	0	3.788715	-1.546185	-1.375776

wA-TS2 (E=-738.944914904)

Sum of electronic and zero-point Energies= -738.738182

Sum of electronic and thermal Energies= -738.724082

Sum of electronic and thermal Enthalpies= -738.723138

Sum of electronic and thermal Free Energies= -738.777269

1	7	0	-1.522116	1.358582	0.473274
2	6	0	-1.953025	0.069700	0.009982
3	6	0	-0.824978	-0.962326	0.273398

4	6	0	0.449898	-0.401575	-0.360389
5	7	0	1.078692	-1.110785	-1.281590
6	1	0	2.877262	-0.262835	0.264907
7	1	0	0.929557	-2.107890	-1.230251
8	7	0	0.645408	0.937937	-0.295384
9	6	0	-0.275947	1.877883	0.172073
10	8	0	0.012969	3.044322	0.301846
11	1	0	-2.829135	-0.226560	0.600760
12	6	0	-0.674530	-1.253359	1.765280
13	1	0	-0.532238	-0.331275	2.327287
14	1	0	-1.592968	-1.730826	2.126829
15	1	0	0.200831	-1.880625	1.923613
16	8	0	-1.157851	-2.155939	-0.447408
17	1	0	-1.425573	-2.825489	0.189482
18	8	0	-2.278827	0.126161	-1.364474
19	1	0	-2.315078	-0.787662	-1.678555
20	1	0	-2.224370	2.071673	0.605046
21	1	0	1.601561	1.254334	-0.511279
22	8	0	2.103383	-0.917227	1.149117
23	1	0	2.121209	-0.401479	1.963454
24	1	0	2.024540	-0.768077	-1.507483
25	8	0	3.226762	0.307817	-0.628615

26	1	0	4.170504	0.473561	-0.593709

wA-IM2 (E=-738.995487236)

Sum of electronic and zero-point Energies= -738.782362

Sum of electronic and thermal Energies= -738.767971

Sum of electronic and thermal Enthalpies= -738.767027

Sum of electronic and thermal Free Energies= -738.821811

1	7	0	-1.258245	1.619099	0.125130
2	6	0	-1.809255	0.350809	-0.281380
3	6	0	-1.009490	-0.813066	0.363276
4	6	0	0.506066	-0.583885	0.045924
5	7	0	0.725484	-0.799544	-1.372135
6	1	0	3.183987	-0.961877	0.097209
7	1	0	0.576269	-1.784495	-1.574434
8	7	0	0.891122	0.754627	0.442847
9	6	0	0.092907	1.879399	0.279397
10	8	0	0.540469	3.007140	0.334124
11	1	0	-2.842852	0.295939	0.066195
12	6	0	-1.270587	-0.915347	1.863426
13	1	0	-0.864179	-0.062407	2.409124
14	1	0	-2.345960	-0.965644	2.042195

15	1	0	-0.834884	-1.840723	2.246121
16	8	0	-1.436059	-2.028970	-0.232662
17	1	0	-1.829831	-1.785114	-1.083672
18	8	0	-1.892024	0.176300	-1.690619
19	1	0	-0.969642	0.081841	-2.002928
20	1	0	-1.789815	2.446559	-0.103393
21	1	0	1.881762	0.949999	0.328215
22	8	0	1.347382	-1.504917	0.761689
23	1	0	1.245784	-1.322529	1.704146
24	1	0	1.688716	-0.562282	-1.601553
25	8	0	3.544472	-0.242797	-0.444128
26	1	0	4.500349	-0.270055	-0.349203

wA-TS3 (E=-738.974479459)

Sum of electronic and zero-point Energies= -738.763752

Sum of electronic and thermal Energies= -738.748966

Sum of electronic and thermal Enthalpies= -738.748022

Sum of electronic and thermal Free Energies= -738.804200

1	7	0	-1.095879	1.699122	0.219638
2	6	0	-1.821476	0.506004	-0.057628
3	6	0	-1.042305	-0.743434	0.419958

4	6	0	0.430178	-0.685573	-0.138695
5	7	0	0.533775	-0.995821	-1.554455
6	1	0	3.228967	-1.073982	-0.198450
7	1	0	-0.377933	-1.033348	-1.989917
8	7	0	0.984753	0.628558	0.182254
9	6	0	0.293798	1.819037	0.202499
10	8	0	0.832553	2.906624	0.249049
11	1	0	-2.782041	0.522955	0.461449
12	6	0	-1.056169	-0.829119	1.946086
13	1	0	-0.475461	-0.029878	2.408648
14	1	0	-2.085147	-0.768153	2.304898
15	1	0	-0.660552	-1.798541	2.253484
16	8	0	-1.710805	-1.897758	-0.053748
17	1	0	-2.102265	-1.670264	-0.906948
18	8	0	-2.172360	0.362284	-1.455859
19	1	0	-1.540422	0.879684	-1.969063
20	1	0	-1.579156	2.584697	0.217466
21	1	0	1.969181	0.728294	-0.065756
22	8	0	1.269641	-1.652835	0.491322
23	1	0	1.384478	-1.376357	1.407665
24	1	0	0.961253	-1.908303	-1.660868
25	8	0	3.770920	-0.284958	-0.337396

26	1	0	4.356810	-0.248155	0.425067

wA-IM3 (E=-738.986315642)

Sum of electronic and zero-point Energies= -738.773881

Sum of electronic and thermal Energies= -738.759228

Sum of electronic and thermal Enthalpies= -738.758284

Sum of electronic and thermal Free Energies= -738.813680

1	7	0	1.141965	1.682599	-0.165191
2	6	0	1.740744	0.488559	0.333103
3	6	0	1.085257	-0.750770	-0.308227
4	6	0	-0.484698	-0.676305	-0.107495
5	7	0	-0.934898	-1.106704	1.212757
6	1	0	-2.871289	-0.661735	0.988513
7	1	0	-0.441503	-0.577373	1.925641
8	7	0	-0.955515	0.669576	-0.375624
9	6	0	-0.237621	1.842994	-0.304072
10	8	0	-0.741552	2.942276	-0.404256
11	1	0	2.806475	0.495945	0.085700
12	6	0	1.462228	-0.844209	-1.785148
13	1	0	1.024482	-0.033621	-2.370126
14	1	0	2.547944	-0.802575	-1.892248

15	1	0	1.125626	-1.804331	-2.176421
16	8	0	1.593945	-1.918494	0.315219
17	1	0	1.729072	-1.698815	1.245955
18	8	0	1.602903	0.311401	1.763509
19	1	0	2.114650	0.990079	2.215115
20	1	0	1.628998	2.560664	-0.064317
21	1	0	-1.965008	0.774682	-0.261574
22	8	0	-1.141350	-1.581610	-0.978605
23	1	0	-1.086737	-1.217247	-1.868271
24	1	0	-0.702614	-2.089485	1.325835
25	8	0	-3.606194	-0.267527	0.479866
26	1	0	-3.728430	-0.904473	-0.232225

wA-TS4 (E=-738.984351555)

Sum of electronic and zero-point Energies= -738.772706

Sum of electronic and thermal Energies= -738.758462

Sum of electronic and thermal Enthalpies= -738.757518

Sum of electronic and thermal Free Energies= -738.812266

1	7	0	1.123790	1.694026	-0.141333
2	6	0	1.727066	0.504499	0.364487
3	6	0	1.105507	-0.737493	-0.302920

4	6	0	-0.467239	-0.686397	-0.139954
5	7	0	-0.944975	-1.140451	1.171782
6	1	0	-2.831442	-0.738657	0.942839
7	1	0	-0.466668	-0.625619	1.907128
8	7	0	-0.957257	0.655360	-0.385818
9	6	0	-0.251069	1.837494	-0.310229
10	8	0	-0.770900	2.928762	-0.419680
11	1	0	2.797952	0.528513	0.142920
12	6	0	1.513544	-0.811263	-1.771063
13	1	0	1.084624	0.006934	-2.350025
14	1	0	2.602376	-0.771215	-1.850499
15	1	0	1.165308	-1.755385	-2.184465
16	8	0	1.613808	-1.903697	0.327243
17	1	0	1.724149	-1.687633	1.261993
18	8	0	1.556216	0.319540	1.790511
19	1	0	2.049766	1.001560	2.256963
20	1	0	1.601726	2.576882	-0.040711
21	1	0	-1.965193	0.759749	-0.266566
22	8	0	-1.033380	-1.589885	-1.074803
23	1	0	-1.668462	-1.095147	-1.600998
24	1	0	-0.709375	-2.124338	1.267002
25	8	0	-3.567757	-0.279643	0.486729

26	1	0	-4.086412	-0.979840	0.080077

wA-IM4 (E=-738.995002143)

Sum of electronic and zero-point Energies= -738.782021

Sum of electronic and thermal Energies= -738.767719

Sum of electronic and thermal Enthalpies= -738.766775

Sum of electronic and thermal Free Energies= -738.821356

1	7	0	-1.538719	1.375901	0.055550
2	6	0	-1.826363	0.028238	-0.319570
3	6	0	-0.829760	-0.927428	0.368245
4	6	0	0.629757	-0.448182	0.091626
5	7	0	1.071891	-0.600877	-1.310268
6	1	0	2.903413	-0.071589	-1.031599
7	1	0	0.455489	-0.060752	-1.913774
8	7	0	0.725787	0.951622	0.464058
9	6	0	-0.264973	1.893610	0.265168
10	8	0	-0.061800	3.089894	0.329490
11	1	0	-2.835881	-0.226189	0.024407
12	6	0	-1.125056	-1.027311	1.865362
13	1	0	-1.021114	-0.061192	2.358836
14	1	0	-2.145413	-1.391242	2.007742

15	1	0	-0.428135	-1.720428	2.336973
16	8	0	-1.032591	-2.193983	-0.266416
17	1	0	-0.481657	-2.834733	0.197949
18	8	0	-1.787573	-0.093441	-1.746572
19	1	0	-1.905742	-1.033421	-1.938778
20	1	0	-2.212050	2.084999	-0.192754
21	1	0	1.662238	1.338198	0.474896
22	8	0	1.461919	-1.254834	0.879612
23	1	0	2.381328	-0.985116	0.691285
24	1	0	0.942924	-1.575000	-1.572481
25	8	0	3.538001	0.117627	-0.305743
26	1	0	4.426601	0.014278	-0.656028

wA-TS5 (E=-738.967232373)

Sum of electronic and zero-point Energies= -738.760302

Sum of electronic and thermal Energies= -738.747112

Sum of electronic and thermal Enthalpies= -738.746168

Sum of electronic and thermal Free Energies= -738.798959

1	7	0	-1.941427	0.737482	-0.079064
2	6	0	-1.669164	-0.633925	-0.367297
3	6	0	-0.427766	-1.093968	0.422492

4	6	0	0.747149	-0.099027	0.220256
5	7	0	1.228455	-0.149378	-1.273350
6	1	0	2.267674	0.380597	-1.164144
7	1	0	0.543870	0.257098	-1.907467
8	7	0	0.274021	1.248685	0.456881
9	6	0	-0.995724	1.721184	0.195863
10	8	0	-1.292926	2.897423	0.248631
11	1	0	-2.526685	-1.239684	-0.052222
12	6	0	-0.745768	-1.246735	1.909338
13	1	0	-1.116317	-0.315167	2.337210
14	1	0	-1.502654	-2.023751	2.037901
15	1	0	0.160385	-1.527503	2.447076
16	8	0	-0.050093	-2.354661	-0.141616
17	1	0	0.704781	-2.663445	0.376222
18	8	0	-1.492592	-0.797341	-1.782791
19	1	0	-1.311786	-1.735527	-1.927419
20	1	0	-2.831075	1.115445	-0.367033
21	1	0	0.978038	1.953929	0.628399
22	8	0	1.815161	-0.445037	0.957722
23	1	0	2.698183	0.166271	0.478391
24	1	0	1.339399	-1.130790	-1.520338
25	8	0	3.274902	0.875262	-0.383658

26	1	0	4.180874	0.614671	-0.568069

wA-PC (E=-739.020891776)

Sum of electronic and zero-point Energies= -738.810874

Sum of electronic and thermal Energies= -738.794786

Sum of electronic and thermal Enthalpies= -738.793842

Sum of electronic and thermal Free Energies= -738.853397

1	7	0	1.130502	1.644059	0.205937
2	6	0	1.537113	0.372865	0.828801
3	6	0	1.313176	-0.740575	-0.230497
4	6	0	-0.127454	-0.654826	-0.736556
5	7	0	-1.859018	-0.391868	2.094288
6	1	0	-2.461564	-0.426206	1.270856
7	1	0	-2.238839	0.318934	2.713107
8	7	0	-0.634396	0.595141	-0.915804
9	6	0	-0.059856	1.804701	-0.447408
10	8	0	-0.613404	2.861638	-0.650107
11	1	0	2.609491	0.444356	1.021793
12	6	0	2.274597	-0.579772	-1.425245
13	1	0	2.189659	0.394685	-1.907657
14	1	0	3.296487	-0.710659	-1.063256

15	1	0	2.071552	-1.362871	-2.158709
16	8	0	1.510397	-1.996913	0.371799
17	1	0	0.810073	-2.570428	0.027951
18	8	0	0.935393	0.145267	2.056977
19	1	0	-0.028451	-0.054208	1.965407
20	1	0	1.435986	2.489777	0.667005
21	1	0	-1.610349	0.664352	-1.198643
22	8	0	-0.764134	-1.678693	-0.974081
23	1	0	-2.607939	-1.264827	-0.970236
24	1	0	-1.954744	-1.282103	2.574664
25	8	0	-3.256525	-0.577031	-0.732584
26	1	0	-4.090250	-0.820635	-1.143848

Path B

wB-RC (E=-738.991536723)

Sum of electronic and zero-point Energies= -738.783042

Sum of electronic and thermal Energies= -738.766620

Sum of electronic and thermal Enthalpies= -738.765676

Sum of electronic and thermal Free Energies= -738.825922

1	7	0	-1.515161	1.341805	0.665351
2	6	0	-2.076614	0.100552	0.230598
3	6	0	-0.948766	-0.951436	0.211179

4	6	0	0.216049	-0.342126	-0.561979
5	7	0	0.927042	-1.173851	-1.325434
6	1	0	1.822641	-0.854990	-1.679463
7	1	0	0.683169	-2.149897	-1.339728
8	7	0	0.549769	0.911163	-0.449948
9	6	0	-0.274738	1.811283	0.228801
10	8	0	0.067553	2.954275	0.447542
11	1	0	-2.842230	-0.208012	0.956800
12	6	0	-0.479013	-1.335342	1.619331
13	1	0	-0.286352	-0.442399	2.213436
14	1	0	-1.263657	-1.911033	2.123553
15	1	0	0.442621	-1.917160	1.575122
16	8	0	-1.398057	-2.107134	-0.513799
17	1	0	-1.779431	-2.726479	0.117551
18	8	0	-2.656122	0.231083	-1.057689
19	1	0	-2.721873	-0.662000	-1.421874
20	1	0	-2.146672	2.076556	0.948590
21	1	0	2.331060	1.028004	-0.810023
22	8	0	3.190285	0.572179	-0.992363
23	1	0	3.805904	1.237495	-1.310728
24	1	0	3.216812	-0.581938	0.521796
25	8	0	2.972588	-1.109525	1.302534

26	1	0	2.974968	-0.466587	2.017802

wB-TS1 (E=-738.942193997)

Sum of electronic and zero-point Energies= -738.735508

Sum of electronic and thermal Energies= -738.721399

Sum of electronic and thermal Enthalpies= -738.720455

Sum of electronic and thermal Free Energies= -738.774702

1	7	0	-1.334486	1.474793	0.525752
2	6	0	-1.924954	0.260479	0.043235
3	6	0	-0.921991	-0.902889	0.262470
4	6	0	0.405910	-0.485953	-0.378432
5	7	0	0.989901	-1.303725	-1.246144
6	1	0	1.963941	-1.063968	-1.473905
7	1	0	0.727647	-2.275091	-1.178408
8	7	0	0.705549	0.830462	-0.411590
9	6	0	-0.062729	1.859257	0.142271
10	8	0	0.363056	2.983648	0.253435
11	1	0	-2.818966	0.055879	0.645815
12	6	0	-0.792229	-1.251874	1.744401
13	1	0	-0.222691	-0.498861	2.280925
14	1	0	-1.793297	-1.359455	2.177906

15	1	0	-0.247576	-2.190866	1.847179
16	8	0	-1.398491	-2.034417	-0.485126
17	1	0	-1.883857	-2.604288	0.120373
18	8	0	-2.270329	0.385499	-1.322430
19	1	0	-2.380958	-0.512220	-1.664168
20	1	0	-1.944549	2.257166	0.712231
21	1	0	1.692277	1.037675	-0.631309
22	8	0	3.241677	-0.007900	-0.635742
23	1	0	4.139913	0.311352	-0.531152
24	1	0	2.809788	-0.336332	0.338698
25	8	0	1.944417	-0.713170	1.295042
26	1	0	2.164898	-1.615103	1.554595

wB-IM1 (E=-738.995652891)

Sum of electronic and zero-point Energies= -738.782615

Sum of electronic and thermal Energies= -738.768171

Sum of electronic and thermal Enthalpies= -738.767227

Sum of electronic and thermal Free Energies= -738.822325

1	7	0	-1.201892	1.637276	0.105485
2	6	0	-1.820781	0.379530	-0.228838
3	6	0	-1.003780	-0.778184	0.398434

4	6	0	0.490226	-0.573441	0.015561
5	7	0	0.642595	-0.699111	-1.438419
6	1	0	1.602329	-0.465030	-1.684579
7	1	0	0.467153	-1.658518	-1.724160
8	7	0	0.928078	0.724315	0.449686
9	6	0	0.156062	1.862919	0.273706
10	8	0	0.625323	2.982343	0.323814
11	1	0	-2.831240	0.362445	0.184825
12	6	0	-1.208886	-0.850890	1.908078
13	1	0	-0.859976	0.055396	2.402049
14	1	0	-2.271889	-0.989313	2.115054
15	1	0	-0.664083	-1.698297	2.323401
16	8	0	-1.430096	-2.016937	-0.168083
17	1	0	-1.872764	-1.788978	-1.000408
18	8	0	-2.001181	0.172029	-1.624713
19	1	0	-1.098187	0.130223	-1.997325
20	1	0	-1.716252	2.480508	-0.101588
21	1	0	1.924345	0.889061	0.342244
22	8	0	3.558598	-0.323517	-0.429720
23	1	0	4.440972	-0.156905	-0.086713
24	1	0	3.154411	-0.985627	0.152227
25	8	0	1.314398	-1.521438	0.712759

26	1	0	0.930327	-2.391775	0.543595

wB-TS2 (E=-738.976371863)

Sum of electronic and zero-point Energies= -738.766176

Sum of electronic and thermal Energies= -738.751220

Sum of electronic and thermal Enthalpies= -738.750275

Sum of electronic and thermal Free Energies= -738.806859

1	7	0	-1.064703	1.688060	0.156256
2	6	0	-1.832179	0.482681	0.130934
3	6	0	-0.950267	-0.726363	0.503287
4	6	0	0.404012	-0.629950	-0.283059
5	7	0	0.261481	-0.777623	-1.724798
6	1	0	0.685350	-1.629750	-2.062011
7	1	0	-0.690834	-0.678274	-2.047051
8	7	0	1.027546	0.629899	0.073794
9	6	0	0.332887	1.810640	0.119510
10	8	0	0.854652	2.906169	0.171117
11	1	0	-2.661322	0.556980	0.840904
12	6	0	-0.732894	-0.770786	2.014889
13	1	0	-0.244763	0.132083	2.378924
14	1	0	-1.700557	-0.885507	2.507333

15	1	0	-0.109315	-1.623739	2.279022
16	8	0	-1.593792	-1.945169	0.153182
17	1	0	-2.031817	-1.806480	-0.696271
18	8	0	-2.421266	0.221944	-1.168597
19	1	0	-2.348164	1.035652	-1.678998
20	1	0	-1.525019	2.562385	0.358645
21	1	0	2.009373	0.716520	-0.185380
22	8	0	3.820356	-0.347280	-0.202180
23	1	0	4.153450	-0.134884	0.675619
24	1	0	3.201644	-1.076932	-0.052740
25	8	0	1.287279	-1.645323	0.182199
26	1	0	0.784520	-2.470476	0.146110

wB-IM2 (E=-738.991566158)

Sum of electronic and zero-point Energies= -738.778713

Sum of electronic and thermal Energies= -738.764324

Sum of electronic and thermal Enthalpies= -738.763380

Sum of electronic and thermal Free Energies= -738.818257

1	7	0	-1.590877	1.338868	0.140677
2	6	0	-1.825239	0.000559	-0.285111
3	6	0	-0.816326	-0.968778	0.364809

4	6	0	0.651777	-0.458835	0.094342
5	7	0	1.170934	-0.818884	-1.239730
6	1	0	1.114554	-1.830717	-1.325202
7	1	0	0.576532	-0.409873	-1.956023
8	7	0	0.707665	0.994032	0.212105
9	6	0	-0.318212	1.901218	0.220930
10	8	0	-0.155584	3.102714	0.314162
11	1	0	-2.835694	-0.294505	0.012615
12	6	0	-1.092500	-1.103948	1.859422
13	1	0	-0.895737	-0.173022	2.390516
14	1	0	-2.134932	-1.393827	2.011440
15	1	0	-0.446814	-1.878621	2.267084
16	8	0	-0.990312	-2.256173	-0.212624
17	1	0	-1.250852	-2.111278	-1.131448
18	8	0	-1.695207	-0.191527	-1.717558
19	1	0	-2.401352	0.290527	-2.159464
20	1	0	-2.327546	2.024445	0.076539
21	1	0	1.635287	1.400132	0.219260
22	8	0	1.479010	-1.069733	1.040132
23	1	0	2.387997	-0.772189	0.852041
24	1	0	2.960777	-0.152789	-0.988851
25	8	0	3.555361	0.219353	-0.300937

26	1	0	4.460574	0.045236	-0.571625

wB-TS3 (E=-738.960406423)

Sum of electronic and zero-point Energies= -738.753804

Sum of electronic and thermal Energies= -738.740521

Sum of electronic and thermal Enthalpies= -738.739577

Sum of electronic and thermal Free Energies= -738.792430

1	7	0	-2.057652	0.558339	-0.085068
2	6	0	-1.622361	-0.778933	-0.295639
3	6	0	-0.323419	-1.084182	0.480822
4	6	0	0.765105	0.019445	0.194200
5	7	0	1.407317	-0.274460	-1.190503
6	1	0	1.630680	-1.269287	-1.198548
7	1	0	0.768211	-0.065802	-1.953056
8	7	0	0.127583	1.342009	0.059906
9	6	0	-1.212586	1.651911	0.057094
10	8	0	-1.642477	2.782839	0.171229
11	1	0	-2.406662	-1.462086	0.044398
12	6	0	-0.583655	-1.169904	1.979901
13	1	0	-0.941323	-0.222293	2.384570
14	1	0	-1.321856	-1.950048	2.178451

