SUPPORTING INFORMATION

Title: Stereoselectivity through a network of non-classical CH weak interactions: a prospective study of a Bicyclic Organocatalytic Scaffold

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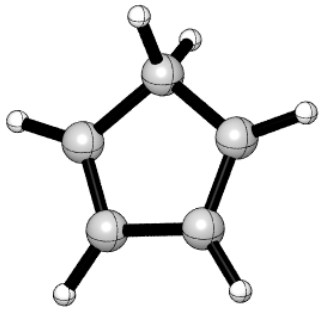
Cyclopentadiene

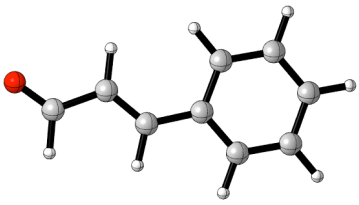


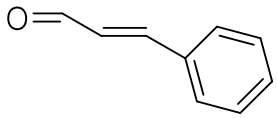
E(RM062X) = -194.072757797

Zero-point correction=	0.093365 (Hartree/Particle)
Thermal correction to Energy=	0.097502
Thermal correction to Enthalpy=	0.098446
Thermal correction to Gibbs Free Energy=	0.066775
Sum of electronic and zero-point Energies=	-193.979393
Sum of electronic and thermal Energies=	-193.975256
Sum of electronic and thermal Enthalpies=	-193.974312
Sum of electronic and thermal Free Energies=	-194.005983

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000007	-0.985916	0.734053
2	6	0	-0.000007	-0.985916	-0.734053
3	6	0	-0.000007	0.279790	-1.174972
4	6	0	0.000043	1.212817	0.000000
5	6	0	-0.000007	0.279790	1.174972
6	1	0	-0.000034	-1.876392	1.346730
7	1	0	-0.000034	-1.876392	-1.346730
8	1	0	-0.000006	0.606220	-2.204472
9	1	0	0.877594	1.868524	0.000000
10	1	0	-0.877596	1.868420	0.000000
11	1	0	-0.000006	0.606220	2.204472

Cinnamonaldehyde



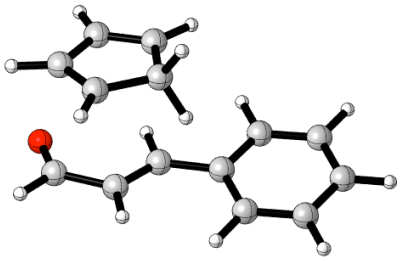


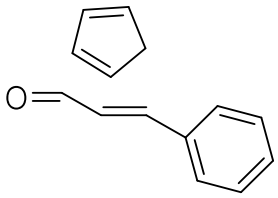
E(RM062X) = -422.930229962

Zero-point correction=	0.144182 (Hartree/Particle)
Thermal correction to Energy=	0.152871
Thermal correction to Enthalpy=	0.153815
Thermal correction to Gibbs Free Energy=	0.109291
Sum of electronic and zero-point Energies=	-422.786048
Sum of electronic and thermal Energies=	-422.777359
Sum of electronic and thermal Enthalpies=	-422.776415
Sum of electronic and thermal Free Energies=	-422.820939

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.293792	1.362913	0.000100
2	6	0	3.224436	0.328176	0.000108
3	6	0	2.790309	-0.989768	0.000059
4	6	0	1.431705	-1.270089	0.000002
5	6	0	0.487190	-0.241241	-0.000004
6	6	0	0.938618	1.082611	0.000044
7	1	0	2.629460	2.391991	0.000136
8	1	0	4.283536	0.551799	0.000151
9	1	0	3.508552	-1.799475	0.000064
10	1	0	1.092612	-2.299629	-0.000037
11	1	0	0.226546	1.897782	0.000036
12	6	0	-0.935126	-0.588871	-0.000060
13	1	0	-1.147752	-1.656781	-0.000126
14	6	0	-1.979080	0.245541	-0.000039
15	1	0	-1.884770	1.324956	0.000027
16	6	0	-3.346423	-0.288594	-0.000108
17	1	0	-3.417878	-1.394651	-0.000163
18	8	0	-4.340352	0.392492	-0.000086

Cinnamonaldehyde and Cyclopentadiene Adduct





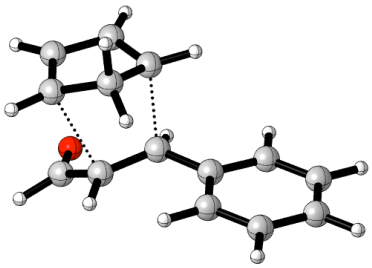
E(RM062X) = -617.009873794

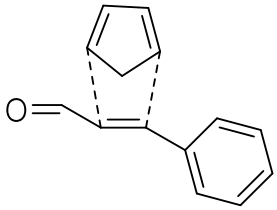
Zero-point correction=	0.238849 (Hartree/Particle)
Thermal correction to Energy=	0.253308
Thermal correction to Enthalpy=	0.254253
Thermal correction to Gibbs Free Energy=	0.195212
Sum of electronic and zero-point Energies=	-616.771024
Sum of electronic and thermal Energies=	-616.756565
Sum of electronic and thermal Enthalpies=	-616.755621
Sum of electronic and thermal Free Energies=	-616.814662

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.305972	-1.447286	-1.182003
2	6	0	-1.010333	-1.934219	-0.602078
3	6	0	-1.180507	-1.672329	0.864727
4	6	0	-2.394046	-1.144047	1.086611
5	6	0	-3.097801	-1.007903	-0.190862
6	6	0	0.044700	1.165200	0.285500
7	6	0	-0.819233	1.464627	-0.688999
8	6	0	-2.176466	1.937300	-0.357900
9	1	0	-0.141436	-1.408756	-1.013120
10	1	0	-0.856656	-3.000064	-0.805204
11	1	0	-0.306086	1.299897	1.305189
12	1	0	-0.587185	1.342016	-1.740654
13	1	0	-0.424196	-1.892454	1.604527
14	1	0	-2.547528	-1.480568	-2.234745
15	1	0	-2.841703	2.114370	-1.222184
16	1	0	-4.094867	-0.603579	-0.297142
17	1	0	-2.800313	-0.842186	2.041244
18	6	0	1.403040	0.640669	0.130343
19	6	0	2.040934	0.546684	-1.111293
20	6	0	2.083406	0.192120	1.264975
21	6	0	3.315853	0.015593	-1.210677
22	1	0	1.541299	0.904093	-2.003066
23	6	0	3.359876	-0.342331	1.166292

24	1	0	1.597421	0.264390	2.231208
25	6	0	3.978838	-0.433904	-0.072830
26	1	0	3.798862	-0.046106	-2.177599
27	1	0	3.871446	-0.686049	2.056213
28	1	0	4.975739	-0.847883	-0.153853
29	8	0	-2.579815	2.125228	0.764793

Uncatalysed TS *E-endo*





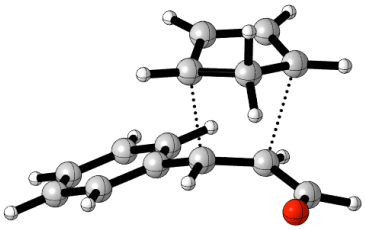
E(RM062X) = -616.981749330

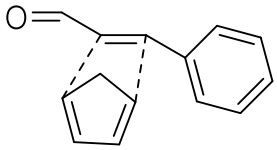
Zero-point correction=	0.241072 (Hartree/Particle)
Thermal correction to Energy=	0.253314
Thermal correction to Enthalpy=	0.254258
Thermal correction to Gibbs Free Energy=	0.202300
Sum of electronic and zero-point Energies=	-616.740677
Sum of electronic and thermal Energies=	-616.728435
Sum of electronic and thermal Enthalpies=	-616.727491
Sum of electronic and thermal Free Energies=	-616.779449

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.264310	-1.088320	-0.950413
2	6	0	-0.975386	-1.765418	-0.589284
3	6	0	-0.819496	-1.282805	0.829091
4	6	0	-2.113289	-1.032360	1.305501
5	6	0	-2.985670	-0.913463	0.224641
6	6	0	-0.194410	0.618036	0.241712
7	6	0	-1.045092	0.897293	-0.833033
8	6	0	-2.225950	1.715237	-0.596646
9	1	0	-0.130138	-1.578590	-1.245625
10	1	0	-1.156330	-2.847921	-0.560817
11	1	0	-0.465398	1.112193	1.167459
12	1	0	-0.717335	0.804864	-1.860307
13	1	0	0.003224	-1.587454	1.462178
14	1	0	-2.690217	-1.099577	-1.944330
15	1	0	-2.791645	2.010975	-1.500106
16	1	0	-4.010924	-0.579989	0.289931
17	1	0	-2.369657	-0.829304	2.335421
18	6	0	1.259902	0.371757	0.089970
19	6	0	1.869266	0.112716	-1.139307
20	6	0	2.067246	0.397489	1.230765
21	6	0	3.235283	-0.119668	-1.222187

22	1	0	1.280679	0.108460	-2.048276
23	6	0	3.431885	0.168452	1.150512
24	1	0	1.609817	0.605212	2.192001
25	6	0	4.022923	-0.095444	-0.079010
26	1	0	3.687034	-0.313553	-2.187002
27	1	0	4.036147	0.198289	2.048490
28	1	0	5.088352	-0.273709	-0.146307
29	8	0	-2.618878	2.046137	0.502926

Uncatalysed TS *E-exo*





E(RM062X) = -616.982302507

Zero-point correction=	0.240925 (Hartree/Particle)
Thermal correction to Energy=	0.253185
Thermal correction to Enthalpy=	0.254129
Thermal correction to Gibbs Free Energy=	0.202055
Sum of electronic and zero-point Energies=	-616.741378
Sum of electronic and thermal Energies=	-616.729118
Sum of electronic and thermal Enthalpies=	-616.728173
Sum of electronic and thermal Free Energies=	-616.780248

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.499889	-2.060256	-0.534464
2	6	0	-0.567069	-1.981018	0.501079
3	6	0	-0.931166	-0.941746	1.359654
4	6	0	-2.377549	-0.638448	1.093820
5	6	0	-2.481590	-1.093154	-0.330358
6	6	0	-0.284419	0.730263	0.183768
7	6	0	-1.176014	0.707457	-0.890107
8	6	0	-2.327963	1.607713	-0.928070
9	1	0	-0.860452	0.333736	-1.854982
10	1	0	-0.535560	1.430848	0.974471
11	1	0	-2.985872	-1.319928	1.703879

12	1	0	-2.698200	0.381436	1.290753
13	1	0	-3.378572	-0.990426	-0.926527
14	1	0	-0.446257	-0.743833	2.306215
15	1	0	-2.835151	1.673034	-1.908922
16	1	0	-1.414870	-2.689333	-1.409530
17	1	0	0.361099	-2.532217	0.549820
18	6	0	1.160362	0.464194	0.025823
19	6	0	1.670684	-0.303255	-1.024448
20	6	0	2.056013	0.978171	0.965160
21	6	0	3.031862	-0.546188	-1.128820
22	1	0	0.997709	-0.724763	-1.761202
23	6	0	3.418799	0.738570	0.860187
24	1	0	1.674329	1.577121	1.784550
25	6	0	3.913321	-0.025977	-0.188090
26	1	0	3.408310	-1.143009	-1.950321
27	1	0	4.095541	1.151357	1.597798
28	1	0	4.975858	-0.213498	-0.273878
29	8	0	-2.748776	2.248941	0.010884

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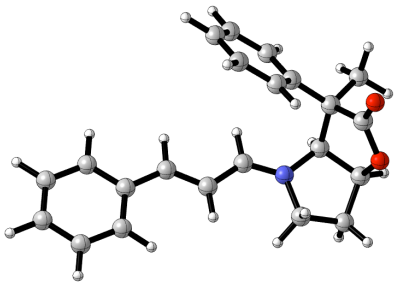
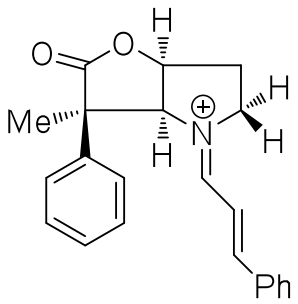
1 - *E*-iminium ion





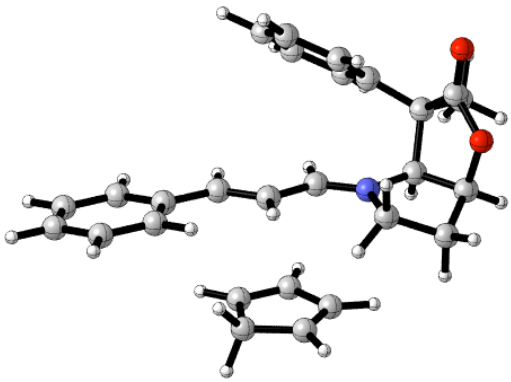
E(RM062X) = -1056.47331306

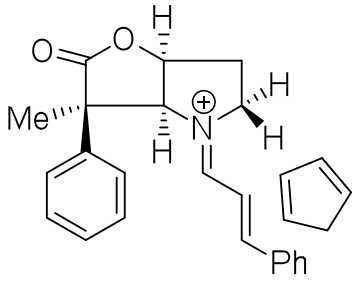
Zero-point correction=	0.396150 (Hartree/Particle)
Thermal correction to Energy=	0.416989
Thermal correction to Enthalpy=	0.417933
Thermal correction to Gibbs Free Energy=	0.344838
Sum of electronic and zero-point Energies=	-1056.077163
Sum of electronic and thermal Energies=	-1056.056324
Sum of electronic and thermal Enthalpies=	-1056.055380
Sum of electronic and thermal Free Energies=	-1056.128475

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.145247	-2.548714	0.120966
2	6	0	2.476040	-3.107552	-0.366996
3	6	0	3.332307	-1.864108	-0.524226

4	6	0	2.382083	-0.758202	-1.012577
5	6	0	3.490893	-0.126771	1.006015
6	6	0	2.869947	0.499446	-0.248170
7	1	0	1.154345	-2.355454	1.196424
8	1	0	2.918931	-3.810996	0.334141
9	8	0	3.770073	-1.436518	0.766033
10	7	0	1.050666	-1.259662	-0.596943
11	1	0	2.390232	-0.612961	-2.092333
12	1	0	4.198130	-2.005116	-1.168640
13	6	0	1.778597	1.502379	0.050331
14	6	0	1.448486	2.483708	-0.884961
15	6	0	1.000802	1.388175	1.203092
16	6	0	0.353015	3.314332	-0.683888
17	1	0	2.041399	2.610895	-1.781421
18	6	0	-0.091398	2.221270	1.406800
19	1	0	1.254869	0.656983	1.960754
20	6	0	-0.424276	3.181123	0.460250
21	1	0	0.116496	4.074983	-1.416858
22	1	0	-0.675288	2.126107	2.313223
23	1	0	-1.269598	3.837233	0.623473
24	1	0	2.354836	-3.595120	-1.335122
25	1	0	0.293958	-3.176369	-0.130951
26	6	0	-0.052800	-0.610980	-0.820189
27	1	0	0.042628	0.304575	-1.396957
28	6	0	-1.341963	-0.984823	-0.372247
29	1	0	-1.471348	-1.877597	0.223355
30	6	0	-2.380445	-0.158813	-0.663028
31	1	0	-2.155594	0.732660	-1.245478
32	6	0	-3.761673	-0.309259	-0.277480
33	6	0	-4.225449	-1.396556	0.480382
34	6	0	-4.671333	0.679259	-0.680274
35	6	0	-5.560498	-1.487288	0.818351
36	1	0	-3.543102	-2.172053	0.803773
37	6	0	-6.009232	0.585387	-0.339219
38	1	0	-4.318286	1.520572	-1.265284
39	6	0	-6.453112	-0.497238	0.409666
40	1	0	-5.915336	-2.326642	1.401293
41	1	0	-6.705149	1.350973	-0.654737
42	1	0	-7.498959	-0.574195	0.677886
43	8	0	3.752287	0.401940	2.034012
44	6	0	4.058649	1.101018	-1.022779
45	1	0	3.762422	1.406138	-2.025421
46	1	0	4.437563	1.967381	-0.482639
47	1	0	4.869990	0.377493	-1.119153

1-*E* and Cyclopentadiene Adduct





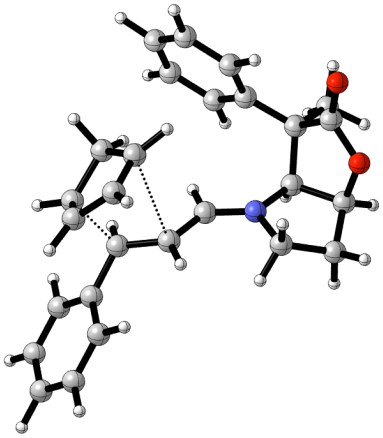
E(RM062X) = -1250.56051309

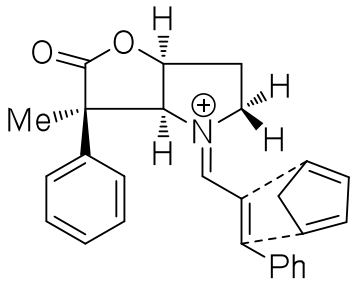
Zero-point correction=	0.490746 (Hartree/Particle)
Thermal correction to Energy=	0.517507
Thermal correction to Enthalpy=	0.518451
Thermal correction to Gibbs Free Energy=	0.430023
Sum of electronic and zero-point Energies=	-1250.069767
Sum of electronic and thermal Energies=	-1250.043006
Sum of electronic and thermal Enthalpies=	-1250.042062
Sum of electronic and thermal Free Energies=	-1250.130490

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.475219	3.379526	0.481400
2	6	0	-2.797484	2.756800	0.816140
3	6	0	-2.506603	1.991963	2.070777
4	6	0	-1.226438	2.188975	2.426505
5	6	0	-0.584095	3.059061	1.435303
6	6	0	-2.109823	-0.505733	0.061296
7	6	0	-1.124733	0.175541	-0.572435
8	6	0	0.131804	0.264768	0.075099
9	7	0	1.169668	0.904505	-0.367463
10	1	0	-3.205639	2.131811	0.015034
11	1	0	-3.547709	3.533880	1.006411
12	1	0	-1.866411	-0.949006	1.024258
13	1	0	-1.273073	0.642492	-1.536052
14	1	0	-3.247373	1.421073	2.612305
15	1	0	-1.316174	4.046115	-0.354862
16	1	0	0.250881	-0.240747	1.029072
17	1	0	0.436179	3.414996	1.501440
18	1	0	-0.743828	1.805206	3.315037
19	6	0	1.179127	1.745253	-1.580837

20	1	0	0.221774	2.255150	-1.669365
21	1	0	1.350336	1.113435	-2.455249
22	6	0	2.341859	2.695925	-1.323407
23	1	0	2.782482	3.082400	-2.239451
24	1	0	2.016659	3.531755	-0.701769
25	6	0	3.325270	1.839229	-0.547566
26	1	0	4.064286	2.412519	0.009491
27	6	0	2.470255	0.920131	0.337881
28	1	0	2.323599	1.290683	1.352746
29	6	0	3.236283	-0.425216	0.305547
30	6	0	3.935333	-0.340936	-1.056517
31	6	0	4.374942	-0.359454	1.341937
32	1	0	3.984568	-0.210046	2.347650
33	1	0	4.940682	-1.289507	1.313102
34	1	0	5.058462	0.462521	1.122679
35	8	0	3.995246	0.960159	-1.452668
36	8	0	4.409893	-1.221710	-1.692050
37	6	0	2.349833	-1.639740	0.466341
38	6	0	2.027340	-2.109299	1.739785
39	6	0	1.740855	-2.233482	-0.639571
40	6	0	1.102359	-3.132587	1.904983
41	1	0	2.493907	-1.682105	2.617961
42	6	0	0.820107	-3.260075	-0.475176
43	1	0	1.996467	-1.908986	-1.640743
44	6	0	0.490950	-3.706964	0.797476
45	1	0	0.870022	-3.488705	2.900451
46	1	0	0.367339	-3.716720	-1.345808
47	1	0	-0.220630	-4.512497	0.925092
48	6	0	-3.470856	-0.702670	-0.385719
49	6	0	-3.938162	-0.232938	-1.622879
50	6	0	-4.358511	-1.369762	0.468687
51	6	0	-5.255254	-0.430253	-1.988799
52	1	0	-3.269081	0.277686	-2.304105
53	6	0	-5.679447	-1.563266	0.100646
54	1	0	-4.001836	-1.735883	1.424555
55	6	0	-6.127611	-1.093261	-1.127128
56	1	0	-5.610150	-0.071666	-2.945853
57	1	0	-6.358217	-2.079279	0.766379
58	1	0	-7.158798	-1.244915	-1.419054

TS1-*E*-*exo*-top





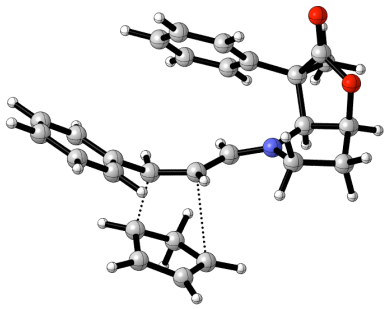
E(RM062X) = -1250.53718004

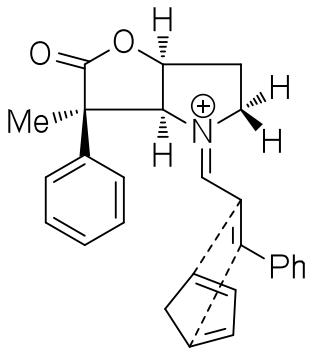
Zero-point correction=	0.492527 (Hartree/Particle)
Thermal correction to Energy=	0.517297
Thermal correction to Enthalpy=	0.518241
Thermal correction to Gibbs Free Energy=	0.437423
Sum of electronic and zero-point Energies=	-1250.044653
Sum of electronic and thermal Energies=	-1250.019883
Sum of electronic and thermal Enthalpies=	-1250.018939
Sum of electronic and thermal Free Energies=	-1250.099757

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.461593	0.456053	2.709220
2	6	0	-2.621548	0.977942	2.110808
3	6	0	-2.285735	1.663616	0.930516
4	6	0	-0.800645	1.925886	1.017641
5	6	0	-0.371632	0.893997	1.996781
6	6	0	-2.326548	0.264010	-0.409709
7	6	0	-1.320019	-0.691780	-0.090409
8	6	0	-0.058321	-0.609219	-0.644674
9	7	0	0.913548	-1.500613	-0.500021
10	1	0	-1.568367	-1.528264	0.547263
11	1	0	-2.048557	0.937742	-1.217475
12	1	0	-0.668514	2.906087	1.497639
13	1	0	-0.239541	1.957003	0.086381
14	1	0	0.662465	0.632792	2.184153
15	1	0	-2.970678	2.372245	0.481834
16	1	0	0.178167	0.234726	-1.281723
17	1	0	-1.438011	-0.210146	3.559169

18	1	0	-3.633102	0.800895	2.450748
19	6	0	0.708634	-2.763095	0.226992
20	1	0	-0.273147	-3.169695	-0.011665
21	1	0	0.769762	-2.584706	1.304603
22	6	0	1.846115	-3.643666	-0.271796
23	1	0	2.148835	-4.398709	0.450006
24	1	0	1.572542	-4.132977	-1.207503
25	6	0	2.268194	-1.381604	-1.079767
26	1	0	2.219920	-1.358480	-2.169429
27	6	0	2.951923	-2.644400	-0.530391
28	1	0	3.752666	-3.022265	-1.162404
29	6	0	3.154026	-0.257202	-0.496312
30	6	0	4.482864	-0.210022	-1.294460
31	1	0	4.284162	0.074298	-2.327874
32	1	0	5.133968	0.541683	-0.850306
33	1	0	5.006073	-1.166395	-1.284977
34	6	0	3.523102	-0.879063	0.853666
35	8	0	3.493657	-2.228939	0.730077
36	8	0	3.841018	-0.353513	1.873083
37	6	0	2.578225	1.148569	-0.486503
38	6	0	2.098516	1.666037	-1.695273
39	6	0	2.639401	1.996732	0.617702
40	6	0	1.667732	2.980057	-1.795293
41	1	0	2.077063	1.038411	-2.580991
42	6	0	2.221282	3.321626	0.511909
43	1	0	3.051688	1.640471	1.550346
44	6	0	1.733267	3.818053	-0.686217
45	1	0	1.308449	3.357804	-2.744117
46	1	0	2.298974	3.970139	1.375713
47	1	0	1.423091	4.851956	-0.765792
48	6	0	-3.758732	-0.139611	-0.484378
49	6	0	-4.585094	0.486471	-1.414425
50	6	0	-4.299047	-1.118963	0.349591
51	6	0	-5.924985	0.135217	-1.519875
52	1	0	-4.176363	1.249493	-2.067901
53	6	0	-5.635559	-1.468776	0.246632
54	1	0	-3.679260	-1.610627	1.091186
55	6	0	-6.452275	-0.842786	-0.690078
56	1	0	-6.554148	0.626021	-2.250805
57	1	0	-6.043988	-2.231774	0.896526
58	1	0	-7.495660	-1.118291	-0.769114