15	1	0	0.352266	-1.422508	2.474068
16	8	0	0.167010	-2.355639	0.053601
17	1	0	-0.216157	-2.522098	-0.817668
18	8	0	-1.328567	-1.078379	-1.687188
19	1	0	-2.142739	-1.002075	-2.195331
20	1	0	-3.036962	0.793188	-0.115859
21	1	0	0.710350	2.106018	0.372451
22	8	0	1.754241	0.028514	1.087919
23	1	0	2.720392	0.464827	0.525531
24	1	0	2.417113	0.329142	-1.113777
25	8	0	3.467896	0.783064	-0.396353
26	1	0	3.642628	1.728583	-0.407499

wB-PC (E=-739.021820520)

Sum of electronic and zero-point Energies= -738.811435

Sum of electronic and thermal Energies= -738.795509

Sum of electronic and thermal Enthalpies= -738.794565

Sum of electronic and thermal Free Energies= -738.853792

1	7	0	2.138644	0.751766	0.444724
2	6	0	0.779909	1.099508	0.791970
3	6	0	-0.055002	-0.194496	0.938901

4	6	0	0.078945	-0.988404	-0.376635
5	7	0	-2.656418	1.744472	-0.824372
6	1	0	-3.276635	2.487580	-0.515952
7	1	0	-2.354298	1.977429	-1.766517
8	7	0	1.339554	-0.964744	-0.927884
9	6	0	2.410287	-0.110058	-0.592182
10	8	0	3.468929	-0.181316	-1.171334
11	1	0	0.794788	1.609993	1.761634
12	6	0	0.440565	-1.066926	2.098627
13	1	0	1.482126	-1.362154	1.978123
14	1	0	0.334290	-0.506296	3.029785
15	1	0	-0.184089	-1.959113	2.163268
16	8	0	-1.397570	0.113024	1.226383
17	1	0	-1.785222	0.645318	0.504796
18	8	0	0.269318	1.947506	-0.221019
19	1	0	-0.699405	2.020624	-0.154937
20	1	0	2.839603	1.472453	0.543727
21	1	0	1.491329	-1.529131	-1.754428
22	8	0	-0.821473	-1.629904	-0.884786
23	1	0	-2.713563	-1.391530	-0.696684
24	1	0	-3.210853	0.881821	-0.891925
25	8	0	-3.609112	-1.049014	-0.529449

26	1	0	-3.679473	-1.107561	0.429388

Path C

wC-RC (E=-738.981367309)

Sum of electronic and zero-point Energies= -738.772996

Sum of electronic and thermal Energies= -738.756490

Sum of electronic and thermal Enthalpies= -738.755546

Sum of electronic and thermal Free Energies= -738.815625

1	7	0	-1.063939	1.607513	0.374188
2	6	0	-1.819348	0.412691	0.575966
3	6	0	-0.854924	-0.792571	0.472569
4	6	0	-0.044941	-0.585598	-0.807000
5	7	0	0.342266	-1.728484	-1.460865
6	1	0	-0.254784	-2.531235	-1.315552
7	1	0	0.666451	-1.574445	-2.407421
8	7	0	0.343467	0.557673	-1.231080
9	6	0	-0.005866	1.712461	-0.509785
10	8	0	0.598449	2.756832	-0.649238
11	1	0	-2.245865	0.438014	1.588352
12	6	0	0.071521	-0.912421	1.684067
13	1	0	0.767389	-0.071521	1.744731
14	1	0	-0.521495	-0.958176	2.604201

15	1	0	0.662045	-1.828217	1.601666
16	8	0	-1.640041	-1.989471	0.299376
17	1	0	-1.770538	-2.389464	1.165840
18	8	0	-2.855651	0.309736	-0.385900
19	1	0	-3.133933	-0.615781	-0.388457
20	1	0	-1.384035	2.477678	0.770051
21	1	0	2.891026	0.400944	0.554326
22	8	0	2.587929	1.123264	1.127941
23	1	0	2.338027	1.832993	0.522974
24	8	0	3.166067	-1.390765	-0.214293
25	1	0	2.343448	-1.700295	-0.620880
26	1	0	3.357028	-2.021556	0.486458

wC-TS1 (E=-738.910065548)

Sum of electronic and zero-point Energies= -738.706006

Sum of electronic and thermal Energies= -738.691743

Sum of electronic and thermal Enthalpies= -738.690799

Sum of electronic and thermal Free Energies= -738.746260

1	7	0	2.248647	0.203210	0.045399
2	6	0	1.331981	1.290666	0.030849
3	6	0	-0.015816	0.781177	0.595458

4	6	0	-0.324572	-0.445529	-0.276585
5	7	0	-1.291010	-0.179358	-1.381355
6	1	0	-0.992179	0.695146	-1.817978
7	1	0	-1.146092	-0.938396	-2.048582
8	7	0	0.569580	-1.317927	-0.583548
9	6	0	1.886794	-1.136574	-0.158720
10	8	0	2.703578	-2.023402	-0.058791
11	1	0	1.705682	2.091514	0.677924
12	6	0	0.106509	0.487658	2.089081
13	1	0	0.824285	-0.308392	2.285911
14	1	0	0.440099	1.394411	2.600936
15	1	0	-0.856199	0.163348	2.478001
16	8	0	-0.965996	1.823944	0.357763
17	1	0	-1.745549	1.625401	0.888602
18	8	0	1.153295	1.803698	-1.300233
19	1	0	0.647544	2.620915	-1.209321
20	1	0	3.237164	0.374351	0.136802
21	1	0	-2.847599	-0.980994	0.331966
22	8	0	-1.779353	-1.241265	0.917667
23	1	0	-1.538913	-2.173754	0.893492
24	8	0	-3.581148	-0.529756	-0.457495
25	1	0	-2.395310	-0.155665	-1.058284

26	1	0	-4.175829	0.120501	-0.074724

wC-IM1 (E=-738.998367467)

Sum of electronic and zero-point Energies= -738.789014

Sum of electronic and thermal Energies= -738.772961

Sum of electronic and thermal Enthalpies= -738.772017

Sum of electronic and thermal Free Energies= -738.831954

1	7	0	-1.823127	-1.323808	0.280111
2	6	0	-0.568595	-1.799332	-0.231830
3	6	0	0.566694	-0.875350	0.261942
4	6	0	0.090011	0.563607	0.050480
5	7	0	3.938755	0.330692	-0.011492
6	1	0	4.499233	0.417396	-0.853802
7	1	0	3.487947	1.226367	0.150936
8	7	0	-1.136960	0.949197	0.062787
9	6	0	-2.183619	0.013770	0.219210
10	8	0	-3.332814	0.376422	0.330407
11	1	0	-0.393572	-2.806986	0.164955
12	6	0	0.863947	-1.092104	1.754164
13	1	0	-0.028452	-0.949625	2.366053
14	1	0	1.233478	-2.110486	1.893084

15	1	0	1.634434	-0.395406	2.090922
16	8	0	1.674072	-1.199701	-0.546969
17	1	0	2.479256	-0.679038	-0.296788
18	8	0	-0.599630	-1.829473	-1.646897
19	1	0	0.328328	-1.829081	-1.924071
20	1	0	-2.614416	-1.947801	0.209441
21	1	0	-1.139774	2.882883	-0.087645
22	8	0	1.064319	1.450404	-0.107767
23	1	0	0.648438	2.355854	-0.207216
24	8	0	-0.488088	3.600198	-0.252291
25	1	0	4.572363	0.147618	0.760000
26	1	0	-0.711448	3.949401	-1.121377

wC-TS2 (E=-738.986447652)

Sum of electronic and zero-point Energies= -738.782555

Sum of electronic and thermal Energies= -738.767718

Sum of electronic and thermal Enthalpies= -738.766774

Sum of electronic and thermal Free Energies= -738.823800

1	7	0	-1.845989	-1.251427	0.287719
2	6	0	-0.599688	-1.757164	-0.219189
3	6	0	0.561894	-0.868948	0.278044

4	6	0	0.159563	0.592383	0.046953
5	7	0	3.904475	0.332360	-0.045985
6	1	0	4.483348	0.414844	-0.875824
7	1	0	3.368310	1.190818	0.048296
8	7	0	-1.099374	0.981687	0.066869
9	6	0	-2.177000	0.091333	0.205929
10	8	0	-3.317630	0.489710	0.284217
11	1	0	-0.455379	-2.770295	0.175506
12	6	0	0.832892	-1.075529	1.776764
13	1	0	-0.057888	-0.885249	2.378057
14	1	0	1.157020	-2.106389	1.935169
15	1	0	1.629911	-0.407309	2.109341
16	8	0	1.664912	-1.246496	-0.512074
17	1	0	2.476232	-0.722173	-0.287358
18	8	0	-0.624909	-1.781731	-1.634965
19	1	0	0.304894	-1.812925	-1.905045
20	1	0	-2.651300	-1.855941	0.206423
21	1	0	-1.069892	2.369010	-0.096577
22	8	0	1.089004	1.464361	-0.119211
23	1	0	0.497396	2.543164	-0.234795
24	8	0	-0.434747	3.299753	-0.240319
25	1	0	4.523087	0.246942	0.753829

26	1	0	-0.598520	3.659939	-1.119431

wC-PC (E=-739.023063182)

Sum of electronic and zero-point Energies= -738.813539

Sum of electronic and thermal Energies= -738.797209

Sum of electronic and thermal Enthalpies= -738.796265

Sum of electronic and thermal Free Energies= -738.856661

1	7	0	-1.758899	-1.410062	0.241152
2	6	0	-0.474336	-1.811623	-0.271213
3	6	0	0.631663	-0.885762	0.278299
4	6	0	0.208522	0.582903	0.065469
5	7	0	3.881184	0.534410	-0.054035
6	1	0	4.470102	0.639709	-0.874085
7	1	0	3.262234	1.340022	-0.003598
8	7	0	-1.131149	0.841267	0.128710
9	6	0	-2.175890	-0.099065	0.210332
10	8	0	-3.329861	0.253181	0.283790
11	1	0	-0.276450	-2.831715	0.078684
12	6	0	0.872720	-1.111278	1.779503
13	1	0	-0.030599	-0.943859	2.369077
14	1	0	1.211376	-2.138405	1.931436
15	1	0	1.652746	-0.434994	2.135212

16	8	0	1.766562	-1.206667	-0.488260
17	1	0	2.539695	-0.622646	-0.269322
18	8	0	-0.486658	-1.766894	-1.685042
19	1	0	0.446852	-1.739130	-1.944219
20	1	0	-2.522334	-2.062330	0.132724
21	1	0	-1.411688	1.825216	0.061366
22	8	0	1.029418	1.480968	-0.093469
23	1	0	0.087198	3.212725	-0.219680
24	8	0	-0.770116	3.671529	-0.218773
25	1	0	4.485102	0.537022	0.761379
26	1	0	-0.903012	3.951083	-1.130076

I.2 At the Mp2/6-311g(d,p) Level
Direct Deaminaiton Mechanism

Path A

A-RE (EUMP2= -0.66079545542378D+03)

Sum of electronic and zero-point Energies= -660.608523

Sum of electronic and thermal Energies= -660.595386

Sum of electronic and thermal Enthalpies= -660.594442

Sum of electronic and thermal Free Energies= -660.647170

1	7	0	-0.859387	1.702999	0.204855
2	6	0	-1.600641	0.631573	-0.378640
3	6	0	-1.110633	-0.663085	0.267683

4	6	0	0.401376	-0.684683	0.111717
5	7	0	0.956757	-1.902597	0.004473
6	1	0	1.960257	-1.933540	-0.181716
7	1	0	0.350315	-2.658882	-0.269177
8	7	0	1.145224	0.383609	0.161077
9	6	0	0.543929	1.649614	0.241014
10	8	0	1.200383	2.661877	0.366919
11	1	0	-2.666663	0.773431	-0.143136
12	6	0	-1.477708	-0.752142	1.743912
13	1	0	-1.057338	0.088998	2.296946
14	1	0	-2.569015	-0.725589	1.855772
15	1	0	-1.095673	-1.688093	2.160284
16	8	0	-1.636019	-1.780334	-0.458192
17	1	0	-2.483211	-1.998880	-0.056656
18	8	0	-1.406741	0.586347	-1.778583
19	1	0	-1.679959	-0.299722	-2.045634
20	1	0	-1.189736	2.637800	0.001918
21	1	0	2.971310	-0.178360	-0.268798
22	8	0	3.594590	-0.915139	-0.403299
23	1	0	4.205913	-0.814903	0.328476

A-TS1 (EUMP2=-0.66076918943108D+03)

Sum of electronic and zero-point Energies= -660.588604

Sum of electronic and thermal Energies= -660.576891

Sum of electronic and thermal Enthalpies= -660.575947

Sum of electronic and thermal Free Energies= -660.625473

1	7	0	-0.555310	1.789463	0.218647
2	6	0	-1.447940	0.833958	-0.358749
3	6	0	-1.161682	-0.523991	0.284119
4	6	0	0.313939	-0.801419	0.084240
5	7	0	0.758537	-2.013494	-0.138787
6	1	0	2.033384	-1.919182	-0.308538
7	1	0	0.025899	-2.698546	-0.278313
8	7	0	1.202877	0.198425	0.192908
9	6	0	0.827861	1.536309	0.230422
10	8	0	1.634128	2.440593	0.311566
11	1	0	-2.480032	1.135050	-0.121899
12	6	0	-1.493766	-0.543906	1.771222
13	1	0	-0.904538	0.199579	2.309485
14	1	0	-2.556156	-0.312094	1.917534
15	1	0	-1.283785	-1.537550	2.177030
16	8	0	-1.881703	-1.539261	-0.417957
17	1	0	-2.744876	-1.608585	0.002479

18	8	0	-1.264497	0.754873	-1.758916
19	1	0	-1.668431	-0.081069	-2.022784
20	1	0	-0.743156	2.758161	-0.006817
21	1	0	2.378510	-0.351363	-0.083791
22	8	0	3.042468	-1.273481	-0.375213
23	1	0	3.626812	-1.472655	0.362874

A-IM1 (EUMP2=-0.66079453254996D+03)

Sum of electronic and zero-point Energies= -660.608139

Sum of electronic and thermal Energies= -660.594519

Sum of electronic and thermal Enthalpies= -660.593574

Sum of electronic and thermal Free Energies= -660.647739

1	7	0	-1.711388	0.370238	0.771050
2	6	0	-1.327901	-0.964309	0.408877
3	6	0	0.197574	-1.031643	0.296027
4	6	0	0.631482	0.009995	-0.718866
5	7	0	1.539248	-0.128988	-1.609116
6	1	0	3.029585	1.047831	-0.431119
7	1	0	1.867516	-1.094883	-1.554610
8	7	0	0.010620	1.241998	-0.552157
9	6	0	-1.239756	1.454672	0.042272

10	8	0	-1.808256	2.523014	-0.026080
11	1	0	-1.660672	-1.641948	1.208283
12	6	0	0.893001	-0.785011	1.629493
13	1	0	0.587745	0.173827	2.050962
14	1	0	0.614493	-1.573225	2.340088
15	1	0	1.975521	-0.770342	1.486916
16	8	0	0.548968	-2.300395	-0.251930
17	1	0	0.776323	-2.872549	0.487166
18	8	0	-1.915910	-1.315451	-0.826346
19	1	0	-1.427142	-2.091395	-1.129196
20	1	0	-2.684163	0.496335	1.020321
21	1	0	0.262503	1.952161	-1.230264
22	8	0	3.224888	1.341889	0.464834
23	1	0	2.465012	1.896766	0.652378

A-TS2 (EUMP2=-0.66070928487688D+03)

Sum of electronic and zero-point Energies= -660.526964

Sum of electronic and thermal Energies= -660.514892

Sum of electronic and thermal Enthalpies= -660.513948

Sum of electronic and thermal Free Energies= -660.564091

1	7	0	1.674751	0.643221	0.564983

2	6	0	0.578328	1.458091	0.128058
3	6	0	-0.713736	0.673011	0.368286
4	6	0	-0.600043	-0.609162	-0.448889
5	7	0	-1.311000	-0.869931	-1.569020
6	1	0	-1.850543	-1.726944	-0.908874
7	1	0	-2.001046	-0.129056	-1.676350
8	7	0	0.604326	-1.258166	-0.294938
9	6	0	1.809694	-0.658231	0.111396
10	8	0	2.858132	-1.264147	0.078320
11	1	0	0.551233	2.363924	0.747004
12	6	0	-0.909085	0.407198	1.855090
13	1	0	-0.147451	-0.274501	2.235245
14	1	0	-0.848901	1.355117	2.399191
15	1	0	-1.884077	-0.060019	2.001739
16	8	0	-1.752354	1.490514	-0.147781
17	1	0	-2.577071	1.137429	0.203073
18	8	0	0.736733	1.782223	-1.237132
19	1	0	-0.101955	2.169047	-1.516331
20	1	0	2.572632	1.101401	0.648144
21	1	0	0.749922	-2.051613	-0.908293
22	8	0	-1.920796	-1.824850	0.414789
23	1	0	-1.603942	-2.586013	0.919067

A-IM2 (EUMP2=-0.66079441570506D+03)

Sum of electronic and zero-point Energies= -660.604575

Sum of electronic and thermal Energies= -660.592801

Sum of electronic and thermal Enthalpies= -660.591857

Sum of electronic and thermal Free Energies= -660.640957

1	7	0	1.399293	1.026942	0.449895
2	6	0	0.067440	1.493406	0.194945
3	6	0	-0.916923	0.336437	0.414795
4	6	0	-0.442193	-0.933540	-0.325787
5	7	0	-0.472355	-0.744674	-1.746134
6	1	0	-0.462337	-1.659679	-2.188673
7	1	0	-1.333833	-0.279582	-2.010051
8	7	0	0.889703	-1.245609	0.152177
9	6	0	1.872188	-0.243979	0.164187
10	8	0	3.056126	-0.496928	0.058606
11	1	0	-0.169211	2.268255	0.939434
12	6	0	-1.072917	0.080168	1.910196
13	1	0	-0.133281	-0.251471	2.356080
14	1	0	-1.394283	1.005702	2.394435
15	1	0	-1.842788	-0.676555	2.087772

16	8	0	-2.151549	0.775949	-0.143301
17	1	0	-2.771698	0.049284	-0.011510
18	8	0	-0.002484	2.055275	-1.095630
19	1	0	-0.941685	2.192655	-1.263401
20	1	0	2.127539	1.723045	0.360564
21	1	0	1.273907	-2.084301	-0.271959
22	8	0	-1.288758	-2.035892	0.003212
23	1	0	-1.021068	-2.326149	0.882621

A-TS3 (EUMP2= -0.66079376826687D+03)

Sum of electronic and zero-point Energies= -660.604292

Sum of electronic and thermal Energies= -660.593101

Sum of electronic and thermal Enthalpies= -660.592157

Sum of electronic and thermal Free Energies= -660.640166

1	7	0	1.403985	1.027134	0.429504
2	6	0	0.071064	1.489116	0.198061
3	6	0	-0.908248	0.335072	0.435751
4	6	0	-0.446152	-0.926686	-0.331959
5	7	0	-0.492274	-0.771417	-1.761577
6	1	0	-0.949256	-1.582892	-2.161756
7	1	0	-0.992066	0.065834	-2.026312

8	7	0	0.889873	-1.249972	0.148576
9	6	0	1.872782	-0.250224	0.154933
10	8	0	3.056876	-0.498678	0.043770
11	1	0	-0.155214	2.278598	0.929628
12	6	0	-1.028990	0.061433	1.931686
13	1	0	-0.080836	-0.272441	2.356724
14	1	0	-1.345780	0.980521	2.431589
15	1	0	-1.794105	-0.698590	2.114481
16	8	0	-2.153202	0.782404	-0.085130
17	1	0	-2.737615	0.015724	-0.055784
18	8	0	-0.032390	2.026812	-1.108788
19	1	0	-0.948644	2.318303	-1.186233
20	1	0	2.133982	1.721248	0.341318
21	1	0	1.267582	-2.063577	-0.328718
22	8	0	-1.293347	-2.023801	-0.012999
23	1	0	-0.995369	-2.349111	0.843894

A-IM3 (EUMP2=-0.660797825919 94D+03)

Sum of electronic and zero-point Energies= -660.607587

Sum of electronic and thermal Energies= -660.595967

Sum of electronic and thermal Enthalpies= -660.595023

Sum of electronic and thermal Free Energies= -660.643621

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1	7	0	1.433113	0.985380	0.478323
2	6	0	0.132834	1.478611	0.152590
3	6	0	-0.893494	0.381626	0.437026
4	6	0	-0.504297	-0.920437	-0.316864
5	7	0	-0.627457	-0.891185	-1.755024
6	1	0	-1.610757	-0.818731	-1.998497
7	1	0	-0.171893	-0.048686	-2.094650
8	7	0	0.851997	-1.254374	0.060154
9	6	0	1.866435	-0.298650	0.162600
10	8	0	3.043824	-0.586957	0.079625
11	1	0	-0.088038	2.336264	0.802399
12	6	0	-1.005408	0.159879	1.942388
13	1	0	-0.089441	-0.269469	2.353567
14	1	0	-1.201927	1.116846	2.433767
15	1	0	-1.844707	-0.506912	2.160483
16	8	0	-2.121891	0.875778	-0.083520
17	1	0	-2.765141	0.169524	0.046238
18	8	0	0.099163	1.903701	-1.205175
19	1	0	-0.828104	2.116195	-1.372469
20	1	0	2.190280	1.654021	0.428139
21	1	0	1.189878	-2.072424	-0.437512

22	8	0	-1.381749	-1.957554	0.081491
23	1	0	-1.074927	-2.241295	0.948556

A-TS4 (EUMP2= -0.66079571368438D+03)

Sum of electronic and zero-point Energies=	-660.606186
Sum of electronic and thermal Energies=	-660.594945
Sum of electronic and thermal Enthalpies=	-660.594001
Sum of electronic and thermal Free Energies=	-660.642032

1	7	0	1.428330	0.989295	0.485949
2	6	0	0.132676	1.478859	0.135019
3	6	0	-0.896189	0.389159	0.429286
4	6	0	-0.508098	-0.922390	-0.302268
5	7	0	-0.619694	-0.924827	-1.745178
6	1	0	-1.599324	-0.818632	-1.991143
7	1	0	-0.129674	-0.111048	-2.108427
8	7	0	0.852782	-1.255491	0.062215
9	6	0	1.863782	-0.292974	0.179291
10	8	0	3.040850	-0.584221	0.100150
11	1	0	-0.094637	2.347375	0.767288
12	6	0	-1.013739	0.186882	1.935110
13	1	0	-0.090868	-0.218941	2.353312

14	1	0	-1.230749	1.148590	2.409439
15	1	0	-1.826790	-0.508912	2.150823
16	8	0	-2.120041	0.880024	-0.109005
17	1	0	-2.793675	0.235109	0.132919
18	8	0	0.119032	1.879115	-1.230788
19	1	0	-0.804398	2.093990	-1.414682
20	1	0	2.186790	1.657095	0.445388
21	1	0	1.207403	-2.031636	-0.489778
22	8	0	-1.418419	-1.904057	0.167001
23	1	0	-0.895964	-2.659928	0.446461

A-IM4 (EUMP2= -0.660801753755 46D+03)

Sum of electronic and zero-point Energies= -660.611295

Sum of electronic and thermal Energies= -660.599729

Sum of electronic and thermal Enthalpies= -660.598785

Sum of electronic and thermal Free Energies= -660.647391

1	7	0	1.448478	0.994347	0.430486
2	6	0	0.144674	1.476816	0.103995
3	6	0	-0.885207	0.398259	0.443336
4	6	0	-0.511553	-0.921946	-0.265088
5	7	0	-0.651947	-0.945571	-1.709092

6	1	0	-1.554359	-0.538069	-1.942572
7	1	0	0.047481	-0.333621	-2.119058
8	7	0	0.851045	-1.244030	0.093298
9	6	0	1.872415	-0.305487	0.171414
10	8	0	3.049400	-0.607636	0.111353
11	1	0	-0.067763	2.357509	0.725102
12	6	0	-0.985865	0.220983	1.952822
13	1	0	-0.043182	-0.135462	2.370433
14	1	0	-1.243581	1.182682	2.406360
15	1	0	-1.764551	-0.507603	2.188850
16	8	0	-2.116019	0.876415	-0.092622
17	1	0	-2.779680	0.229845	0.172882
18	8	0	0.100740	1.848551	-1.268555
19	1	0	-0.824767	2.063369	-1.438363
20	1	0	2.206440	1.657977	0.346061
21	1	0	1.186771	-2.131229	-0.261745
22	8	0	-1.415422	-1.884581	0.233815
23	1	0	-1.452227	-2.552357	-0.461606

A-TS5 (EUMP2=-0.66074932196131D+03)

Sum of electronic and zero-point Energies= -660.564553

Sum of electronic and thermal Energies= -660.552934

Sum of electronic and thermal Enthalpies= -660.551990

Sum of electronic and thermal Free Energies= -660.601407

1	7	0	1.391094	1.088844	0.135254
2	6	0	0.020586	1.490472	0.095212
3	6	0	-0.861042	0.325761	0.548080
4	6	0	-0.434112	-0.970124	-0.149068
5	7	0	-0.696734	-0.885367	-1.692628
6	1	0	-1.231871	-0.060036	-1.952890
7	1	0	0.143381	-0.957585	-2.263125
8	7	0	0.952337	-1.196075	0.115155
9	6	0	1.910604	-0.198774	0.093977
10	8	0	3.108323	-0.415439	0.083048
11	1	0	-0.122268	2.333670	0.785748
12	6	0	-0.801973	0.136533	2.057462
13	1	0	0.228012	0.067959	2.413428
14	1	0	-1.297449	0.985763	2.536497
15	1	0	-1.325797	-0.786978	2.317129
16	8	0	-2.186298	0.623910	0.127942
17	1	0	-2.656570	-0.211540	0.267646
18	8	0	-0.308652	1.916233	-1.225620
19	1	0	-1.229938	2.198113	-1.166569

20	1	0	2.098270	1.803548	0.049632
21	1	0	1.285779	-2.149240	0.078740
22	8	0	-1.254872	-2.016455	0.069370
23	1	0	-1.290816	-1.844699	-1.282593

A-PC (EUMP2=-0.66082185618707D+03)

Sum of electronic and zero-point Energies= -660.634297

Sum of electronic and thermal Energies= -660.621052

Sum of electronic and thermal Enthalpies= -660.620107

Sum of electronic and thermal Free Energies= -660.673511

1	7	0	-1.056220	-1.193843	0.785946
2	6	0	0.329440	-0.831461	0.569595
3	6	0	0.396997	0.699819	0.525976
4	6	0	-0.503732	1.162210	-0.609649
5	7	0	3.540554	-1.188020	-0.455510
6	1	0	3.499693	-0.278347	-0.005151
7	1	0	4.144167	-1.787652	0.095997
8	7	0	-1.703980	0.501993	-0.692626
9	6	0	-2.026577	-0.727514	-0.079581
10	8	0	-3.092232	-1.266494	-0.284385
11	1	0	0.905005	-1.181660	1.438844

12	6	0	-0.057435	1.342451	1.836839
13	1	0	-1.088873	1.085844	2.085031
14	1	0	0.599682	1.001348	2.642616
15	1	0	0.038579	2.428332	1.748703
16	8	0	1.720608	1.102292	0.230651
17	1	0	1.604861	1.785190	-0.447941
18	8	0	0.778187	-1.411576	-0.618032
19	1	0	1.763213	-1.394358	-0.601666
20	1	0	-1.215205	-2.169132	1.005434
21	1	0	-2.351579	0.800269	-1.411926
22	8	0	-0.180532	2.082208	-1.343509
23	1	0	3.997572	-1.055209	-1.351477

Path B

B-RE (EUMP2=-0.660790375398 53D+03)

Sum of electronic and zero-point Energies= -660.604304

Sum of electronic and thermal Energies= -660.590626

Sum of electronic and thermal Enthalpies= -660.589682

Sum of electronic and thermal Free Energies= -660.643485

1	7	0	0.507425	1.456967	0.544637
2	6	0	-0.894891	1.213101	0.582618
3	6	0	-1.096293	-0.295705	0.442849

4	6	0	-0.331927	-0.711216	-0.800976
5	7	0	-0.878801	-1.727175	-1.502754
6	1	0	-0.454549	-1.938652	-2.393982
7	1	0	-1.864039	-1.894539	-1.373264
8	7	0	0.817387	-0.218686	-1.141364
9	6	0	1.340225	0.850282	-0.391392
10	8	0	2.489546	1.225096	-0.532765
11	1	0	-1.283113	1.539492	1.559232
12	6	0	-0.570198	-1.078348	1.640384
13	1	0	0.516002	-0.997666	1.718300
14	1	0	-1.028433	-0.699507	2.562385
15	1	0	-0.828517	-2.134480	1.516508
16	8	0	-2.488006	-0.555108	0.217928
17	1	0	-2.877028	-0.740165	1.078562
18	8	0	-1.554541	1.897173	-0.465309
19	1	0	-2.424962	1.484932	-0.524562
20	1	0	0.844793	2.355637	0.859953
21	1	0	2.421548	-1.537787	-0.080546
22	8	0	2.792760	-1.473347	0.804963
23	1	0	3.256639	-0.634204	0.734346

B-TS1 (EUMP2= -0.660713112794 29D+03)

Sum of electronic and zero-point Energies= -660.531093

Sum of electronic and thermal Energies= -660.519000

Sum of electronic and thermal Enthalpies= -660.518056

Sum of electronic and thermal Free Energies= -660.567729

1	7	0	-1.313888	-1.149173	0.463148
2	6	0	0.032602	-1.535324	0.217991
3	6	0	0.934995	-0.305545	0.460711
4	6	0	0.389847	0.739541	-0.495368
5	7	0	1.091983	0.922071	-1.623819
6	1	0	0.635519	1.425576	-2.369196
7	1	0	2.095083	0.829290	-1.599040
8	7	0	-0.981292	0.951158	-0.594532
9	6	0	-1.870226	0.042333	-0.029678
10	8	0	-3.064131	0.250098	0.058726
11	1	0	0.315259	-2.305771	0.951905
12	6	0	0.916623	0.110748	1.919181
13	1	0	-0.066636	0.475513	2.212447
14	1	0	1.168932	-0.757599	2.540650
15	1	0	1.636005	0.915022	2.076855
16	8	0	2.262745	-0.634099	0.031626
17	1	0	2.751485	-0.886385	0.820228

18	8	0	0.194604	-2.029199	-1.097117
19	1	0	1.147639	-2.040177	-1.247279
20	1	0	-1.998425	-1.881289	0.587743
21	1	0	-0.711037	2.020253	-0.009019
22	8	0	0.383059	2.385429	0.499123
23	1	0	0.815309	3.048823	-0.054765

B-IM1 (EUMP2=-0.66080775667630D+03)

Sum of electronic and zero-point Energies= -660.616845

Sum of electronic and thermal Energies= -660.605526

Sum of electronic and thermal Enthalpies= -660.604582

Sum of electronic and thermal Free Energies= -660.652695

1	7	0	1.366899	1.077494	0.374025
2	6	0	-0.003960	1.478160	0.199488
3	6	0	-0.923892	0.278274	0.489895
4	6	0	-0.409954	-0.936027	-0.306372
5	7	0	-0.485031	-0.611236	-1.738385
6	1	0	-0.051310	-1.371916	-2.256382
7	1	0	-1.465412	-0.583584	-2.011915
8	7	0	0.944565	-1.194323	0.075280
9	6	0	1.894176	-0.184831	0.146125

10	8	0	3.090910	-0.399766	0.098031
11	1	0	-0.233680	2.272752	0.915727
12	6	0	-0.991631	-0.011669	1.978969
13	1	0	-0.004301	-0.250492	2.377044
14	1	0	-1.389728	0.870730	2.486963
15	1	0	-1.658274	-0.854989	2.166359
16	8	0	-2.239221	0.568153	0.028221
17	1	0	-2.123529	1.294785	-0.601189
18	8	0	-0.281956	2.042246	-1.069986
19	1	0	-0.119990	1.303635	-1.686361
20	1	0	2.066170	1.804678	0.317639
21	1	0	1.323718	-2.097079	-0.178725
22	8	0	-1.127215	-2.106828	0.009525
23	1	0	-2.057281	-1.865953	-0.080563

B-TS2 (EUMP2= -0.66079052139961D+03)

Sum of electronic and zero-point Energies= -660.601727

Sum of electronic and thermal Energies= -660.590213

Sum of electronic and thermal Enthalpies= -660.589269

Sum of electronic and thermal Free Energies= -660.637939

1	7	0	1.373897	1.066588	0.231304

2	6	0	0.004849	1.472518	0.249552
3	6	0	-0.894325	0.260633	0.505315
4	6	0	-0.413735	-0.931691	-0.361346
5	7	0	-0.488343	-0.687541	-1.796032
6	1	0	-1.171773	-1.304787	-2.214148
7	1	0	-0.693540	0.278047	-2.013687
8	7	0	0.939896	-1.228563	0.055739
9	6	0	1.889305	-0.229299	0.102513
10	8	0	3.089362	-0.425904	0.099964
11	1	0	-0.149854	2.212494	1.043107
12	6	0	-0.878743	-0.082512	1.987451
13	1	0	0.139667	-0.234767	2.346748
14	1	0	-1.345480	0.740471	2.535478
15	1	0	-1.447050	-0.995875	2.165908
16	8	0	-2.242288	0.549666	0.167456
17	1	0	-2.210419	1.082692	-0.635751
18	8	0	-0.412782	2.080153	-0.988598
19	1	0	0.396841	2.348552	-1.433293
20	1	0	2.087012	1.740613	0.468706
21	1	0	1.313948	-2.088187	-0.329128
22	8	0	-1.166647	-2.078517	-0.052386
23	1	0	-2.082769	-1.773711	-0.083417

B-IM2 (EUMP2= -0.66079776580198D+03)

Sum of electronic and zero-point Energies= -660.607539

Sum of electronic and thermal Energies= -660.595865

Sum of electronic and thermal Enthalpies= -660.594921

Sum of electronic and thermal Free Energies= -660.643841

1	7	0	-1.479492	-0.946450	0.494471
2	6	0	-0.211930	-1.450503	0.081558
3	6	0	0.888364	-0.448806	0.434597
4	6	0	0.579810	0.922615	-0.237376
5	7	0	0.964218	1.043395	-1.630414
6	1	0	1.936090	0.754489	-1.709129
7	1	0	0.401811	0.408586	-2.187986
8	7	0	-0.840442	1.195417	-0.140610
9	6	0	-1.880716	0.341515	0.136510
10	8	0	-3.050676	0.677856	0.115731
11	1	0	-0.010530	-2.384769	0.618458
12	6	0	1.007823	-0.313404	1.944319
13	1	0	0.144832	0.205110	2.364611
14	1	0	1.087783	-1.308989	2.390830
15	1	0	1.910540	0.253705	2.170510

16	8	0	2.125917	-0.947873	-0.043600
17	1	0	1.911204	-1.388347	-0.874788
18	8	0	-0.100264	-1.686148	-1.333003
19	1	0	-0.635195	-2.458162	-1.538358
20	1	0	-2.259457	-1.587411	0.540935
21	1	0	-1.139994	2.105853	-0.462006
22	8	0	1.324913	1.886359	0.465078
23	1	0	1.443703	2.603350	-0.168497

B-TS3 (EUMP2= -0.66073988931902D+03)

Sum of electronic and zero-point Energies=	-660.555479
Sum of electronic and thermal Energies=	-660.543708
Sum of electronic and thermal Enthalpies=	-660.542763
Sum of electronic and thermal Free Energies=	-660.592349

1	7	0	-1.491448	-1.042090	0.173750
2	6	0	-0.147672	-1.473108	0.018203
3	6	0	0.827270	-0.419413	0.545001
4	6	0	0.535474	0.957196	-0.103106
5	7	0	1.180758	1.050294	-1.517630
6	1	0	1.947713	0.388685	-1.612585
7	1	0	0.536069	1.008532	-2.303433

8	7	0	-0.899154	1.162930	-0.249042
9	6	0	-1.918953	0.268621	0.007161
10	8	0	-3.091790	0.583239	0.087803
11	1	0	-0.009088	-2.401004	0.587597
12	6	0	0.736317	-0.271608	2.052287
13	1	0	-0.241862	0.106657	2.356758
14	1	0	0.921283	-1.239100	2.528014
15	1	0	1.499812	0.444209	2.359329
16	8	0	2.154148	-0.831102	0.226304
17	1	0	2.053325	-1.461998	-0.496528
18	8	0	0.239952	-1.696790	-1.350728
19	1	0	-0.298504	-2.422322	-1.679807
20	1	0	-2.235755	-1.710087	0.299963
21	1	0	-1.162831	2.129389	-0.100648
22	8	0	1.166995	2.014572	0.414539
23	1	0	1.509697	2.029611	-0.928826

B-PC (EUMP2= -0.660814624377 89D+03)

Sum of electronic and zero-point Energies= -660.628205

Sum of electronic and thermal Energies= -660.614453

Sum of electronic and thermal Enthalpies= -660.613509

Sum of electronic and thermal Free Energies= -660.667849

1	7	0	-1.679931	0.540884	0.823078
2	6	0	-0.281629	0.790949	1.084036
3	6	0	0.477015	0.896374	-0.243835
4	6	0	0.242741	-0.414839	-1.002212
5	7	0	3.050844	-1.224234	0.601558
6	1	0	3.010492	-1.704042	-0.291862
7	1	0	3.985567	-1.342402	0.975840
8	7	0	-1.055688	-0.904871	-0.888849
9	6	0	-2.054738	-0.512449	0.010466
10	8	0	-3.146687	-1.041954	0.031333
11	1	0	-0.194471	1.747994	1.610182
12	6	0	-0.077482	2.040853	-1.095668
13	1	0	-1.137998	1.921694	-1.321573
14	1	0	0.076460	2.979441	-0.555037
15	1	0	0.499657	2.078506	-2.022484
16	8	0	1.825023	1.170359	-0.035304
17	1	0	2.284082	0.346300	0.254629
18	8	0	0.334881	-0.253765	1.825150
19	1	0	-0.015633	-0.210287	2.718940
20	1	0	-2.344935	0.708335	1.566082
21	1	0	-1.274823	-1.729681	-1.434001
22	8	0	1.069613	-0.972972	-1.695485

23	1	0	2.406938	-1.696996	1.226500

Path C

C-RE (EUMP2=-0.66078558877222D+03)

Sum of electronic and zero-point Energies= -660.599471

Sum of electronic and thermal Energies= -660.585756

Sum of electronic and thermal Enthalpies= -660.584812

Sum of electronic and thermal Free Energies= -660.640003

1	7	0	1.888816	0.021769	0.769979
2	6	0	1.170881	1.190582	0.375011
3	6	0	-0.301680	0.800269	0.249020
4	6	0	-0.340448	-0.422405	-0.653894
5	7	0	-1.482115	-0.549349	-1.414516
6	1	0	-1.381927	-1.237246	-2.151788
7	1	0	-1.872642	0.340202	-1.700352
8	7	0	0.555369	-1.345882	-0.690393
9	6	0	1.720902	-1.194596	0.099385
10	8	0	2.530674	-2.088472	0.208635
11	1	0	1.276101	1.950627	1.163280
12	6	0	-0.936528	0.483054	1.597423
13	1	0	-0.383793	-0.315100	2.096402
14	1	0	-0.897587	1.374355	2.236289

15	1	0	-1.975626	0.175815	1.457202
16	8	0	-0.998019	1.860783	-0.417524
17	1	0	-1.509193	2.328345	0.249836
18	8	0	1.657606	1.684497	-0.857647
19	1	0	0.990531	2.314326	-1.156766
20	1	0	2.838967	0.154602	1.090377
21	1	0	-3.108964	-1.013284	-0.189333
22	8	0	-3.809477	-0.995385	0.474878
23	1	0	-3.635380	-1.791213	0.980967

C-TS1 (EUMP2=-0.660706321513 09D+03)

Sum of electronic and zero-point Energies= -660.522795

Sum of electronic and thermal Energies= -660.510764

Sum of electronic and thermal Enthalpies= -660.509820

Sum of electronic and thermal Free Energies= -660.560072

1	7	0	1.698214	0.743082	0.269932
2	6	0	0.497719	1.478399	0.085414
3	6	0	-0.645948	0.556190	0.512921
4	6	0	-0.460762	-0.684458	-0.348932
5	7	0	-1.398566	-0.796108	-1.519185
6	1	0	-0.860456	-1.101950	-2.327123

7	1	0	-1.885538	0.084812	-1.675348
8	7	0	0.695258	-1.223582	-0.580738
9	6	0	1.829176	-0.624586	-0.023194
10	8	0	2.892349	-1.189141	0.130240
11	1	0	0.509504	2.362490	0.737128
12	6	0	-0.571031	0.252649	2.001140
13	1	0	0.310726	-0.344667	2.239177
14	1	0	-0.524116	1.193414	2.558927
15	1	0	-1.455863	-0.314780	2.294028
16	8	0	-1.865391	1.224805	0.190051
17	1	0	-2.548974	0.756161	0.682654
18	8	0	0.333286	1.877833	-1.274766
19	1	0	-0.455861	2.431543	-1.278482
20	1	0	2.570370	1.232115	0.399904
21	1	0	-1.963792	-1.572018	-0.910165
22	8	0	-1.772879	-1.799237	0.456686
23	1	0	-1.254188	-2.574110	0.707450

C-IM1 (EUMP2=-0.660789203420 15D+03)

Sum of electronic and zero-point Energies= -660.601881

Sum of electronic and thermal Energies= -660.588610

Sum of electronic and thermal Enthalpies= -660.587666

Sum of electronic and thermal Free Energies= -660.641029

1	7	0	-1.710843	0.574782	0.661312
2	6	0	-0.382414	0.853122	1.113246
3	6	0	0.564298	0.934485	-0.093864
4	6	0	0.209245	-0.212582	-1.016051
5	7	0	2.248503	-1.865276	0.694140
6	1	0	1.296557	-2.171212	0.876840
7	1	0	2.822286	-2.243086	1.441649
8	7	0	-0.892320	-0.866643	-1.069173
9	6	0	-1.945301	-0.509335	-0.185947
10	8	0	-3.012862	-1.078379	-0.223344
11	1	0	-0.380917	1.825748	1.622423
12	6	0	0.372386	2.245519	-0.850052
13	1	0	-0.673083	2.381489	-1.137002
14	1	0	0.681800	3.067064	-0.197359
15	1	0	1.007506	2.245676	-1.738170
16	8	0	1.902126	0.881775	0.349109
17	1	0	2.144903	-0.068101	0.441561
18	8	0	0.033191	-0.165775	2.012630
19	1	0	0.958186	0.040598	2.195290
20	1	0	-2.433272	0.650081	1.367093

21	1	0	2.547044	-2.318152	-0.163441
22	8	0	1.180745	-0.512076	-1.894467
23	1	0	0.776723	-1.181763	-2.468259

C-TS2 (EUMP2=-0.66074482562771D+03)

Sum of electronic and zero-point Energies= -660.562470

Sum of electronic and thermal Energies= -660.549430

Sum of electronic and thermal Enthalpies= -660.548486

Sum of electronic and thermal Free Energies= -660.601541

1	7	0	-1.907009	-0.717688	0.424649
2	6	0	-0.722059	-1.380399	-0.052869
3	6	0	0.526944	-0.570558	0.337078
4	6	0	0.222001	0.839201	-0.092989
5	7	0	3.765607	0.510890	-0.173567
6	1	0	4.375887	0.444467	-0.981733
7	1	0	4.366366	0.568485	0.641816
8	7	0	-0.991036	1.353131	-0.148068
9	6	0	-2.168050	0.611781	0.077485
10	8	0	-3.276560	1.090119	0.036781
11	1	0	-0.662740	-2.361585	0.436854
12	6	0	0.769086	-0.587959	1.846087

13	1	0	-0.096223	-0.201312	2.389761
14	1	0	0.961528	-1.620123	2.152068
15	1	0	1.646957	0.018640	2.085804
16	8	0	1.586239	-1.147650	-0.383218
17	1	0	2.402475	-0.600459	-0.255117
18	8	0	-0.779344	-1.518258	-1.455523
19	1	0	0.136035	-1.690997	-1.715295
20	1	0	-2.752291	-1.273571	0.385039
21	1	0	3.262301	1.390747	-0.250192
22	8	0	1.051143	1.764992	-0.422083
23	1	0	-0.132587	2.315362	-0.506509

C-PC (EUMP2=-0.66082280682515D+03)