TS1-*E-exo*





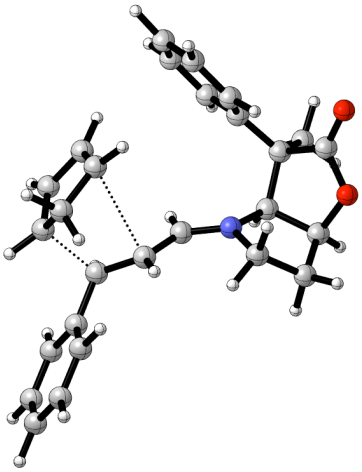
E(RM062X) = -1250.53643061

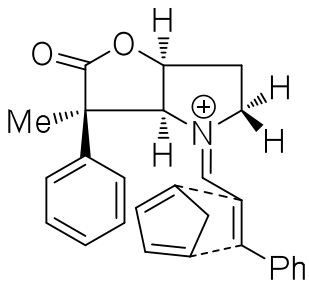
Zero-point correction=	0.492184 (Hartree/Particle)
Thermal correction to Energy=	0.517072
Thermal correction to Enthalpy=	0.518016
Thermal correction to Gibbs Free Energy=	0.436607
Sum of electronic and zero-point Energies=	-1250.044246
Sum of electronic and thermal Energies=	-1250.019359
Sum of electronic and thermal Enthalpies=	-1250.018414
Sum of electronic and thermal Free Energies=	-1250.099824

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.574164	3.391669	0.276316
2	6	0	-3.524863	2.395915	0.557585
3	6	0	-3.032079	1.532423	1.549952
4	6	0	-1.899896	2.279775	2.216089
5	6	0	-1.523427	3.249042	1.150220
6	6	0	-2.021306	0.237227	0.520064
7	6	0	-0.937969	0.912381	-0.108356
8	6	0	0.330909	0.824853	0.437982
9	7	0	1.454498	1.235026	-0.124024
10	1	0	-1.056051	1.302857	-1.109654
11	1	0	-1.720705	-0.342117	1.391656
12	1	0	-2.335216	2.855264	3.044858
13	1	0	-1.089652	1.679698	2.621963
14	1	0	-0.627405	3.854770	1.168313
15	1	0	-3.692221	0.875949	2.102817
16	1	0	0.450715	0.333280	1.399633
17	1	0	-2.639581	4.113350	-0.524845
18	1	0	-4.453461	2.250421	0.022702
19	6	0	-3.035856	-0.484965	-0.296805
20	6	0	-3.442738	-0.034932	-1.552755

21	6	0	-3.590363	-1.656660	0.213798
22	6	0	-4.378451	-0.749152	-2.284278
23	1	0	-3.033687	0.880329	-1.966069
24	6	0	-4.527438	-2.373940	-0.518935
25	1	0	-3.279857	-2.012686	1.190216
26	6	0	-4.922039	-1.921992	-1.769706
27	1	0	-4.685257	-0.393284	-3.259254
28	1	0	-4.948472	-3.284016	-0.111852
29	1	0	-5.651633	-2.478129	-2.343472
30	6	0	1.508652	1.985642	-1.383959
31	1	0	1.409432	1.304011	-2.233759
32	1	0	0.694417	2.710154	-1.412764
33	6	0	2.790457	0.916968	0.405170
34	1	0	2.896730	1.309815	1.417251
35	6	0	2.889216	2.631452	-1.328926
36	1	0	3.292099	2.863106	-2.312137
37	1	0	2.860542	3.543206	-0.730565
38	6	0	3.728563	1.584973	-0.617498
39	1	0	4.642553	1.978766	-0.176320
40	6	0	3.191222	-0.580182	0.329168
41	6	0	3.733475	-0.683895	-1.100134
42	8	0	4.067087	0.554872	-1.547982
43	8	0	3.904194	-1.662251	-1.748889
44	6	0	4.416187	-0.802150	1.236076
45	1	0	4.185546	-0.564858	2.273937
46	1	0	4.734375	-1.841554	1.169180
47	1	0	5.250131	-0.169315	0.927201
48	6	0	2.054801	-1.538537	0.609763
49	6	0	1.779527	-1.945971	1.914815
50	6	0	1.187895	-1.933715	-0.409747
51	6	0	0.653626	-2.710507	2.197071
52	1	0	2.441164	-1.673133	2.726691
53	6	0	0.062387	-2.696666	-0.130185
54	1	0	1.392072	-1.651425	-1.435289
55	6	0	-0.211496	-3.082433	1.175639
56	1	0	0.462777	-3.027045	3.214624
57	1	0	-0.599578	-2.992320	-0.934418
58	1	0	-1.080498	-3.690975	1.391942

TS1-*E*-endo-top





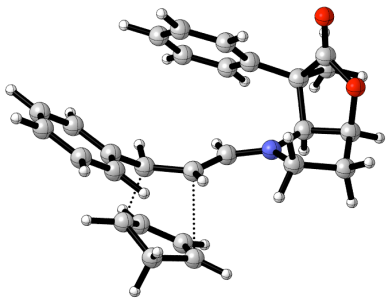
E(RM062X) = -1250.53110292

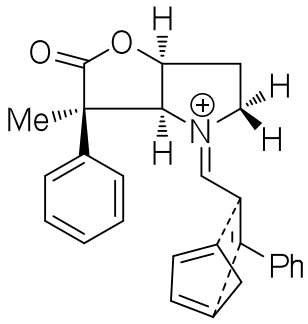
Zero-point correction=	0.492645 (Hartree/Particle)
Thermal correction to Energy=	0.517396
Thermal correction to Enthalpy=	0.518341
Thermal correction to Gibbs Free Energy=	0.437708
Sum of electronic and zero-point Energies=	-1250.038458
Sum of electronic and thermal Energies=	-1250.013707
Sum of electronic and thermal Enthalpies=	-1250.012762
Sum of electronic and thermal Free Energies=	-1250.093395

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.843602	2.042974	-1.156594
2	6	0	2.316892	1.997832	-1.348745
3	6	0	2.799301	2.048826	0.082326
4	6	0	1.751265	2.642815	0.812644
5	6	0	0.557577	2.566145	0.085863
6	6	0	2.598740	0.193003	0.582668
7	6	0	1.502813	-0.351321	-0.156027
8	6	0	0.259315	-0.508812	0.434549
9	7	0	-0.727547	-1.293487	0.033772
10	1	0	2.696842	1.188809	-1.965859
11	1	0	2.614605	2.942754	-1.825029
12	1	0	2.408430	0.307019	1.644127
13	1	0	1.690969	-0.803923	-1.118659
14	1	0	3.836432	2.236784	0.325596
15	1	0	0.116964	1.837533	-1.929856
16	1	0	0.058878	0.022337	1.363346

17	1	0	-0.428981	2.813299	0.449906
18	1	0	1.841731	3.006659	1.828080
19	6	0	-0.604023	-2.295768	-1.035500
20	1	0	-1.139948	-1.959750	-1.926390
21	1	0	0.441735	-2.453680	-1.284495
22	6	0	-1.914948	-1.543397	0.869067
23	1	0	-1.611628	-1.549874	1.916218
24	6	0	-1.259266	-3.523015	-0.410142
25	1	0	-1.614785	-4.242825	-1.143929
26	1	0	-0.560896	-4.014855	0.268408
27	6	0	-2.409153	-2.925367	0.380401
28	1	0	-2.768204	-3.563604	1.185799
29	6	0	-3.147021	-0.634928	0.657961
30	6	0	-3.903768	-1.367317	-0.460074
31	6	0	-4.048871	-0.799063	1.897825
32	1	0	-4.310115	-1.847536	2.050971
33	1	0	-3.542774	-0.447064	2.796696
34	1	0	-4.970878	-0.235898	1.760818
35	8	0	-3.489660	-2.657820	-0.512612
36	8	0	-4.757048	-0.941587	-1.165377
37	6	0	-2.903923	0.817290	0.296360
38	6	0	-3.072175	1.840301	1.228556
39	6	0	-2.612793	1.167045	-1.023940
40	6	0	-2.992916	3.175198	0.845203
41	1	0	-3.314215	1.611397	2.257606
42	6	0	-2.543077	2.497482	-1.410679
43	1	0	-2.509344	0.393439	-1.776820
44	6	0	-2.745271	3.508383	-0.478602
45	1	0	-3.157200	3.952613	1.580299
46	1	0	-2.367315	2.746371	-2.450042
47	1	0	-2.719783	4.546099	-0.785083
48	6	0	3.981814	-0.313339	0.333728
49	6	0	4.898675	-0.278327	1.384805
50	6	0	4.398537	-0.797028	-0.906419
51	6	0	6.200033	-0.722840	1.205807
52	1	0	4.587269	0.095628	2.354076
53	6	0	5.701281	-1.238512	-1.086690
54	1	0	3.712899	-0.846496	-1.743400
55	6	0	6.605427	-1.202298	-0.032641
56	1	0	6.896580	-0.696256	2.033557
57	1	0	6.010659	-1.615680	-2.052745
58	1	0	7.620168	-1.549407	-0.175951

TS1-*E-endo*





E(RM062X) = -1250.53499870

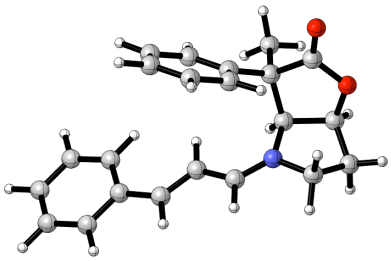
Zero-point correction=	0.492422 (Hartree/Particle)
Thermal correction to Energy=	0.517310
Thermal correction to Enthalpy=	0.518254
Thermal correction to Gibbs Free Energy=	0.436382
Sum of electronic and zero-point Energies=	-1250.042577
Sum of electronic and thermal Energies=	-1250.017689
Sum of electronic and thermal Enthalpies=	-1250.016745
Sum of electronic and thermal Free Energies=	-1250.098617

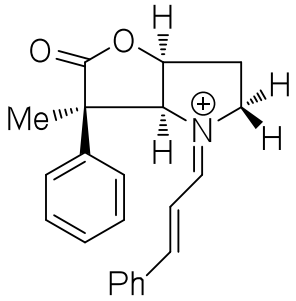
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.438603	3.229453	0.911253
2	6	0	-2.793694	2.821074	0.450071
3	6	0	-3.042746	1.618336	1.332799
4	6	0	-2.242275	1.824982	2.478461
5	6	0	-1.237774	2.751211	2.193202
6	6	0	-2.051041	0.285760	0.384032
7	6	0	-0.964584	0.944874	-0.270009
8	6	0	0.309733	0.859017	0.271306
9	7	0	1.441349	1.195118	-0.317253
10	1	0	-2.917653	2.675955	-0.618745
11	1	0	-3.495509	3.606055	0.765386
12	1	0	-1.739112	-0.357417	1.200992
13	1	0	-1.084080	1.300090	-1.284186
14	1	0	-4.024334	1.169682	1.409358
15	1	0	-0.813726	3.951717	0.403257
16	1	0	0.414072	0.443779	1.269932
17	1	0	-0.410849	3.005898	2.840228
18	1	0	-2.333089	1.265237	3.400040
19	6	0	1.520009	1.827574	-1.640304
20	1	0	0.723905	2.564695	-1.743532
21	1	0	1.410421	1.072624	-2.423979

22	6	0	2.913427	2.447486	-1.633554
23	1	0	3.327335	2.577688	-2.630737
24	1	0	2.899732	3.411949	-1.123907
25	6	0	3.725976	1.456248	-0.819701
26	1	0	4.645026	1.871736	-0.410063
27	6	0	2.768020	0.907327	0.253543
28	1	0	2.873010	1.395782	1.223148
29	6	0	3.141698	-0.596477	0.326058
30	6	0	3.687417	-0.847749	-1.083707
31	6	0	4.359982	-0.749012	1.256357
32	1	0	4.131048	-0.404374	2.264108
33	1	0	4.658462	-1.795646	1.295665
34	1	0	5.206737	-0.166281	0.889408
35	8	0	4.048654	0.335751	-1.645491
36	8	0	3.840120	-1.886864	-1.634932
37	6	0	1.990310	-1.507040	0.692827
38	6	0	1.712634	-1.794206	2.028943
39	6	0	1.117012	-1.981298	-0.286902
40	6	0	0.580349	-2.520477	2.378640
41	1	0	2.378356	-1.457572	2.812959
42	6	0	-0.014135	-2.707944	0.059887
43	1	0	1.322122	-1.793732	-1.333762
44	6	0	-0.288901	-2.975397	1.394944
45	1	0	0.388230	-2.743872	3.420377
46	1	0	-0.676959	-3.070602	-0.715568
47	1	0	-1.161971	-3.555930	1.665399
48	6	0	-3.120397	-0.366037	-0.429851
49	6	0	-3.509207	0.099654	-1.685324
50	6	0	-3.763187	-1.484039	0.102673
51	6	0	-4.516518	-0.542404	-2.391389
52	1	0	-3.024987	0.958719	-2.133605
53	6	0	-4.767995	-2.127950	-0.604116
54	1	0	-3.466749	-1.853698	1.078478
55	6	0	-5.148521	-1.656525	-1.853648
56	1	0	-4.805911	-0.174324	-3.367107
57	1	0	-5.253124	-2.997607	-0.180318
58	1	0	-5.931973	-2.156123	-2.408019

---

1 - *Z*-iminium ion





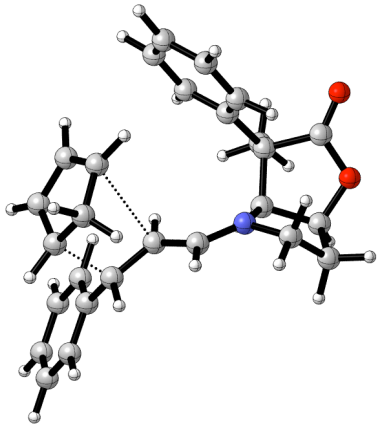
E(RM062X) = -1056.47219360

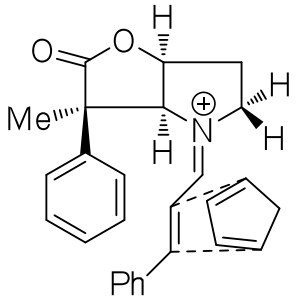
Zero-point correction=	0.396479 (Hartree/Particle)
Thermal correction to Energy=	0.416979
Thermal correction to Enthalpy=	0.417923
Thermal correction to Gibbs Free Energy=	0.346964
Sum of electronic and zero-point Energies=	-1056.075714
Sum of electronic and thermal Energies=	-1056.055214
Sum of electronic and thermal Enthalpies=	-1056.054270
Sum of electronic and thermal Free Energies=	-1056.125230

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.692849	-2.115711	-1.088012
2	6	0	-3.695768	-2.388213	0.024447
3	6	0	-3.517058	-1.176316	0.926155
4	6	0	-2.014294	-0.822249	0.863120
5	6	0	-3.389249	1.006097	0.144800
6	6	0	-2.008018	0.728560	0.753804
7	1	0	-3.071848	-1.365947	-1.786713
8	1	0	-4.718544	-2.465374	-0.336759
9	8	0	-4.198757	-0.068391	0.342877
10	7	0	-1.552097	-1.540710	-0.340853
11	1	0	-1.453111	-1.175683	1.727279
12	1	0	-3.881054	-1.324417	1.941085
13	6	0	-0.888505	1.313584	-0.078436
14	6	0	0.248053	1.863137	0.511500
15	6	0	-0.951297	1.247097	-1.471127
16	6	0	1.317666	2.285375	-0.267896
17	1	0	0.312200	1.969941	1.586908
18	6	0	0.116788	1.663983	-2.251478
19	1	0	-1.851536	0.886508	-1.956971
20	6	0	1.262451	2.171427	-1.649752
21	1	0	2.193437	2.708689	0.207274
22	1	0	0.046332	1.613880	-3.330491
23	1	0	2.094304	2.504180	-2.256904
24	1	0	-3.432660	-3.298540	0.564688
25	1	0	-2.369881	-2.996922	-1.636365
26	6	0	-0.312660	-1.685062	-0.699130
27	1	0	-0.157009	-2.210521	-1.637856

28	6	0	0.822841	-1.238747	0.014226
29	1	0	0.695576	-0.775034	0.981264
30	6	0	2.042215	-1.338017	-0.572370
31	1	0	2.089901	-1.792797	-1.559704
32	6	0	3.304069	-0.885401	-0.038142
33	6	0	4.461675	-1.094327	-0.800273
34	6	0	3.411416	-0.237562	1.202810
35	6	0	5.696385	-0.675756	-0.334489
36	1	0	4.384814	-1.591126	-1.760426
37	6	0	4.644197	0.177291	1.665227
38	1	0	2.529596	-0.056746	1.804336
39	6	0	5.787525	-0.040479	0.897324
40	1	0	6.585212	-0.843135	-0.927780
41	1	0	4.724544	0.672929	2.623591
42	1	0	6.751458	0.287316	1.264811
43	6	0	-2.081241	1.292740	2.183897
44	1	0	-2.144795	2.379348	2.144526
45	1	0	-2.963795	0.918090	2.705381
46	1	0	-1.203721	1.005561	2.763407
47	8	0	-3.761344	1.996649	-0.387359

TS1-*Z*-*exo*-top





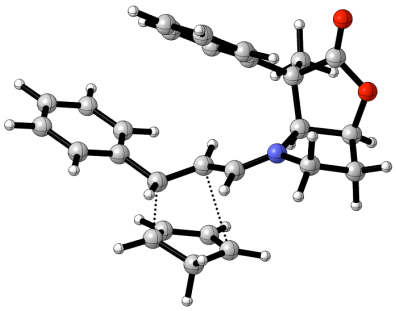
E(RM062X) = -1250.53111571

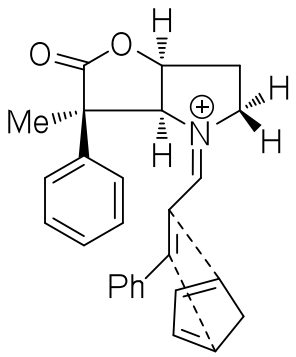
Zero-point correction=	0.492388 (Hartree/Particle)
Thermal correction to Energy=	0.517120
Thermal correction to Enthalpy=	0.518064
Thermal correction to Gibbs Free Energy=	0.437558
Sum of electronic and zero-point Energies=	-1250.038727
Sum of electronic and thermal Energies=	-1250.013996
Sum of electronic and thermal Enthalpies=	-1250.013051
Sum of electronic and thermal Free Energies=	-1250.093558

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.438427	2.635394	0.201077
2	6	0	2.776950	2.274338	-0.053831
3	6	0	2.886138	1.726572	-1.334380
4	6	0	1.626796	2.119612	-2.065249
5	6	0	0.705563	2.429393	-0.937964
6	6	0	2.470732	-0.187460	-0.944638
7	6	0	1.117313	-0.293414	-0.523372
8	6	0	0.144936	-0.671612	-1.431711
9	7	0	-1.062962	-1.146003	-1.168952
10	1	0	0.871269	-0.244307	0.528858
11	1	0	2.636493	-0.466409	-1.982550
12	1	0	1.836982	3.063606	-2.587367
13	1	0	1.248354	1.422367	-2.808474
14	1	0	-0.361206	2.573238	-1.038890
15	1	0	3.840668	1.610209	-1.831070
16	1	0	0.391372	-0.651258	-2.490414
17	1	0	1.046111	2.972767	1.148209
18	1	0	3.584543	2.321959	0.664124
19	6	0	3.580297	-0.627370	-0.058885
20	6	0	3.507194	-0.527411	1.331467
21	6	0	4.732812	-1.153185	-0.638760
22	6	0	4.563111	-0.951582	2.121138
23	1	0	2.627421	-0.105885	1.804678
24	6	0	5.790877	-1.581566	0.152646
25	1	0	4.801278	-1.235472	-1.718057
26	6	0	5.707889	-1.481842	1.533340
27	1	0	4.496609	-0.870681	3.198349
28	1	0	6.677770	-1.993046	-0.311068
29	1	0	6.530447	-1.814267	2.152760
30	6	0	-1.910707	-1.768165	-2.199631
31	1	0	-2.827532	-1.188818	-2.325304
32	1	0	-1.382979	-1.802785	-3.149983
33	6	0	-1.471190	-1.588846	0.168052
34	1	0	-0.575748	-1.872872	0.720967
35	6	0	-2.204329	-3.135028	-1.589989
36	1	0	-3.090801	-3.612184	-2.001724
37	1	0	-1.346013	-3.796393	-1.715963
38	6	0	-2.391862	-2.805824	-0.115602
39	1	0	-2.200451	-3.647774	0.547491
40	6	0	-2.361991	-0.635009	0.999386
41	6	0	-3.782610	-1.135035	0.685349
42	8	0	-3.725897	-2.354841	0.097487
43	8	0	-4.807024	-0.591340	0.932280
44	6	0	-2.142985	-0.971374	2.483585
45	1	0	-1.120275	-0.741922	2.785803

46	1	0	-2.837898	-0.405381	3.102432
47	1	0	-2.313580	-2.034720	2.663806
48	6	0	-2.270788	0.849882	0.694817
49	6	0	-1.717916	1.756234	1.594989
50	6	0	-2.863551	1.350502	-0.467202
51	6	0	-1.777396	3.125753	1.353328
52	1	0	-1.274591	1.410326	2.519631
53	6	0	-2.924836	2.713540	-0.711903
54	1	0	-3.348260	0.673546	-1.161292
55	6	0	-2.387178	3.609798	0.206007
56	1	0	-1.373912	3.815618	2.084266
57	1	0	-3.422256	3.078317	-1.601348
58	1	0	-2.459893	4.675916	0.034276

TS1-*Z-exo*





E(RM062X) = -1250.53457159

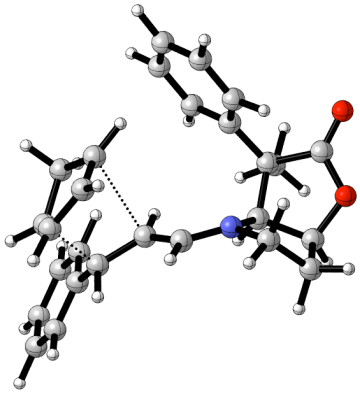
Zero-point correction=	0.492168 (Hartree/Particle)
Thermal correction to Energy=	0.516850
Thermal correction to Enthalpy=	0.517794
Thermal correction to Gibbs Free Energy=	0.437827
Sum of electronic and zero-point Energies=	-1250.042404
Sum of electronic and thermal Energies=	-1250.017722
Sum of electronic and thermal Enthalpies=	-1250.016778
Sum of electronic and thermal Free Energies=	-1250.096745

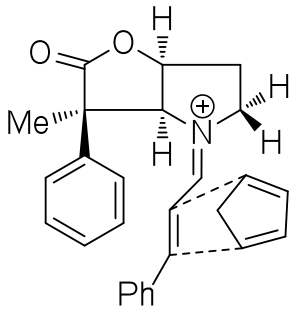
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.642816	3.257359	1.370853
2	6	0	-2.848162	2.713202	0.901397
3	6	0	-2.795408	2.575226	-0.497528
4	6	0	-1.680976	3.490830	-0.950800

5	6	0	-0.858755	3.580349	0.287460
6	6	0	-1.935287	0.858905	-0.746752
7	6	0	-0.617602	0.931493	-0.216599
8	6	0	0.477485	1.204891	-1.021562
9	7	0	1.747151	1.115146	-0.674949
10	1	0	-0.445243	0.589057	0.794189
11	1	0	-1.978133	0.905280	-1.832815
12	1	0	-2.126675	4.480728	-1.120404
13	1	0	-1.155015	3.210309	-1.859161
14	1	0	0.135054	4.005570	0.329837
15	1	0	-3.696549	2.435922	-1.081616
16	1	0	0.311511	1.506950	-2.052257
17	1	0	-1.362234	3.360125	2.409034
18	1	0	-3.658756	2.359924	1.523470
19	6	0	2.871114	1.531078	-1.528538
20	1	0	2.538321	2.267126	-2.257150
21	1	0	3.278553	0.664236	-2.055024
22	6	0	3.865944	2.067444	-0.505142
23	1	0	4.891993	2.074297	-0.865704
24	1	0	3.587208	3.075483	-0.194119
25	6	0	2.206885	0.687239	0.646957
26	1	0	1.619160	1.196699	1.413363
27	6	0	3.696231	1.102805	0.660409
28	1	0	4.020844	1.509948	1.616576
29	6	0	2.244853	-0.849849	0.881017
30	6	0	2.193946	-1.103328	2.395382
31	1	0	1.250175	-0.754343	2.816066
32	1	0	2.302666	-2.168415	2.595763
33	1	0	3.003001	-0.574600	2.903590
34	6	0	3.676416	-1.207935	0.456490
35	8	0	4.437508	-0.083852	0.393283
36	8	0	4.117152	-2.286854	0.241271
37	6	0	1.227884	-1.646562	0.089029
38	6	0	0.069245	-2.150030	0.673230
39	6	0	1.424699	-1.845082	-1.278207
40	6	0	-0.886228	-2.804620	-0.095235
41	1	0	-0.106271	-2.038976	1.735800
42	6	0	0.472120	-2.493774	-2.048578
43	1	0	2.345322	-1.514664	-1.746759
44	6	0	-0.693595	-2.968379	-1.458110
45	1	0	-1.786967	-3.179568	0.375251
46	1	0	0.649332	-2.648512	-3.105234
47	1	0	-1.437693	-3.480945	-2.054222
48	6	0	-2.887959	-0.141557	-0.186462
49	6	0	-3.707398	-0.854025	-1.056433
50	6	0	-2.953745	-0.412516	1.180190
51	6	0	-4.567418	-1.833587	-0.573827
52	1	0	-3.660368	-0.656893	-2.121618

53	6	0	-3.814928	-1.383471	1.664586
54	1	0	-2.328016	0.137266	1.875822
55	6	0	-4.621758	-2.101393	0.786074
56	1	0	-5.195007	-2.384809	-1.261965
57	1	0	-3.858958	-1.584915	2.727228
58	1	0	-5.293308	-2.860908	1.164458

TS1-*Z-endo*-top





E(RM062X) = -1250.53251228

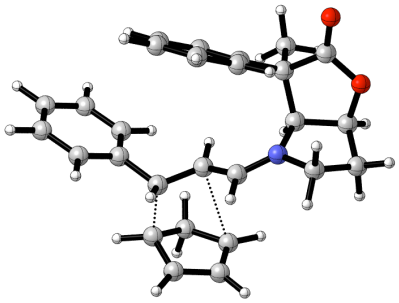
Zero-point correction=	0.492726 (Hartree/Particle)
Thermal correction to Energy=	0.517408
Thermal correction to Enthalpy=	0.518353
Thermal correction to Gibbs Free Energy=	0.437882
Sum of electronic and zero-point Energies=	-1250.039786
Sum of electronic and thermal Energies=	-1250.015104
Sum of electronic and thermal Enthalpies=	-1250.014160
Sum of electronic and thermal Free Energies=	-1250.094630

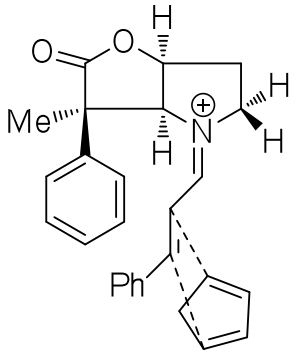
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.709230	2.278979	1.137408
2	6	0	-1.908576	2.219386	0.262732
3	6	0	-2.909268	1.549443	1.176693
4	6	0	-2.450132	1.804037	2.485988
5	6	0	-1.103677	2.183000	2.455297
6	6	0	-2.426354	-0.306297	0.956426
7	6	0	-1.040665	-0.359670	0.611387
8	6	0	-0.048944	-0.551345	1.554990
9	7	0	1.195936	-0.937871	1.312172

10	1	0	-1.753363	1.777795	-0.716949
11	1	0	-2.248873	3.253637	0.109153
12	1	0	-2.660281	-0.680263	1.946586
13	1	0	-0.757901	-0.352025	-0.433078
14	1	0	-3.966459	1.531305	0.948102
15	1	0	0.287430	2.500819	0.784279
16	1	0	-0.292558	-0.427628	2.607043
17	1	0	-0.467031	2.321839	3.317266
18	1	0	-3.032614	1.635427	3.382770
19	6	0	2.162131	-1.249800	2.374871
20	1	0	1.682337	-1.185528	3.349299
21	1	0	2.989315	-0.536959	2.340611
22	6	0	2.623909	-2.652097	1.991363
23	1	0	3.589221	-2.923002	2.412999
24	1	0	1.878652	-3.389414	2.292837
25	6	0	2.689284	-2.577604	0.472368
26	1	0	2.586816	-3.544773	-0.016812
27	6	0	1.594202	-1.564575	0.047253
28	1	0	0.717483	-2.057054	-0.375171
29	6	0	2.297440	-0.680056	-1.007900
30	6	0	3.788034	-0.924813	-0.721845
31	6	0	2.057611	-1.318433	-2.388445
32	1	0	0.995523	-1.325271	-2.635704
33	1	0	2.603282	-0.767044	-3.152814
34	1	0	2.405245	-2.353607	-2.397386
35	8	0	3.934225	-2.003868	0.082948
36	8	0	4.713209	-0.317648	-1.149654
37	6	0	1.989165	0.808180	-0.983291
38	6	0	1.069244	1.376991	-1.863088
39	6	0	2.699639	1.657333	-0.131897
40	6	0	0.886071	2.755125	-1.913538
41	1	0	0.519161	0.754595	-2.558206
42	6	0	2.528729	3.033773	-0.187991
43	1	0	3.446461	1.251483	0.540101
44	6	0	1.626667	3.589538	-1.087828
45	1	0	0.189246	3.176545	-2.627383
46	1	0	3.121461	3.673531	0.453072
47	1	0	1.512643	4.663886	-1.152830
48	6	0	-3.440613	-0.748356	-0.046914
49	6	0	-3.262630	-0.576179	-1.419961
50	6	0	-4.621461	-1.331281	0.411717
51	6	0	-4.242546	-0.985937	-2.311711
52	1	0	-2.357230	-0.125539	-1.809435
53	6	0	-5.600003	-1.744971	-0.480514
54	1	0	-4.772386	-1.468713	1.476750
55	6	0	-5.413321	-1.571317	-1.845043
56	1	0	-4.092228	-0.850098	-3.374857
57	1	0	-6.507355	-2.203412	-0.109623

58	1	0	-6.175244	-1.891620	-2.543333

TS1-*Z-endo*





E(RM062X) = -1250.53391661

Zero-point correction=	0.492537 (Hartree/Particle)
Thermal correction to Energy=	0.517156
Thermal correction to Enthalpy=	0.518100
Thermal correction to Gibbs Free Energy=	0.438260
Sum of electronic and zero-point Energies=	-1250.041380
Sum of electronic and thermal Energies=	-1250.016761
Sum of electronic and thermal Enthalpies=	-1250.015817
Sum of electronic and thermal Free Energies=	-1250.095657

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.900748	3.425006	0.745741
2	6	0	-2.176290	2.820856	1.217272
3	6	0	-2.834461	2.485556	-0.103371
4	6	0	-2.282938	3.397831	-1.033651
5	6	0	-1.086764	3.913608	-0.536461
6	6	0	-1.939444	0.852320	-0.527714
7	6	0	-0.626008	0.926226	0.029159
8	6	0	0.466431	1.310825	-0.737526
9	7	0	1.738380	1.176346	-0.423074
10	1	0	-2.091305	2.015427	1.939282
11	1	0	-2.767112	3.624713	1.678702
12	1	0	-1.966871	0.889054	-1.611357
13	1	0	-0.446894	0.484713	0.999592
14	1	0	-3.876328	2.197613	-0.155424
15	1	0	-0.053553	3.636986	1.384292
16	1	0	0.282060	1.766228	-1.707173

17	1	0	-0.392895	4.537591	-1.081652
18	1	0	-2.680349	3.581593	-2.023163
19	6	0	2.846589	1.740524	-1.211322
20	1	0	3.242868	0.980490	-1.889531
21	1	0	2.498875	2.592273	-1.791779
22	6	0	2.222458	0.533173	0.800844
23	1	0	1.656225	0.907710	1.655578
24	6	0	3.861327	2.092151	-0.129683
25	1	0	4.879981	2.165457	-0.503599
26	1	0	3.589125	3.028636	0.359658
27	6	0	3.713906	0.937087	0.850579
28	1	0	4.064462	1.167012	1.855355
29	6	0	2.258117	-1.020647	0.772722
30	6	0	3.671685	-1.301379	0.243122
31	6	0	2.261579	-1.523817	2.224693
32	1	0	3.094726	-1.091511	2.782565
33	1	0	1.338096	-1.246751	2.734310
34	1	0	2.366489	-2.607873	2.239368
35	8	0	4.439363	-0.185540	0.357325
36	8	0	4.096643	-2.325251	-0.175971
37	6	0	1.205974	-1.672162	-0.100956
38	6	0	0.061184	-2.253673	0.436545
39	6	0	1.352097	-1.647254	-1.488693
40	6	0	-0.930985	-2.764709	-0.391843
41	1	0	-0.075580	-2.314952	1.508717
42	6	0	0.363013	-2.153224	-2.318044
43	1	0	2.259873	-1.251669	-1.931064
44	6	0	-0.788746	-2.706335	-1.769497
45	1	0	-1.821492	-3.200497	0.045088
46	1	0	0.500830	-2.136235	-3.391684
47	1	0	-1.561022	-3.108005	-2.412991
48	6	0	-2.890881	-0.170887	0.002859
49	6	0	-3.802574	-0.748847	-0.878944
50	6	0	-2.891876	-0.581898	1.335271
51	6	0	-4.683378	-1.730123	-0.446618
52	1	0	-3.808655	-0.441820	-1.918940
53	6	0	-3.776622	-1.557573	1.771071
54	1	0	-2.189388	-0.164425	2.046589
55	6	0	-4.672386	-2.137877	0.880782
56	1	0	-5.377401	-2.176722	-1.146775
57	1	0	-3.764066	-1.869918	2.807347
58	1	0	-5.358955	-2.901756	1.221352

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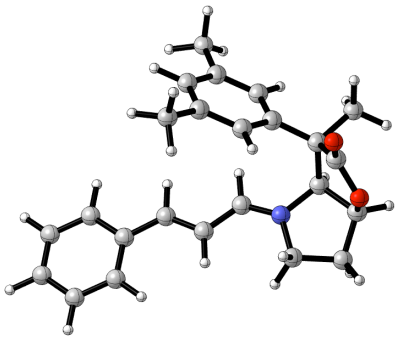
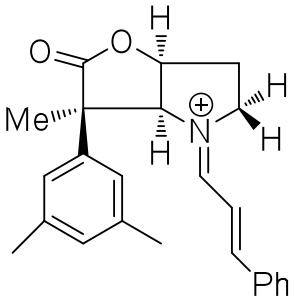
2 - *E*-iminium ion





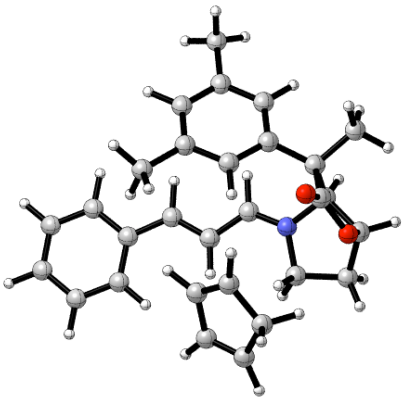
E(RM062X) = -1135.09555028

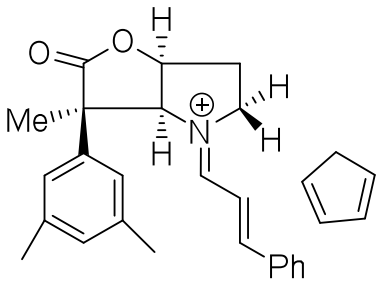
Zero-point correction=	0.451371 (Hartree/Particle)
Thermal correction to Energy=	0.475804
Thermal correction to Enthalpy=	0.476748
Thermal correction to Gibbs Free Energy=	0.395687
Sum of electronic and zero-point Energies=	-1134.644179
Sum of electronic and thermal Energies=	-1134.619746
Sum of electronic and thermal Enthalpies=	-1134.618802
Sum of electronic and thermal Free Energies=	-1134.699863

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.287408	-2.804014	-0.171312
2	6	0	2.669301	-3.266025	-0.616291
3	6	0	3.480203	-1.983283	-0.598974
4	6	0	2.519651	-0.872106	-1.052356
5	6	0	3.462842	-0.386996	1.086187
6	1	0	1.217064	-2.718627	0.915858
7	1	0	3.094775	-4.016553	0.045682
8	8	0	3.808765	-1.661021	0.753188
9	7	0	1.186597	-1.453740	-0.765010
10	1	0	2.587816	-0.630850	-2.112559
11	1	0	4.393394	-2.032360	-1.189300
12	6	0	1.766012	1.270128	0.146173
13	6	0	1.475359	2.318040	-0.727187
14	6	0	0.895037	1.009220	1.200600
15	6	0	0.324063	3.086114	-0.570882
16	1	0	2.141511	2.550652	-1.548911
17	6	0	-0.269529	1.755211	1.376069
18	1	0	1.114801	0.213818	1.904546
19	6	0	-0.545579	2.778570	0.475509
20	1	0	2.632441	-3.663350	-1.631419
21	1	0	0.481126	-3.432333	-0.542158
22	6	0	0.073927	-0.810537	-0.955658
23	1	0	0.159455	0.162394	-1.431386
24	6	0	-1.216770	-1.259995	-0.582585
25	1	0	-1.338819	-2.219487	-0.099629
26	6	0	-2.260816	-0.414083	-0.775317

27	1	0	-2.040059	0.545366	-1.239495
28	6	0	-3.641688	-0.618300	-0.409195
29	6	0	-4.102209	-1.799156	0.194055
30	6	0	-4.551755	0.417354	-0.664128
31	6	0	-5.435362	-1.934595	0.525688
32	1	0	-3.419450	-2.613676	0.399244
33	6	0	-5.887506	0.279109	-0.328812
34	1	0	-4.200615	1.330745	-1.130326
35	6	0	-6.328670	-0.896285	0.265748
36	1	0	-5.787857	-2.847024	0.987767
37	1	0	-6.583922	1.081952	-0.530042
38	1	0	-7.372793	-1.008563	0.528114
39	8	0	3.629834	0.053278	2.173831
40	6	0	2.911124	0.329395	-0.151389
41	6	0	4.130492	1.025825	-0.785905
42	1	0	3.896264	1.400953	-1.781120
43	1	0	4.437467	1.857572	-0.153582
44	1	0	4.972519	0.337577	-0.876694
45	1	0	-1.448678	3.367154	0.602485
46	6	0	-1.195403	1.458335	2.523000
47	1	0	-0.814933	1.903860	3.444377
48	1	0	-2.191125	1.861911	2.342480
49	1	0	-1.283126	0.383981	2.690479
50	6	0	0.042666	4.245183	-1.487072
51	1	0	-1.028336	4.388685	-1.628114
52	1	0	0.443599	5.166828	-1.059919
53	1	0	0.505728	4.104839	-2.463252

2-*E* and Cyclopentadiene Adduct





E(RM062X) = -1329.18410204

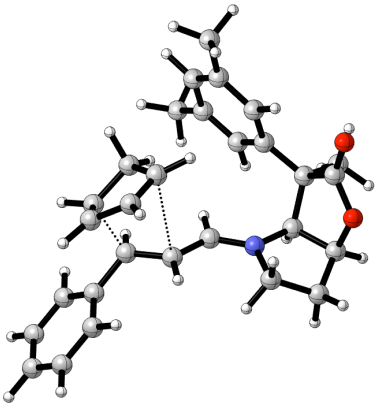
Zero-point correction=	0.546006 (Hartree/Particle)
Thermal correction to Energy=	0.576238
Thermal correction to Enthalpy=	0.577182
Thermal correction to Gibbs Free Energy=	0.481940
Sum of electronic and zero-point Energies=	-1328.638096
Sum of electronic and thermal Energies=	-1328.607864

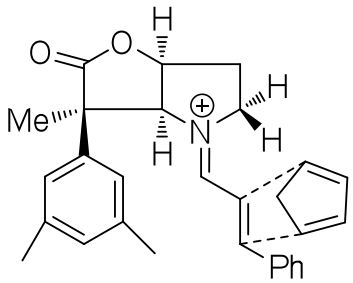
Sum of electronic and thermal Enthalpies= -1328.606920
Sum of electronic and thermal Free Energies= -1328.702162

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.658003	-2.456339	-1.970004
2	6	0	-1.353037	-3.703988	-1.515571
3	6	0	-0.321790	-4.380289	-0.662472
4	6	0	0.799036	-3.639967	-0.654039
5	6	0	0.588149	-2.433882	-1.465787
6	6	0	2.278988	0.492695	1.110696
7	6	0	1.211859	-0.320230	1.300303
8	6	0	-0.064595	0.280753	1.459530
9	7	0	-1.181831	-0.373532	1.553238
10	1	0	-2.290684	-3.488931	-0.987314
11	1	0	-1.631993	-4.331857	-2.369378
12	1	0	2.102300	1.566102	1.154568
13	1	0	1.288199	-1.397680	1.233692
14	1	0	-0.468257	-5.334181	-0.176942
15	1	0	-1.115056	-1.735290	-2.632943
16	1	0	-0.128811	1.364623	1.485112
17	1	0	1.338173	-1.673305	-1.643320
18	1	0	1.726199	-3.900960	-0.161316
19	6	0	-1.267795	-1.851319	1.613919
20	1	0	-1.107550	-2.249848	0.612093
21	1	0	-0.499036	-2.235549	2.280356
22	6	0	-2.521262	0.261905	1.504081
23	1	0	-2.653396	0.916239	2.365193
24	6	0	-2.683887	-2.091000	2.115865
25	1	0	-3.073994	-3.060517	1.813597
26	1	0	-2.733887	-2.009824	3.202566
27	6	0	-3.461013	-0.953555	1.483998
28	1	0	-4.427460	-0.763560	1.946995
29	6	0	-2.841262	0.974166	0.163973
30	6	0	-3.248821	-0.218274	-0.708318
31	6	0	-4.135216	1.792812	0.350487
32	1	0	-4.975295	1.150897	0.619412
33	1	0	-4.018548	2.538342	1.135670
34	1	0	-4.376922	2.296243	-0.584324
35	8	0	-3.649813	-1.241684	0.094232
36	8	0	-3.284171	-0.292698	-1.892284
37	6	0	-1.695741	1.793839	-0.384773
38	6	0	-1.501695	3.101662	0.058144
39	6	0	-0.736153	1.211288	-1.208048
40	6	0	-0.361227	3.819585	-0.295797
41	1	0	-2.236766	3.584456	0.690519

42	6	0	0.418191	1.901919	-1.570628
43	1	0	-0.870278	0.197743	-1.563135
44	6	0	0.594792	3.198843	-1.099216
45	1	0	1.485959	3.750559	-1.382021
46	6	0	3.636904	0.099272	0.808170
47	6	0	4.590751	1.106563	0.610236
48	6	0	4.024292	-1.243129	0.677763
49	6	0	5.900612	0.784030	0.298277
50	1	0	4.294932	2.144963	0.706620
51	6	0	5.331478	-1.561683	0.366497
52	1	0	3.303159	-2.037107	0.825233
53	6	0	6.270441	-0.549314	0.176007
54	1	0	6.631902	1.567238	0.150185
55	1	0	5.627717	-2.597677	0.269258
56	1	0	7.293574	-0.804880	-0.067825
57	6	0	1.467450	1.235222	-2.417274
58	1	0	1.025690	0.482051	-3.069827
59	1	0	1.996113	1.958999	-3.036671
60	1	0	2.210311	0.736884	-1.785938
61	6	0	-0.185109	5.247118	0.143598
62	1	0	0.867559	5.492983	0.280235
63	1	0	-0.585786	5.925079	-0.613055
64	1	0	-0.711392	5.445337	1.076770

TS2-*E*-*exo*-top





E(RM062X) = -1329.15885592

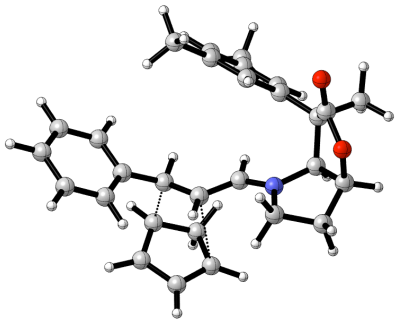
Zero-point correction=	0.547314 (Hartree/Particle)
Thermal correction to Energy=	0.575883
Thermal correction to Enthalpy=	0.576827
Thermal correction to Gibbs Free Energy=	0.487089
Sum of electronic and zero-point Energies=	-1328.611542

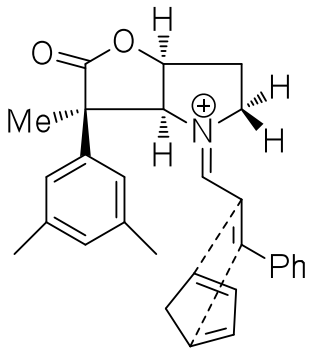
Sum of electronic and thermal Energies= -1328.582973
Sum of electronic and thermal Enthalpies= -1328.582029
Sum of electronic and thermal Free Energies= -1328.671767

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.659747	0.465858	-2.751157
2	6	0	2.770485	1.030202	-2.099538
3	6	0	2.364350	1.637005	-0.899023
4	6	0	0.868037	1.809258	-1.010336
5	6	0	0.528758	0.800432	-2.047298
6	6	0	2.454090	0.177053	0.374043
7	6	0	1.501194	-0.810935	-0.004478
8	6	0	0.241811	-0.838936	0.565001
9	7	0	-0.665913	-1.790328	0.401788
10	1	0	1.799005	-1.602328	-0.677277
11	1	0	2.132097	0.796600	1.208431
12	1	0	0.680463	2.802823	-1.443190
13	1	0	0.286005	1.753415	-0.093571
14	1	0	-0.482227	0.484255	-2.269375
15	1	0	2.993493	2.362755	-0.398953
16	1	0	-0.048745	-0.038643	1.237531
17	1	0	1.698494	-0.161066	-3.629964
18	1	0	3.798817	0.932145	-2.420528
19	6	0	-0.396103	-3.017495	-0.363632
20	1	0	0.635891	-3.328427	-0.210024
21	1	0	-0.561062	-2.835086	-1.429124
22	6	0	-1.397905	-4.012273	0.208144
23	1	0	-1.676090	-4.791345	-0.497850
24	1	0	-1.003894	-4.474682	1.114097
25	6	0	-1.988701	-1.804256	1.059863
26	1	0	-1.871800	-1.763070	2.143853
27	6	0	-2.578460	-3.134121	0.562448
28	1	0	-3.276952	-3.591725	1.260175
29	6	0	-3.014278	-0.773257	0.538862
30	6	0	-4.263941	-0.815756	1.454652
31	1	0	-4.005037	-0.490849	2.461723
32	1	0	-5.016209	-0.137458	1.054527
33	1	0	-4.697006	-1.815273	1.509575
34	6	0	-3.471403	-1.451980	-0.755566
35	8	0	-3.269944	-2.789081	-0.642837
36	8	0	-3.986092	-0.977815	-1.717210
37	6	0	-2.542414	0.666835	0.434662
38	6	0	-2.127862	1.303896	1.612738
39	6	0	-2.592099	1.405689	-0.738666
40	6	0	-1.783120	2.647834	1.630953