Sum of electronic and zero-point Energies= -660.635264

Sum of electronic and thermal Energies= -660.621989

Sum of electronic and thermal Enthalpies= -660.621045

Sum of electronic and thermal Free Energies= -660.674539

1	7	0	-1.911278	-0.751770	0.431880
2	6	0	-0.698264	-1.367935	-0.031134
3	6	0	0.504327	-0.498759	0.339827
4	6	0	0.267266	0.916338	-0.196221

5	7	0	3.859954	0.447412	-0.114760
6	1	0	3.370734	1.312276	-0.327076
7	1	0	4.402689	0.597304	0.728776
8	7	0	-1.049482	1.329637	-0.167573
9	6	0	-2.194233	0.554348	0.082219
10	8	0	-3.305926	1.035156	0.040307
11	1	0	-0.595216	-2.336399	0.475143
12	6	0	0.708885	-0.418973	1.852330
13	1	0	-0.155655	0.023316	2.353462
14	1	0	0.874343	-1.428607	2.239163
15	1	0	1.594920	0.186203	2.065537
16	8	0	1.589612	-1.114229	-0.306828
17	1	0	2.408347	-0.575870	-0.174212
18	8	0	-0.750388	-1.533738	-1.432437
19	1	0	0.172679	-1.679523	-1.682574
20	1	0	-2.741377	-1.329389	0.400511
21	1	0	4.523349	0.281579	-0.864240
22	8	0	1.161511	1.660953	-0.559719
23	1	0	-1.235513	2.276915	-0.474026

Water-Mediated Deamination Mechanism

Path A

wA-RC (EUMP2 = -0.73708233191336D+03)

Sum of electronic and zero-point Energies=	-736.869701
Sum of electronic and thermal Energies=	-736.853831
Sum of electronic and thermal Enthalpies=	-736.852886
Sum of electronic and thermal Free Energies=	-736.912282

1	7	0	1.423272	1.613001	-0.250878
2	6	0	2.026588	0.497028	0.405658
3	6	0	1.439452	-0.768451	-0.216660
4	6	0	-0.074534	-0.645111	-0.127428
5	7	0	-0.741891	-1.791537	0.009458
6	1	0	-1.770131	-1.792759	0.064489
7	1	0	-0.207861	-2.605835	0.267935
8	7	0	-0.699746	0.493904	-0.259581
9	6	0	0.025897	1.687504	-0.347467
10	8	0	-0.531303	2.753057	-0.528631
11	1	0	3.110896	0.523900	0.217130
12	6	0	1.854315	-0.944961	-1.672537
13	1	0	1.534240	-0.091435	-2.271747
14	1	0	2.946985	-1.020723	-1.739176
15	1	0	1.405788	-1.858389	-2.072451
16	8	0	1.828982	-1.902002	0.566021

17	1	0	2.673326	-2.204350	0.215915
18	8	0	1.766156	0.528537	1.794620
19	1	0	1.929973	-0.369835	2.106539
20	1	0	1.831061	2.518797	-0.056766
21	1	0	-2.439614	0.924102	0.220918
22	8	0	-3.384630	0.988545	0.463450
23	1	0	-3.689482	1.736170	-0.052904
24	8	0	-3.573380	-1.672353	0.066366
25	1	0	-3.973651	-1.767377	-0.799541
26	1	0	-3.699885	-0.722168	0.262671

wA-TS1 (EUMP2= -0.73705565387759D+03)

Sum of electronic and zero-point Energies= -736.850618

Sum of electronic and thermal Energies= -736.836842

Sum of electronic and thermal Enthalpies= -736.835898

Sum of electronic and thermal Free Energies= -736.890632

1	7	0	-1.452979	1.574450	0.232698
2	6	0	-2.002731	0.409319	-0.383299
3	6	0	-1.335487	-0.808500	0.252390
4	6	0	0.171059	-0.646826	0.090497
5	7	0	0.914578	-1.704399	-0.107132

6	1	0	2.263398	-1.658758	-0.121384
7	1	0	0.342944	-2.534131	-0.230574
8	7	0	0.710221	0.573627	0.226376
9	6	0	-0.059015	1.726470	0.288133
10	8	0	0.446996	2.827624	0.420157
11	1	0	-3.083271	0.380318	-0.173041
12	6	0	-1.677868	-0.948879	1.730927
13	1	0	-1.337576	-0.078286	2.293046
14	1	0	-2.764701	-1.034963	1.856459
15	1	0	-1.198702	-1.848097	2.128587
16	8	0	-1.722157	-1.979394	-0.472468
17	1	0	-2.545334	-2.287733	-0.079842
18	8	0	-1.773359	0.417689	-1.779141
19	1	0	-1.884887	-0.498959	-2.059947
20	1	0	-1.908245	2.450986	0.012001
21	1	0	2.041249	0.818224	-0.098974
22	8	0	3.113733	0.870440	-0.382013
23	1	0	3.531527	1.491798	0.219701
24	8	0	3.390057	-1.471702	-0.112444
25	1	0	3.719355	-1.738013	0.749679
26	1	0	3.403606	-0.274892	-0.223920

wA-IM1 (EUMP2=-0.73708341052085D+03)

Sum of electronic and zero-point Energies= -736.870417

Sum of electronic and thermal Energies= -736.854530

Sum of electronic and thermal Enthalpies= -736.853586

Sum of electronic and thermal Free Energies= -736.912177

1	7	0	-0.819458	1.722855	0.256108
2	6	0	-1.844406	0.734652	0.122852
3	6	0	-1.232063	-0.632698	0.436049
4	6	0	-0.048501	-0.861308	-0.485449
5	7	0	0.353000	-2.010451	-0.897654
6	1	0	2.852240	-0.225766	0.943795
7	1	0	-0.315566	-2.709313	-0.573561
8	7	0	0.664783	0.273735	-0.800414
9	6	0	0.408257	1.564282	-0.354583
10	8	0	1.222975	2.460188	-0.478819
11	1	0	-2.623814	0.952216	0.867691
12	6	0	-0.745301	-0.734534	1.878990
13	1	0	0.145631	-0.124188	2.043461
14	1	0	-1.537679	-0.417791	2.568011
15	1	0	-0.482739	-1.777094	2.084528
16	8	0	-2.194533	-1.641973	0.130181

17	1	0	-2.684418	-1.810371	0.941407
18	8	0	-2.384565	0.744986	-1.181669
19	1	0	-2.835476	-0.103947	-1.272435
20	1	0	-1.092493	2.690020	0.356954
21	1	0	1.594572	0.130013	-1.184723
22	8	0	2.534205	0.380543	1.624682
23	1	0	2.562728	1.226879	1.170446
24	1	0	2.266573	-1.842843	-0.896291
25	8	0	3.043852	-1.270742	-0.758196
26	1	0	3.758761	-1.697161	-1.232161

wA-TS2 (EUMP2=-0.73702365961472D+03)

Sum of electronic and zero-point Energies= -736.814052

Sum of electronic and thermal Energies= -736.800186

Sum of electronic and thermal Enthalpies= -736.799242

Sum of electronic and thermal Free Energies= -736.852919

1	7	0	-1.564835	1.291405	0.478839
2	6	0	-1.921599	0.006601	-0.045336
3	6	0	-0.787690	-0.979332	0.280130
4	6	0	0.469371	-0.393790	-0.337171
5	7	0	1.099523	-1.072654	-1.280075

6	1	0	2.782078	-0.231363	0.305568
7	1	0	0.984201	-2.074326	-1.211650
8	7	0	0.623571	0.950231	-0.267080
9	6	0	-0.335627	1.862994	0.177908
10	8	0	-0.092564	3.043401	0.294842
11	1	0	-2.828804	-0.333861	0.472820
12	6	0	-0.669009	-1.206471	1.778149
13	1	0	-0.461816	-0.269719	2.294771
14	1	0	-1.624845	-1.600280	2.147542
15	1	0	0.153455	-1.894511	1.971579
16	8	0	-1.063740	-2.199328	-0.408105
17	1	0	-1.336653	-2.837661	0.256909
18	8	0	-2.135910	0.083225	-1.437325
19	1	0	-2.134114	-0.830656	-1.748748
20	1	0	-2.299807	1.983983	0.531882
21	1	0	1.572060	1.288340	-0.486901
22	8	0	2.052304	-0.869089	1.139727
23	1	0	2.020016	-0.300853	1.916382
24	1	0	2.040473	-0.692953	-1.484019
25	8	0	3.163252	0.362522	-0.599742
26	1	0	4.106527	0.505133	-0.525174

wA-IM2 (EUMP2=-0.73709034424669D+03)

Sum of electronic and zero-point Energies= -736.873600

Sum of electronic and thermal Energies= -736.859397

Sum of electronic and thermal Enthalpies= -736.858453

Sum of electronic and thermal Free Energies= -736.912885

1	7	0	-1.260538	1.605552	0.169275
2	6	0	-1.796833	0.350040	-0.286123
3	6	0	-1.006317	-0.808524	0.348812
4	6	0	0.495222	-0.588306	0.048671
5	7	0	0.714819	-0.760118	-1.373350
6	1	0	3.161185	-0.968231	0.087820
7	1	0	0.582997	-1.746007	-1.589324
8	7	0	0.883690	0.729256	0.488463
9	6	0	0.097603	1.862469	0.289748
10	8	0	0.558402	2.987793	0.314981
11	1	0	-2.836372	0.278391	0.047464
12	6	0	-1.271688	-0.904753	1.842285
13	1	0	-0.842190	-0.057612	2.381835
14	1	0	-2.350820	-0.927286	2.013518
15	1	0	-0.858290	-1.843787	2.220902
16	8	0	-1.429693	-2.021645	-0.247987

17	1	0	-1.804878	-1.759451	-1.099898
18	8	0	-1.851493	0.210286	-1.694053
19	1	0	-0.917957	0.102436	-1.962695
20	1	0	-1.773187	2.431972	-0.109186
21	1	0	1.872642	0.922570	0.349952
22	8	0	1.316947	-1.532635	0.736381
23	1	0	1.199901	-1.349788	1.676185
24	1	0	1.680882	-0.514437	-1.583336
25	8	0	3.523286	-0.239106	-0.430523
26	1	0	4.472762	-0.294700	-0.314703

wA-TS3 (EUMP2=-0.73706778816504D+03)

Sum of electronic and zero-point Energies= -736.853379

Sum of electronic and thermal Energies= -736.838807

Sum of electronic and thermal Enthalpies= -736.837863

Sum of electronic and thermal Free Energies= -736.893662

1	7	0	-1.154299	1.660028	0.275632
2	6	0	-1.808881	0.462867	-0.129204
3	6	0	-1.038421	-0.759094	0.387385
4	6	0	0.438213	-0.678421	-0.094772
5	7	0	0.621407	-0.980353	-1.503503

6	1	0	3.188779	-1.025786	-0.181854
7	1	0	-0.272072	-1.043107	-1.973424
8	7	0	0.950460	0.637427	0.252493
9	6	0	0.233233	1.818531	0.231271
10	8	0	0.752743	2.918345	0.246295
11	1	0	-2.816337	0.426835	0.295321
12	6	0	-1.114279	-0.824801	1.905990
13	1	0	-0.526004	-0.032915	2.374336
14	1	0	-2.156555	-0.725800	2.220265
15	1	0	-0.757352	-1.804480	2.232780
16	8	0	-1.663880	-1.929366	-0.100201
17	1	0	-1.997270	-1.705663	-0.976947
18	8	0	-2.013042	0.365887	-1.549957
19	1	0	-1.278927	0.836371	-1.961330
20	1	0	-1.650157	2.533111	0.158570
21	1	0	1.926289	0.763330	-0.016941
22	8	0	1.257118	-1.630101	0.571037
23	1	0	1.341113	-1.310781	1.476109
24	1	0	1.056338	-1.893962	-1.575523
25	8	0	3.719016	-0.238839	-0.345800
26	1	0	4.344335	-0.238751	0.381285

wA-IM3 (EUMP2=-0.73708116313071D+03)

Sum of electronic and zero-point Energies= -736.864782

Sum of electronic and thermal Energies= -736.850477

Sum of electronic and thermal Enthalpies= -736.849533

Sum of electronic and thermal Free Energies= -736.904038

1	7	0	1.240072	1.612170	-0.228101
2	6	0	1.748294	0.403583	0.330238
3	6	0	1.034899	-0.794958	-0.297652
4	6	0	-0.507417	-0.649946	-0.091758
5	7	0	-0.975209	-1.036376	1.230525
6	1	0	-2.880671	-0.535904	0.973376
7	1	0	-0.446826	-0.515849	1.925087
8	7	0	-0.908284	0.705761	-0.383859
9	6	0	-0.137505	1.847982	-0.302004
10	8	0	-0.595237	2.971948	-0.364834
11	1	0	2.818658	0.329001	0.104926
12	6	0	1.390159	-0.894026	-1.773603
13	1	0	0.932808	-0.086532	-2.350118
14	1	0	2.475401	-0.840243	-1.893905
15	1	0	1.054153	-1.862930	-2.148177
16	8	0	1.497095	-1.984241	0.314780

17	1	0	1.622216	-1.758785	1.244143
18	8	0	1.560201	0.279311	1.750816
19	1	0	2.144184	0.912499	2.178199
20	1	0	1.756311	2.465675	-0.061976
21	1	0	-1.908017	0.862451	-0.251530
22	8	0	-1.206668	-1.534521	-0.944211
23	1	0	-1.115808	-1.172131	-1.831164
24	1	0	-0.771855	-2.025477	1.353928
25	8	0	-3.594291	-0.158780	0.432174
26	1	0	-3.635983	-0.808211	-0.273866

wA-TS4 (EUMP2=-0.737078446398l4D+03)

Sum of electronic and zero-point Energies= -736.862976

Sum of electronic and thermal Energies= -736.849008

Sum of electronic and thermal Enthalpies= -736.848064

Sum of electronic and thermal Free Energies= -736.902189

1	7	0	1.241048	1.612547	-0.205309
2	6	0	1.744322	0.400463	0.351015
3	6	0	1.042679	-0.792001	-0.299428
4	6	0	-0.499998	-0.652974	-0.114782
5	7	0	-0.988283	-1.052299	1.204251

6	1	0	-2.836841	-0.597864	0.917093
7	1	0	-0.471051	-0.542213	1.916376
8	7	0	-0.905568	0.705465	-0.380718
9	6	0	-0.131591	1.847286	-0.302330
10	8	0	-0.593648	2.969378	-0.373350
11	1	0	2.817562	0.330642	0.139484
12	6	0	1.413753	-0.871987	-1.771362
13	1	0	0.955794	-0.060234	-2.339102
14	1	0	2.501332	-0.815972	-1.875092
15	1	0	1.066007	-1.827378	-2.163540
16	8	0	1.495845	-1.987431	0.310867
17	1	0	1.611648	-1.768910	1.243062
18	8	0	1.537113	0.267922	1.768425
19	1	0	2.116792	0.897445	2.206775
20	1	0	1.758107	2.465721	-0.042083
21	1	0	-1.901771	0.873485	-0.243568
22	8	0	-1.124347	-1.538737	-1.024117
23	1	0	-1.733081	-0.999455	-1.535905
24	1	0	-0.784732	-2.042945	1.315078
25	8	0	-3.552355	-0.146769	0.431864
26	1	0	-4.045997	-0.871933	0.045661

wA-IM4 (EUMP2=-0.73708954665623D+03)

Sum of electronic and zero-point Energies= -736.872777

Sum of electronic and thermal Energies= -736.858735

Sum of electronic and thermal Enthalpies= -736.857791

Sum of electronic and thermal Free Energies= -736.911875

1	7	0	1.524883	1.374796	-0.107133
2	6	0	1.817441	0.043556	0.312777
3	6	0	0.833106	-0.920554	-0.353031
4	6	0	-0.615372	-0.460864	-0.084091
5	7	0	-1.051209	-0.569790	1.316170
6	1	0	-2.872401	-0.064974	1.014009
7	1	0	-0.431072	-0.001054	1.889562
8	7	0	-0.733970	0.914999	-0.508768
9	6	0	0.236405	1.876891	-0.279085
10	8	0	0.008156	3.071727	-0.313856
11	1	0	2.829593	-0.217719	-0.024221
12	6	0	1.119233	-1.016848	-1.845794
13	1	0	0.954140	-0.057524	-2.338211
14	1	0	2.158982	-1.325989	-1.988608
15	1	0	0.456585	-1.755065	-2.301906
16	8	0	1.049761	-2.176009	0.286694

17	1	0	0.469896	-2.798648	-0.166374
18	8	0	1.768864	-0.036027	1.735541
19	1	0	1.884889	-0.973813	1.933886
20	1	0	2.173723	2.093670	0.182055
21	1	0	-1.676036	1.290993	-0.477569
22	8	0	-1.429947	-1.311392	-0.840135
23	1	0	-2.343744	-1.035664	-0.649698
24	1	0	-0.894408	-1.532973	1.606108
25	8	0	-3.503788	0.100969	0.287251
26	1	0	-4.377320	0.011498	0.670469

wA-TS5 (EUMP2=-0.73705817157268D+03)

Sum of electronic and zero-point Energies= -736.847349

Sum of electronic and thermal Energies= -736.834479

Sum of electronic and thermal Enthalpies= -736.833535

Sum of electronic and thermal Free Energies= -736.885564

1	7	0	-1.837947	0.894727	-0.033119
2	6	0	-1.709937	-0.489423	-0.351398
3	6	0	-0.515141	-1.070904	0.405776
4	6	0	0.731161	-0.197300	0.205923
5	7	0	1.142987	-0.188751	-1.287283

6	1	0	2.194522	0.291442	-1.178972
7	1	0	0.453130	0.276628	-1.875365
8	7	0	0.405999	1.163155	0.555412
9	6	0	-0.792361	1.777149	0.235524
10	8	0	-0.958109	2.982069	0.258570
11	1	0	-2.619172	-1.013207	-0.027388
12	6	0	-0.825804	-1.201846	1.889839
13	1	0	-1.115228	-0.240128	2.316868
14	1	0	-1.641953	-1.918952	2.016943
15	1	0	0.064631	-1.559407	2.411150
16	8	0	-0.255391	-2.346497	-0.174857
17	1	0	0.527379	-2.663475	0.295458
18	8	0	-1.570383	-0.642191	-1.765610
19	1	0	-1.447530	-1.590155	-1.901573
20	1	0	-2.668380	1.369456	-0.357455
21	1	0	1.195597	1.792993	0.644822
22	8	0	1.786724	-0.701283	0.868604
23	1	0	2.673174	-0.058648	0.403251
24	1	0	1.206496	-1.160836	-1.586218
25	8	0	3.215572	0.709439	-0.380472
26	1	0	4.125255	0.472011	-0.570457

wA-PC (EUMP2=-0.73710323094342D+03)

Sum of electronic and zero-point Energies= -736.889924

Sum of electronic and thermal Energies= -736.873861

Sum of electronic and thermal Enthalpies= -736.872917

Sum of electronic and thermal Free Energies= -736.932445

1	7	0	1.332880	1.543427	0.232619
2	6	0	1.625506	0.199074	0.738836
3	6	0	1.201161	-0.782484	-0.363629
4	6	0	-0.255247	-0.530322	-0.722037
5	7	0	-1.631033	-0.812845	1.999302
6	1	0	-2.330462	-0.541659	1.310878
7	1	0	-1.973361	-0.491325	2.899868
8	7	0	-0.656945	0.770857	-0.720127
9	6	0	0.074761	1.871491	-0.211137
10	8	0	-0.401516	2.986429	-0.229655
11	1	0	2.711752	0.137189	0.855305
12	6	0	2.044028	-0.599503	-1.631470
13	1	0	1.958700	0.407859	-2.043921
14	1	0	3.089686	-0.801398	-1.382348
15	1	0	1.717664	-1.329042	-2.378650
16	8	0	1.329151	-2.096106	0.124151

17	1	0	0.607589	-2.579053	-0.300789
18	8	0	1.074523	-0.056463	1.984928
19	1	0	0.122572	-0.286822	1.892079
20	1	0	1.740648	2.301359	0.765896
21	1	0	-1.641308	0.954259	-0.908394
22	8	0	-0.988270	-1.469956	-1.033773
23	1	0	-2.807524	-0.862114	-0.965264
24	1	0	-1.639776	-1.827747	2.033242
25	8	0	-3.363493	-0.148727	-0.618264
26	1	0	-4.214897	-0.262525	-1.042930

Path B

wB-RC (EUMP2=-0.73707668553981D+03)

Sum of electronic and zero-point Energies= -736.864491

Sum of electronic and thermal Energies= -736.848252

Sum of electronic and thermal Enthalpies= -736.847307

Sum of electronic and thermal Free Energies= -736.907013

1	7	0	-1.381092	1.435962	0.619572
2	6	0	-2.033135	0.262169	0.135430
3	6	0	-1.030626	-0.888262	0.230830
4	6	0	0.213966	-0.429365	-0.503958
5	7	0	0.855609	-1.359194	-1.217209

6	1	0	1.791460	-1.145438	-1.545603
7	1	0	0.527189	-2.309167	-1.168112
8	7	0	0.666081	0.792539	-0.441578
9	6	0	-0.098374	1.788123	0.183848
10	8	0	0.337733	2.907251	0.364497
11	1	0	-2.894347	0.047186	0.786371
12	6	0	-0.676275	-1.240184	1.671319
13	1	0	-0.355165	-0.350367	2.213977
14	1	0	-1.564642	-1.643624	2.174223
15	1	0	0.131977	-1.973991	1.693642
16	8	0	-1.551227	-2.026696	-0.461661
17	1	0	-2.049582	-2.536221	0.185375
18	8	0	-2.455063	0.432497	-1.203376
19	1	0	-2.600016	-0.460858	-1.538893
20	1	0	-1.960916	2.243323	0.805061
21	1	0	2.448842	0.741625	-0.900725
22	8	0	3.250342	0.197705	-1.059196
23	1	0	3.897853	0.798087	-1.430994
24	1	0	3.070629	-0.675673	0.677078
25	8	0	2.667770	-0.965575	1.506654
26	1	0	2.322757	-0.136376	1.842945

wB-TS1 (EUMP2=-0.737020955316 95D+03)