41	1	0	-2.094207	0.747504	2.545263
42	6	0	-2.250951	2.764181	-0.747912
43	1	0	-2.946954	0.949728	-1.653013
44	6	0	-1.856804	3.368534	0.434995
45	1	0	-1.604992	4.424263	0.438038
46	6	0	3.903211	-0.160707	0.454284
47	6	0	4.684257	0.458674	1.426851
48	6	0	4.502933	-1.072381	-0.415199
49	6	0	6.037973	0.167297	1.538773
50	1	0	4.229137	1.169055	2.108434
51	6	0	5.853200	-1.362298	-0.305869
52	1	0	3.918691	-1.557210	-1.189401
53	6	0	6.624573	-0.743583	0.673158
54	1	0	6.631448	0.652089	2.302822
55	1	0	6.307875	-2.072992	-0.983787
56	1	0	7.678753	-0.972563	0.757223
57	6	0	-2.327101	3.538771	-2.035592
58	1	0	-1.722542	3.066319	-2.813839
59	1	0	-3.353364	3.573903	-2.404679
60	1	0	-1.978853	4.562449	-1.905348
61	6	0	-1.383496	3.333975	2.909146
62	1	0	-2.191022	3.978318	3.262043
63	1	0	-1.163121	2.614622	3.697110
64	1	0	-0.506298	3.964828	2.761091

TS2-*E-exo*





E(RM062X) = -1329.15946294

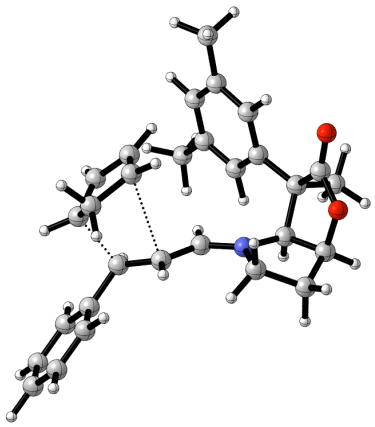
Zero-point correction=	0.547039 (Hartree/Particle)
Thermal correction to Energy=	0.575529
Thermal correction to Enthalpy=	0.576473
Thermal correction to Gibbs Free Energy=	0.487382
Sum of electronic and zero-point Energies=	-1328.612424
Sum of electronic and thermal Energies=	-1328.583934

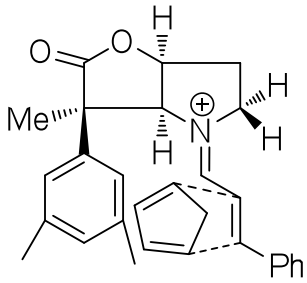
Sum of electronic and thermal Enthalpies= -1328.582990
Sum of electronic and thermal Free Energies= -1328.672081

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.456183	3.644546	0.527691
2	6	0	-3.428576	2.654994	0.749159
3	6	0	-2.946680	1.711606	1.671550
4	6	0	-1.789948	2.382106	2.375905
5	6	0	-1.398725	3.412916	1.374685
6	6	0	-1.973221	0.474467	0.536149
7	6	0	-0.878573	1.171667	-0.045822
8	6	0	0.391473	1.002668	0.481956
9	7	0	1.522380	1.437491	-0.041693
10	1	0	-0.990449	1.646726	-1.010645
11	1	0	-1.679973	-0.178358	1.356726
12	1	0	-2.203008	2.909465	3.246976
13	1	0	-0.991752	1.734795	2.729694
14	1	0	-0.487754	3.993996	1.424968
15	1	0	-3.615918	1.031049	2.182786
16	1	0	0.502272	0.418915	1.391855
17	1	0	-2.511610	4.422674	-0.219608
18	1	0	-4.365375	2.569609	0.215572
19	6	0	-3.009227	-0.159827	-0.324571
20	6	0	-3.393932	0.379608	-1.552187
21	6	0	-3.593659	-1.349108	0.104474
22	6	0	-4.330022	-0.270385	-2.341070
23	1	0	-2.962291	1.311114	-1.901049
24	6	0	-4.533261	-2.000496	-0.684385
25	1	0	-3.299675	-1.774518	1.058066
26	6	0	-4.899204	-1.465068	-1.910718
27	1	0	-4.616909	0.152558	-3.295120
28	1	0	-4.976554	-2.926471	-0.341495
29	1	0	-5.627851	-1.971750	-2.529725
30	6	0	1.600128	2.298306	-1.226586
31	1	0	1.490568	1.699448	-2.135663
32	1	0	0.802734	3.041015	-1.191941
33	6	0	2.847585	1.020436	0.442692
34	1	0	2.964364	1.293648	1.492192
35	6	0	2.995823	2.901940	-1.106061
36	1	0	3.408367	3.219983	-2.060693
37	1	0	2.985759	3.750407	-0.420357
38	6	0	3.807723	1.769394	-0.500683
39	1	0	4.725810	2.096629	-0.015675
40	6	0	3.196328	-0.472895	0.201053
41	6	0	3.766161	-0.436226	-1.220768

42	8	0	4.134534	0.835115	-1.530216
43	8	0	3.933047	-1.343860	-1.966176
44	6	0	4.392211	-0.843157	1.097581
45	1	0	4.144016	-0.725952	2.151679
46	1	0	4.679895	-1.876767	0.910880
47	1	0	5.251823	-0.204842	0.884169
48	6	0	2.016769	-1.409877	0.348340
49	6	0	1.691552	-1.944534	1.595754
50	6	0	1.166210	-1.647228	-0.726370
51	6	0	0.531340	-2.691981	1.777004
52	1	0	2.343634	-1.790215	2.447053
53	6	0	-0.003458	-2.391714	-0.575993
54	1	0	1.410484	-1.259245	-1.709366
55	6	0	-0.309988	-2.896119	0.682605
56	1	0	-1.210480	-3.488818	0.809859
57	6	0	0.214563	-3.311794	3.111185
58	1	0	-0.860535	-3.341799	3.289700
59	1	0	0.580308	-4.340165	3.146383
60	1	0	0.686394	-2.765987	3.927811
61	6	0	-0.901983	-2.630593	-1.758279
62	1	0	-1.715678	-3.308808	-1.505684
63	1	0	-1.345820	-1.693108	-2.103553
64	1	0	-0.339468	-3.059619	-2.588551

TS2-*E*-*endo*-top





E(RM062X) = -1329.15312061

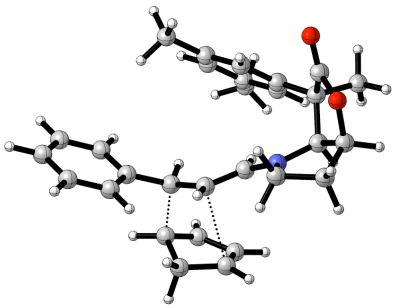
Zero-point correction=	0.547680 (Hartree/Particle)
Thermal correction to Energy=	0.576291
Thermal correction to Enthalpy=	0.577235
Thermal correction to Gibbs Free Energy=	0.487091

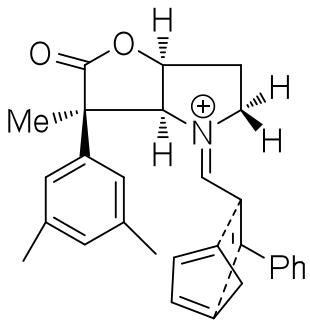
Sum of electronic and zero-point Energies=	-1328.605441
Sum of electronic and thermal Energies=	-1328.576830
Sum of electronic and thermal Enthalpies=	-1328.575886
Sum of electronic and thermal Free Energies=	-1328.666030

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.762282	-0.892787	-2.098900
2	6	0	-2.237984	-1.016657	-2.237974
3	6	0	-2.587604	-1.758088	-0.965936
4	6	0	-1.406420	-2.430334	-0.588642
5	6	0	-0.302462	-1.851371	-1.221574
6	6	0	-2.627902	-0.309716	0.294923
7	6	0	-1.691949	0.676960	-0.145253
8	6	0	-0.433465	0.772972	0.425171
9	7	0	0.418894	1.776009	0.277910
10	1	0	-2.782337	-0.097728	-2.434580
11	1	0	-2.433092	-1.700863	-3.075663
12	1	0	-2.330445	-0.830526	1.199059
13	1	0	-2.020263	1.441146	-0.834150
14	1	0	-3.560990	-2.208777	-0.825102
15	1	0	-0.140367	-0.250457	-2.708888
16	1	0	-0.101822	-0.023973	1.082766
17	1	0	0.732175	-2.069317	-1.007412
18	1	0	-1.353131	-3.206423	0.164243
19	6	0	0.065260	3.000619	-0.461866
20	1	0	0.322821	2.883710	-1.517354
21	1	0	-1.002108	3.191009	-0.370876
22	6	0	1.697278	1.909180	1.016083
23	1	0	1.517419	1.814453	2.087694
24	6	0	0.905914	4.074564	0.213792
25	1	0	1.133723	4.912785	-0.440669
26	1	0	0.406014	4.444960	1.109828
27	6	0	2.155375	3.319817	0.607779
28	1	0	2.752602	3.820904	1.366733
29	6	0	2.880688	1.038772	0.539344
30	6	0	3.316023	1.810532	-0.709962
31	6	0	4.050315	1.228151	1.542970
32	1	0	4.341124	2.273451	1.651088
33	1	0	3.764438	0.835199	2.518806
34	1	0	4.912405	0.667197	1.184975
35	8	0	2.950450	3.110409	-0.563414
36	8	0	3.924958	1.441287	-1.661921
37	6	0	2.653461	-0.456610	0.402871
38	6	0	2.075124	-1.132071	1.483517
39	6	0	3.163662	-1.201985	-0.654239

40	6	0	1.989255	-2.518067	1.515419
41	1	0	1.721846	-0.572355	2.345628
42	6	0	3.103661	-2.599812	-0.640399
43	1	0	3.646243	-0.704412	-1.483454
44	6	0	2.515062	-3.239876	0.442408
45	1	0	2.475594	-4.324186	0.463760
46	6	0	-4.088061	0.008907	0.310331
47	6	0	-4.897322	-0.633988	1.247268
48	6	0	-4.675734	0.902761	-0.584627
49	6	0	-6.260847	-0.385553	1.296468
50	1	0	-4.452602	-1.331424	1.948798
51	6	0	-6.040268	1.148821	-0.538140
52	1	0	-4.078308	1.427228	-1.320144
53	6	0	-6.836620	0.505818	0.400942
54	1	0	-6.873015	-0.886619	2.034901
55	1	0	-6.482771	1.848555	-1.235169
56	1	0	-7.900151	0.701668	0.436141
57	6	0	3.653127	-3.385042	-1.800002
58	1	0	2.942508	-3.393311	-2.630299
59	1	0	4.578806	-2.942694	-2.167216
60	1	0	3.850619	-4.418513	-1.519349
61	6	0	1.405957	-3.232395	2.705080
62	1	0	0.830440	-4.106317	2.398675
63	1	0	2.201330	-3.583853	3.365469
64	1	0	0.758323	-2.577282	3.287943

TS2-*E-endo*





E(RM062X) = -1329.15795587

Zero-point correction=	0.547499 (Hartree/Particle)
Thermal correction to Energy=	0.575854
Thermal correction to Enthalpy=	0.576798
Thermal correction to Gibbs Free Energy=	0.488031
Sum of electronic and zero-point Energies=	-1328.610457

Sum of electronic and thermal Energies= -1328.582102
Sum of electronic and thermal Enthalpies= -1328.581158
Sum of electronic and thermal Free Energies= -1328.669924

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.308530	3.416976	1.152738
2	6	0	-2.674652	3.080918	0.664291
3	6	0	-2.958020	1.827650	1.460912
4	6	0	-2.156718	1.930245	2.618345
5	6	0	-1.126423	2.846420	2.399481
6	6	0	-1.979059	0.546173	0.406791
7	6	0	-0.876056	1.236949	-0.179388
8	6	0	0.394709	1.048534	0.349078
9	7	0	1.538272	1.409933	-0.194650
10	1	0	-2.802271	3.012795	-0.412030
11	1	0	-3.354050	3.861765	1.034074
12	1	0	-1.687889	-0.166189	1.172439
13	1	0	-0.977297	1.690913	-1.155406
14	1	0	-3.948138	1.393181	1.497671
15	1	0	-0.664743	4.159002	0.699973
16	1	0	0.481403	0.519169	1.294168
17	1	0	-0.294825	3.032666	3.063610
18	1	0	-2.265309	1.309910	3.498182
19	6	0	1.654683	2.179737	-1.438579
20	1	0	0.885839	2.951432	-1.467534
21	1	0	1.529627	1.518928	-2.301408
22	6	0	3.069829	2.741960	-1.349168
23	1	0	3.498930	2.975438	-2.320765
24	1	0	3.084768	3.637910	-0.726985
25	6	0	3.838057	1.629241	-0.656337
26	1	0	4.762993	1.959973	-0.187008
27	6	0	2.846052	0.983486	0.329510
28	1	0	2.965129	1.327415	1.357512
29	6	0	3.142611	-0.535079	0.197612
30	6	0	3.726546	-0.619683	-1.216825
31	6	0	4.315301	-0.881447	1.133007
32	1	0	4.060257	-0.681032	2.172908
33	1	0	4.569190	-1.934802	1.023504
34	1	0	5.198608	-0.289302	0.886034
35	8	0	4.140523	0.613047	-1.612703
36	8	0	3.867667	-1.583876	-1.893030
37	6	0	1.930573	-1.421058	0.391090
38	6	0	1.588353	-1.889290	1.660117
39	6	0	1.071235	-1.676361	-0.672704
40	6	0	0.404563	-2.590632	1.872272

41	1	0	2.245477	-1.719621	2.504459
42	6	0	-0.122780	-2.373881	-0.491514
43	1	0	1.327665	-1.339856	-1.671727
44	6	0	-0.444100	-2.814333	0.787354
45	6	0	-3.056960	-0.013134	-0.460482
46	6	0	-3.390244	0.528189	-1.701592
47	6	0	-3.751909	-1.134323	-0.006188
48	6	0	-4.388067	-0.048685	-2.474476
49	1	0	-2.865765	1.392916	-2.089528
50	6	0	-4.749074	-1.711440	-0.778258
51	1	0	-3.498061	-1.562558	0.957782
52	6	0	-5.068564	-1.170086	-2.016815
53	1	0	-4.631843	0.375935	-3.439658
54	1	0	-5.274671	-2.585193	-0.415194
55	1	0	-5.843763	-1.619470	-2.623324
56	1	0	-1.364609	-3.369193	0.940006
57	6	0	-1.025791	-2.637634	-1.665135
58	1	0	-1.914151	-3.191142	-1.364629
59	1	0	-1.355316	-1.700711	-2.121032
60	1	0	-0.501828	-3.214176	-2.429125
61	6	0	0.068931	-3.140704	3.232135
62	1	0	0.404643	-4.176656	3.313868
63	1	0	0.556257	-2.572871	4.024289
64	1	0	-1.006663	-3.131718	3.409660

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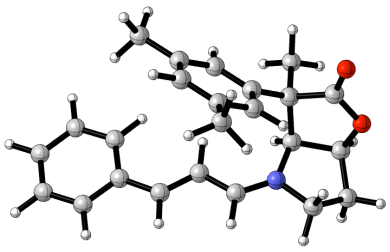
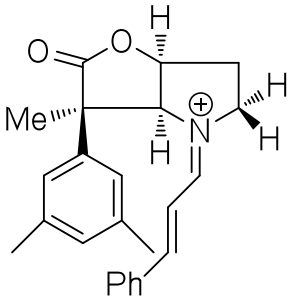
2 - *Z*-iminium ion





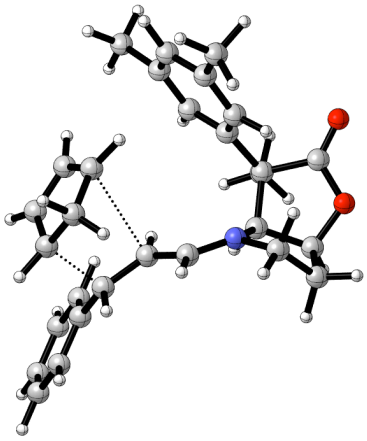
E(RM062X) = -1135.09530871

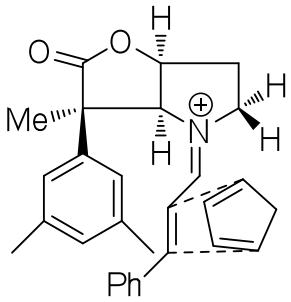
Zero-point correction=	0.451595 (Hartree/Particle)
Thermal correction to Energy=	0.475559
Thermal correction to Enthalpy=	0.476503
Thermal correction to Gibbs Free Energy=	0.398580
Sum of electronic and zero-point Energies=	-1134.643713
Sum of electronic and thermal Energies=	-1134.619750
Sum of electronic and thermal Enthalpies=	-1134.618806
Sum of electronic and thermal Free Energies=	-1134.696728

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.028527	-1.367590	1.799599
2	6	0	4.053331	-2.042590	0.898360
3	6	0	3.732596	-1.446672	-0.464395
4	6	0	2.200263	-1.254257	-0.489039
5	6	0	3.365271	0.815766	-0.837645
6	6	0	2.013517	0.151451	-1.134360
7	1	0	3.320908	-0.340063	2.030070
8	1	0	5.079063	-1.831193	1.191021
9	8	0	4.288348	-0.136188	-0.534528
10	7	0	1.828443	-1.341296	0.935531
11	1	0	1.679846	-2.032231	-1.045993
12	1	0	4.104722	-2.035857	-1.300474
13	6	0	0.853192	0.963026	-0.598885
14	6	0	-0.349967	1.063671	-1.294697
15	6	0	0.957287	1.562132	0.655144
16	6	0	-1.452966	1.701146	-0.733156
17	1	0	-0.449726	0.641224	-2.287203
18	6	0	-0.128279	2.204130	1.243682
19	1	0	1.905468	1.552261	1.184452
20	6	0	-1.331985	2.241316	0.544876
21	1	0	3.897235	-3.121949	0.880404
22	1	0	2.810246	-1.902183	2.720534
23	6	0	0.611842	-1.358253	1.386732
24	1	0	0.510385	-1.330989	2.468721
25	6	0	-0.560967	-1.418644	0.598145
26	1	0	-0.471399	-1.554885	-0.469669
27	6	0	-1.761495	-1.181367	1.178267
28	1	0	-1.779607	-0.981654	2.247518
29	6	0	-3.040766	-1.116943	0.506124
30	6	0	-4.145141	-0.635294	1.220823
31	6	0	-3.208070	-1.497218	-0.833579
32	6	0	-5.383458	-0.522518	0.610601
33	1	0	-4.022760	-0.343968	2.257589
34	6	0	-4.447880	-1.397671	-1.435163
35	1	0	-2.372715	-1.887606	-1.401212
36	6	0	-5.535447	-0.905448	-0.716585
37	1	0	-6.230276	-0.145690	1.168465
38	1	0	-4.575254	-1.703428	-2.465229
39	1	0	-6.504062	-0.827273	-1.193227
40	8	0	3.632833	1.968395	-0.890628
41	6	0	1.988146	-0.042948	-2.660258
42	1	0	1.132049	-0.646289	-2.962590
43	1	0	1.932776	0.927970	-3.150627
44	1	0	2.892970	-0.548156	-3.003253
45	1	0	-2.189556	2.734362	0.992539
46	6	0	0.009477	2.885319	2.577832
47	1	0	0.272812	3.935773	2.438275
48	1	0	-0.924843	2.852281	3.137853
49	1	0	0.793774	2.429314	3.182023
50	6	0	-2.752016	1.820022	-1.481377
51	1	0	-3.587642	1.482969	-0.863818
52	1	0	-2.940700	2.859613	-1.755736
53	1	0	-2.742332	1.225650	-2.394178

TS2-*Z*-*exo*-top





E(RM062X) = -1329.15272716

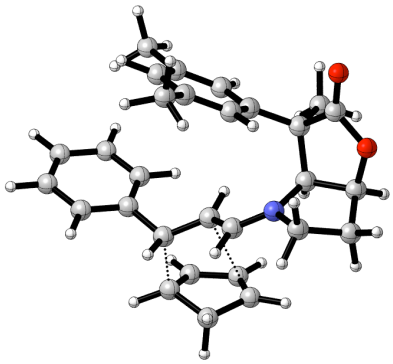
Zero-point correction=	0.547363 (Hartree/Particle)
Thermal correction to Energy=	0.575783
Thermal correction to Enthalpy=	0.576727
Thermal correction to Gibbs Free Energy=	0.487773
Sum of electronic and zero-point Energies=	-1328.605364
Sum of electronic and thermal Energies=	-1328.576944
Sum of electronic and thermal Enthalpies=	-1328.576000
Sum of electronic and thermal Free Energies=	-1328.664954

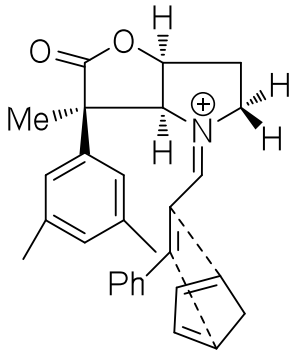
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.327935	2.516307	-0.007023
2	6	0	2.693393	2.301888	-0.281231
3	6	0	2.837102	1.690309	-1.529177
4	6	0	1.523952	1.888391	-2.244107
5	6	0	0.597823	2.151372	-1.108469
6	6	0	2.648526	-0.232255	-1.011940
7	6	0	1.325349	-0.456027	-0.545868
8	6	0	0.376860	-0.989936	-1.401146
9	7	0	-0.764986	-1.571906	-1.073743
10	1	0	1.098822	-0.368944	0.508280
11	1	0	2.821969	-0.556998	-2.035138
12	1	0	1.608284	2.818943	-2.822686
13	1	0	1.216035	1.109447	-2.937011
14	1	0	-0.481079	2.158927	-1.182243

15	1	0	3.787185	1.652001	-2.046119
16	1	0	0.593357	-1.007603	-2.466395
17	1	0	0.920467	2.861270	0.931346
18	1	0	3.506075	2.488430	0.407717
19	6	0	3.819468	-0.487434	-0.132706
20	6	0	3.764789	-0.308176	1.250528
21	6	0	5.012488	-0.914681	-0.711670
22	6	0	4.879262	-0.557853	2.034298
23	1	0	2.852296	0.039131	1.722009
24	6	0	6.129572	-1.168093	0.073963
25	1	0	5.067007	-1.057386	-1.785466
26	6	0	6.065004	-0.990325	1.447846
27	1	0	4.826546	-0.416682	3.106077
28	1	0	7.048032	-1.504510	-0.388847
29	1	0	6.933411	-1.186362	2.062865
30	6	0	-1.573979	-2.332436	-2.040107
31	1	0	-2.546329	-1.852494	-2.167074
32	1	0	-1.070832	-2.371125	-3.003590
33	6	0	-1.093087	-1.971323	0.298661
34	1	0	-0.159404	-2.131843	0.837785
35	6	0	-1.714347	-3.683251	-1.345937
36	1	0	-2.560098	-4.267735	-1.701065
37	1	0	-0.798534	-4.264249	-1.462953
38	6	0	-1.893446	-3.288035	0.113261
39	1	0	-1.599197	-4.066360	0.815342
40	6	0	-2.052550	-1.061870	1.103392
41	6	0	-3.422515	-1.723225	0.875373
42	8	0	-3.259612	-2.960745	0.345843
43	8	0	-4.489427	-1.278320	1.139823
44	6	0	-1.753055	-1.279669	2.595735
45	1	0	-0.749921	-0.930639	2.843973
46	1	0	-2.481603	-0.746513	3.204801
47	1	0	-1.808848	-2.341128	2.846289
48	6	0	-2.126881	0.402951	0.706711
49	6	0	-1.626674	1.412232	1.523764
50	6	0	-2.811041	0.762507	-0.453959
51	6	0	-1.827147	2.757288	1.214373
52	1	0	-1.107921	1.168447	2.442831
53	6	0	-3.030765	2.094784	-0.788375
54	1	0	-3.251231	-0.005199	-1.082046
55	6	0	-2.531909	3.081273	0.059805
56	1	0	-2.709701	4.125218	-0.178568
57	6	0	-1.331833	3.842890	2.132644
58	1	0	-0.845326	4.643641	1.573074
59	1	0	-2.163953	4.289011	2.680440
60	1	0	-0.626375	3.454215	2.867660
61	6	0	-3.842974	2.461141	-2.000754
62	1	0	-3.782777	1.690722	-2.769161