Sum of electronic and zero-point Energies= -736.811416

Sum of electronic and thermal Energies= -736.797594

Sum of electronic and thermal Enthalpies= -736.796649

Sum of electronic and thermal Free Energies= -736.845801

1	7	0	-1.365059	1.430922	0.533492
2	6	0	-1.903058	0.221536	-0.010913
3	6	0	-0.899873	-0.909190	0.266646
4	6	0	0.421720	-0.479133	-0.353423
5	7	0	1.004999	-1.282842	-1.234915
6	1	0	1.977952	-1.019172	-1.450116
7	1	0	0.766473	-2.258984	-1.139623
8	7	0	0.695039	0.841150	-0.394396
9	6	0	-0.098650	1.854087	0.152974
10	8	0	0.298522	2.991330	0.264127
11	1	0	-2.833969	-0.009531	0.525672
12	6	0	-0.802067	-1.199081	1.756325
13	1	0	-0.282479	-0.402090	2.281673
14	1	0	-1.817157	-1.323811	2.155764
15	1	0	-0.231305	-2.116794	1.907878
16	8	0	-1.328237	-2.069837	-0.453809

17	1	0	-1.847617	-2.594847	0.163107
18	8	0	-2.144057	0.356277	-1.394202
19	1	0	-2.223913	-0.545745	-1.728881
20	1	0	-2.003532	2.205828	0.653474
21	1	0	1.685582	1.053705	-0.604211
22	8	0	3.181587	0.042274	-0.605692
23	1	0	4.089596	0.306808	-0.459184
24	1	0	2.716523	-0.324417	0.374487
25	8	0	1.896898	-0.717823	1.275393
26	1	0	2.112857	-1.642655	1.434513

wB-IM1 (EUMP2=-0.73709075564845D+03)

Sum of electronic and zero-point Energies= -736.874098

Sum of electronic and thermal Energies= -736.859852

Sum of electronic and thermal Enthalpies= -736.858908

Sum of electronic and thermal Free Energies= -736.913559

1	7	0	-1.208838	1.617967	0.137366
2	6	0	-1.811647	0.366316	-0.235994
3	6	0	-0.995136	-0.778607	0.384434
4	6	0	0.486315	-0.566923	0.025879
5	7	0	0.644374	-0.632620	-1.428031

6	1	0	1.608357	-0.386315	-1.648799
7	1	0	0.494569	-1.591343	-1.735021
8	7	0	0.917673	0.708271	0.515059
9	6	0	0.152509	1.848673	0.287663
10	8	0	0.626526	2.969014	0.308472
11	1	0	-2.827600	0.329779	0.168584
12	6	0	-1.209897	-0.851641	1.886155
13	1	0	-0.861839	0.059212	2.375125
14	1	0	-2.277375	-0.988805	2.078876
15	1	0	-0.667583	-1.702240	2.302206
16	8	0	-1.401935	-2.017623	-0.187307
17	1	0	-1.828436	-1.773588	-1.021703
18	8	0	-1.968099	0.185260	-1.632062
19	1	0	-1.050142	0.152089	-1.963266
20	1	0	-1.708907	2.456292	-0.125286
21	1	0	1.910054	0.880172	0.379561
22	8	0	3.529867	-0.324091	-0.432380
23	1	0	4.401311	-0.183793	-0.059120
24	1	0	3.124572	-0.997088	0.128638
25	8	0	1.290505	-1.541394	0.688848
26	1	0	0.862783	-2.385923	0.496059

wB-TS2 (EUMP2=-0.73706936865186D+03)

Sum of electronic and zero-point Energies= -736.855642

Sum of electronic and thermal Energies= -736.840792

Sum of electronic and thermal Enthalpies= -736.839848

Sum of electronic and thermal Free Energies= -736.896473

1	7	0	-1.093809	1.651638	0.124203
2	6	0	-1.840736	0.436058	0.097424
3	6	0	-0.936863	-0.734610	0.488802
4	6	0	0.419657	-0.600641	-0.248386
5	7	0	0.317617	-0.676319	-1.696972
6	1	0	0.765439	-1.513628	-2.043910
7	1	0	-0.637465	-0.611711	-2.021233
8	7	0	1.022256	0.637708	0.185192
9	6	0	0.300398	1.810173	0.144086
10	8	0	0.795402	2.920007	0.183005
11	1	0	-2.677016	0.499995	0.803213
12	6	0	-0.756866	-0.756914	1.999396
13	1	0	-0.369804	0.194906	2.364665
14	1	0	-1.727816	-0.962246	2.458295
15	1	0	-0.058891	-1.545664	2.282105
16	8	0	-1.523678	-1.976304	0.129587

17	1	0	-1.944683	-1.837267	-0.727160
18	8	0	-2.396670	0.147888	-1.200443
19	1	0	-2.415326	0.988340	-1.668221
20	1	0	-1.578957	2.519426	0.299530
21	1	0	1.989526	0.752176	-0.114383
22	8	0	3.808309	-0.339653	-0.244690
23	1	0	4.140409	-0.173850	0.639840
24	1	0	3.180173	-1.056677	-0.101457
25	8	0	1.284847	-1.631215	0.198254
26	1	0	0.752744	-2.435176	0.128121

wB-IM2 (EUMP2=-0.737085249155555D+03)

Sum of electronic and zero-point Energies= -736.868513

Sum of electronic and thermal Energies= -736.854441

Sum of electronic and thermal Enthalpies= -736.853497

Sum of electronic and thermal Free Energies= -736.907611

1	7	0	-1.608023	1.304494	0.207843
2	6	0	-1.803817	-0.010125	-0.300188
3	6	0	-0.805602	-0.974565	0.342778
4	6	0	0.645449	-0.469214	0.088821
5	7	0	1.178522	-0.812161	-1.236849

6	1	0	1.122931	-1.824928	-1.322783
7	1	0	0.574290	-0.402788	-1.945208
8	7	0	0.692780	0.973252	0.221460
9	6	0	-0.335380	1.881210	0.234086
10	8	0	-0.172834	3.086032	0.302233
11	1	0	-2.816284	-0.343526	-0.044394
12	6	0	-1.085926	-1.102667	1.831211
13	1	0	-0.819155	-0.188088	2.362211
14	1	0	-2.148271	-1.317416	1.981059
15	1	0	-0.493113	-1.927587	2.225560
16	8	0	-0.981021	-2.258721	-0.233448
17	1	0	-1.205127	-2.090756	-1.156558
18	8	0	-1.618123	-0.132064	-1.724099
19	1	0	-2.352507	0.320625	-2.148570
20	1	0	-2.334802	1.991421	0.063341
21	1	0	1.617701	1.387592	0.204510
22	8	0	1.459798	-1.092523	1.036119
23	1	0	2.357862	-0.768699	0.855823
24	1	0	2.936581	-0.116356	-0.954772
25	8	0	3.514231	0.266153	-0.265857
26	1	0	4.412205	0.122557	-0.567226

wB-TS3 (EUMP2=-0.73704958995781D+03)

Sum of electronic and zero-point Energies= -736.839399

Sum of electronic and thermal Energies= -736.826301

Sum of electronic and thermal Enthalpies= -736.825357

Sum of electronic and thermal Free Energies= -736.877949

1	7	0	-2.036530	0.573827	-0.070157
2	6	0	-1.611337	-0.755207	-0.322232
3	6	0	-0.343331	-1.077601	0.472535
4	6	0	0.765481	-0.024037	0.187568
5	7	0	1.407240	-0.334773	-1.172374
6	1	0	1.665243	-1.321674	-1.150586
7	1	0	0.759291	-0.163503	-1.937940
8	7	0	0.165489	1.306975	0.025742
9	6	0	-1.170036	1.652090	0.056710
10	8	0	-1.570213	2.794711	0.180918
11	1	0	-2.403734	-1.446074	-0.010329
12	6	0	-0.630011	-1.110544	1.962624
13	1	0	-0.896354	-0.120861	2.338800
14	1	0	-1.446474	-1.811464	2.159740
15	1	0	0.274578	-1.445714	2.469735
16	8	0	0.112773	-2.371181	0.091258

17	1	0	-0.231400	-2.510771	-0.799123
18	8	0	-1.286616	-1.015499	-1.705250
19	1	0	-2.103478	-0.938204	-2.207104
20	1	0	-3.010094	0.826873	-0.138007
21	1	0	0.759684	2.050696	0.369291
22	8	0	1.743505	-0.038123	1.092966
23	1	0	2.694381	0.452568	0.513477
24	1	0	2.383441	0.306334	-1.099872
25	8	0	3.402019	0.808925	-0.382039
26	1	0	3.525187	1.760733	-0.356613

wB-PC (EUMP2=-0.73710388394841D+03)

Sum of electronic and zero-point Energies= -736.890119

Sum of electronic and thermal Energies= -736.874234

Sum of electronic and thermal Enthalpies= -736.873289

Sum of electronic and thermal Free Energies= -736.932491

1	7	0	2.153768	0.596405	0.609016
2	6	0	0.797930	0.962451	0.929462
3	6	0	-0.078018	-0.295481	0.892706
4	6	0	0.037319	-0.880821	-0.514807
5	7	0	-2.524808	1.816853	-0.725064

6	1	0	-3.082887	2.619570	-0.451181
7	1	0	-2.178011	2.005902	-1.661035
8	7	0	1.316985	-0.849078	-1.026672
9	6	0	2.407834	-0.084144	-0.566648
10	8	0	3.468041	-0.086654	-1.152299
11	1	0	0.780194	1.365783	1.949651
12	6	0	0.379956	-1.339706	1.906072
13	1	0	1.402084	-1.669128	1.716553
14	1	0	0.320494	-0.904948	2.908032
15	1	0	-0.298985	-2.194825	1.855441
16	8	0	-1.410131	0.019204	1.216955
17	1	0	-1.757171	0.624543	0.536069
18	8	0	0.362669	1.924645	-0.011123
19	1	0	-0.604400	1.995153	0.031835
20	1	0	2.856989	1.303021	0.783437
21	1	0	1.453392	-1.272468	-1.936952
22	8	0	-0.887318	-1.385936	-1.131538
23	1	0	-2.803199	-1.251403	-0.745484
24	1	0	-3.163516	1.021501	-0.810608
25	8	0	-3.681187	-0.938123	-0.487554
26	1	0	-3.633329	-1.030847	0.467048

Path C

wC-RC (EUMP2=-0.737069225996l2D+03)

Sum of electronic and zero-point Energies= -736.857059

Sum of electronic and thermal Energies= -736.840820

Sum of electronic and thermal Enthalpies= -736.839876

Sum of electronic and thermal Free Energies= -736.899217

1	7	0	-0.938854	1.608703	0.460445
2	6	0	-1.774203	0.462059	0.583009
3	6	0	-0.876041	-0.773717	0.473779
4	6	0	-0.064931	-0.587536	-0.795990
5	7	0	0.279308	-1.748311	-1.454853
6	1	0	-0.389438	-2.498086	-1.336490
7	1	0	0.583487	-1.581026	-2.407354
8	7	0	0.378861	0.540497	-1.223298
9	6	0	0.069466	1.706183	-0.484143
10	8	0	0.673158	2.744742	-0.665541
11	1	0	-2.244895	0.476282	1.577341
12	6	0	0.046848	-0.936773	1.673751
13	1	0	0.755884	-0.107638	1.741648
14	1	0	-0.550971	-0.983246	2.592849
15	1	0	0.611277	-1.867774	1.568477
16	8	0	-1.707019	-1.929614	0.291617
17	1	0	-1.844686	-2.310331	1.164757

18	8	0	-2.758892	0.448363	-0.431774
19	1	0	-3.096547	-0.455518	-0.439577
20	1	0	-1.264788	2.495594	0.815974
21	1	0	2.821096	0.312039	0.526599
22	8	0	2.595189	1.064948	1.088701
23	1	0	2.418134	1.768001	0.457871
24	8	0	2.998134	-1.493997	-0.197145
25	1	0	2.180476	-1.802387	-0.608061
26	1	0	3.174375	-2.148969	0.480624

wC-TS1 (EUMP2=-0.73699558185038D+03)

Sum of electronic and zero-point Energies= -736.787980

Sum of electronic and thermal Energies= -736.773974

Sum of electronic and thermal Enthalpies= -736.773030

Sum of electronic and thermal Free Energies= -736.827839

1	7	0	2.233392	0.331097	-0.124920
2	6	0	1.243466	1.338093	0.087284
3	6	0	0.003511	0.648466	0.670139
4	6	0	-0.292844	-0.432367	-0.353753
5	7	0	-1.297686	-0.068541	-1.379383
6	1	0	-0.971661	0.817821	-1.774025

7	1	0	-1.202835	-0.786835	-2.100697
8	7	0	0.621482	-1.223375	-0.797885
9	6	0	1.919131	-1.025975	-0.286737
10	8	0	2.742420	-1.899331	-0.124448
11	1	0	1.623047	2.072941	0.808614
12	6	0	0.308845	0.114385	2.064015
13	1	0	1.018451	-0.715619	2.041015
14	1	0	0.730216	0.925871	2.666587
15	1	0	-0.613375	-0.249013	2.514235
16	8	0	-1.038649	1.612538	0.706441
17	1	0	-1.777635	1.154725	1.124577
18	8	0	0.914410	1.991832	-1.140906
19	1	0	0.323071	2.709561	-0.882589
20	1	0	3.181835	0.507157	0.169608
21	1	0	-2.817873	-0.993420	0.261730
22	8	0	-1.744281	-1.306761	0.804685
23	1	0	-1.513548	-2.239181	0.744904
24	8	0	-3.555885	-0.451692	-0.443160
25	1	0	-2.382560	-0.041272	-1.013331
26	1	0	-4.134228	0.134697	0.048101

wC-IM1 (EUMP2=-0.737080541116 93D+03)

Sum of electronic and zero-point Energies= -736.867521

Sum of electronic and thermal Energies= -736.851558

Sum of electronic and thermal Enthalpies= -736.850614

Sum of electronic and thermal Free Energies= -736.910431

1	7	0	-1.788076	-1.329710	0.363671
2	6	0	-0.573191	-1.777995	-0.250098
3	6	0	0.571510	-0.878261	0.217556
4	6	0	0.097669	0.553130	0.027393
5	7	0	3.892947	0.281633	0.056459
6	1	0	4.486950	0.431871	-0.752665
7	1	0	3.455667	1.172529	0.269397
8	7	0	-1.129064	0.951598	0.072492
9	6	0	-2.167553	0.005177	0.260238
10	8	0	-3.319611	0.363371	0.375235
11	1	0	-0.372019	-2.804822	0.083458
12	6	0	0.898115	-1.101167	1.693929
13	1	0	0.020123	-0.931021	2.321614
14	1	0	1.243844	-2.131100	1.822718
15	1	0	1.697422	-0.421823	2.003180
16	8	0	1.654610	-1.203272	-0.619550
17	1	0	2.454239	-0.696420	-0.340681

18	8	0	-0.690571	-1.723471	-1.656752
19	1	0	0.223393	-1.741714	-1.970963
20	1	0	-2.582774	-1.950447	0.277843
21	1	0	-1.103757	2.894888	-0.071977
22	8	0	1.080916	1.429252	-0.149933
23	1	0	0.657125	2.326143	-0.230269
24	8	0	-0.444972	3.596156	-0.237667
25	1	0	4.506695	0.048367	0.829799
26	1	0	-0.719838	3.977316	-1.074577

wC-TS2 (EUMP2=-0.73706711033337D+03)

Sum of electronic and zero-point Energies= -736.859630

Sum of electronic and thermal Energies= -736.844892

Sum of electronic and thermal Enthalpies= -736.843948

Sum of electronic and thermal Free Energies= -736.900859

1	7	0	-1.803658	-1.271431	0.358149
2	6	0	-0.589947	-1.733211	-0.249986
3	6	0	0.573122	-0.864824	0.230796
4	6	0	0.165841	0.586983	0.021662
5	7	0	3.869648	0.306816	0.043079
6	1	0	4.503552	0.427526	-0.739904

7	1	0	3.349227	1.172889	0.144829
8	7	0	-1.096079	0.972774	0.090938
9	6	0	-2.161419	0.068426	0.257744
10	8	0	-3.307018	0.454147	0.353704
11	1	0	-0.412298	-2.767383	0.073739
12	6	0	0.866373	-1.079785	1.715332
13	1	0	-0.009445	-0.856326	2.329181
14	1	0	1.160131	-2.122707	1.866289
15	1	0	1.694295	-0.434421	2.022534
16	8	0	1.658967	-1.235697	-0.582230
17	1	0	2.459867	-0.721375	-0.320074
18	8	0	-0.693543	-1.660998	-1.657896
19	1	0	0.223374	-1.703206	-1.961741
20	1	0	-2.607415	-1.877608	0.254187
21	1	0	-1.061667	2.348404	-0.073927
22	8	0	1.092620	1.455363	-0.172423
23	1	0	0.473508	2.526958	-0.263042
24	8	0	-0.438418	3.272810	-0.238831
25	1	0	4.444282	0.189753	0.870591
26	1	0	-0.631458	3.609845	-1.119693

wC-PC (EUMP2=-0.73710388242455D+03)

Sum of electronic and zero-point Energies= -736.890975

Sum of electronic and thermal Energies= -736.874626

Sum of electronic and thermal Enthalpies= -736.873682

Sum of electronic and thermal Free Energies= -736.934266

1	7	0	-1.697176	-1.458207	0.296671
2	6	0	-0.441926	-1.787242	-0.317821
3	6	0	0.656085	-0.873293	0.226338
4	6	0	0.210387	0.578835	0.042047
5	7	0	3.859317	0.545486	0.051228
6	1	0	4.518434	0.666402	-0.710573
7	1	0	3.270426	1.372763	0.077000
8	7	0	-1.132125	0.808113	0.184959
9	6	0	-2.154522	-0.153746	0.271876
10	8	0	-3.318091	0.169190	0.366931
11	1	0	-0.193879	-2.823443	-0.053942
12	6	0	0.918780	-1.116077	1.712392
13	1	0	0.027192	-0.927335	2.315117
14	1	0	1.234905	-2.154407	1.847921
15	1	0	1.725174	-0.458608	2.050180
16	8	0	1.779772	-1.168962	-0.563548
17	1	0	2.535808	-0.592125	-0.295103
18	8	0	-0.537407	-1.632956	-1.718977

19	1	0	0.383777	-1.603776	-2.012393
20	1	0	-2.451130	-2.115908	0.146114
21	1	0	-1.437970	1.782464	0.120714
22	8	0	1.009873	1.491071	-0.155384
23	1	0	0.003108	3.201432	-0.259730
24	8	0	-0.854013	3.647609	-0.221904
25	1	0	4.402356	0.524546	0.907596
26	1	0	-1.002213	3.921774	-1.128839

II. Gas Structures of Cis-(5R,6R)-mCg

II.1 At the B3lyp/6-311g(d,p) Level

(5R,6R)-mCg-RC (E=-739.004932980)

Sum of electronic and zero-point Energies=	-738.795809
Sum of electronic and thermal Energies=	-738.779795
Sum of electronic and thermal Enthalpies=	-738.778851
Sum of electronic and thermal Free Energies=	-738.838543

1	7	0	1.439957	1.595755	0.196598
2	6	0	2.092711	0.433047	-0.313481
3	6	0	1.408512	-0.814322	0.266490
4	6	0	-0.111985	-0.619536	0.092838
5	7	0	-0.807068	-1.737230	-0.086170

6	1	0	-1.837400	-1.733262	-0.143242
7	1	0	-0.284740	-2.590023	-0.217305
8	7	0	-0.701016	0.546087	0.169143
9	6	0	0.048812	1.706975	0.305471
10	8	0	-0.462620	2.789322	0.514535
11	1	0	3.146734	0.453925	-0.017130
12	6	0	1.738258	-1.006528	1.748130
13	1	0	1.433676	-0.142538	2.338579
14	1	0	1.223733	-1.891955	2.124514
15	1	0	2.813711	-1.160434	1.858944
16	8	0	1.851043	-1.979102	-0.414324
17	1	0	1.940341	-1.728642	-1.345384
18	8	0	1.997531	0.269932	-1.737520
19	1	0	2.390536	1.032844	-2.172336
20	1	0	1.924994	2.480690	0.204726
21	1	0	-2.448680	0.980933	-0.242823
22	8	0	-3.413089	1.040768	-0.437397
23	1	0	-3.738934	1.722968	0.156765
24	8	0	-3.647835	-1.626206	-0.122172
25	1	0	-3.991746	-1.752163	0.767440
26	1	0	-3.753431	-0.660163	-0.291414

(5R,6R)-mCg-TS1 (E=-738.978794586)

Sum of electronic and zero-point Energies= -738.778239

Sum of electronic and thermal Energies= -738.764149

Sum of electronic and thermal Enthalpies= -738.763205

Sum of electronic and thermal Free Energies= -738.818525

1	7	0	1.467772	1.554670	0.174618
2	6	0	2.053733	0.345573	-0.312307
3	6	0	1.305201	-0.851763	0.293347
4	6	0	-0.207621	-0.620728	0.084082
5	7	0	-0.973760	-1.657762	-0.098733
6	1	0	-2.258441	-1.614201	-0.163825
7	1	0	-0.442913	-2.519791	-0.167643
8	7	0	-0.709382	0.622881	0.152177
9	6	0	0.087730	1.750740	0.252947
10	8	0	-0.375713	2.862942	0.413465
11	1	0	3.107102	0.315808	-0.014661
12	6	0	1.599047	-1.006423	1.787112
13	1	0	1.300373	-0.120314	2.346793
14	1	0	1.056222	-1.870250	2.173784
15	1	0	2.667891	-1.180087	1.928872
16	8	0	1.720452	-2.052279	-0.335860
17	1	0	1.802478	-1.848294	-1.278456

18	8	0	1.947285	0.160889	-1.731583
19	1	0	2.406072	0.876990	-2.181375
20	1	0	1.999411	2.412191	0.159768
21	1	0	-1.978940	0.858806	-0.080854
22	8	0	-3.132040	0.935351	-0.339158
23	1	0	-3.563073	1.498131	0.311060
24	8	0	-3.451246	-1.433867	-0.208640
25	1	0	-3.843261	-1.730821	0.618452
26	1	0	-3.443784	-0.205370	-0.265231

(5R,6R)-mCg-IM1(E=-738.998609379)

Sum of electronic and zero-point Energies= -738.788907

Sum of electronic and thermal Energies= -738.772824

Sum of electronic and thermal Enthalpies= -738.771879

Sum of electronic and thermal Free Energies= -738.830997

1	7	0	0.878052	1.727806	0.152756
2	6	0	1.884276	0.702580	0.141550
3	6	0	1.243488	-0.659003	0.464329
4	6	0	0.029530	-0.866643	-0.455109
5	7	0	-0.400556	-2.008426	-0.829185
6	1	0	0.232300	-2.735516	-0.498803
7	7	0	-0.670216	0.275199	-0.793868