63	1	0	-4.894430	2.573681	-1.728571
64	1	0	-3.510648	3.406100	-2.429993

TS2-*Z-exo*





E(RM062X) = -1329.15508257

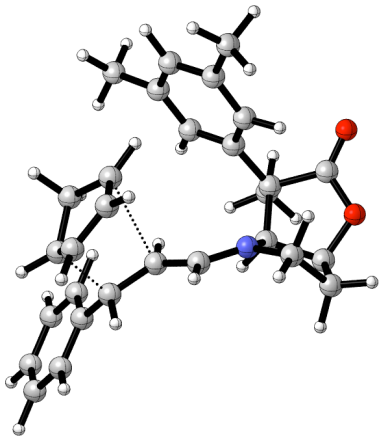
Zero-point correction=	0.547805 (Hartree/Particle)
Thermal correction to Energy=	0.575816
Thermal correction to Enthalpy=	0.576760
Thermal correction to Gibbs Free Energy=	0.489761
Sum of electronic and zero-point Energies=	-1328.607278
Sum of electronic and thermal Energies=	-1328.579267
Sum of electronic and thermal Enthalpies=	-1328.578322
Sum of electronic and thermal Free Energies=	-1328.665322

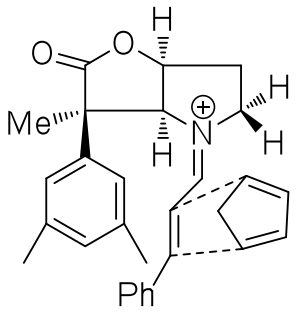
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.517772	3.548403	-1.043538
2	6	0	2.732058	3.031376	-0.579926
3	6	0	2.625628	2.728506	0.794522
4	6	0	1.449383	3.539444	1.289405
5	6	0	0.665605	3.692452	0.031924
6	6	0	1.858383	0.967601	0.804984
7	6	0	0.554152	1.047550	0.237655
8	6	0	-0.573814	1.231945	1.026531
9	7	0	-1.829168	1.208134	0.625051
10	1	0	0.420344	0.811905	-0.808706
11	1	0	1.860484	0.874377	1.889080
12	1	0	1.832789	4.532909	1.559060
13	1	0	0.914809	3.149487	2.150553
14	1	0	-0.351992	4.057368	-0.013393

15	1	0	3.510310	2.579135	1.401167
16	1	0	-0.445448	1.415818	2.089798
17	1	0	1.271999	3.747622	-2.076527
18	1	0	3.586695	2.792715	-1.197376
19	6	0	-2.978278	1.552054	1.476487
20	1	0	-2.663668	2.206714	2.286468
21	1	0	-3.414824	0.643404	1.898793
22	6	0	-3.929067	2.203532	0.478119
23	1	0	-4.967691	2.187569	0.800335
24	1	0	-3.629375	3.234418	0.282674
25	6	0	-2.243399	0.923264	-0.747824
26	1	0	-1.619899	1.496881	-1.437091
27	6	0	-3.725963	1.361182	-0.773931
28	1	0	-4.008121	1.870423	-1.694047
29	6	0	-2.287846	-0.582740	-1.134636
30	6	0	-2.165956	-0.687098	-2.661884
31	1	0	-1.195150	-0.321555	-2.998875
32	1	0	-2.284729	-1.724264	-2.972510
33	1	0	-2.938425	-0.091597	-3.153107
34	6	0	-3.741865	-0.958624	-0.814434
35	8	0	-4.491097	0.165690	-0.659770
36	8	0	-4.207189	-2.045936	-0.739597
37	6	0	-1.321121	-1.467139	-0.373265
38	6	0	-0.162722	-1.967619	-0.959334
39	6	0	-1.574817	-1.754622	0.965754
40	6	0	0.747362	-2.719954	-0.220113
41	1	0	0.045734	-1.793548	-2.008086
42	6	0	-0.677422	-2.488557	1.733801
43	1	0	-2.503984	-1.429054	1.423348
44	6	0	0.488238	-2.947945	1.127718
45	1	0	1.195490	-3.530148	1.710383
46	6	0	2.912545	0.125418	0.164782
47	6	0	3.875047	-0.477578	0.970525
48	6	0	3.010580	-0.012411	-1.220113
49	6	0	4.926743	-1.190491	0.406205
50	1	0	3.807186	-0.383264	2.048825
51	6	0	4.061655	-0.717912	-1.784541
52	1	0	2.275584	0.451337	-1.869357
53	6	0	5.027599	-1.304073	-0.972616
54	1	0	5.669145	-1.649809	1.045868
55	1	0	4.130356	-0.812155	-2.860803
56	1	0	5.850142	-1.850309	-1.415224
57	6	0	-0.987440	-2.830319	3.165933
58	1	0	-1.478019	-3.804124	3.224195
59	1	0	-0.078908	-2.883094	3.765573
60	1	0	-1.658156	-2.098206	3.615846
61	6	0	1.977986	-3.300978	-0.857423
62	1	0	2.069965	-2.994742	-1.898531

63	1	0	2.875930	-2.977698	-0.328210
64	1	0	1.945729	-4.391489	-0.825149

TS2-*Z*-*endo*-top





E(RM062X) = -1329.15433616

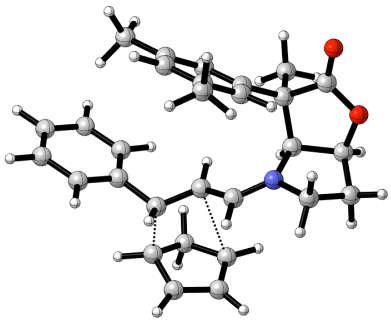
Zero-point correction=	0.547706 (Hartree/Particle)
Thermal correction to Energy=	0.576105
Thermal correction to Enthalpy=	0.577050
Thermal correction to Gibbs Free Energy=	0.488084
Sum of electronic and zero-point Energies=	-1328.606630
Sum of electronic and thermal Energies=	-1328.578231
Sum of electronic and thermal Enthalpies=	-1328.577287
Sum of electronic and thermal Free Energies=	-1328.666252

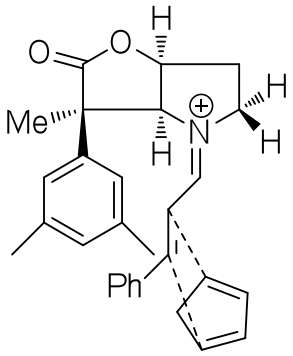
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.604296	1.762476	-1.644785
2	6	0	1.821453	1.973912	-0.818841
3	6	0	2.856352	1.214930	-1.618171
4	6	0	2.353971	1.171969	-2.936070
5	6	0	0.982391	1.444929	-2.933292
6	6	0	2.527115	-0.590947	-1.018592
7	6	0	1.156247	-0.674839	-0.626354
8	6	0	0.157911	-1.103385	-1.481686
9	7	0	-1.052888	-1.509460	-1.126292
10	1	0	1.723034	1.726495	0.233683
11	1	0	2.076501	3.041616	-0.885189
12	1	0	2.777457	-1.136224	-1.921313

13	1	0	0.893769	-0.484423	0.405630
14	1	0	3.915713	1.321400	-1.426280
15	1	0	-0.400660	1.967883	-1.304262
16	1	0	0.368055	-1.168269	-2.546025
17	1	0	0.320722	1.361781	-3.783573
18	1	0	2.931286	0.874867	-3.802271
19	6	0	-2.023947	-2.061795	-2.081121
20	1	0	-1.574544	-2.144024	-3.068608
21	1	0	-2.893758	-1.403340	-2.141651
22	6	0	-2.384936	-3.397175	-1.439026
23	1	0	-3.339390	-3.797434	-1.773373
24	1	0	-1.599516	-4.130347	-1.627539
25	6	0	-2.423103	-3.051048	0.042623
26	1	0	-2.254624	-3.905633	0.695713
27	6	0	-1.382422	-1.918561	0.244488
28	1	0	-0.467071	-2.275763	0.718020
29	6	0	-2.116609	-0.901888	1.148494
30	6	0	-3.594727	-1.267094	0.944129
31	6	0	-1.831051	-1.290556	2.612581
32	1	0	-0.766909	-1.213922	2.836301
33	1	0	-2.388432	-0.638298	3.283110
34	1	0	-2.135567	-2.321920	2.803057
35	8	0	-3.692171	-2.483880	0.356828
36	8	0	-4.548193	-0.643871	1.277034
37	6	0	-1.870120	0.573589	0.876667
38	6	0	-0.890540	1.278957	1.575671
39	6	0	-2.668263	1.267298	-0.030010
40	6	0	-0.723007	2.650833	1.404587
41	1	0	-0.265641	0.773601	2.303775
42	6	0	-2.539039	2.644259	-0.207689
43	1	0	-3.455185	0.751497	-0.568578
44	6	0	-1.563064	3.320840	0.518087
45	6	0	3.585082	-0.742677	0.024894
46	6	0	3.412035	-0.301006	1.337215
47	6	0	4.800377	-1.323299	-0.335734
48	6	0	4.431059	-0.445343	2.266720
49	1	0	2.479928	0.155906	1.649672
50	6	0	5.818383	-1.471659	0.595297
51	1	0	4.947655	-1.668919	-1.352967
52	6	0	5.636527	-1.030981	1.898924
53	1	0	4.284479	-0.101800	3.282552
54	1	0	6.752653	-1.932377	0.302163
55	1	0	6.429042	-1.144095	2.626838
56	1	0	-1.459460	4.394444	0.396728
57	6	0	-3.471838	3.384646	-1.126807
58	1	0	-4.390025	3.646809	-0.597107
59	1	0	-3.022237	4.308514	-1.488997
60	1	0	-3.752958	2.774134	-1.984865

61	6	0	0.311598	3.405954	2.195865
62	1	0	1.061302	2.734889	2.616952
63	1	0	0.820086	4.146987	1.577556
64	1	0	-0.155369	3.940145	3.025598

TS2-*Z-endo*





E(RM062X) = -1329.15517312

Zero-point correction=	0.547941 (Hartree/Particle)
Thermal correction to Energy=	0.575956
Thermal correction to Enthalpy=	0.576900
Thermal correction to Gibbs Free Energy=	0.490080
Sum of electronic and zero-point Energies=	-1328.607232
Sum of electronic and thermal Energies=	-1328.579217
Sum of electronic and thermal Enthalpies=	-1328.578273
Sum of electronic and thermal Free Energies=	-1328.665093

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.660581	3.584098	-0.533875
2	6	0	2.014031	3.138137	-0.963139
3	6	0	2.601919	2.728480	0.370340
4	6	0	1.923590	3.521831	1.330699
5	6	0	0.730554	3.990857	0.792697
6	6	0	1.820956	1.002814	0.545317
7	6	0	0.526665	1.067616	-0.059846
8	6	0	-0.607169	1.357370	0.693651
9	7	0	-1.863692	1.245589	0.319906
10	1	0	2.052921	2.398942	-1.756865
11	1	0	2.560675	4.029439	-1.301234
12	1	0	1.804296	0.903699	1.625640
13	1	0	0.398456	0.714059	-1.073320

14	1	0	3.658495	2.518659	0.474459
15	1	0	-0.160078	3.784111	-1.210062
16	1	0	-0.466035	1.729041	1.705303
17	1	0	-0.043894	4.516906	1.333078
18	1	0	2.241952	3.650515	2.356729
19	6	0	-3.001654	1.740759	1.112035
20	1	0	-3.403947	0.933321	1.729500
21	1	0	-2.683233	2.558986	1.754412
22	6	0	-2.302478	0.677379	-0.956159
23	1	0	-1.720135	1.113692	-1.769819
24	6	0	-3.992341	2.146360	0.027113
25	1	0	-5.021611	2.181107	0.376684
26	1	0	-3.722041	3.115897	-0.394316
27	6	0	-3.799697	1.057427	-1.018630
28	1	0	-4.131229	1.342397	-2.015693
29	6	0	-2.309858	-0.875493	-1.024510
30	6	0	-3.726606	-1.211791	-0.538797
31	6	0	-2.282294	-1.285005	-2.505193
32	1	0	-3.112221	-0.829009	-3.048834
33	1	0	-1.353935	-0.964208	-2.978933
34	1	0	-2.371664	-2.367120	-2.590836
35	8	0	-4.514727	-0.105508	-0.610916
36	8	0	-4.140730	-2.263967	-0.184124
37	6	0	-1.258925	-1.557554	-0.174134
38	6	0	-0.117821	-2.123982	-0.733676
39	6	0	-1.409027	-1.576431	1.210777
40	6	0	0.877345	-2.675934	0.069638
41	1	0	0.011319	-2.159010	-1.808568
42	6	0	-0.423374	-2.101685	2.039781
43	1	0	-2.320859	-1.197652	1.662415
44	6	0	0.722414	-2.630429	1.451676
45	1	0	1.497436	-3.052650	2.084067
46	6	0	2.890623	0.152940	-0.065276
47	6	0	3.926045	-0.295746	0.755936
48	6	0	2.942783	-0.140886	-1.427117
49	6	0	4.997363	-1.002230	0.228941
50	1	0	3.894405	-0.081193	1.818764
51	6	0	4.016988	-0.843556	-1.956613
52	1	0	2.145914	0.167802	-2.093123
53	6	0	5.051241	-1.268745	-1.133544
54	1	0	5.791955	-1.340653	0.881264
55	1	0	4.044350	-1.061565	-3.016580
56	1	0	5.889122	-1.812465	-1.549565
57	6	0	-0.617824	-2.153664	3.531025
58	1	0	0.332032	-2.060939	4.057437
59	1	0	-1.284691	-1.363140	3.875648
60	1	0	-1.063132	-3.107603	3.820935
61	6	0	2.084722	-3.337517	-0.532346

62	1	0	2.121277	-3.193987	-1.611307
63	1	0	3.002672	-2.932485	-0.103858
64	1	0	2.068420	-4.410726	-0.333066

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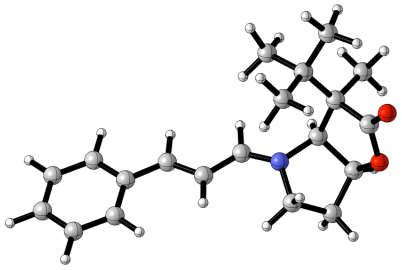
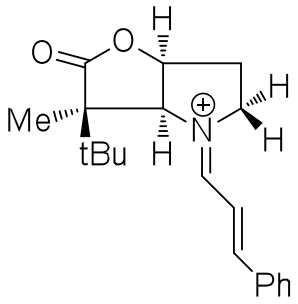
3 - *E*-iminium ion





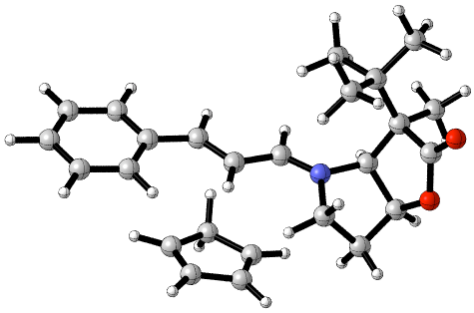
E(RM062X) = -982.660110783

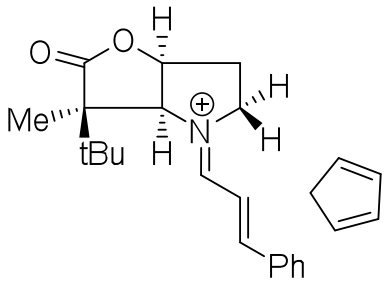
Zero-point correction=	0.428752 (Hartree/Particle)
Thermal correction to Energy=	0.450063
Thermal correction to Enthalpy=	0.451007
Thermal correction to Gibbs Free Energy=	0.378536
Sum of electronic and zero-point Energies=	-982.231359
Sum of electronic and thermal Energies=	-982.210048
Sum of electronic and thermal Enthalpies=	-982.209104
Sum of electronic and thermal Free Energies=	-982.281575

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.745019	-2.025541	0.572114
2	6	0	1.659629	-2.928227	-0.251168
3	6	0	2.680778	-1.943053	-0.804444
4	6	0	1.922840	-0.599874	-0.994715
5	6	0	3.742725	-0.403335	0.563832
6	6	0	2.877846	0.452818	-0.367130
7	1	0	2.143944	-3.699799	0.342671
8	8	0	3.656414	-1.709585	0.201696
9	7	0	0.624038	-0.864469	-0.329576
10	1	0	1.717463	-0.367790	-2.038893
11	1	0	3.178799	-2.288491	-1.708156
12	1	0	1.096716	-3.393044	-1.061627
13	1	0	-0.229940	-2.453507	0.780684
14	6	0	-0.488141	-0.317734	-0.710802
15	1	0	-0.404644	0.365099	-1.550950
16	6	0	-1.766487	-0.506100	-0.133291
17	1	0	-1.876855	-1.121726	0.747886
18	6	0	-2.826668	0.141594	-0.685233
19	1	0	-2.632726	0.760623	-1.559246
20	6	0	-4.199399	0.113673	-0.249481
21	6	0	-4.629349	-0.630036	0.861985

22	6	0	-5.137308	0.866864	-0.971685
23	6	0	-5.958053	-0.615700	1.233419
24	1	0	-3.925528	-1.218572	1.436278
25	6	0	-6.468979	0.877999	-0.596572
26	1	0	-4.811498	1.442824	-1.830020
27	6	0	-6.878522	0.137536	0.505270
28	1	0	-6.286719	-1.188584	2.090124
29	1	0	-7.186504	1.460668	-1.158283
30	1	0	-7.919524	0.144410	0.801808
31	8	0	4.451036	-0.051851	1.449817
32	6	0	3.841057	0.839090	-1.515642
33	1	0	3.352092	1.519674	-2.213111
34	1	0	4.730318	1.323151	-1.119221
35	1	0	4.164728	-0.043518	-2.070835
36	1	0	1.218649	-1.709141	1.504311
37	6	0	2.284913	1.709512	0.351422
38	6	0	1.219657	2.404479	-0.515929
39	6	0	1.659090	1.349339	1.707148
40	6	0	3.405655	2.732873	0.610220
41	1	0	1.447196	2.368306	-1.583941
42	1	0	0.222065	1.998804	-0.348888
43	1	0	1.164739	3.457737	-0.237965
44	1	0	2.405038	0.965136	2.402379
45	1	0	1.228953	2.250121	2.148408
46	1	0	0.848208	0.623869	1.616993
47	1	0	3.006407	3.528905	1.240362
48	1	0	4.254158	2.286111	1.124662
49	1	0	3.748775	3.194448	-0.316401

3-*E* and Cyclopentadiene Adduct





E(RM062X) = -1176.74652161

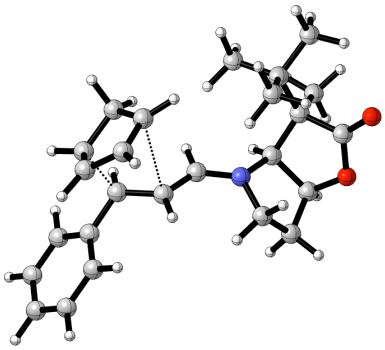
Zero-point correction=	0.523341 (Hartree/Particle)
Thermal correction to Energy=	0.550489
Thermal correction to Enthalpy=	0.551433
Thermal correction to Gibbs Free Energy=	0.464675
Sum of electronic and zero-point Energies=	-1176.223180
Sum of electronic and thermal Energies=	-1176.196033
Sum of electronic and thermal Enthalpies=	-1176.195088

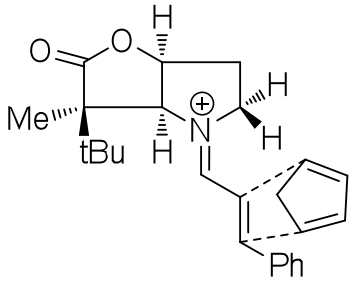
Sum of electronic and thermal Free Energies= -1176.281846

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.705705	3.200984	-0.187008
2	6	0	-3.039490	2.700558	-0.539890
3	6	0	-3.606951	2.162029	0.549895
4	6	0	-2.673362	2.295609	1.714377
5	6	0	-1.466849	2.953167	1.112229
6	6	0	-2.259903	-0.911192	0.499258
7	6	0	-1.288536	-0.251414	-0.179906
8	6	0	-0.037105	-0.064816	0.455826
9	7	0	1.019314	0.487211	-0.053382
10	1	0	-1.444062	0.104095	-1.188069
11	1	0	-2.022110	-1.253605	1.505232
12	1	0	-3.110099	2.933634	2.491768
13	1	0	-2.453970	1.337387	2.198357
14	1	0	-0.595807	3.249068	1.680816
15	1	0	-4.591188	1.720668	0.614210
16	1	0	0.081420	-0.449141	1.464482
17	1	0	-1.055098	3.732969	-0.869172
18	1	0	-3.488771	2.787293	-1.519440
19	6	0	-3.591789	-1.230919	0.043691
20	6	0	-4.074552	-0.840469	-1.215334
21	6	0	-4.435198	-1.942533	0.907467
22	6	0	-5.361417	-1.163299	-1.595091
23	1	0	-3.445140	-0.276574	-1.891520
24	6	0	-5.727375	-2.261866	0.524904
25	1	0	-4.068292	-2.246069	1.881220
26	6	0	-6.189470	-1.873194	-0.725614
27	1	0	-5.730091	-0.863587	-2.567043
28	1	0	-6.371859	-2.812660	1.196677
29	1	0	-7.198278	-2.122371	-1.028744
30	6	0	1.043636	1.324253	-1.266069
31	1	0	0.031642	1.556054	-1.583016
32	6	0	2.300978	0.605767	0.680747
33	1	0	2.067972	0.691109	1.741525
34	6	0	1.820349	2.535534	-0.759813
35	1	0	2.243331	3.138397	-1.560145
36	1	0	1.172151	3.153617	-0.137619
37	6	0	2.915586	1.901743	0.085333
38	1	0	3.328357	2.568580	0.839801
39	6	0	3.399907	-0.466116	0.435638
40	6	0	4.212565	0.153252	-0.706625
41	8	0	3.960404	1.484864	-0.783098
42	8	0	5.003744	-0.369199	-1.422155

43	6	0	4.337401	-0.351651	1.661867
44	1	0	3.891393	-0.835239	2.531424
45	1	0	5.295953	-0.820748	1.453569
46	1	0	4.528720	0.693297	1.913870
47	1	0	1.578445	0.796833	-2.059504
48	6	0	2.992522	-1.948173	0.143814
49	6	0	1.967763	-2.465754	1.170303
50	6	0	2.404648	-2.111517	-1.265915
51	6	0	4.234719	-2.852983	0.240053
52	1	0	2.118397	-2.053512	2.170976
53	1	0	0.940826	-2.278948	0.857394
54	1	0	2.062936	-3.548969	1.255040
55	1	0	3.140478	-1.877640	-2.034793
56	1	0	2.101373	-3.150873	-1.403776
57	1	0	1.515249	-1.498790	-1.425153
58	1	0	3.962793	-3.849044	-0.112241
59	1	0	5.053829	-2.487078	-0.375747
60	1	0	4.576896	-2.955953	1.270492

TS3-*E-exo*-top





E(RM062X) = -1176.72479265

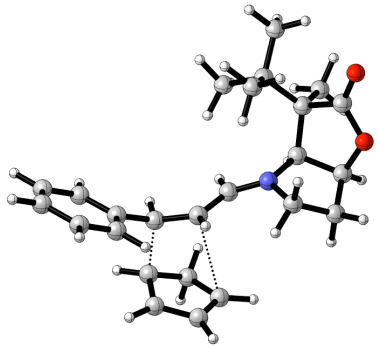
Zero-point correction=	0.524670 (Hartree/Particle)
Thermal correction to Energy=	0.550026
Thermal correction to Enthalpy=	0.550970
Thermal correction to Gibbs Free Energy=	0.470385
Sum of electronic and zero-point Energies=	-1176.200123
Sum of electronic and thermal Energies=	-1176.174767
Sum of electronic and thermal Enthalpies=	-1176.173823
Sum of electronic and thermal Free Energies=	-1176.254408