8	6	0	-0.388673	1.561693	-0.362209
9	8	0	-1.202365	2.462738	-0.434171
10	1	0	2.631723	0.943963	0.903372
11	6	0	0.757828	-0.732017	1.916574
12	1	0	-0.134742	-0.125959	2.079488
13	1	0	0.506024	-1.770191	2.138068
14	1	0	1.554850	-0.419512	2.595190
15	8	0	2.189881	-1.694213	0.278124
16	1	0	2.653473	-1.496952	-0.547507
17	8	0	2.514501	0.526282	-1.129184
18	1	0	2.984607	1.331834	-1.365893
19	1	0	1.092821	2.664293	0.456571
20	1	0	-1.613987	0.133442	-1.148423
21	8	0	-2.676721	0.425100	1.574887
22	1	0	-2.648096	1.269819	1.110191
23	1	0	-2.989476	-0.197173	0.900090
24	8	0	-3.077629	-1.241702	-0.821887
25	1	0	-2.295237	-1.829510	-0.911562
26	1	0	-3.765251	-1.595885	-1.391660

(5R,6R)-mCg-TS2(E=-738.947024367)

Sum of electronic and zero-point Energies= -738.740240

Sum of electronic and thermal Energies= -738.726249

Sum of electronic and thermal Enthalpies= -738.725305

Sum of electronic and thermal Free Energies= -738.779186

1	7	0	1.395895	1.428405	0.490887
2	6	0	1.934523	0.168617	0.060318
3	6	0	0.886531	-0.947371	0.282800
4	6	0	-0.432746	-0.457662	-0.353034
5	7	0	-1.034545	-1.255891	-1.222626
6	1	0	-0.849142	-2.239959	-1.084954
7	7	0	-0.686794	0.877193	-0.397481
8	6	0	0.129854	1.867122	0.140417
9	8	0	-0.237779	3.011164	0.277964
10	1	0	2.819743	-0.053270	0.662752
11	6	0	0.747725	-1.268612	1.770144
12	1	0	0.560499	-0.364666	2.349031
13	1	0	-0.093097	-1.941328	1.916940
14	1	0	1.680354	-1.730063	2.103072
15	8	0	1.310015	-2.133175	-0.363440
16	1	0	1.696956	-1.862462	-1.208478
17	8	0	2.258517	0.119146	-1.331120
18	1	0	3.009578	0.693948	-1.507967
19	1	0	2.016817	2.167544	0.783417

20	1	0	-1.667118	1.121921	-0.617577
21	8	0	-2.034848	-0.893869	1.180084
22	1	0	-2.038782	-0.337091	1.966878
23	1	0	-2.835465	-0.342245	0.292898
24	8	0	-3.226902	0.150998	-0.649648
25	1	0	-1.997481	-0.973525	-1.456515
26	1	0	-4.172086	0.306563	-0.609553

(5R,6R)-mCg-IM2(E=-738.981273516)

Sum of electronic and zero-point Energies= -738.769556

Sum of electronic and thermal Energies= -738.754548

Sum of electronic and thermal Enthalpies= -738.753604

Sum of electronic and thermal Free Energies= -738.810085

1	7	0	1.335679	1.545236	0.289665
2	6	0	1.855456	0.281287	-0.143718
3	6	0	0.940224	-0.880004	0.327801
4	6	0	-0.565191	-0.566999	-0.021813
5	7	0	-0.823339	-0.903474	-1.388458
6	1	0	-0.738600	-1.907417	-1.505955
7	7	0	-0.881972	0.818604	0.257176
8	6	0	-0.010982	1.885848	0.245695
9	8	0	-0.383695	3.042243	0.279605

10	1	0	2.835036	0.138584	0.324299
11	6	0	1.138783	-1.115646	1.824199
12	1	0	0.791211	-0.266881	2.417124
13	1	0	0.605400	-2.018622	2.121511
14	1	0	2.198844	-1.271254	2.031381
15	8	0	1.344869	-2.062701	-0.334550
16	1	0	1.570897	-1.785654	-1.234955
17	8	0	2.005160	0.166402	-1.563372
18	1	0	2.831791	0.586083	-1.819197
19	1	0	1.933865	2.355415	0.218760
20	1	0	-1.850834	1.069400	0.082056
21	8	0	-1.458954	-1.367669	0.807051
22	1	0	-1.377212	-1.051672	1.715549
23	1	0	-3.222986	-0.758607	0.109558
24	8	0	-3.612703	-0.070360	-0.453936
25	1	0	-1.762998	-0.615486	-1.645641
26	1	0	-4.534133	0.013308	-0.194525

(5R,6R)-mCg-TS3(E=-738.975003382)

Sum of electronic and zero-point Energies= -738.763623

Sum of electronic and thermal Energies= -738.749226

Sum of electronic and thermal Enthalpies= -738.748281

Sum of electronic and thermal Free Energies= -738.804197

1	7	0	-0.333640	1.939699	-0.135291
2	6	0	-1.203948	1.109162	0.632496
3	6	0	-1.370213	-0.265808	-0.042620
4	6	0	0.055232	-0.904445	-0.391409
5	7	0	1.034591	0.130315	-0.700417
6	6	0	0.925673	1.494416	-0.537472
7	8	0	1.830686	2.267528	-0.772386
8	1	0	-2.185119	1.592707	0.682747
9	6	0	-2.222754	-0.127712	-1.301437
10	1	0	-1.734261	0.496507	-2.051858
11	1	0	-2.409629	-1.114498	-1.720733
12	1	0	-3.179698	0.327954	-1.040134
13	8	0	-2.083225	-1.112039	0.852598
14	1	0	-1.887285	-0.784080	1.742565
15	8	0	-0.747330	0.833963	1.968395
16	1	0	-0.740103	1.652258	2.474770
17	1	0	-0.351165	2.936131	0.027043
18	1	0	2.002732	-0.186063	-0.669410
19	1	0	2.409979	-1.189559	1.161469
20	1	0	0.078279	-1.204804	-2.316709
21	8	0	3.282062	-0.980830	0.780533
22	1	0	3.766808	-1.811213	0.796949

23	8	0	-0.039125	-1.757460	-1.535920
24	7	0	0.521287	-1.767097	0.687331
25	1	0	0.914664	-2.591249	0.240575
26	1	0	-0.289343	-2.087490	1.208251

(5R,6R)-mCg-IM3(E= -738.986315628)

Sum of electronic and zero-point Energies= -738.773883

Sum of electronic and thermal Energies= -738.759229

Sum of electronic and thermal Enthalpies= -738.758284

Sum of electronic and thermal Free Energies= -738.813682

1	7	0	-1.144322	1.681214	-0.165982
2	6	0	-1.741617	0.486427	0.332315
3	6	0	-1.084038	-0.752101	-0.308428
4	6	0	0.485726	-0.675406	-0.106837
5	7	0	0.954773	0.671194	-0.374475
6	6	0	0.235170	1.843583	-0.303694
7	8	0	0.737620	2.943571	-0.403546
8	1	0	-2.807245	0.492215	0.084385
9	6	0	-1.460155	-0.846286	-1.785532
10	1	0	-1.022938	-0.035390	-2.370483
11	1	0	-1.122475	-1.806196	-2.176416
12	1	0	-2.545854	-0.805731	-1.893206

13	8	0	-1.591437	-1.920424	0.314939
14	1	0	-1.727377	-1.700786	1.245569
15	8	0	-1.604185	0.309764	1.762809
16	1	0	-2.116406	0.988343	2.214003
17	1	0	-1.632685	2.558587	-0.065521
18	1	0	1.964044	0.777740	-0.259931
19	1	0	2.872760	-0.658925	0.989017
20	1	0	1.087688	-1.216440	-1.867701
21	8	0	3.606789	-0.265090	0.478894
22	1	0	3.725621	-0.901272	-0.234455
23	8	0	1.144200	-1.579699	-0.977702
24	7	0	0.935872	-1.105279	1.213552
25	1	0	0.704260	-2.088199	1.326783
26	1	0	0.441938	-0.576133	1.926196

(5R,6R)-mCg-TS4(E= -738.984351110)

Sum of electronic and zero-point Energies= -738.772700

Sum of electronic and thermal Energies= -738.758461

Sum of electronic and thermal Enthalpies= -738.757517

Sum of electronic and thermal Free Energies= -738.812256

1	7	0	-1.124266	1.693758	-0.142946
2	6	0	-1.726932	0.504546	0.364400

3	6	0	-1.105490	-0.737784	-0.302417
4	6	0	0.467349	-0.686394	-0.140030
5	7	0	0.957239	0.655434	-0.385947
6	6	0	0.250766	1.837446	-0.310605
7	8	0	0.770525	2.928802	-0.419482
8	1	0	-2.797973	0.528107	0.143536
9	6	0	-1.514066	-0.812635	-1.770347
10	1	0	-1.085441	0.005212	-2.350013
11	1	0	-1.165872	-1.756990	-2.183252
12	1	0	-2.602934	-0.772745	-1.849401
13	8	0	-1.613458	-1.903609	0.328770
14	1	0	-1.723433	-1.686866	1.263408
15	8	0	-1.554996	0.320782	1.790434
16	1	0	-2.048880	1.002659	2.256741
17	1	0	-1.602034	2.576646	-0.041622
18	1	0	1.964954	0.760185	-0.264864
19	1	0	2.830968	-0.741146	0.941002
20	1	0	1.668779	-1.094896	-1.600916
21	8	0	3.566661	-0.279272	0.486682
22	1	0	4.087362	-0.977061	0.078514
23	8	0	1.033351	-1.589717	-1.075203
24	7	0	0.945639	-1.140678	1.171355

25	1	0	0.709311	-2.124348	1.266941
26	1	0	0.468489	-0.625314	1.907078

(5R,6R)-mCg-IM4(E= -738.991566391)

Sum of electronic and zero-point Energies= -738.778712

Sum of electronic and thermal Energies= -738.764324

Sum of electronic and thermal Enthalpies= -738.763380

Sum of electronic and thermal Free Energies= -738.818253

1	7	0	1.590539	1.339217	0.141259
2	6	0	1.825250	0.001089	-0.285081
3	6	0	0.816645	-0.968777	0.364578
4	6	0	-0.651520	-0.459068	0.094496
5	7	0	-0.707945	0.993637	0.214143
6	6	0	0.317666	1.901197	0.221528
7	8	0	0.154666	3.102688	0.314053
8	1	0	2.835788	-0.293831	0.012487
9	6	0	1.092980	-1.104453	1.859120
10	1	0	0.896121	-0.173747	2.390566
11	1	0	0.447440	-1.879378	2.266543
12	1	0	2.135466	-1.394236	2.010939
13	8	0	0.990828	-2.255885	-0.213390
14	1	0	1.251107	-2.110569	-1.132218

15	8	0	1.695255	-0.190412	-1.717613
16	1	0	2.402209	0.290691	-2.159258
17	1	0	2.326715	2.025231	0.075840
18	1	0	-1.635636	1.399621	0.220628
19	1	0	-2.960276	-0.152445	-0.988444
20	1	0	-2.387760	-0.773746	0.851543
21	8	0	-3.555975	0.218793	-0.300983
22	1	0	-4.460775	0.044388	-0.572903
23	8	0	-1.478764	-1.071343	1.039397
24	7	0	-1.170386	-0.817812	-1.240107
25	1	0	-1.114286	-1.829586	-1.326384
26	1	0	-0.575774	-0.408338	-1.955955

(5R,6R)-mCg-TS5(E= -738.961418554)

Sum of electronic and zero-point Energies= -738.754325

Sum of electronic and thermal Energies= -738.741065

Sum of electronic and thermal Enthalpies= -738.740121

Sum of electronic and thermal Free Energies= -738.793051

1	7	0	1.926010	0.838308	0.062706
2	6	0	1.720613	-0.525272	-0.278908
3	6	0	0.474598	-1.099064	0.427025
4	6	0	-0.764722	-0.162508	0.191431

5	7	0	-0.359951	1.243230	0.144496
6	6	0	0.900567	1.780139	0.146786
7	8	0	1.133930	2.969317	0.230137
8	1	0	2.599081	-1.102953	0.023687
9	6	0	0.715374	-1.261361	1.923089
10	1	0	0.906810	-0.301981	2.404517
11	1	0	-0.175628	-1.698890	2.368728
12	1	0	1.567259	-1.925561	2.084808
13	8	0	0.201742	-2.392453	-0.112930
14	1	0	0.610262	-2.416999	-0.988185
15	8	0	1.497377	-0.746063	-1.700829
16	1	0	2.294375	-0.496950	-2.180044
17	1	0	2.846697	1.244481	0.003838
18	1	0	-1.114295	1.905330	0.276785
19	1	0	-2.352577	0.103693	-1.146063
20	1	0	-2.668902	0.175815	0.560218
21	8	0	-3.297514	0.783177	-0.348340
22	1	0	-4.231010	0.563111	-0.395381
23	8	0	-1.761297	-0.385186	1.050395
24	7	0	-1.355432	-0.458116	-1.231221
25	1	0	-1.509000	-1.464194	-1.276465
26	1	0	-0.719947	-0.170795	-1.972308

(5R,6R)-mCg-PC(E= -739.017492602)

Sum of electronic and zero-point Energies= -738.807681

Sum of electronic and thermal Energies= -738.791464

Sum of electronic and thermal Enthalpies= -738.790520

Sum of electronic and thermal Free Energies= -738.852215

1	7	0	-2.069506	0.665552	0.332245
2	6	0	-1.602653	-0.678041	0.559732
3	6	0	-0.564120	-1.104947	-0.519622
4	6	0	0.389482	0.051204	-0.873125
5	7	0	0.025207	1.308137	-0.467575
6	6	0	-1.196804	1.704019	0.107179
7	8	0	-1.440690	2.869049	0.316435
8	1	0	-2.468169	-1.346094	0.479420
9	6	0	-1.264078	-1.573149	-1.797280
10	1	0	-1.950886	-0.814325	-2.179754
11	1	0	-0.515075	-1.801106	-2.555678
12	1	0	-1.825810	-2.483469	-1.577045
13	8	0	0.188142	-2.185660	-0.004128
14	1	0	0.994312	-1.833232	0.456927
15	8	0	-1.048091	-0.764062	1.861887
16	1	0	-0.585512	-1.614302	1.878416

17	1	0	-2.881911	0.956938	0.858162
18	1	0	0.699834	2.052804	-0.606057
19	1	0	2.693493	-0.241544	1.084398
20	1	0	2.790154	0.936690	-0.857474
21	8	0	3.119811	1.484434	-0.122346
22	1	0	3.986844	1.802389	-0.388793
23	8	0	1.430366	-0.151871	-1.477350
24	7	0	2.272269	-1.058521	1.532124
25	1	0	3.026726	-1.697841	1.764587
26	1	0	1.872956	-0.732712	2.408044

II.2 At the Mp2/6-311g(d,p) Level

(5R,6R)-mCg-RC （EUMP2 = -0.73708682026122D+03）

Sum of electronic and zero-point Energies= -736.874244

Sum of electronic and thermal Energies= -736.858226

Sum of electronic and thermal Enthalpies= -736.857282

Sum of electronic and thermal Free Energies= -736.917154

1	7	0	1.424502	1.591787	0.240551
2	6	0	2.049472	0.459212	-0.360482
3	6	0	1.431841	-0.795900	0.242832
4	6	0	-0.084330	-0.636436	0.112940
5	7	0	-0.755725	-1.772034	-0.055840

6	1	0	-1.784479	-1.782505	-0.092985
7	1	0	-0.212365	-2.608334	-0.204691
8	7	0	-0.708583	0.510804	0.216658
9	6	0	0.028216	1.687959	0.337665
10	8	0	-0.503933	2.764754	0.533831
11	1	0	3.125340	0.485877	-0.148013
12	6	0	1.803191	-0.964313	1.709743
13	1	0	1.457501	-0.114459	2.300390
14	1	0	1.345603	-1.881091	2.090275
15	1	0	2.890024	-1.053711	1.794782
16	8	0	1.891668	-1.947603	-0.442296
17	1	0	1.908478	-1.687945	-1.373423
18	8	0	1.829798	0.325675	-1.766298
19	1	0	2.237081	1.080117	-2.200240
20	1	0	1.877953	2.492309	0.167474
21	1	0	-2.444888	0.937628	-0.246115
22	8	0	-3.394797	1.013072	-0.469405
23	1	0	-3.687107	1.740245	0.082454
24	8	0	-3.586488	-1.652486	-0.075739
25	1	0	-3.984162	-1.751383	0.790903
26	1	0	-3.710658	-0.701076	-0.267331

(5R,6R)-mCg-TS1 (EUMP2=-0.73705984800602D+03)

Sum of electronic and zero-point Energies= -736.855008

Sum of electronic and thermal Energies= -736.841082

Sum of electronic and thermal Enthalpies= -736.840138

Sum of electronic and thermal Free Energies= -736.895285

1	7	0	1.458878	1.548095	0.234186
2	6	0	2.020254	0.369896	-0.342453
3	6	0	1.326782	-0.839567	0.271247
4	6	0	-0.180672	-0.638735	0.086877
5	7	0	-0.933142	-1.688312	-0.110579
6	1	0	-2.276971	-1.638165	-0.135171
7	1	0	-0.363389	-2.526475	-0.189362
8	7	0	-0.713791	0.591656	0.193277
9	6	0	0.068362	1.728119	0.284547
10	8	0	-0.410548	2.841190	0.425185
11	1	0	3.093729	0.336678	-0.118447
12	6	0	1.642667	-0.981156	1.753815
13	1	0	1.285243	-0.116552	2.315078
14	1	0	1.158007	-1.885591	2.131046
15	1	0	2.724074	-1.082025	1.885386
16	8	0	1.768622	-2.025372	-0.363638

17	1	0	1.789078	-1.805161	-1.304447
18	8	0	1.808024	0.228228	-1.749119
19	1	0	2.275116	0.943968	-2.188279
20	1	0	1.958833	2.420745	0.131406
21	1	0	-2.035218	0.838988	-0.114394
22	8	0	-3.118994	0.898879	-0.385217
23	1	0	-3.529011	1.506450	0.235615
24	8	0	-3.405799	-1.445250	-0.136247
25	1	0	-3.746121	-1.718385	0.719412
26	1	0	-3.411774	-0.247296	-0.237952

(5R,6R)-mCg-IM1(EUMP2=-0.73708605614901D+03)

Sum of electronic and zero-point Energies= -736.873225

Sum of electronic and thermal Energies= -736.857158

Sum of electronic and thermal Enthalpies= -736.856214

Sum of electronic and thermal Free Energies= -736.915241

1	7	0	0.831500	1.715568	0.200343
2	6	0	1.853945	0.716181	0.127292
3	6	0	1.243173	-0.640578	0.466406
4	6	0	0.051408	-0.871187	-0.455744
5	7	0	-0.355359	-2.029450	-0.835156
6	1	0	0.303100	-2.719742	-0.470519

7	7	0	-0.658107	0.258154	-0.817209
8	6	0	-0.415159	1.546229	-0.365256
9	8	0	-1.237207	2.439886	-0.462845
10	1	0	2.630693	0.958342	0.861840
11	6	0	0.749714	-0.695776	1.908206
12	1	0	-0.152404	-0.096379	2.048553
13	1	0	0.513530	-1.737634	2.140613
14	1	0	1.541541	-0.357962	2.583551
15	8	0	2.206305	-1.661664	0.303583
16	1	0	2.636334	-1.468467	-0.539497
17	8	0	2.421761	0.551258	-1.167699
18	1	0	2.882178	1.364592	-1.391820
19	1	0	1.053230	2.666762	0.452146
20	1	0	-1.593540	0.101944	-1.184814
21	8	0	-2.593622	0.429630	1.575984
22	1	0	-2.601991	1.257487	1.088123
23	1	0	-2.897085	-0.200708	0.911021
24	8	0	-3.039454	-1.275960	-0.783880
25	1	0	-2.260696	-1.855878	-0.878188
26	1	0	-3.741869	-1.716679	-1.263421

(5R,6R)-mCg-TS2 (EUMP2 =-0.73702541721187D+03)

Sum of electronic and zero-point Energies= -736.815744

Sum of electronic and thermal Energies= -736.801982

Sum of electronic and thermal Enthalpies= -736.801038

Sum of electronic and thermal Free Energies= -736.854540

1	7	0	1.384404	1.412102	0.498491
2	6	0	1.903459	0.168825	0.009827
3	6	0	0.880014	-0.938703	0.290740
4	6	0	-0.438335	-0.467955	-0.332455
5	7	0	-1.022497	-1.267723	-1.214710
6	1	0	-0.846463	-2.249821	-1.047235
7	7	0	-0.691254	0.865083	-0.398674
8	6	0	0.119956	1.859608	0.141604
9	8	0	-0.248629	3.006510	0.273771
10	1	0	2.826057	-0.060848	0.554355
11	6	0	0.778696	-1.204078	1.783970
12	1	0	0.505724	-0.296199	2.321742
13	1	0	0.013993	-1.957407	1.962224
14	1	0	1.756579	-1.555726	2.127334
15	8	0	1.300258	-2.140653	-0.319961
16	1	0	1.633836	-1.877369	-1.188229
17	8	0	2.127063	0.131382	-1.395113
18	1	0	2.872549	0.704948	-1.592667
19	1	0	2.023707	2.160331	0.725824

20	1	0	-1.681805	1.090200	-0.609923
21	8	0	-1.951302	-0.891177	1.175539
22	1	0	-1.920872	-0.274580	1.914494
23	1	0	-2.725317	-0.376917	0.339347
24	8	0	-3.167055	0.123657	-0.621389
25	1	0	-1.988148	-0.977276	-1.436801
26	1	0	-4.109831	0.260487	-0.531107

(5R,6R)-mCg-IM2 (EUMP2=-0.737074764101 94D+03)

Sum of electronic and zero-point Energies= -736.859257

Sum of electronic and thermal Energies= -736.844496

Sum of electronic and thermal Enthalpies= -736.843552

Sum of electronic and thermal Free Energies= -736.899599

1	7	0	1.370254	1.503644	0.341260
2	6	0	1.838355	0.249605	-0.170912
3	6	0	0.925931	-0.888739	0.314443
4	6	0	-0.560606	-0.566436	-0.012530
5	7	0	-0.823229	-0.864306	-1.388742
6	1	0	-0.791139	-1.873002	-1.503511
7	7	0	-0.857102	0.810138	0.302332
8	6	0	0.027743	1.870638	0.259017
9	8	0	-0.331687	3.033009	0.261085

10	1	0	2.835827	0.062578	0.245923
11	6	0	1.132998	-1.103606	1.806466
12	1	0	0.742927	-0.261600	2.384475
13	1	0	0.638010	-2.030079	2.104335
14	1	0	2.200822	-1.206656	2.014597
15	8	0	1.309887	-2.080616	-0.338808
16	1	0	1.492709	-1.799543	-1.246178
17	8	0	1.906402	0.181373	-1.591611
18	1	0	2.737267	0.588321	-1.850920
19	1	0	1.971926	2.304741	0.200353
20	1	0	-1.817812	1.078595	0.106514
21	8	0	-1.444676	-1.375548	0.793789
22	1	0	-1.343622	-1.057534	1.698676
23	1	0	-3.205587	-0.722779	0.107095
24	8	0	-3.591241	-0.018793	-0.430827
25	1	0	-1.760317	-0.546245	-1.620703
26	1	0	-4.506459	0.032692	-0.152537

(5R,6R)-mCg-TS3 （EUMP2=-0.73706812008358D+03）

Sum of electronic and zero-point Energies= -736.853199

Sum of electronic and thermal Energies= -736.838913

Sum of electronic and thermal Enthalpies= -736.837969

Sum of electronic and thermal Free Energies= -736.893450

1	7	0	-0.236541	1.931004	-0.110589
2	6	0	-1.173345	1.135385	0.609826
3	6	0	-1.372568	-0.204042	-0.098705
4	6	0	0.004436	-0.917051	-0.318192
5	7	0	0.979209	0.049133	-0.797350
6	6	0	0.989494	1.409643	-0.530062
7	8	0	1.952953	2.120528	-0.734520
8	1	0	-2.136718	1.660947	0.625281
9	6	0	-2.066893	0.012940	-1.434845
10	1	0	-1.410564	0.518721	-2.146633
11	1	0	-2.371585	-0.956448	-1.831862
12	1	0	-2.961205	0.622722	-1.283003
13	8	0	-2.229458	-1.008477	0.695223
14	1	0	-2.089551	-0.701261	1.600148
15	8	0	-0.791350	0.812314	1.950950
16	1	0	-0.828963	1.622820	2.466490
17	1	0	-0.157275	2.907293	0.140809
18	1	0	1.930250	-0.318057	-0.804180
19	1	0	2.418870	-1.058191	1.140074
20	1	0	-0.026984	-1.471658	-2.157136
21	8	0	3.263070	-0.992613	0.669981

22	1	0	3.700029	-1.818243	0.883684
23	8	0	-0.103549	-1.925756	-1.311384
24	7	0	0.464377	-1.603384	0.881251
25	1	0	0.804462	-2.507164	0.559042
26	1	0	-0.340158	-1.807973	1.463974

(5R,6R)-mCg-IM3 （EUMP2=-0.73708116317191D+03）

Sum of electronic and zero-point Energies= -736.864779

Sum of electronic and thermal Energies= -736.850475

Sum of electronic and thermal Enthalpies= -736.849531

Sum of electronic and thermal Free Energies= -736.904034

1	7	0	-1.240073	1.612133	-0.228490
2	6	0	-1.748159	0.403756	0.330361
3	6	0	-1.035007	-0.794938	-0.297525
4	6	0	0.507381	-0.649998	-0.091879
5	7	0	0.908268	0.705703	-0.383833
6	6	0	0.137506	1.847915	-0.302124
7	8	0	0.595262	2.971876	-0.364893
8	1	0	-2.818595	0.329213	0.105405
9	6	0	-1.390619	-0.894254	-1.773367
10	1	0	-0.933752	-0.086614	-2.350053
11	1	0	-1.054345	-1.863048	-2.147975

12	1	0	-2.475918	-0.840923	-1.893352
13	8	0	-1.497153	-1.984091	0.315198
14	1	0	-1.622101	-1.758472	1.244547
15	8	0	-1.559624	0.279669	1.750939
16	1	0	-2.143530	0.912842	2.178446
17	1	0	-1.755955	2.465689	-0.061597
18	1	0	1.908047	0.862315	-0.251803
19	1	0	2.880496	-0.536132	0.973062
20	1	0	1.115648	-1.172055	-1.831372
21	8	0	3.594230	-0.158818	0.432119
22	1	0	3.636074	-0.808042	-0.274105
23	8	0	1.206524	-1.534531	-0.944456
24	7	0	0.975299	-1.036533	1.230330
25	1	0	0.771905	-2.025626	1.353721
26	1	0	0.447033	-0.515992	1.924973

(5R,6R)-mCg-TS4 （EUMP2=-0.73707844639520D+03）

Sum of electronic and zero-point Energies= -736.862976

Sum of electronic and thermal Energies= -736.849008

Sum of electronic and thermal Enthalpies= -736.848064

Sum of electronic and thermal Free Energies= -736.902191

1	7	0	-1.241243	1.612423	-0.205160

2	6	0	-1.744332	0.400275	0.351167
3	6	0	-1.042640	-0.792090	-0.299386
4	6	0	0.500042	-0.652905	-0.114886
5	7	0	0.905463	0.705617	-0.380688
6	6	0	0.131344	1.847348	-0.302309
7	8	0	0.593251	2.969496	-0.373423
8	1	0	-2.817587	0.330372	0.139748
9	6	0	-1.413883	-0.872053	-1.771282
10	1	0	-0.956137	-0.060183	-2.339025
11	1	0	-1.066014	-1.827349	-2.163577
12	1	0	-2.501485	-0.816227	-1.874863
13	8	0	-1.495619	-1.987592	0.310908
14	1	0	-1.611341	-1.769146	1.243130
15	8	0	-1.536953	0.267698	1.768549
16	1	0	-2.116207	0.897582	2.206945
17	1	0	-1.758505	2.465519	-0.042195
18	1	0	1.901649	0.873772	-0.243602
19	1	0	2.836932	-0.597218	0.917242
20	1	0	1.733428	-0.999251	-1.535787
21	8	0	3.552624	-0.146572	0.431869
22	1	0	4.045535	-0.872114	0.045437
23	8	0	1.124346	-1.538515	-1.024392

24	7	0	0.988492	-1.052297	1.204078
25	1	0	0.785266	-2.043027	1.314744
26	1	0	0.471093	-0.542497	1.916289

(5R,6R)-mCg-IM4 （EUMP2=-0.73708524915700D+03）

Sum of electronic and zero-point Energies= -736.868512

Sum of electronic and thermal Energies= -736.854441

Sum of electronic and thermal Enthalpies= -736.853497

Sum of electronic and thermal Free Energies= -736.907610

1	7	0	1.608012	1.304500	0.208010
2	6	0	1.803818	-0.010075	-0.300151
3	6	0	0.805622	-0.974594	0.342743
4	6	0	-0.645443	-0.469224	0.088825
5	7	0	-0.692797	0.973239	0.221625
6	6	0	0.335358	1.881203	0.234154
7	8	0	0.172806	3.086027	0.302218
8	1	0	2.816296	-0.343472	-0.044409
9	6	0	1.085955	-1.102854	1.831162
10	1	0	0.819090	-0.188367	2.362266
11	1	0	0.493222	-1.927878	2.225407
12	1	0	2.148317	-1.317529	1.980996
13	8	0	0.981060	-2.258684	-0.233624

14	1	0	1.205171	-2.090628	-1.156718
15	8	0	1.618106	-0.131893	-1.724076
16	1	0	2.352601	0.320626	-2.148540
17	1	0	2.334728	1.991459	0.063358
18	1	0	-1.617721	1.387572	0.204621
19	1	0	-2.936595	-0.116272	-0.954796
20	1	0	-2.357885	-0.768817	0.855753
21	8	0	-3.514262	0.266105	-0.265818
22	1	0	-4.412239	0.122559	-0.567210
23	8	0	-1.459810	-1.092629	1.036038
24	7	0	-1.178485	-0.812029	-1.236901
25	1	0	-1.122903	-1.824785	-1.322954
26	1	0	-0.574245	-0.402580	-1.945209

(5R,6R)-mCg-TS5 （EUMP2=-0.73705080032699D+03）

Sum of electronic and zero-point Energies= -736.839904

Sum of electronic and thermal Energies= -736.826972

Sum of electronic and thermal Enthalpies= -736.826028

Sum of electronic and thermal Free Energies= -736.878031

1	7	0	1.920671	0.817334	0.126572
2	6	0	1.699207	-0.518700	-0.295447
3	6	0	0.472512	-1.103498	0.406423

4	6	0	-0.763176	-0.190467	0.182477
5	7	0	-0.366314	1.210993	0.148716
6	6	0	0.889890	1.761256	0.165270
7	8	0	1.113537	2.955344	0.233352
8	1	0	2.575397	-1.124404	-0.035407
9	6	0	0.717489	-1.254674	1.896335
10	1	0	0.816490	-0.280724	2.378422
11	1	0	-0.137879	-1.774967	2.327040
12	1	0	1.626926	-1.841231	2.056573
13	8	0	0.215436	-2.398269	-0.127797
14	1	0	0.595071	-2.386177	-1.014680
15	8	0	1.440830	-0.662271	-1.712249
16	1	0	2.251067	-0.429613	-2.175388
17	1	0	2.830344	1.233888	-0.009440
18	1	0	-1.128494	1.869097	0.266983
19	1	0	-2.316968	0.121913	-1.136139
20	1	0	-2.640137	0.187483	0.540342
21	8	0	-3.219818	0.829288	-0.324639
22	1	0	-4.163323	0.657992	-0.329099
23	8	0	-1.755349	-0.434953	1.040920
24	7	0	-1.345377	-0.464713	-1.224997
25	1	0	-1.527531	-1.466942	-1.268656

26	1	0	-0.696427	-0.188226	-1.959630

(5R,6R)-mCg-PC (EUMP2=-0.73710004517192D+03)

Sum of electronic and zero-point Energies= -736.886467

Sum of electronic and thermal Energies= -736.870528

Sum of electronic and thermal Enthalpies= -736.869583

Sum of electronic and thermal Free Energies= -736.928831

1	7	0	-1.827036	1.147587	0.095306
2	6	0	-1.733803	-0.231633	0.488703
3	6	0	-0.806387	-1.005074	-0.468743
4	6	0	0.441199	-0.190761	-0.814900
5	7	0	0.438310	1.132365	-0.447124
6	6	0	-0.662667	1.888225	-0.012559
7	8	0	-0.579601	3.082120	0.171637
8	1	0	-2.738282	-0.668180	0.416517
9	6	0	-1.531048	-1.356558	-1.760486
10	1	0	-1.940102	-0.460027	-2.234953
11	1	0	-0.829810	-1.848369	-2.437350
12	1	0	-2.345889	-2.048193	-1.528227
13	8	0	-0.412849	-2.208259	0.162624
14	1	0	0.420881	-2.007577	0.650219
15	8	0	-1.266656	-0.307213	1.823559

16	1	0	-1.057305	-1.243871	1.935994
17	1	0	-2.548533	1.680542	0.565441
18	1	0	1.311908	1.642185	-0.549665
19	1	0	2.398065	-0.675130	1.207139
20	1	0	2.963515	0.194291	-0.865495
21	8	0	3.340084	0.804763	-0.214067
22	1	0	4.236557	0.961538	-0.513783
23	8	0	1.397126	-0.710610	-1.375927
24	7	0	1.739996	-1.260795	1.719822
25	1	0	2.299467	-1.927116	2.243513
26	1	0	1.302052	-0.645791	2.399916

III. Gas Structures of Cis-(5S,6S)-mCg

III.1 At the B3lyp/6-311g(d,p) Level

Cg-RC (E=-699.670459881)

Sum of electronic and zero-point Energies= -699.488786

Sum of electronic and thermal Energies= -699.474303

Sum of electronic and thermal Enthalpies= -699.473359

Sum of electronic and thermal Free Energies= -699.530026

1	7	0	1.672102	1.435709	-0.362292
2	6	0	2.261278	0.202769	0.053611
3	6	0	1.444448	-0.924785	-0.583793

4	6	0	-0.034109	-0.683561	-0.306015
5	7	0	-0.792476	-1.769025	-0.181179
6	1	0	-1.813361	-1.696976	-0.043370
7	1	0	-0.330767	-2.663111	-0.135619
8	7	0	-0.535877	0.518418	-0.253032
9	6	0	0.288378	1.640377	-0.334332
10	8	0	-0.170154	2.762803	-0.394702
11	1	0	3.293393	0.165935	-0.322244
12	8	0	1.823295	-2.196706	-0.056479
13	1	0	2.574301	-2.528886	-0.558184
14	8	0	2.258091	0.078817	1.467232
15	1	0	2.366721	-0.860286	1.668437
16	1	0	2.198339	2.283375	-0.204986
17	1	0	-2.211702	1.038024	0.344796
18	8	0	-3.149189	1.132328	0.631237
19	1	0	-3.471108	1.909570	0.165828
20	8	0	-3.602005	-1.461833	0.077559
21	1	0	-4.011416	-1.468979	-0.793023
22	1	0	-3.623876	-0.513563	0.349614
23	1	0	1.582952	-0.892894	-1.671323

Cg-TS1(E=-699.644921355)

Sum of electronic and zero-point Energies= -699.471483

Sum of electronic and thermal Energies= -699.458977

Sum of electronic and thermal Enthalpies= -699.458033

Sum of electronic and thermal Free Energies= -699.510237

1	7	0	1.692918	1.381835	-0.350428
2	6	0	2.210025	0.105425	0.030122
3	6	0	1.316977	-0.958491	-0.613798
4	6	0	-0.146768	-0.676452	-0.286035
5	7	0	-0.973331	-1.673628	-0.140236
6	1	0	-2.257872	-1.535949	0.022828
7	1	0	-0.509835	-2.573993	-0.176432
8	7	0	-0.548042	0.597809	-0.213468
9	6	0	0.329303	1.672873	-0.276285
10	8	0	-0.067881	2.820920	-0.289414
11	1	0	3.231223	0.015136	-0.366160
12	8	0	1.654225	-2.260164	-0.137922
13	1	0	2.372057	-2.609056	-0.675226
14	8	0	2.224586	-0.048083	1.440622
15	1	0	2.269299	-0.997144	1.618894
16	1	0	2.272956	2.192009	-0.185766
17	1	0	-1.792559	0.912780	0.156499

18	8	0	-2.894512	1.041828	0.508548
19	1	0	-3.319243	1.711764	-0.035733
20	8	0	-3.413069	-1.268903	0.162220
21	1	0	-3.874067	-1.448559	-0.663177
22	1	0	-3.303540	-0.057803	0.340185
23	1	0	1.426762	-0.896204	-1.703440

Cg-IM1(E=-699.664740746)

Sum of electronic and zero-point Energies= -699.483203

Sum of electronic and thermal Energies= -699.468201

Sum of electronic and thermal Enthalpies= -699.467257

Sum of electronic and thermal Free Energies= -699.525177

1	7	0	-1.444319	1.339711	0.530934
2	6	0	-1.987090	0.017048	0.425826
3	6	0	-0.835398	-0.990592	0.512885
4	6	0	0.259102	-0.648132	-0.480539
5	7	0	0.985702	-1.501037	-1.088670
6	1	0	2.729534	-0.278426	1.114717
7	1	0	0.671165	-2.441822	-0.860300
8	7	0	0.493407	0.702430	-0.614857
9	6	0	-0.290062	1.739880	-0.116135
10	8	0	0.040578	2.900239	-0.227650

11	1	0	-2.668135	-0.136249	1.273355
12	8	0	-1.313883	-2.302549	0.233680
13	1	0	-1.482206	-2.752350	1.066423
14	8	0	-2.687169	-0.141713	-0.797026
15	1	0	-2.789029	-1.093648	-0.933410
16	1	0	-2.079593	2.102200	0.713862
17	1	0	1.369873	0.983121	-1.041155
18	8	0	2.195534	-0.283289	1.928529
19	1	0	2.198572	0.638921	2.202495
20	1	0	2.702651	-0.797611	-1.074332
21	8	0	3.316260	-0.114150	-0.721343
22	1	0	4.171968	-0.260740	-1.132776
23	1	0	-0.358196	-0.928646	1.497532

Cg-TS2(E=-699.617288667)

Sum of electronic and zero-point Energies= -699.438790

Sum of electronic and thermal Energies= -699.425892

Sum of electronic and thermal Enthalpies= -699.424948

Sum of electronic and thermal Free Energies= -699.477135

1	7	0	-1.516341	1.266295	0.549485
2	6	0	-1.959473	-0.081589	0.338676
3	6	0	-0.763060	-1.018773	0.545642

4	6	0	0.424584	-0.529112	-0.258252
5	7	0	1.102663	-1.377193	-1.011329
6	1	0	2.716544	-0.183924	0.497143
7	1	0	0.996187	-2.348509	-0.756665
8	7	0	0.537386	0.802268	-0.477421
9	6	0	-0.347764	1.770649	0.007757
10	8	0	-0.091470	2.950200	-0.045235
11	1	0	-2.721096	-0.310052	1.094833
12	8	0	-1.104937	-2.338247	0.134286
13	1	0	-1.198426	-2.888302	0.916970
14	8	0	-2.496722	-0.231826	-0.963033
15	1	0	-2.562483	-1.181517	-1.131710
16	1	0	-2.217339	1.976076	0.704016
17	1	0	1.484925	1.110511	-0.742500
18	8	0	1.928591	-0.622849	1.419150
19	1	0	1.864029	0.098402	2.056315
20	1	0	2.049059	-1.039041	-1.258099
21	8	0	3.134570	0.201700	-0.510838
22	1	0	4.071061	0.401927	-0.466906
23	1	0	-0.434393	-0.994045	1.583873

Cg-IM2(E=-699.667348222)

Sum of electronic and zero-point Energies= -699.481605

Sum of electronic and thermal Energies= -699.468591

Sum of electronic and thermal Enthalpies= -699.467647

Sum of electronic and thermal Free Energies= -699.519910

1	7	0	1.497281	1.418547	-0.239547
2	6	0	1.940659	0.058626	-0.079457
3	6	0	0.926644	-0.901853	-0.728799
4	6	0	-0.496609	-0.580541	-0.215734
5	7	0	-0.595869	-0.957577	1.181394
6	1	0	-3.181702	-0.663972	-0.067675
7	1	0	-0.543964	-1.971098	1.243975
8	7	0	-0.761144	0.827254	-0.415591
9	6	0	0.176554	1.834404	-0.223681
10	8	0	-0.138762	3.001574	-0.110748
11	1	0	2.906719	-0.055703	-0.574348
12	8	0	1.282877	-2.237285	-0.447766
13	1	0	1.807811	-2.202521	0.365673
14	8	0	2.175693	-0.331780	1.269025
15	1	0	1.297429	-0.361450	1.696645
16	1	0	2.143600	2.153054	0.008762
17	1	0	-1.708222	1.111639	-0.182004
18	8	0	-1.487906	-1.324164	-0.946255
19	1	0	-1.412423	-1.078311	-1.877043

20	1	0	-1.498217	-0.658506	1.546147
21	8	0	-3.412685	0.004365	0.595940
22	1	0	-4.368198	0.104194	0.574192
23	1	0	0.938073	-0.760395	-1.813643

Cg-TS3(E=-699.647238189)

Sum of electronic and zero-point Energies= -699.464214

Sum of electronic and thermal Energies= -699.450682

Sum of electronic and thermal Enthalpies= -699.449737

Sum of electronic and thermal Free Energies= -699.503779

1	7	0	1.261726	1.585596	-0.280194
2	6	0	1.922962	0.325674	-0.242778
3	6	0	0.990189	-0.789886	-0.736750
4	6	0	-0.400026	-0.716485	-0.045227
5	7	0	-0.403122	-1.168923	1.333878
6	1	0	-3.196988	-0.938926	0.099284
7	1	0	0.539045	-1.292615	1.680933
8	7	0	-0.885907	0.652031	-0.194962
9	6	0	-0.113954	1.791510	-0.162454
10	8	0	-0.574617	2.911703	-0.076964
11	1	0	2.809971	0.343357	-0.879481
12	8	0	1.605719	-2.044514	-0.584063

13	1	0	2.089676	-2.018380	0.251551
14	8	0	2.421818	-0.023231	1.072471
15	1	0	1.935907	0.510344	1.712291
16	1	0	1.803442	2.436271	-0.270638
17	1	0	-1.845774	0.789275	0.121157
18	8	0	-1.334639	-1.570734	-0.704785
19	1	0	-1.430878	-1.245909	-1.607818
20	1	0	-0.880368	-2.060399	1.393670
21	8	0	-3.686924	-0.155478	0.386773
22	1	0	-4.303858	0.028604	-0.328385
23	1	0	0.825069	-0.639407	-1.807818

Cg-IM3 (E=-699.658816042)

Sum of electronic and zero-point Energies= -699.473976

Sum of electronic and thermal Energies= -699.460581

Sum of electronic and thermal Enthalpies= -699.459637

Sum of electronic and thermal Free Energies= -699.512872

1	7	0	1.489723	1.414061	-0.318067
2	6	0	1.925357	0.083893	-0.045911
3	6	0	0.958392	-0.916155	-0.681811
4	6	0	-0.520404	-0.628174	-0.266417
5	7	0	-0.898287	-1.177923	1.030703

6	1	0	-2.766402	-0.404757	1.089664
7	1	0	-0.258071	-0.834820	1.740739
8	7	0	-0.767587	0.798285	-0.290786
9	6	0	0.155092	1.817760	-0.230049
10	8	0	-0.147304	2.990109	-0.151524
11	1	0	2.924824	-0.056946	-0.468306
12	8	0	1.331767	-2.240262	-0.377864
13	1	0	1.633875	-2.230893	0.539640
14	8	0	1.960197	-0.264870	1.357069
15	1	0	2.656365	0.238351	1.791137
16	1	0	2.136794	2.180644	-0.209158
17	1	0	-1.725237	1.054569	-0.048280
18	8	0	-1.401465	-1.285407	-1.163916
19	1	0	-1.286885	-0.881007	-2.030926
20	1	0	-0.821696	-2.190253	0.987372
21	8	0	-3.457131	0.159788	0.694519
22	1	0	-3.689695	-0.333471	-0.099799
23	1	0	1.030047	-0.801187	-1.766183

Cg-TS4 (E= -699.656880784)