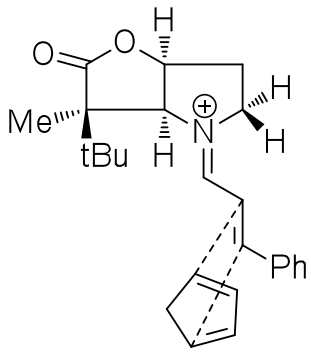
Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.912602	2.440709	-1.626574
2	6	0	3.125862	2.227438	-0.945231
3	6	0	2.889485	2.116451	0.434269
4	6	0	1.508756	2.686578	0.660298
5	6	0	0.914523	2.592952	-0.698743
6	6	0	2.560850	0.224432	0.664702
7	6	0	1.403326	-0.155776	-0.076560
8	6	0	0.174469	-0.291453	0.537732
9	7	0	-0.915225	-0.861131	0.038983
10	1	0	1.518064	-0.460494	-1.107172
11	1	0	2.382969	0.314644	1.734397
12	1	0	1.631359	3.753874	0.892994
13	1	0	0.922027	2.249728	1.464890
14	1	0	-0.135308	2.739869	-0.912517
15	1	0	3.689805	2.249443	1.151410
16	1	0	0.065718	0.068856	1.558247
17	1	0	1.787649	2.449161	-2.699384
18	1	0	4.088529	2.079649	-1.415939
19	6	0	-0.893081	-1.796853	-1.094702
20	1	0	0.120333	-1.939463	-1.455913
21	6	0	-1.494112	-3.047142	-0.456971
22	1	0	-1.873246	-3.765954	-1.179850
23	1	0	-0.752251	-3.529285	0.181283
24	6	0	-2.145891	-1.055873	0.827752
25	1	0	-1.884216	-1.012582	1.885313
26	6	0	-2.622963	-2.470428	0.383287
27	1	0	-2.927225	-3.106569	1.212007
28	6	0	-3.386196	-0.161591	0.538954
29	6	0	-4.280047	-0.292944	1.795330
30	1	0	-3.874573	0.293604	2.619824
31	1	0	-5.290878	0.048472	1.584368
32	1	0	-4.344341	-1.332796	2.121002
33	6	0	-4.136266	-0.969763	-0.522377
34	8	0	-3.743448	-2.264919	-0.471811
35	8	0	-4.985756	-0.606180	-1.271666
36	6	0	3.878646	-0.409844	0.374183
37	6	0	4.759551	-0.636549	1.429037
38	6	0	4.257899	-0.780265	-0.916422
39	6	0	5.993904	-1.232692	1.203780
40	1	0	4.476074	-0.352892	2.436819
41	6	0	5.489649	-1.372653	-1.142344
42	1	0	3.595225	-0.602539	-1.756134
43	6	0	6.360817	-1.601794	-0.081582
44	1	0	6.666072	-1.408174	2.033437
45	1	0	5.773238	-1.658729	-2.146860
46	1	0	7.321793	-2.065729	-0.260605

47	1	0	-1.516781	-1.416257	-1.907364
48	6	0	-3.172509	1.326386	0.121647
49	6	0	-2.229385	2.033855	1.101528
50	6	0	-2.591684	1.432135	-1.296400
51	6	0	-4.508198	2.089086	0.143231
52	1	0	-2.551061	1.929646	2.138909
53	1	0	-1.206589	1.672577	1.015586
54	1	0	-2.215471	3.102814	0.875971
55	1	0	-3.271602	1.008215	-2.035302
56	1	0	-2.457994	2.486810	-1.550055
57	1	0	-1.620586	0.940985	-1.385442
58	1	0	-4.347742	3.086434	-0.269987
59	1	0	-5.267533	1.590708	-0.456025
60	1	0	-4.881289	2.216282	1.160084

TS3-*E*-exo





E(RM062X) = -1176.72249185

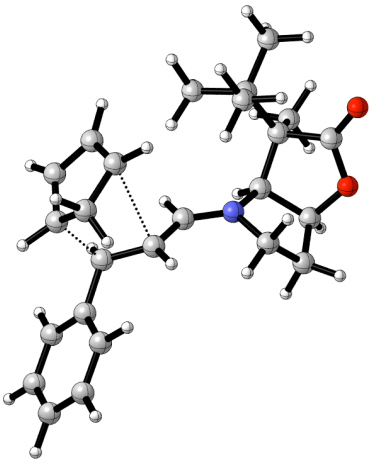
Zero-point correction=	0.524327 (Hartree/Particle)
Thermal correction to Energy=	0.549917
Thermal correction to Enthalpy=	0.550862
Thermal correction to Gibbs Free Energy=	0.468489
Sum of electronic and zero-point Energies=	-1176.198165
Sum of electronic and thermal Energies=	-1176.172574
Sum of electronic and thermal Enthalpies=	-1176.171630
Sum of electronic and thermal Free Energies=	-1176.254003

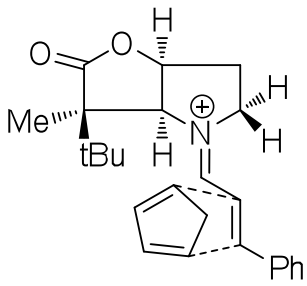
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.866000	3.006633	-0.462826
2	6	0	-3.842403	2.140398	0.054489

3	6	0	-3.389732	1.573051	1.261347
4	6	0	-2.264544	2.468826	1.730042
5	6	0	-1.843318	3.101242	0.450413
6	6	0	-2.414782	0.034793	0.681019
7	6	0	-1.286541	0.463220	-0.079920
8	6	0	-0.033164	0.545131	0.500835
9	7	0	1.108332	0.812861	-0.107342
10	1	0	-1.374387	0.552118	-1.153701
11	1	0	-2.157575	-0.285744	1.689176
12	1	0	-2.714433	3.254425	2.352839
13	1	0	-1.474709	2.000196	2.311194
14	1	0	-0.934979	3.675618	0.326027
15	1	0	-4.086831	1.121737	1.956683
16	1	0	0.064375	0.326151	1.560742
17	1	0	-2.896875	3.480352	-1.433211
18	1	0	-4.762000	1.866822	-0.444707
19	6	0	-3.438529	-0.858458	0.064278
20	6	0	-3.801363	-0.756494	-1.278730
21	6	0	-4.053672	-1.821379	0.860063
22	6	0	-4.754422	-1.607989	-1.813857
23	1	0	-3.343910	-0.007814	-1.916163
24	6	0	-5.008668	-2.676305	0.324221
25	1	0	-3.779043	-1.910414	1.905566
26	6	0	-5.360152	-2.571310	-1.013048
27	1	0	-5.025689	-1.524064	-2.858203
28	1	0	-5.475046	-3.423608	0.952679
29	1	0	-6.103211	-3.235874	-1.433698
30	6	0	1.210213	1.475130	-1.411525
31	1	0	0.236763	1.851673	-1.717295
32	6	0	2.411915	0.792865	0.575081
33	1	0	2.255614	1.056340	1.621859
34	6	0	2.223477	2.576235	-1.104733
35	1	0	2.711327	2.977363	-1.990204
36	1	0	1.738974	3.388767	-0.560507
37	6	0	3.223584	1.865796	-0.203980
38	1	0	3.786998	2.537003	0.441535
39	6	0	3.299717	-0.479638	0.461380
40	6	0	4.148497	-0.178891	-0.777014
41	8	0	4.133819	1.154507	-1.033038
42	8	0	4.798174	-0.926218	-1.434413
43	6	0	4.305119	-0.371501	1.632628
44	1	0	3.826402	-0.642636	2.574059
45	1	0	5.155491	-1.029539	1.470613
46	1	0	4.688265	0.646520	1.727472
47	1	0	1.582134	0.778275	-2.167053
48	6	0	2.625301	-1.888968	0.394666
49	6	0	1.581271	-2.066912	1.510927
50	6	0	1.941945	-2.130339	-0.959542

51	6	0	3.690651	-2.983950	0.584782
52	1	0	1.879749	-1.598939	2.451997
53	1	0	0.600992	-1.691677	1.219900
54	1	0	1.452346	-3.131698	1.710473
55	1	0	2.665423	-2.141291	-1.774386
56	1	0	1.451267	-3.105221	-0.939490
57	1	0	1.170907	-1.388860	-1.175057
58	1	0	3.229017	-3.952472	0.386478
59	1	0	4.527499	-2.860220	-0.099846
60	1	0	4.064493	-3.006742	1.609268

TS3-*E-endo*-top





E(RM062X) = -1176.72256139

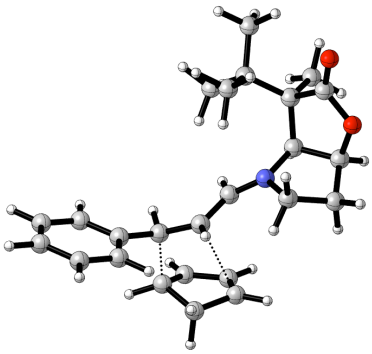
Zero-point correction=	0.524885 (Hartree/Particle)
Thermal correction to Energy=	0.550261
Thermal correction to Enthalpy=	0.551206
Thermal correction to Gibbs Free Energy=	0.470586
Sum of electronic and zero-point Energies=	-1176.197677
Sum of electronic and thermal Energies=	-1176.172300
Sum of electronic and thermal Enthalpies=	-1176.171356
Sum of electronic and thermal Free Energies=	-1176.251976

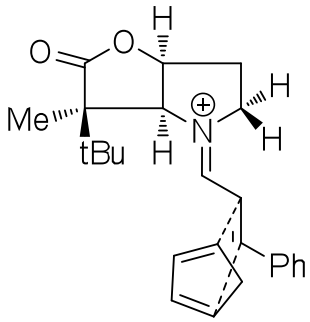
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.079448	2.213604	-1.470331
2	6	0	2.536805	1.944063	-1.555079
3	6	0	2.945793	2.055952	-0.101211

4	6	0	1.950194	2.860353	0.500971
5	6	0	0.802789	2.883292	-0.297827
6	6	0	2.566697	0.325941	0.534788
7	6	0	1.427844	-0.191953	-0.169625
8	6	0	0.196578	-0.270376	0.452201
9	7	0	-0.881337	-0.920498	0.038325
10	1	0	2.829177	1.039926	-2.080868
11	1	0	2.991477	2.792707	-2.086052
12	1	0	2.371347	0.526745	1.583958
13	1	0	1.572840	-0.668549	-1.127591
14	1	0	3.985003	2.175909	0.175733
15	1	0	0.377858	2.037330	-2.274789
16	1	0	0.084152	0.223447	1.413377
17	1	0	-0.149182	3.316181	-0.030818
18	1	0	2.037904	3.312530	1.480617
19	6	0	-0.851228	-1.921801	-1.037438
20	1	0	-1.449471	-1.577807	-1.885233
21	1	0	0.167355	-2.101291	-1.365629
22	6	0	-2.107572	-1.073678	0.852919
23	1	0	-1.830168	-1.019493	1.906045
24	6	0	-1.483443	-3.126164	-0.348689
25	1	0	-1.861283	-3.874880	-1.041149
26	1	0	-0.763837	-3.586553	0.329864
27	6	0	-2.614404	-2.484685	0.434995
28	1	0	-2.970452	-3.084199	1.270098
29	6	0	-3.345319	-0.174702	0.563939
30	6	0	-4.049276	-0.955747	-0.547263
31	6	0	-4.276482	-0.366139	1.787371
32	1	0	-4.356214	-1.418237	2.063111
33	1	0	-3.897207	0.179118	2.651040
34	1	0	-5.279332	-0.011281	1.561103
35	8	0	-3.693364	-2.261727	-0.470800
36	8	0	-4.835882	-0.571214	-1.352474
37	6	0	3.898299	-0.339013	0.363509
38	6	0	4.810410	-0.274647	1.417087
39	6	0	4.267783	-1.000516	-0.806851
40	6	0	6.061804	-0.862000	1.308357
41	1	0	4.534622	0.235317	2.333893
42	6	0	5.521616	-1.584719	-0.917636
43	1	0	3.581301	-1.083871	-1.640315
44	6	0	6.421872	-1.516530	0.137669
45	1	0	6.754606	-0.810454	2.138062
46	1	0	5.793996	-2.099943	-1.829553
47	1	0	7.397619	-1.975638	0.049276
48	6	0	-3.142607	1.332309	0.223565
49	6	0	-2.285314	2.016147	1.295092
50	6	0	-2.483149	1.511134	-1.151980
51	6	0	-4.494499	2.067216	0.194430

52	1	0	-2.682753	1.869142	2.299737
53	1	0	-1.249840	1.681283	1.280688
54	1	0	-2.280956	3.093117	1.111657
55	1	0	-3.130142	1.139433	-1.946741
56	1	0	-2.317386	2.576016	-1.335309
57	1	0	-1.518745	1.006165	-1.216212
58	1	0	-4.331499	3.081037	-0.175659
59	1	0	-5.208325	1.576500	-0.463969
60	1	0	-4.926964	2.153260	1.191776

TS3-*E-endo*





E(RM062X) = -1176.72103474

Zero-point correction=	0.524831 (Hartree/Particle)
Thermal correction to Energy=	0.550256
Thermal correction to Enthalpy=	0.551201
Thermal correction to Gibbs Free Energy=	0.469505
Sum of electronic and zero-point Energies=	-1176.196204
Sum of electronic and thermal Energies=	-1176.170778
Sum of electronic and thermal Enthalpies=	-1176.169834
Sum of electronic and thermal Free Energies=	-1176.251529

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.789680	3.005963	0.055288
2	6	0	-3.141705	2.476917	-0.267818
3	6	0	-3.423501	1.653004	0.970723
4	6	0	-2.648639	2.252568	1.994806
5	6	0	-1.625140	3.010992	1.430833
6	6	0	-2.461672	0.081645	0.569223
7	6	0	-1.333953	0.453019	-0.234672

8	6	0	-0.072011	0.570734	0.329743
9	7	0	1.076141	0.732051	-0.296754
10	1	0	-3.249693	1.973475	-1.223549
11	1	0	-3.835664	3.329277	-0.256509
12	1	0	-2.194968	-0.257422	1.565540
13	1	0	-1.426082	0.436007	-1.311229
14	1	0	-4.418143	1.280302	1.178163
15	1	0	-1.141161	3.496975	-0.658330
16	1	0	0.013174	0.494493	1.410126
17	1	0	-0.810739	3.475380	1.968208
18	1	0	-2.772646	2.056959	3.051925
19	6	0	1.205194	1.195887	-1.682556
20	1	0	0.238496	1.507908	-2.069161
21	6	0	2.200025	2.343064	-1.516633
22	1	0	2.701078	2.620946	-2.441129
23	1	0	1.696008	3.217791	-1.101420
24	6	0	3.188228	1.778893	-0.505755
25	1	0	3.734166	2.541203	0.047067
26	6	0	2.368561	0.821191	0.404079
27	1	0	2.190332	1.230534	1.398936
28	6	0	3.263186	-0.447908	0.488351
29	6	0	4.138334	-0.317974	-0.761409
30	6	0	4.241145	-0.170627	1.654768
31	1	0	3.742050	-0.311473	2.614016
32	1	0	5.097526	-0.838867	1.604915
33	1	0	4.618133	0.853367	1.614901
34	8	0	4.119122	0.964848	-1.206827
35	8	0	4.808565	-1.144904	-1.289901
36	6	0	-3.529151	-0.786553	-0.020570
37	6	0	-3.852173	-0.771977	-1.376786
38	6	0	-4.244546	-1.626207	0.833013
39	6	0	-4.865590	-1.583721	-1.866228
40	1	0	-3.311509	-0.142014	-2.072463
41	6	0	-5.255501	-2.439786	0.343653
42	1	0	-4.002089	-1.648002	1.889972
43	6	0	-5.570327	-2.418315	-1.008500
44	1	0	-5.101938	-1.567841	-2.922198
45	1	0	-5.795234	-3.091954	1.017745
46	1	0	-6.358253	-3.051934	-1.393700
47	1	0	1.605232	0.398704	-2.314062
48	6	0	2.593929	-1.856621	0.604325
49	6	0	1.521381	-1.880180	1.707593
50	6	0	1.946165	-2.291126	-0.718876
51	6	0	3.656296	-2.907295	0.974720
52	1	0	1.791496	-1.276634	2.577432
53	1	0	0.546969	-1.560915	1.339480
54	1	0	1.393081	-2.905498	2.057422
55	1	0	2.690078	-2.412243	-1.505920

56	1	0	1.458360	-3.256755	-0.573508
57	1	0	1.178035	-1.592980	-1.055684
58	1	0	3.202051	-3.896809	0.904534
59	1	0	4.510189	-2.877323	0.300686
60	1	0	4.004045	-2.782097	2.001027

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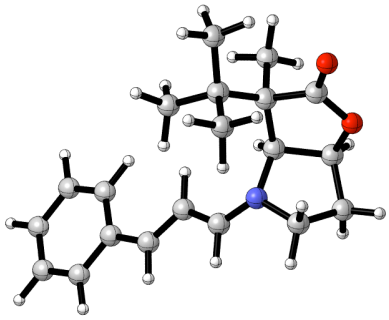
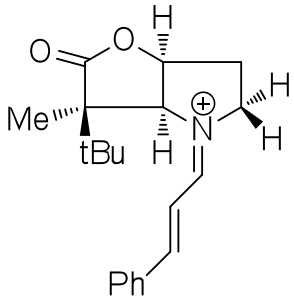
3 - *Z*-iminium ion





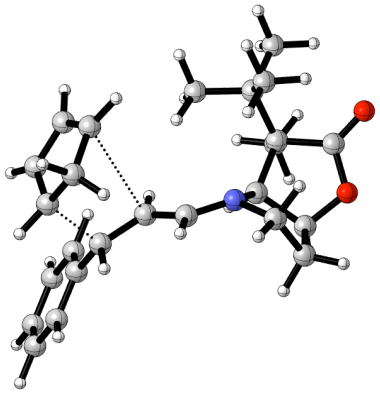
E(RM062X) = -982.658332811

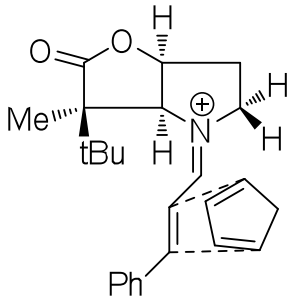
Zero-point correction=	0.428919 (Hartree/Particle)
Thermal correction to Energy=	0.450073
Thermal correction to Enthalpy=	0.451017
Thermal correction to Gibbs Free Energy=	0.379093
Sum of electronic and zero-point Energies=	-982.229414
Sum of electronic and thermal Energies=	-982.208260
Sum of electronic and thermal Enthalpies=	-982.207315
Sum of electronic and thermal Free Energies=	-982.279240

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.818706	2.357292	0.896587
2	6	0	-2.298491	2.895466	-0.446106
3	6	0	-2.480482	1.612131	-1.250605
4	6	0	-1.422684	0.599901	-0.706994
5	6	0	-3.685377	-0.165125	-0.380490
6	6	0	-2.249583	-0.696187	-0.462862
7	1	0	-3.234121	3.445689	-0.380705
8	8	0	-3.753485	1.073777	-0.930817
9	7	0	-0.849632	1.335373	0.445448
10	1	0	-0.620861	0.421005	-1.419178
11	1	0	-2.417995	1.755623	-2.327486
12	1	0	-1.532694	3.529505	-0.894983
13	1	0	-1.330376	3.081116	1.543345
14	6	0	0.412662	1.411601	0.745034
15	1	0	0.654854	2.131977	1.522099
16	6	0	1.484990	0.690329	0.168823
17	1	0	1.293364	-0.049306	-0.594500

18	6	0	2.745106	0.944964	0.610166
19	1	0	2.860701	1.694555	1.390604
20	6	0	3.970334	0.332866	0.163401
21	6	0	5.176711	0.787229	0.716845
22	6	0	4.000975	-0.695624	-0.792925
23	6	0	6.382928	0.236431	0.321800
24	1	0	5.159018	1.577599	1.458189
25	6	0	5.205571	-1.244220	-1.182236
26	1	0	3.082743	-1.070757	-1.226587
27	6	0	6.396958	-0.778182	-0.626965
28	1	0	7.309232	0.593137	0.751403
29	1	0	5.226953	-2.038048	-1.916789
30	1	0	7.338641	-1.212833	-0.936735
31	6	0	-2.216149	-1.439054	-1.820462
32	1	0	-2.999633	-2.191883	-1.861270
33	1	0	-2.378931	-0.747270	-2.649566
34	1	0	-1.252309	-1.926901	-1.967708
35	8	0	-4.655211	-0.714523	0.028611
36	1	0	-2.625920	1.863966	1.441566
37	6	0	-1.893973	-1.636383	0.734640
38	6	0	-0.394693	-1.956854	0.764940
39	6	0	-2.284960	-1.009714	2.080347
40	6	0	-2.645686	-2.971978	0.594027
41	1	0	-0.001235	-2.220222	-0.219950
42	1	0	0.194705	-1.140310	1.177000
43	1	0	-0.229934	-2.818289	1.413819
44	1	0	-3.359425	-0.840204	2.148759
45	1	0	-2.008171	-1.693452	2.884481
46	1	0	-1.759447	-0.072378	2.270366
47	1	0	-2.493466	-3.550247	1.506430
48	1	0	-3.715479	-2.827450	0.459004
49	1	0	-2.255920	-3.565597	-0.233867

TS3-*Z*-*exo*-top





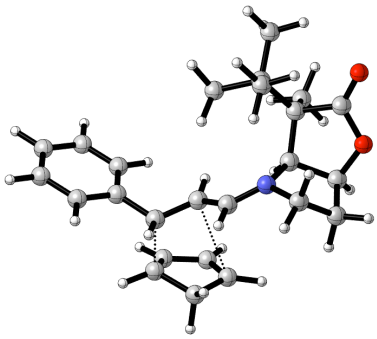
E(RM062X) = -1176.72114325

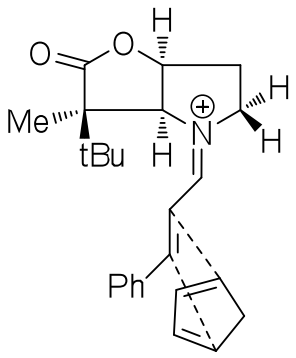
Zero-point correction=	0.524709 (Hartree/Particle)
Thermal correction to Energy=	0.550052
Thermal correction to Enthalpy=	0.550996
Thermal correction to Gibbs Free Energy=	0.470218
Sum of electronic and zero-point Energies=	-1176.196434
Sum of electronic and thermal Energies=	-1176.171092
Sum of electronic and thermal Enthalpies=	-1176.170147
Sum of electronic and thermal Free Energies=	-1176.250925

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.790807	2.922495	0.300782
2	6	0	3.060376	2.331204	0.161357
3	6	0	3.187972	1.757728	-1.114801
4	6	0	2.088647	2.374021	-1.950133
5	6	0	1.148257	2.857162	-0.907880
6	6	0	2.537009	-0.029800	-0.854976
7	6	0	1.163387	-0.018676	-0.454609
8	6	0	0.164635	-0.190758	-1.387408
9	7	0	-1.128976	-0.460085	-1.202377
10	1	0	0.923171	-0.008720	0.599864
11	1	0	2.681339	-0.300202	-1.898856
12	1	0	2.515062	3.256276	-2.448109
13	1	0	1.648312	1.752260	-2.725785
14	1	0	0.137569	3.189494	-1.106353
15	1	0	4.163710	1.536299	-1.529167
16	1	0	0.446875	-0.144771	-2.436516
17	1	0	1.380181	3.323103	1.215955
18	1	0	3.799281	2.246248	0.946943

19	6	0	3.556171	-0.671427	0.024989
20	6	0	3.487490	-0.598245	1.416603
21	6	0	4.613148	-1.360169	-0.565065
22	6	0	4.452811	-1.210626	2.199119
23	1	0	2.681421	-0.055448	1.898297
24	6	0	5.580229	-1.976657	0.218854
25	1	0	4.677551	-1.423234	-1.645927
26	6	0	5.501530	-1.903133	1.601349
27	1	0	4.389897	-1.150043	3.277842
28	1	0	6.393052	-2.513431	-0.252408
29	1	0	6.253821	-2.381292	2.214688
30	6	0	-1.922613	-0.963696	-2.338615
31	1	0	-1.399067	-0.792769	-3.275860
32	6	0	-1.671808	-1.044212	0.041889
33	1	0	-0.831813	-1.299792	0.685859
34	6	0	-2.101161	-2.428570	-1.956219
35	1	0	-2.904184	-2.930803	-2.490787
36	1	0	-1.166511	-2.971817	-2.105785
37	6	0	-2.423916	-2.316423	-0.472156
38	1	0	-2.193531	-3.212281	0.101028
39	6	0	-2.771419	-0.295299	0.849323
40	6	0	-4.066477	-0.859108	0.261544
41	8	0	-3.814902	-2.041250	-0.350258
42	8	0	-5.169869	-0.422177	0.341272
43	6	0	-2.721500	-0.915584	2.266415
44	1	0	-1.859509	-0.541935	2.819487
45	1	0	-3.626006	-0.677083	2.821343
46	1	0	-2.643341	-2.003169	2.213072
47	1	0	-2.881719	-0.442027	-2.369590
48	6	0	-2.757546	1.262530	0.887969
49	6	0	-1.359763	1.760602	1.257082
50	6	0	-3.144825	1.861596	-0.471683
51	6	0	-3.742001	1.792628	1.942910
52	1	0	-1.007964	1.350638	2.206680
53	1	0	-0.638165	1.518436	0.481750
54	1	0	-1.382526	2.848188	1.363250
55	1	0	-4.154469	1.571733	-0.763240
56	1	0	-3.126217	2.951142	-0.401374
57	1	0	-2.446866	1.571727	-1.258541
58	1	0	-3.782103	2.880591	1.865854
59	1	0	-4.746805	1.403866	1.789702
60	1	0	-3.416087	1.551324	2.955362

TS3-*Z-exo*





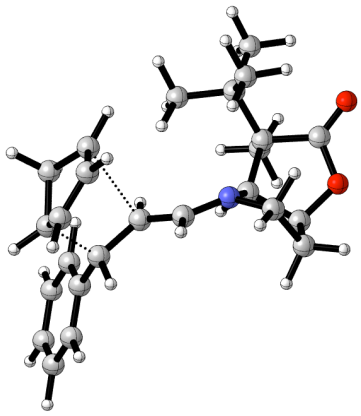
E(RM062X) = -1176.72121723

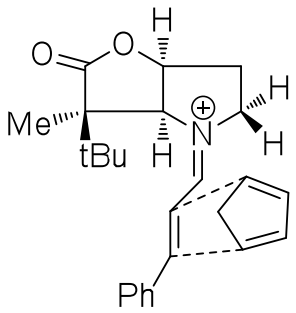
Zero-point correction=	0.524535 (Hartree/Particle)
Thermal correction to Energy=	0.549950
Thermal correction to Enthalpy=	0.550895
Thermal correction to Gibbs Free Energy=	0.469270
Sum of electronic and zero-point Energies=	-1176.196682
Sum of electronic and thermal Energies=	-1176.171267
Sum of electronic and thermal Enthalpies=	-1176.170323
Sum of electronic and thermal Free Energies=	-1176.251948

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.044534	2.384875	1.866341
2	6	0	-3.254324	1.905453	1.337788
3	6	0	-3.290154	2.124043	-0.051632
4	6	0	-2.236147	3.173113	-0.324653
5	6	0	-1.350743	3.013444	0.860586
6	6	0	-2.432646	0.550975	-0.750807
7	6	0	-1.078226	0.539665	-0.306341
8	6	0	-0.058778	0.974632	-1.132717
9	7	0	1.249253	0.885105	-0.935123
10	1	0	-0.832777	0.032346	0.614644
11	1	0	-2.546805	0.852574	-1.790316
12	1	0	-2.726076	4.153211	-0.241059
13	1	0	-1.745331	3.134171	-1.293703
14	1	0	-0.372023	3.464780	0.954649
15	1	0	-4.226131	2.097959	-0.595732
16	1	0	-0.329513	1.414191	-2.089667
17	1	0	-1.702171	2.241838	2.880882
18	1	0	-4.004530	1.357946	1.892089
19	6	0	2.194739	1.670512	-1.746128
20	1	0	1.676993	2.161049	-2.566622

21	6	0	2.780844	2.609534	-0.697635
22	1	0	3.723885	3.064388	-0.992243
23	1	0	2.062877	3.394481	-0.452228
24	6	0	1.860444	0.584582	0.369674
25	1	0	1.094280	0.708319	1.134627
26	6	0	2.975931	1.671092	0.487544
27	1	0	2.981352	2.175784	1.452495
28	6	0	2.633700	-0.749991	0.582289
29	6	0	2.634293	-0.974340	2.112385
30	1	0	1.659764	-1.332493	2.446283
31	1	0	3.390391	-1.703518	2.393615
32	1	0	2.856745	-0.045567	2.642484
33	6	0	4.081338	-0.352311	0.274519
34	8	0	4.214410	0.998085	0.320299
35	8	0	5.017119	-1.057356	0.076757
36	6	0	-3.349434	-0.570396	-0.395960
37	6	0	-4.353516	-0.923677	-1.294232
38	6	0	-3.236877	-1.272295	0.804515
39	6	0	-5.226689	-1.964600	-1.005428
40	1	0	-4.449193	-0.386942	-2.231936
41	6	0	-4.108468	-2.309922	1.094035
42	1	0	-2.469570	-1.011334	1.524872
43	6	0	-5.105707	-2.659235	0.188855
44	1	0	-5.998579	-2.232095	-1.715033
45	1	0	-4.010451	-2.850947	2.026244
46	1	0	-5.783861	-3.471001	0.416637
47	1	0	2.961328	1.007787	-2.153325
48	6	0	2.194822	-2.029149	-0.202928
49	6	0	0.683043	-2.257891	-0.089334
50	6	0	2.560392	-1.928950	-1.690489
51	6	0	2.894166	-3.270982	0.377144
52	1	0	0.319762	-2.154898	0.936569
53	1	0	0.115137	-1.590564	-0.734252
54	1	0	0.453687	-3.276476	-0.406439
55	1	0	3.638516	-1.861042	-1.835869
56	1	0	2.215168	-2.828740	-2.202690
57	1	0	2.076004	-1.080444	-2.175096
58	1	0	2.681582	-4.121246	-0.272648
59	1	0	3.973768	-3.145147	0.428660
60	1	0	2.513951	-3.519033	1.369166

TS3-*Z-endo*-top





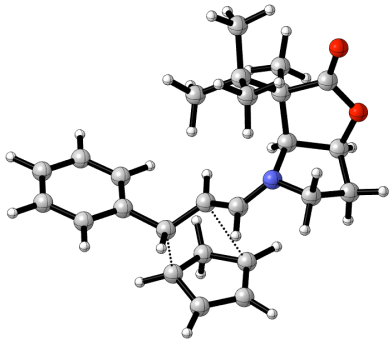
E(RM062X) = -1176.72053293

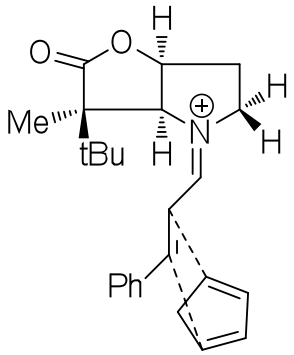
Zero-point correction=	0.525452 (Hartree/Particle)
Thermal correction to Energy=	0.550544
Thermal correction to Enthalpy=	0.551488
Thermal correction to Gibbs Free Energy=	0.471349
Sum of electronic and zero-point Energies=	-1176.195081
Sum of electronic and thermal Energies=	-1176.169989
Sum of electronic and thermal Enthalpies=	-1176.169045
Sum of electronic and thermal Free Energies=	-1176.249183

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.072958	2.806388	-0.426055
2	6	0	-2.248532	2.198372	-1.096968
3	6	0	-3.148565	1.907672	0.094393
4	6	0	-2.727775	2.845109	1.089276
5	6	0	-1.449223	3.311396	0.805544
6	6	0	-2.586178	0.335706	0.728589
7	6	0	-1.181450	0.147769	0.412093
8	6	0	-0.180111	0.490416	1.289040
9	7	0	1.119121	0.178527	1.247249
10	1	0	-2.030508	1.370221	-1.764525
11	1	0	-2.731528	2.988523	-1.689145
12	1	0	-2.772760	0.425634	1.794396
13	1	0	-0.937173	-0.389357	-0.493307
14	1	0	-4.210946	1.759357	-0.059315
15	1	0	-0.109881	2.955798	-0.896599
16	1	0	-0.457539	1.078941	2.160165
17	1	0	-0.837003	3.924498	1.450883

18	1	0	-3.289400	3.068725	1.987863
19	6	0	1.946846	0.385394	2.447878
20	1	0	1.420233	1.001633	3.172410
21	6	0	2.204103	-1.050407	2.891069
22	1	0	3.039612	-1.159093	3.578802
23	1	0	1.303003	-1.471182	3.340427
24	6	0	2.504247	-1.726785	1.560765
25	1	0	2.329123	-2.800730	1.558627
26	6	0	1.667073	-0.960234	0.483938
27	1	0	0.830434	-1.554130	0.117247
28	6	0	2.707685	-0.720678	-0.649857
29	6	0	4.039571	-0.795286	0.099951
30	6	0	2.695581	-2.022737	-1.487309
31	1	0	1.805445	-2.069181	-2.114728
32	1	0	3.576967	-2.078976	-2.122152
33	1	0	2.698038	-2.902269	-0.841134
34	8	0	3.873603	-1.485183	1.253630
35	8	0	5.107733	-0.393518	-0.236047
36	6	0	-3.547384	-0.656304	0.130490
37	6	0	-3.417820	-1.122778	-1.176857
38	6	0	-4.623423	-1.093027	0.899834
39	6	0	-4.343379	-2.014558	-1.698861
40	1	0	-2.592271	-0.803286	-1.802187
41	6	0	-5.547688	-1.988324	0.379081
42	1	0	-4.736047	-0.737009	1.917884
43	6	0	-5.410489	-2.449609	-0.922527
44	1	0	-4.230579	-2.372510	-2.713957
45	1	0	-6.373535	-2.325661	0.991669
46	1	0	-6.130193	-3.146409	-1.331402
47	1	0	2.876448	0.886736	2.167705
48	6	0	2.590288	0.551161	-1.543105
49	6	0	1.171943	0.673047	-2.104510
50	6	0	2.913910	1.824947	-0.749307
51	6	0	3.555909	0.471897	-2.737422
52	1	0	0.863361	-0.217757	-2.655449
53	1	0	0.453460	0.861785	-1.311453
54	1	0	1.131580	1.512779	-2.802678
55	1	0	3.937660	1.811505	-0.374762
56	1	0	2.819768	2.691990	-1.407084
57	1	0	2.229926	1.967648	0.089290
58	1	0	3.526039	1.422772	-3.272464
59	1	0	4.580614	0.293137	-2.418634
60	1	0	3.260030	-0.305509	-3.442786

TS3-*Z-endo*





E(RM062X) = -1176.72051097

Zero-point correction=	0.525006 (Hartree/Particle)
Thermal correction to Energy=	0.550269
Thermal correction to Enthalpy=	0.551213
Thermal correction to Gibbs Free Energy=	0.470281
Sum of electronic and zero-point Energies=	-1176.195505
Sum of electronic and thermal Energies=	-1176.170242
Sum of electronic and thermal Enthalpies=	-1176.169298
Sum of electronic and thermal Free Energies=	-1176.250230

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.402042	2.786283	1.087799
2	6	0	-2.615576	2.032655	1.504201
3	6	0	-3.360176	1.950725	0.189370
4	6	0	-2.910908	3.064414	-0.560443
5	6	0	-1.696850	3.520266	-0.048806
6	6	0	-2.457156	0.492412	-0.625861
7	6	0	-1.106116	0.509847	-0.153528
8	6	0	-0.090236	1.052816	-0.925408
9	7	0	1.216458	0.968561	-0.742226
10	1	0	-2.449933	1.096599	2.029019
11	1	0	-3.195900	2.690925	2.166097
12	1	0	-2.562227	0.752870	-1.673960
13	1	0	-0.849483	-0.072776	0.718558
14	1	0	-4.395110	1.637097	0.150335
15	1	0	-0.515900	2.899362	1.698713
16	1	0	-0.377460	1.606123	-1.816207
17	1	0	-1.066082	4.275873	-0.495231
18	1	0	-3.389499	3.433559	-1.458077
19	6	0	2.138618	1.883489	-1.437394

20	1	0	1.602721	2.474326	-2.176009
21	6	0	1.845986	0.497320	0.503722
22	1	0	1.087297	0.494968	1.285222
23	6	0	2.710256	2.674620	-0.266223
24	1	0	3.636801	3.195326	-0.497146
25	1	0	1.972371	3.392069	0.098899
26	6	0	2.943379	1.576654	0.764698
27	1	0	2.957627	1.933724	1.793316
28	6	0	2.645172	-0.837665	0.516555
29	6	0	4.077871	-0.371916	0.236625
30	6	0	2.685362	-1.266407	2.002287
31	1	0	2.904982	-0.414320	2.649301
32	1	0	1.725402	-1.685914	2.305138
33	1	0	3.459943	-2.011972	2.165357
34	8	0	4.189621	0.959949	0.479083
35	8	0	5.019299	-1.021153	-0.085299
36	6	0	-3.345934	-0.655540	-0.265700
37	6	0	-4.389246	-0.980674	-1.132852
38	6	0	-3.187197	-1.397566	0.904223
39	6	0	-5.251769	-2.027013	-0.843198
40	1	0	-4.522009	-0.412713	-2.047307
41	6	0	-4.051944	-2.443091	1.195644
42	1	0	-2.382635	-1.182086	1.596867
43	6	0	-5.086042	-2.760118	0.324505
44	1	0	-6.050980	-2.271729	-1.530488
45	1	0	-3.914494	-3.015118	2.103997
46	1	0	-5.756992	-3.577542	0.553246
47	1	0	2.916272	1.303017	-1.938373
48	6	0	2.206836	-2.006495	-0.424039
49	6	0	0.701720	-2.275160	-0.306793
50	6	0	2.535314	-1.700354	-1.892006
51	6	0	2.939336	-3.301751	-0.032691
52	1	0	0.363328	-2.320532	0.731615
53	1	0	0.107171	-1.535651	-0.839269
54	1	0	0.478194	-3.244243	-0.755740
55	1	0	3.609159	-1.601717	-2.050365
56	1	0	2.184800	-2.525627	-2.514259
57	1	0	2.034027	-0.798595	-2.245696
58	1	0	2.725112	-4.060428	-0.786901
59	1	0	4.017796	-3.162980	0.011934
60	1	0	2.587199	-3.688703	0.924605

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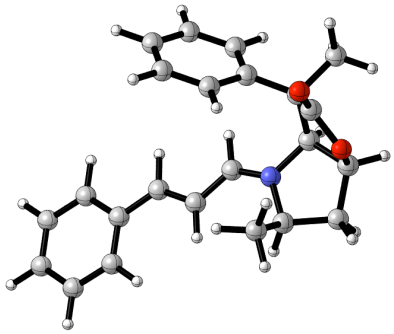
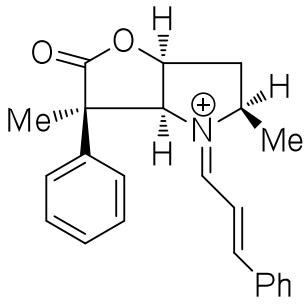
4 - *E*-iminium ion





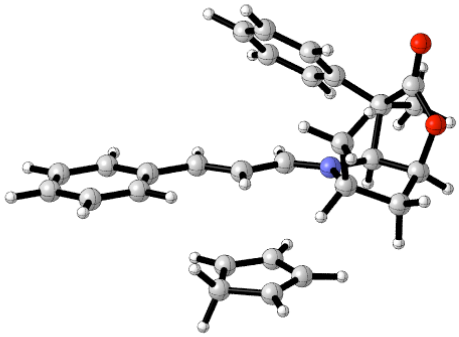
E(RM062X) = -1095.78498722

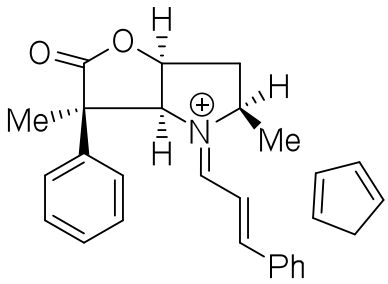
Zero-point correction=	0.424695 (Hartree/Particle)
Thermal correction to Energy=	0.446780
Thermal correction to Enthalpy=	0.447724
Thermal correction to Gibbs Free Energy=	0.372668
Sum of electronic and zero-point Energies=	-1095.360292
Sum of electronic and thermal Energies=	-1095.338207
Sum of electronic and thermal Enthalpies=	-1095.337263
Sum of electronic and thermal Free Energies=	-1095.412319

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.062098	-2.455936	-0.104128
2	6	0	2.408653	-2.962432	-0.627585
3	6	0	3.264760	-1.714217	-0.770214
4	6	0	2.299522	-0.578287	-1.143736
5	6	0	3.512190	-0.067908	0.846009
6	6	0	2.831305	0.631994	-0.333956
7	1	0	2.870413	-3.681111	0.046765
8	8	0	3.809681	-1.348330	0.498706
9	7	0	0.981207	-1.098989	-0.714508
10	1	0	2.265037	-0.367826	-2.212269
11	1	0	4.080671	-1.832369	-1.481088
12	6	0	1.764391	1.623397	0.071415
13	6	0	1.416394	2.669864	-0.782922
14	6	0	1.024443	1.440058	1.240203
15	6	0	0.340102	3.497981	-0.488680
16	1	0	1.980528	2.852142	-1.688196
17	6	0	-0.048810	2.269995	1.536902
18	1	0	1.293676	0.655644	1.936406
19	6	0	-0.400518	3.295755	0.669121
20	1	0	0.090149	4.309584	-1.159919
21	1	0	-0.602685	2.120777	2.454845
22	1	0	-1.231018	3.948542	0.905407
23	1	0	2.287743	-3.426453	-1.607226
24	1	0	0.240698	-3.042586	-0.515762
25	6	0	-0.122318	-0.433326	-0.875260

26	1	0	-0.029049	0.536772	-1.355334
27	6	0	-1.417053	-0.857467	-0.486214
28	1	0	-1.556774	-1.825918	-0.026992
29	6	0	-2.451342	0.002323	-0.671868
30	1	0	-2.219499	0.967278	-1.118981
31	6	0	-3.837661	-0.200465	-0.327327
32	6	0	-4.310775	-1.387949	0.253360
33	6	0	-4.741959	0.839311	-0.586475
34	6	0	-5.649367	-1.524834	0.560841
35	1	0	-3.633234	-2.206060	0.461500
36	6	0	-6.083397	0.699275	-0.275850
37	1	0	-4.382118	1.757998	-1.034998
38	6	0	-6.536503	-0.482016	0.297536
39	1	0	-6.011095	-2.441800	1.006497
40	1	0	-6.774852	1.505802	-0.479296
41	1	0	-7.585046	-0.595309	0.541166
42	8	0	3.799943	0.386678	1.902942
43	6	0	3.985499	1.268166	-1.134007
44	1	0	3.642585	1.624356	-2.104455
45	1	0	4.395819	2.105049	-0.570746
46	1	0	4.786007	0.546771	-1.306211
47	6	0	0.952466	-2.395901	1.416210
48	1	0	0.918665	-3.413170	1.806823
49	1	0	1.811433	-1.897478	1.863375
50	1	0	0.043787	-1.878766	1.726822

4-*E* and Cyclopentadiene Adduct





E(RM062X) = -1289.87229874

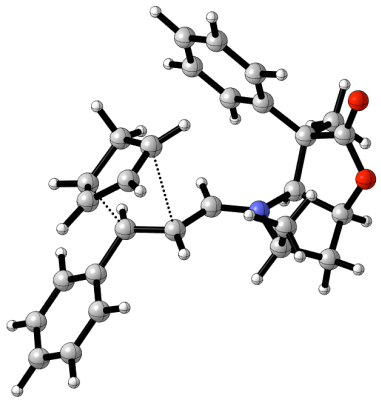
Zero-point correction=	0.518854 (Hartree/Particle)
Thermal correction to Energy=	0.547006
Thermal correction to Enthalpy=	0.547950
Thermal correction to Gibbs Free Energy=	0.456841
Sum of electronic and zero-point Energies=	-1289.353445
Sum of electronic and thermal Energies=	-1289.325293

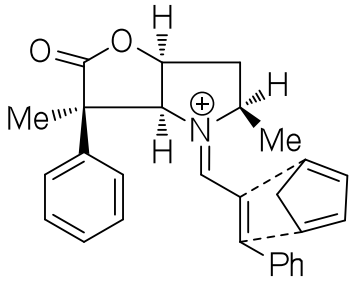
Sum of electronic and thermal Enthalpies= -1289.324349
Sum of electronic and thermal Free Energies= -1289.415458

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.483837	3.338995	0.805689
2	6	0	-2.716255	2.641244	1.298095
3	6	0	-2.207281	1.812685	2.437949
4	6	0	-0.894946	2.044481	2.605777
5	6	0	-0.445079	3.001837	1.588420
6	6	0	-2.213421	-0.527692	0.052327
7	6	0	-1.225905	0.196616	-0.525824
8	6	0	0.040176	0.205560	0.114188
9	7	0	1.091985	0.847542	-0.287392
10	1	0	-3.227817	2.053750	0.528978
11	1	0	-3.449459	3.373832	1.657189
12	1	0	-1.960656	-1.077400	0.956634
13	1	0	-1.383167	0.767495	-1.430172
14	1	0	-2.833989	1.178686	3.048809
15	1	0	-1.478333	4.056727	-0.002616
16	1	0	0.144494	-0.361603	1.034280
17	1	0	0.560042	3.398496	1.520964
18	1	0	-0.268480	1.630308	3.384554
19	6	0	1.119323	1.738772	-1.477738
20	1	0	0.190322	2.310449	-1.460008
21	6	0	2.316132	2.644702	-1.176659
22	1	0	2.803461	3.002229	-2.081859
23	1	0	2.001336	3.504655	-0.583804
24	6	0	3.257725	1.786577	-0.347737
25	1	0	3.940591	2.368950	0.268621
26	6	0	2.362088	0.843246	0.468396
27	1	0	2.167144	1.191537	1.483411
28	6	0	3.135192	-0.498949	0.450875
29	6	0	3.918268	-0.377637	-0.860422
30	6	0	4.206658	-0.449083	1.557614
31	1	0	3.752517	-0.323369	2.539572
32	1	0	4.781162	-1.374174	1.545603
33	1	0	4.894873	0.382718	1.398349
34	8	0	4.022550	0.934473	-1.202827
35	8	0	4.415802	-1.242382	-1.501791
36	6	0	2.249861	-1.722335	0.526366
37	6	0	1.880973	-2.249427	1.763845
38	6	0	1.687739	-2.269060	-0.627792
39	6	0	0.956087	-3.283122	1.847312
40	1	0	2.310938	-1.860721	2.677711
41	6	0	0.766720	-3.304879	-0.545284

42	1	0	1.979451	-1.898094	-1.602439
43	6	0	0.391007	-3.809503	0.692852
44	1	0	0.687964	-3.684442	2.816221
45	1	0	0.351015	-3.724697	-1.452213
46	1	0	-0.320416	-4.622742	0.756607
47	6	0	-3.587276	-0.648646	-0.383170
48	6	0	-4.081535	0.003228	-1.523503
49	6	0	-4.459429	-1.430308	0.385753
50	6	0	-5.408751	-0.131695	-1.880848
51	1	0	-3.427070	0.612200	-2.134495
52	6	0	-5.790070	-1.563134	0.025511
53	1	0	-4.082737	-1.935452	1.267647
54	6	0	-6.264447	-0.913868	-1.106778
55	1	0	-5.785102	0.369811	-2.762516
56	1	0	-6.456078	-2.170150	0.623979
57	1	0	-7.303654	-1.015992	-1.391721
58	6	0	1.235422	0.941306	-2.772415
59	1	0	1.157358	1.624841	-3.618131
60	1	0	2.195424	0.430971	-2.844099
61	1	0	0.437312	0.202189	-2.853160