Sum of electronic and zero-point Energies= -699.472573

Sum of electronic and thermal Energies= -699.459698

Sum of electronic and thermal Enthalpies= -699.458754

Sum of electronic and thermal Free Energies= -699.511095

1	7	0	1.465169	1.439243	-0.316904
2	6	0	1.923188	0.123750	-0.004540
3	6	0	1.008052	-0.905963	-0.663044
4	6	0	-0.493242	-0.649482	-0.315739
5	7	0	-0.923338	-1.244160	0.954107
6	1	0	-2.726283	-0.519101	1.031166
7	1	0	-0.308925	-0.930839	1.701940
8	7	0	-0.775937	0.768174	-0.294061
9	6	0	0.123442	1.811352	-0.245223
10	8	0	-0.213310	2.974965	-0.175299
11	1	0	2.941894	0.003662	-0.385001
12	8	0	1.399505	-2.217953	-0.324200
13	1	0	1.663318	-2.189744	0.604471
14	8	0	1.907420	-0.199195	1.404445
15	1	0	2.568084	0.332469	1.859462
16	1	0	2.093057	2.222052	-0.210974
17	1	0	-1.731514	1.006447	-0.026764
18	8	0	-1.262207	-1.296063	-1.321156
19	1	0	-1.818025	-0.622932	-1.724842
20	1	0	-0.841947	-2.253880	0.873611
21	8	0	-3.408828	0.128640	0.758151

22	1	0	-4.049249	-0.383386	0.255465
23	1	0	1.099044	-0.808636	-1.744778

Cg-IM4 (E= -699.667833040)

Sum of electronic and zero-point Energies= -699.482151

Sum of electronic and thermal Energies= -699.469254

Sum of electronic and thermal Enthalpies= -699.468310

Sum of electronic and thermal Free Energies= -699.520419

1	7	0	1.810023	1.046838	-0.224895
2	6	0	1.900697	-0.367174	-0.057839
3	6	0	0.690106	-1.022138	-0.718940
4	6	0	-0.634921	-0.397784	-0.238029
5	7	0	-1.009827	-0.720904	1.153304
6	1	0	-2.762558	0.100417	1.105072
7	1	0	-0.283151	-0.378696	1.778324
8	7	0	-0.527827	1.039463	-0.379467
9	6	0	0.626737	1.779178	-0.216813
10	8	0	0.625317	2.990445	-0.124527
11	1	0	2.810206	-0.727187	-0.552420
12	8	0	0.738105	-2.407656	-0.414228
13	1	0	0.003068	-2.821707	-0.881618
14	8	0	1.974852	-0.694321	1.336888

15	1	0	1.975028	-1.659543	1.388213
16	1	0	2.616678	1.604525	0.011297
17	1	0	-1.383088	1.566499	-0.252509
18	8	0	-1.615016	-0.943110	-1.082343
19	1	0	-2.475195	-0.584426	-0.791338
20	1	0	-1.020408	-1.733552	1.249729
21	8	0	-3.393322	0.493068	0.463425
22	1	0	-4.269164	0.466364	0.857394
23	1	0	0.746796	-0.850372	-1.798744

Cg-TS5 (E= -699.638854332)

Sum of electronic and zero-point Energies= -699.459355

Sum of electronic and thermal Energies= -699.447585

Sum of electronic and thermal Enthalpies= -699.446641

Sum of electronic and thermal Free Energies= -699.496912

1	7	0	2.077628	0.377043	-0.092665
2	6	0	1.628185	-0.976363	-0.059199
3	6	0	0.297311	-1.073771	-0.803447
4	6	0	-0.716160	-0.015496	-0.344398
5	7	0	-1.153244	-0.310533	1.135997
6	1	0	-2.148115	0.318674	1.183599
7	1	0	-0.411870	-0.095758	1.798875
8	7	0	-0.067475	1.276369	-0.341700

9	6	0	1.277022	1.514614	-0.142068
10	8	0	1.746962	2.630162	-0.048894
11	1	0	2.367061	-1.611692	-0.560674
12	8	0	-0.233991	-2.373550	-0.601732
13	1	0	-1.074552	-2.385399	-1.080077
14	8	0	1.499222	-1.412582	1.303591
15	1	0	1.217584	-2.336243	1.268793
16	1	0	3.033918	0.574414	0.158317
17	1	0	-0.658350	2.093973	-0.397919
18	8	0	-1.834807	-0.082013	-1.084438
19	1	0	-2.650019	0.487746	-0.432080
20	1	0	-1.353181	-1.307162	1.200174
21	8	0	-3.135716	1.022742	0.576934
22	1	0	-4.045812	0.765398	0.746620
23	1	0	0.473461	-0.876078	-1.866061

Cg-PC (E= -699.693286398)

Sum of electronic and zero-point Energies=	-699.510596
Sum of electronic and thermal Energies=	-699.496043
Sum of electronic and thermal Enthalpies=	-699.495098
Sum of electronic and thermal Free Energies=	-699.551627

1	7	0	1.536502	1.377675	-0.080803

2	6	0	1.864847	0.000346	0.322686
3	6	0	1.256115	-0.907123	-0.768066
4	6	0	-0.228034	-0.608537	-0.904641
5	7	0	-1.263917	-0.361894	2.281543
6	1	0	-2.029975	-0.280695	1.611456
7	1	0	-1.374113	0.392022	2.953930
8	7	0	-0.572202	0.706764	-0.848099
9	6	0	0.275044	1.769511	-0.439453
10	8	0	-0.133251	2.908374	-0.434198
11	1	0	2.950847	-0.095240	0.279007
12	8	0	1.470134	-2.261852	-0.504283
13	1	0	0.617794	-2.700789	-0.641345
14	8	0	1.497685	-0.313357	1.622156
15	1	0	0.515445	-0.330974	1.738807
16	1	0	2.065068	2.120954	0.353884
17	1	0	-1.564505	0.932565	-0.883689
18	8	0	-1.039121	-1.518417	-1.053838
19	1	0	-2.757357	-0.882158	-0.588174
20	1	0	-1.398890	-1.230993	2.790426
21	8	0	-3.232518	-0.146767	-0.159496
22	1	0	-4.161531	-0.239818	-0.387381
23	1	0	1.723274	-0.611707	-1.721289

III.2 At the Mp2/6-311g(d,p) Level

Cg-RC(EUMP2=-0.69787680382396D+03)

Sum of electronic and zero-point Energies=	-697.692008
Sum of electronic and thermal Energies=	-697.677496
Sum of electronic and thermal Enthalpies=	-697.676552
Sum of electronic and thermal Free Energies=	-697.733404

1	7	0	1.669895	1.429724	-0.401494
2	6	0	2.230847	0.219522	0.105546
3	6	0	1.479785	-0.920406	-0.565440
4	6	0	-0.005478	-0.696147	-0.343686
5	7	0	-0.751757	-1.796008	-0.252456
6	1	0	-1.768188	-1.726104	-0.104044
7	1	0	-0.271090	-2.675395	-0.151874
8	7	0	-0.538090	0.495203	-0.306607
9	6	0	0.281366	1.627814	-0.367938
10	8	0	-0.189347	2.747412	-0.417195
11	1	0	3.293585	0.182670	-0.174363
12	8	0	1.846249	-2.178098	-0.006209
13	1	0	2.628326	-2.481824	-0.474933
14	8	0	2.088930	0.133999	1.510012
15	1	0	2.212132	-0.798291	1.725925

16	1	0	2.174209	2.281979	-0.194226
17	1	0	-2.196539	1.012946	0.347044
18	8	0	-3.113810	1.125439	0.666340
19	1	0	-3.396348	1.931531	0.231694
20	8	0	-3.546716	-1.470239	0.071817
21	1	0	-4.026426	-1.460444	-0.758131
22	1	0	-3.578641	-0.533902	0.354242
23	1	0	1.667076	-0.888399	-1.646456

Cg-TS1(EUMP2=-0.69785014243762D+03)

Sum of electronic and zero-point Energies= -697.672941

Sum of electronic and thermal Energies= -697.660519

Sum of electronic and thermal Enthalpies= -697.659575

Sum of electronic and thermal Free Energies= -697.711797

1	7	0	1.687434	1.380390	-0.394786
2	6	0	2.183696	0.125986	0.069703
3	6	0	1.349777	-0.953961	-0.602358
4	6	0	-0.118407	-0.692079	-0.304860
5	7	0	-0.934012	-1.701136	-0.146138
6	1	0	-2.266711	-1.545648	-0.001195
7	1	0	-0.434174	-2.583890	-0.174521
8	7	0	-0.551031	0.575479	-0.260805

9	6	0	0.314505	1.658028	-0.309222
10	8	0	-0.093286	2.806327	-0.308897
11	1	0	3.234826	0.031827	-0.240241
12	8	0	1.692051	-2.243529	-0.106288
13	1	0	2.446956	-2.551254	-0.615129
14	8	0	2.076015	0.013524	1.476265
15	1	0	2.131199	-0.931815	1.662124
16	1	0	2.243224	2.195258	-0.169976
17	1	0	-1.826518	0.897201	0.192887
18	8	0	-2.867106	1.009878	0.563659
19	1	0	-3.270664	1.714996	0.051124
20	8	0	-3.368305	-1.266257	0.110810
21	1	0	-3.791607	-1.420454	-0.737510
22	1	0	-3.266914	-0.088898	0.329591
23	1	0	1.491275	-0.887836	-1.689011

Cg-IM1 (EUMP2 =-0.69787667626477D+03)

Sum of electronic and zero-point Energies= -697.691995

Sum of electronic and thermal Energies= -697.677132

Sum of electronic and thermal Enthalpies= -697.676188

Sum of electronic and thermal Free Energies= -697.733704

1	7	0	-1.352794	1.370450	0.547776

2	6	0	-1.958022	0.083217	0.395271
3	6	0	-0.865975	-0.967577	0.542040
4	6	0	0.238108	-0.698760	-0.454531
5	7	0	0.933921	-1.599859	-1.045939
6	1	0	2.592217	-0.234545	1.150501
7	1	0	0.567295	-2.508101	-0.761421
8	7	0	0.514306	0.636807	-0.647192
9	6	0	-0.206026	1.717942	-0.151042
10	8	0	0.167678	2.863866	-0.296904
11	1	0	-2.696688	-0.040894	1.198938
12	8	0	-1.391985	-2.262802	0.285046
13	1	0	-1.608203	-2.654897	1.134437
14	8	0	-2.576937	-0.036748	-0.870342
15	1	0	-2.721188	-0.983431	-0.992534
16	1	0	-1.969834	2.159740	0.681343
17	1	0	1.389114	0.870719	-1.103558
18	8	0	2.030560	-0.174540	1.936655
19	1	0	1.957732	0.774660	2.053230
20	1	0	2.680324	-0.920425	-0.997606
21	8	0	3.288770	-0.235070	-0.661669
22	1	0	4.149574	-0.469749	-1.010441
23	1	0	-0.401580	-0.891430	1.531884

Cg-TS2 (EUMP2=-0.69781948176975D+03)

Sum of electronic and zero-point Energies= -697.638285

Sum of electronic and thermal Energies= -697.625512

Sum of electronic and thermal Enthalpies= -697.624568

Sum of electronic and thermal Free Energies= -697.676876

1	7	0	-1.553514	1.205306	0.577821
2	6	0	-1.942629	-0.143164	0.292933
3	6	0	-0.736943	-1.032309	0.568336
4	6	0	0.441193	-0.513224	-0.222728
5	7	0	1.116316	-1.337628	-1.005430
6	1	0	2.652283	-0.136650	0.497858
7	1	0	1.045524	-2.308013	-0.732750
8	7	0	0.510212	0.819069	-0.450710
9	6	0	-0.404955	1.760011	0.031603
10	8	0	-0.191796	2.950289	-0.024828
11	1	0	-2.752212	-0.416647	0.982187
12	8	0	-1.017436	-2.366499	0.173849
13	1	0	-1.071010	-2.894913	0.973249
14	8	0	-2.360999	-0.274361	-1.049117
15	1	0	-2.387070	-1.223821	-1.220716
16	1	0	-2.291517	1.887452	0.686705

17	1	0	1.445865	1.149149	-0.729326
18	8	0	1.902426	-0.575341	1.392478
19	1	0	1.798801	0.181257	1.979628
20	1	0	2.052812	-0.959250	-1.244744
21	8	0	3.079259	0.266199	-0.521228
22	1	0	4.016292	0.447052	-0.452154
23	1	0	-0.452495	-0.963020	1.618210

Cg-IM2 (EUMP2=-0.69788552967445D+03)

Sum of electronic and zero-point Energies= -697.696610

Sum of electronic and thermal Energies= -697.683726

Sum of electronic and thermal Enthalpies= -697.682782

Sum of electronic and thermal Free Energies= -697.734828

1	7	0	1.493257	1.410421	-0.274380
2	6	0	1.931505	0.056166	-0.077030
3	6	0	0.926569	-0.905308	-0.720900
4	6	0	-0.487719	-0.580806	-0.226056
5	7	0	-0.577633	-0.907327	1.182235
6	1	0	-3.159420	-0.676773	-0.043596
7	1	0	-0.544508	-1.921275	1.266673
8	7	0	-0.759520	0.811747	-0.474786
9	6	0	0.169805	1.822249	-0.235267

10	8	0	-0.154875	2.985056	-0.090361
11	1	0	2.903149	-0.071359	-0.561263
12	8	0	1.273796	-2.235744	-0.414453
13	1	0	1.783763	-2.168037	0.403892
14	8	0	2.145404	-0.304588	1.276357
15	1	0	1.250293	-0.330086	1.664581
16	1	0	2.126975	2.138180	0.026814
17	1	0	-1.703516	1.091378	-0.220752
18	8	0	-1.465613	-1.352560	-0.924776
19	1	0	-1.377979	-1.113086	-1.855101
20	1	0	-1.480881	-0.591836	1.531648
21	8	0	-3.390262	0.006880	0.597401
22	1	0	-4.345906	0.067898	0.566406
23	1	0	0.946729	-0.775047	-1.808606

Cg-TS3 （EUMP2=-0.69786361405175D+03）

Sum of electronic and zero-point Energies= -697.677264

Sum of electronic and thermal Energies= -697.663892

Sum of electronic and thermal Enthalpies= -697.662947

Sum of electronic and thermal Free Energies= -697.716819

1	7	0	1.317809	1.543092	-0.330814
2	6	0	1.924247	0.265031	-0.194278

3	6	0	0.984509	-0.815883	-0.724088
4	6	0	-0.412384	-0.697533	-0.086734
5	7	0	-0.475960	-1.123503	1.297995
6	1	0	-3.159851	-0.877510	0.120509
7	1	0	0.454203	-1.279192	1.664189
8	7	0	-0.854912	0.672856	-0.272635
9	6	0	-0.048900	1.792589	-0.192442
10	8	0	-0.480287	2.923304	-0.075043
11	1	0	2.854812	0.224446	-0.766346
12	8	0	1.552368	-2.088419	-0.543777
13	1	0	1.981083	-2.057916	0.318953
14	8	0	2.307572	-0.052237	1.157407
15	1	0	1.733514	0.475271	1.723661
16	1	0	1.889213	2.369204	-0.227401
17	1	0	-1.799815	0.837654	0.073620
18	8	0	-1.342757	-1.535263	-0.759205
19	1	0	-1.416671	-1.176806	-1.650622
20	1	0	-0.970225	-2.007808	1.339975
21	8	0	-3.626641	-0.097622	0.439581
22	1	0	-4.305228	0.041158	-0.223566
23	1	0	0.863530	-0.658949	-1.801248

Cg-IM3 （EUMP2=-0.69787702144614D+03）

Sum of electronic and zero-point Energies= -697.688584

Sum of electronic and thermal Energies= -697.675505

Sum of electronic and thermal Enthalpies= -697.674561

Sum of electronic and thermal Free Energies= -697.726961

1	7	0	1.569652	1.326499	-0.378795
2	6	0	1.911213	-0.015273	-0.042707
3	6	0	0.901877	-0.961590	-0.675163
4	6	0	-0.544228	-0.599236	-0.256649
5	7	0	-0.942584	-1.112493	1.042858
6	1	0	-2.767787	-0.271955	1.074287
7	1	0	-0.272550	-0.791682	1.735952
8	7	0	-0.712022	0.831233	-0.296621
9	6	0	0.262079	1.804298	-0.230437
10	8	0	0.020619	2.989897	-0.119013
11	1	0	2.909139	-0.238389	-0.436345
12	8	0	1.206106	-2.300570	-0.365792
13	1	0	1.480168	-2.282025	0.558327
14	8	0	1.879143	-0.313845	1.362401
15	1	0	2.616240	0.143950	1.776250
16	1	0	2.254863	2.050696	-0.212438
17	1	0	-1.649252	1.139779	-0.040375

18	8	0	-1.461395	-1.217032	-1.138786
19	1	0	-1.301868	-0.824293	-2.003173
20	1	0	-0.903079	-2.128048	1.004354
21	8	0	-3.436511	0.289453	0.650011
22	1	0	-3.600770	-0.217688	-0.148955
23	1	0	0.980226	-0.849438	-1.760811

Cg-TS4 （EUMP2=-0.69787435285809D+03）

Sum of electronic and zero-point Energies= -697.686664

Sum of electronic and thermal Energies= -697.674001

Sum of electronic and thermal Enthalpies= -697.673057

Sum of electronic and thermal Free Energies= -697.724905

1	7	0	1.569190	1.328734	-0.378809
2	6	0	1.912176	-0.007146	-0.015183
3	6	0	0.928271	-0.964381	-0.665319
4	6	0	-0.531133	-0.607600	-0.293366
5	7	0	-0.974015	-1.155840	0.985627
6	1	0	-2.726766	-0.356322	1.000321
7	1	0	-0.320050	-0.866774	1.709445
8	7	0	-0.708038	0.820209	-0.278658
9	6	0	0.261974	1.800551	-0.236641
10	8	0	0.007907	2.984322	-0.132264

11	1	0	2.922607	-0.225194	-0.378271
12	8	0	1.229540	-2.300059	-0.332645
13	1	0	1.475616	-2.271395	0.598942
14	8	0	1.840301	-0.285367	1.392266
15	1	0	2.558160	0.187545	1.822455
16	1	0	2.251124	2.058472	-0.223973
17	1	0	-1.638697	1.127170	0.001063
18	8	0	-1.362019	-1.207847	-1.272603
19	1	0	-1.866832	-0.486287	-1.656452
20	1	0	-0.940642	-2.169929	0.913017
21	8	0	-3.387225	0.289134	0.688348
22	1	0	-3.995391	-0.253060	0.183245
23	1	0	1.015149	-0.865942	-1.748672

Cg-IM4 （EUMP2=-0.69788552353098D+03）

Sum of electronic and zero-point Energies= -697.696446

Sum of electronic and thermal Energies= -697.683781

Sum of electronic and thermal Enthalpies= -697.682837

Sum of electronic and thermal Free Energies= -697.734437

1	7	0	1.783016	1.065503	-0.261957
2	6	0	1.895204	-0.340206	-0.060718
3	6	0	0.702257	-1.019354	-0.711798

4	6	0	-0.621602	-0.416213	-0.238132
5	7	0	-0.973585	-0.699097	1.160268
6	1	0	-2.718846	0.099850	1.092586
7	1	0	-0.238957	-0.322113	1.755779
8	7	0	-0.551532	1.009723	-0.432937
9	6	0	0.584073	1.774746	-0.229707
10	8	0	0.554318	2.984899	-0.109026
11	1	0	2.813025	-0.696108	-0.545701
12	8	0	0.769426	-2.394988	-0.381866
13	1	0	0.016959	-2.800406	-0.826759
14	8	0	1.961195	-0.633429	1.334616
15	1	0	1.956236	-1.597487	1.385584
16	1	0	2.569458	1.635393	0.015473
17	1	0	-1.414322	1.517183	-0.270974
18	8	0	-1.593123	-1.015665	-1.050527
19	1	0	-2.445010	-0.649185	-0.756343
20	1	0	-0.946396	-1.709327	1.283340
21	8	0	-3.354781	0.472117	0.452027
22	1	0	-4.209388	0.449237	0.884467
23	1	0	0.756068	-0.857250	-1.794740

Cg-TS5 (EUMP2=-0.69785300729586D+03)

Sum of electronic and zero-point Energies= -697.669866

Sum of electronic and thermal Energies= -697.658396

Sum of electronic and thermal Enthalpies= -697.657451

Sum of electronic and thermal Free Energies= -697.707018

1	7	0	2.005690	0.522550	-0.143465
2	6	0	1.681401	-0.861925	-0.065592
3	6	0	0.363409	-1.093619	-0.786878
4	6	0	-0.718839	-0.117736	-0.343303
5	7	0	-1.059727	-0.343190	1.150983
6	1	0	-2.040235	0.279410	1.205608
7	1	0	-0.286326	-0.091005	1.764208
8	7	0	-0.202127	1.220174	-0.458916
9	6	0	1.103797	1.584957	-0.187427
10	8	0	1.465286	2.738732	-0.057554
11	1	0	2.471628	-1.443132	-0.557109
12	8	0	-0.059658	-2.418557	-0.527255
13	1	0	-0.925409	-2.470508	-0.954548
14	8	0	1.597654	-1.264136	1.304711
15	1	0	1.354137	-2.197891	1.275310
16	1	0	2.928283	0.808268	0.150010
17	1	0	-0.880409	1.971227	-0.416072
18	8	0	-1.859340	-0.340899	-1.017996
19	1	0	-2.633064	0.308735	-0.375676

20	1	0	-1.248000	-1.337448	1.272267
21	8	0	-3.029241	0.962398	0.570563
22	1	0	-3.952147	0.797689	0.773658
23	1	0	0.508471	-0.912451	-1.858418

Cg-PC (EUMP2 =-0.69789955147849D+03)

Sum of electronic and zero-point Energies= -697.713909

Sum of electronic and thermal Energies= -697.699325

Sum of electronic and thermal Enthalpies= -697.698381

Sum of electronic and thermal Free Energies= -697.755442

1	7	0	1.690189	1.265774	-0.087772
2	6	0	1.882434	-0.152045	0.228712
3	6	0	1.128408	-0.916362	-0.861055
4	6	0	-0.323695	-0.475520	-0.876352
5	7	0	-1.200752	-0.786529	2.096114
6	1	0	-1.974316	-0.407689	1.553057
7	1	0	-1.283906	-0.390537	3.027720
8	7	0	-0.535888	0.853224	-0.670246
9	6	0	0.433959	1.796998	-0.250911
10	8	0	0.131959	2.960782	-0.096058
11	1	0	2.950786	-0.356889	0.125394
12	8	0	1.217898	-2.298244	-0.671101

13	1	0	0.341727	-2.630980	-0.905729
14	8	0	1.533689	-0.500710	1.523864
15	1	0	0.555611	-0.561502	1.611332
16	1	0	2.305962	1.911457	0.389699
17	1	0	-1.502255	1.172407	-0.630072
18	8	0	-1.221630	-1.290832	-1.086196
19	1	0	-2.896328	-0.483543	-0.597800
20	1	0	-1.377099	-1.782071	2.191758
21	8	0	-3.272206	0.254413	-0.095269
22	1	0	-4.195927	0.288257	-0.347866
23	1	0	1.556576	-0.607894	-1.828444