TS4-*E-exo*-top





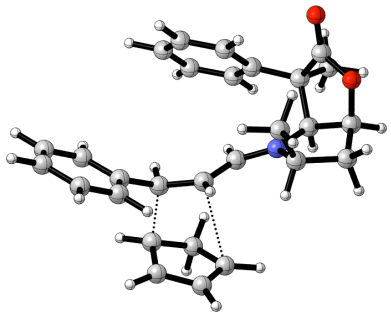
E(RM062X) = -1289.84828047

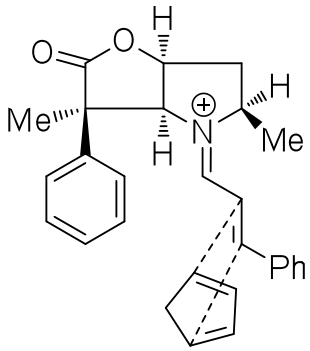
Zero-point correction=	0.520561 (Hartree/Particle)
Thermal correction to Energy=	0.546785
Thermal correction to Enthalpy=	0.547730
Thermal correction to Gibbs Free Energy=	0.464191
Sum of electronic and zero-point Energies=	-1289.327719
Sum of electronic and thermal Energies=	-1289.301495
Sum of electronic and thermal Enthalpies=	-1289.300551
Sum of electronic and thermal Free Energies=	-1289.384090

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.727586	0.769969	2.665922
2	6	0	-2.871390	1.201677	1.970642
3	6	0	-2.494901	1.819275	0.766417
4	6	0	-1.028165	2.148713	0.913753
5	6	0	-0.617649	1.205292	1.984957
6	6	0	-2.398078	0.323794	-0.462968
7	6	0	-1.360214	-0.552868	-0.033923
8	6	0	-0.097369	-0.473736	-0.590132
9	7	0	0.900099	-1.329134	-0.412412
10	1	0	-1.594121	-1.356585	0.649770
11	1	0	-2.117170	0.951528	-1.306043
12	1	0	-0.958391	3.165677	1.325301
13	1	0	-0.415548	2.131109	0.015316
14	1	0	0.413356	0.998939	2.239958
15	1	0	-3.180285	2.463102	0.229558
16	1	0	0.116225	0.338776	-1.277654
17	1	0	-1.727676	0.161873	3.558964
18	1	0	-3.893099	1.004356	2.266056
19	6	0	0.741541	-2.581823	0.363039
20	1	0	-0.256463	-2.969997	0.151467
21	6	0	1.804717	-3.492972	-0.255238
22	1	0	2.200953	-4.217400	0.453980
23	1	0	1.396372	-4.027934	-1.113593
24	6	0	2.167378	-1.255922	-1.163981
25	1	0	1.963151	-1.220149	-2.235573
26	6	0	2.885687	-2.544393	-0.732562
27	1	0	3.522107	-2.965820	-1.508476
28	6	0	3.159415	-0.154963	-0.728876
29	6	0	4.305878	-0.089759	-1.769039
30	1	0	3.924282	0.221946	-2.740371
31	1	0	5.045715	0.636873	-1.436288
32	1	0	4.800278	-1.055121	-1.885246
33	6	0	3.807731	-0.809441	0.493140
34	8	0	3.703749	-2.155655	0.376333
35	8	0	4.383475	-0.302686	1.402287
36	6	0	2.585261	1.236704	-0.530354
37	6	0	2.089446	1.911228	-1.652264
38	6	0	2.600292	1.907767	0.690260
39	6	0	1.641978	3.220787	-1.564503
40	1	0	2.072169	1.416673	-2.617842
41	6	0	2.161053	3.227400	0.775666
42	1	0	3.009724	1.427838	1.567533
43	6	0	1.690544	3.890875	-0.346195

44	1	0	1.281558	3.726392	-2.451358
45	1	0	2.214351	3.741845	1.727295
46	1	0	1.372842	4.923561	-0.279206
47	6	0	-3.802584	-0.161483	-0.573115
48	6	0	-4.615894	0.362478	-1.575117
49	6	0	-4.330704	-1.116179	0.296477
50	6	0	-5.930233	-0.064666	-1.715612
51	1	0	-4.216498	1.105435	-2.256924
52	6	0	-5.641918	-1.541718	0.158370
53	1	0	-3.721687	-1.529425	1.092770
54	6	0	-6.445354	-1.017390	-0.849635
55	1	0	-6.548894	0.347219	-2.502128
56	1	0	-6.040850	-2.285021	0.836391
57	1	0	-7.468743	-1.352275	-0.955968
58	6	0	0.892888	-2.351864	1.862716
59	1	0	0.721029	-3.289410	2.392397
60	1	0	1.893539	-2.001033	2.113934
61	1	0	0.162673	-1.622990	2.216843

TS4-*E-exo*





E(RM062X) = -1289.84740254

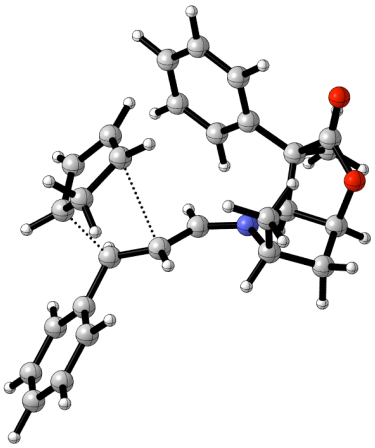
Zero-point correction=	0.520531 (Hartree/Particle)
Thermal correction to Energy=	0.546760
Thermal correction to Enthalpy=	0.547704
Thermal correction to Gibbs Free Energy=	0.463723
Sum of electronic and zero-point Energies=	-1289.326872
Sum of electronic and thermal Energies=	-1289.300643
Sum of electronic and thermal Enthalpies=	-1289.299698
Sum of electronic and thermal Free Energies=	-1289.383679

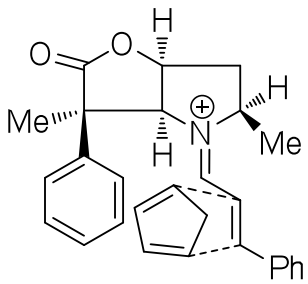
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.627243	-3.267192	0.792016
2	6	0	3.581458	-2.250648	0.964462
3	6	0	3.066292	-1.252515	1.807625
4	6	0	1.904355	-1.890286	2.533470
5	6	0	1.547940	-2.992935	1.597986
6	6	0	2.095046	-0.114427	0.565872
7	6	0	1.026127	-0.871271	0.011997
8	6	0	-0.256032	-0.710758	0.514315
9	7	0	-1.377559	-1.156210	-0.021024
10	1	0	1.171537	-1.401039	-0.918398
11	1	0	1.775721	0.588117	1.334092
12	1	0	2.306728	-2.350751	3.446429
13	1	0	1.091669	-1.231631	2.828399
14	1	0	0.645189	-3.584384	1.669972
15	1	0	3.713180	-0.525395	2.282110
16	1	0	-0.381381	-0.125181	1.420997
17	1	0	2.709223	-4.094527	0.102252
18	1	0	4.528956	-2.189216	0.446903
19	6	0	3.139029	0.470080	-0.321002
20	6	0	3.579090	-0.172562	-1.478483
21	6	0	3.689011	1.704458	0.017169
22	6	0	4.544454	0.412679	-2.282063
23	1	0	3.174575	-1.139779	-1.755792
24	6	0	4.656041	2.292611	-0.788391
25	1	0	3.351900	2.211078	0.915117
26	6	0	5.084771	1.648206	-1.939465
27	1	0	4.877458	-0.093192	-3.179053
28	1	0	5.073442	3.253081	-0.515512
29	1	0	5.837855	2.103524	-2.569004
30	6	0	-1.425754	-1.998423	-1.235424
31	1	0	-0.633720	-2.745517	-1.140504
32	6	0	-2.702406	-0.867706	0.549644
33	1	0	-2.747677	-1.223986	1.579813
34	6	0	-2.808003	-2.649077	-1.117238
35	1	0	-3.235143	-2.903454	-2.085528
36	1	0	-2.755236	-3.552618	-0.508150
37	6	0	-3.658633	-1.615345	-0.395355
38	1	0	-4.518935	-2.045750	0.114467
39	6	0	-3.170299	0.607442	0.442009
40	6	0	-3.784551	0.631090	-0.959962
41	8	0	-4.124133	-0.632992	-1.324067
42	8	0	-3.998318	1.570378	-1.653314
43	6	0	-4.360635	0.807251	1.399299
44	1	0	-4.072566	0.608609	2.430975
45	1	0	-4.724242	1.830858	1.320669
46	1	0	-5.180818	0.132903	1.146948
47	6	0	-2.063293	1.619038	0.638615

48	6	0	-1.761147	2.097530	1.913219
49	6	0	-1.240929	1.990309	-0.425782
50	6	0	-0.649719	2.905528	2.123528
51	1	0	-2.389480	1.846458	2.757778
52	6	0	-0.129808	2.796144	-0.217956
53	1	0	-1.468698	1.653142	-1.429078
54	6	0	0.173826	3.250325	1.059368
55	1	0	-0.437776	3.276012	3.118449
56	1	0	0.495555	3.074190	-1.056857
57	1	0	1.031466	3.891444	1.219853
58	6	0	-1.221090	-1.191377	-2.515548
59	1	0	-1.145381	-1.875010	-3.361782
60	1	0	-2.059816	-0.522013	-2.704124
61	1	0	-0.305360	-0.600606	-2.468775

TS4-*E-endo*-top





E(RM062X) = -1289.84289668

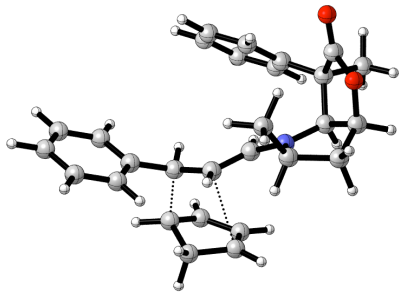
Zero-point correction=	0.520979 (Hartree/Particle)
Thermal correction to Energy=	0.547164
Thermal correction to Enthalpy=	0.548108
Thermal correction to Gibbs Free Energy=	0.464709
Sum of electronic and zero-point Energies=	-1289.321918
Sum of electronic and thermal Energies=	-1289.295733
Sum of electronic and thermal Enthalpies=	-1289.294789
Sum of electronic and thermal Free Energies=	-1289.378187

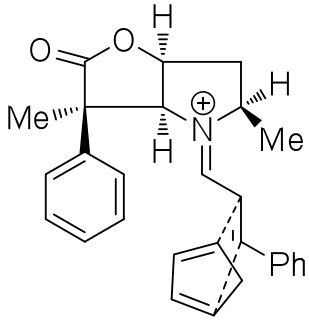
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.704865	1.159888	2.008601
2	6	0	-2.181052	1.073386	2.169830
3	6	0	-2.651291	1.797434	0.926238
4	6	0	-1.579015	2.637738	0.556777
5	6	0	-0.395518	2.196875	1.155772
6	6	0	-2.514690	0.424734	-0.394279
7	6	0	-1.484885	-0.479756	0.017854
8	6	0	-0.208958	-0.416802	-0.513417
9	7	0	0.738165	-1.338393	-0.387982
10	1	0	-2.588276	0.081622	2.344113
11	1	0	-2.455505	1.698613	3.031064
12	1	0	-2.263097	1.011100	-1.271599
13	1	0	-1.749412	-1.308402	0.658322
14	1	0	-3.678229	2.120268	0.818274
15	1	0	0.012563	0.593432	2.587970
16	1	0	0.054785	0.441570	-1.122902
17	1	0	0.596107	2.562779	0.940438
18	1	0	-1.646999	3.436200	-0.171075
19	6	0	0.465000	-2.639744	0.271885
20	1	0	-0.555818	-2.925152	0.011939
21	6	0	2.012271	-1.316190	-1.140349
22	1	0	1.811147	-1.200964	-2.206723
23	6	0	1.459901	-3.580807	-0.408576
24	1	0	1.786814	-4.388923	0.243242
25	1	0	1.024031	-4.011084	-1.311156
26	6	0	2.617283	-2.686856	-0.795849
27	1	0	3.236585	-3.098522	-1.590300
28	6	0	3.110495	-0.348051	-0.647013
29	6	0	3.641448	-1.118678	0.563651
30	6	0	4.276715	-0.382386	-1.672251
31	1	0	4.667190	-1.389152	-1.822372
32	1	0	3.937930	0.013409	-2.629810
33	1	0	5.085518	0.248536	-1.306162
34	8	0	3.433270	-2.442629	0.355281
35	8	0	4.201512	-0.724240	1.536280
36	6	0	2.740563	1.111470	-0.449012
37	6	0	2.122898	1.780881	-1.511017
38	6	0	3.162067	1.859820	0.649535
39	6	0	1.921596	3.152729	-1.478175
40	1	0	1.829821	1.230171	-2.399779
41	6	0	2.977295	3.240425	0.672780
42	1	0	3.671980	1.376040	1.469129
43	6	0	2.361008	3.892202	-0.384905
44	1	0	1.455351	3.648500	-2.320333
45	1	0	3.333818	3.806509	1.523915
46	1	0	2.235039	4.967055	-0.367161
47	6	0	-3.929652	-0.055143	-0.456462

48	6	0	-4.779688	0.506008	-1.409069
49	6	0	-4.437291	-1.018540	0.414833
50	6	0	-6.105472	0.107717	-1.498231
51	1	0	-4.397374	1.257141	-2.091515
52	6	0	-5.763890	-1.414523	0.328130
53	1	0	-3.804922	-1.478822	1.164186
54	6	0	-6.601566	-0.852971	-0.627564
55	1	0	-6.750023	0.546689	-2.248521
56	1	0	-6.144398	-2.166649	1.006935
57	1	0	-7.635345	-1.165375	-0.693964
58	6	0	0.601930	-2.557558	1.787899
59	1	0	1.616740	-2.293990	2.084060
60	1	0	-0.089024	-1.821752	2.201773
61	1	0	0.361765	-3.526963	2.225706

TS4-*E-endo*





E(RM062X) = -1289.84635486

Zero-point correction=	0.520776 (Hartree/Particle)
Thermal correction to Energy=	0.546976
Thermal correction to Enthalpy=	0.547920
Thermal correction to Gibbs Free Energy=	0.463748
Sum of electronic and zero-point Energies=	-1289.325579
Sum of electronic and thermal Energies=	-1289.299379
Sum of electronic and thermal Enthalpies=	-1289.298435
Sum of electronic and thermal Free Energies=	-1289.382607

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.456297	-2.927248	1.531406
2	6	0	2.834044	-2.633411	1.049434
3	6	0	3.074344	-1.284452	1.689117
4	6	0	2.236100	-1.255370	2.825740

5	6	0	1.227248	-2.210315	2.692518
6	6	0	2.123758	-0.160681	0.455261
7	6	0	1.047135	-0.933545	-0.075623
8	6	0	-0.237162	-0.742077	0.419884
9	7	0	-1.367289	-1.150640	-0.119851
10	1	0	2.997144	-2.700269	-0.021908
11	1	0	3.509973	-3.349788	1.537239
12	1	0	1.802370	0.636146	1.118535
13	1	0	1.185548	-1.486759	-0.993640
14	1	0	4.057916	-0.833829	1.704548
15	1	0	0.836556	-3.729228	1.153356
16	1	0	-0.342112	-0.172040	1.339104
17	1	0	0.377502	-2.327072	3.349676
18	1	0	2.306555	-0.527070	3.622846
19	6	0	-1.439343	-1.963065	-1.354472
20	1	0	-0.669749	-2.734960	-1.278845
21	6	0	-2.838320	-2.579359	-1.250661
22	1	0	-3.273223	-2.795461	-2.224759
23	1	0	-2.808579	-3.500627	-0.667148
24	6	0	-3.660357	-1.544352	-0.498762
25	1	0	-4.530752	-1.966272	0.000942
26	6	0	-2.683779	-0.848317	0.464682
27	1	0	-2.733663	-1.234455	1.483751
28	6	0	-3.115877	0.640190	0.401192
29	6	0	-3.731949	0.719372	-0.998410
30	6	0	-4.299405	0.839471	1.366952
31	1	0	-4.013451	0.605798	2.391887
32	1	0	-4.640463	1.872641	1.317822
33	1	0	-5.134941	0.190822	1.098269
34	8	0	-4.100895	-0.525115	-1.399094
35	8	0	-3.924426	1.683643	-1.662900
36	6	0	-1.987734	1.623547	0.621755
37	6	0	-1.682115	2.075780	1.904836
38	6	0	-1.155410	1.999096	-0.433706
39	6	0	-0.559703	2.864126	2.131658
40	1	0	-2.317188	1.821016	2.743139
41	6	0	-0.033783	2.785880	-0.209485
42	1	0	-1.384815	1.682546	-1.443378
43	6	0	0.271497	3.215832	1.075904
44	1	0	-0.345832	3.215343	3.133117
45	1	0	0.597259	3.069374	-1.042330
46	1	0	1.137344	3.842383	1.249597
47	6	0	3.222265	0.299803	-0.445206
48	6	0	3.628409	-0.411325	-1.574008
49	6	0	3.875379	1.491684	-0.129521
50	6	0	4.663574	0.062178	-2.367661
51	1	0	3.137345	-1.335040	-1.855470
52	6	0	4.907986	1.966820	-0.924234

53	1	0	3.565207	2.052723	0.745554
54	6	0	5.306346	1.250753	-2.045356
55	1	0	4.966502	-0.496786	-3.243492
56	1	0	5.400696	2.896072	-0.669365
57	1	0	6.111694	1.618087	-2.667617
58	6	0	-1.209908	-1.129991	-2.612757
59	1	0	-1.159672	-1.792571	-3.477358
60	1	0	-2.025350	-0.426943	-2.780085
61	1	0	-0.273447	-0.573665	-2.551942

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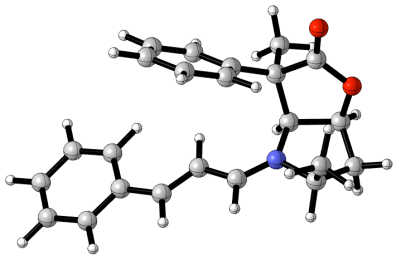
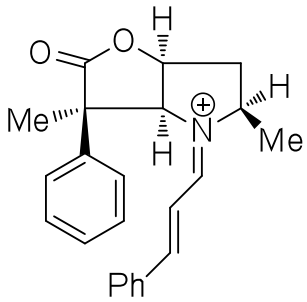
4 - *Z*-iminium ion





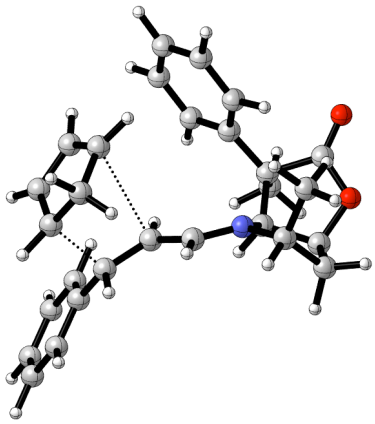
E(RM062X) = -1095.78308154

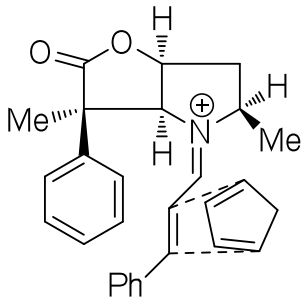
Zero-point correction=	0.424731 (Hartree/Particle)
Thermal correction to Energy=	0.446592
Thermal correction to Enthalpy=	0.447536
Thermal correction to Gibbs Free Energy=	0.374017
Sum of electronic and zero-point Energies=	-1095.358351
Sum of electronic and thermal Energies=	-1095.336490
Sum of electronic and thermal Enthalpies=	-1095.335546
Sum of electronic and thermal Free Energies=	-1095.409064

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.648256	-2.240609	0.430694
2	6	0	3.653948	-2.116227	-0.715787
3	6	0	3.387470	-0.745482	-1.318290
4	6	0	1.878182	-0.486116	-1.139278
5	6	0	3.196674	1.216685	-0.097223
6	6	0	1.814884	1.013204	-0.730214
7	1	0	4.684062	-2.200547	-0.375063
8	8	0	4.047910	0.258859	-0.549965
9	7	0	1.487244	-1.459904	-0.101744
10	1	0	1.302471	-0.684046	-2.043492
11	1	0	3.712265	-0.662752	-2.354029
12	6	0	0.686300	1.397749	0.201236
13	6	0	-0.475356	2.002187	-0.277290
14	6	0	0.766361	1.093108	1.560463
15	6	0	-1.550436	2.242956	0.568398

16	1	0	-0.555932	2.293016	-1.316980
17	6	0	-0.307389	1.329405	2.406485
18	1	0	1.681204	0.684183	1.970603
19	6	0	-1.476910	1.891034	1.908813
20	1	0	-2.445159	2.711304	0.178447
21	1	0	-0.222992	1.094329	3.459829
22	1	0	-2.313968	2.081038	2.568079
23	1	0	3.467930	-2.882123	-1.469812
24	1	0	2.306169	-3.269054	0.543397
25	6	0	0.265718	-1.709237	0.260667
26	1	0	0.160163	-2.440157	1.059443
27	6	0	-0.910656	-1.155060	-0.294263
28	1	0	-0.836551	-0.494511	-1.145252
29	6	0	-2.102460	-1.425235	0.294561
30	1	0	-2.096792	-2.075732	1.166815
31	6	0	-3.399833	-0.928870	-0.098206
32	6	0	-4.518025	-1.330825	0.644917
33	6	0	-3.579432	-0.057249	-1.183978
34	6	0	-5.784086	-0.880369	0.311812
35	1	0	-4.385595	-2.002151	1.485383
36	6	0	-4.843299	0.388574	-1.515011
37	1	0	-2.728999	0.273142	-1.766856
38	6	0	-5.946603	-0.021334	-0.767361
39	1	0	-6.642035	-1.197134	0.889405
40	1	0	-4.979241	1.056969	-2.354873
41	1	0	-6.935221	0.331515	-1.031488
42	6	0	1.850084	1.840529	-2.029416
43	1	0	1.866211	2.901889	-1.785465
44	1	0	2.742459	1.611223	-2.614033
45	1	0	0.979978	1.629457	-2.651184
46	8	0	3.540123	2.074142	0.645591
47	6	0	3.134219	-1.717455	1.775367
48	1	0	2.324816	-1.716680	2.507210
49	1	0	3.918678	-2.380370	2.141292
50	1	0	3.555440	-0.715653	1.703247

TS4-*Z-exo*-top





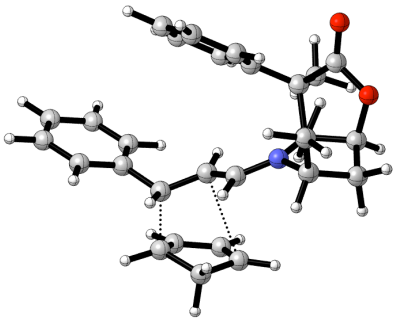
E(RM062X) = -1289.84008764

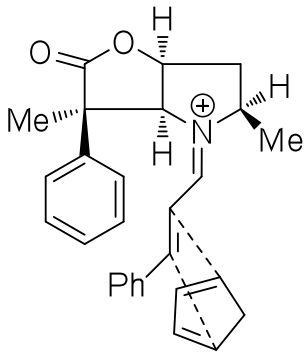
Zero-point correction=	0.520534 (Hartree/Particle)
Thermal correction to Energy=	0.546723
Thermal correction to Enthalpy=	0.547667
Thermal correction to Gibbs Free Energy=	0.463638
Sum of electronic and zero-point Energies=	-1289.319553
Sum of electronic and thermal Energies=	-1289.293364
Sum of electronic and thermal Enthalpies=	-1289.292420
Sum of electronic and thermal Free Energies=	-1289.376450

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.724403	2.613584	0.720568
2	6	0	-2.994541	2.004884	0.771545
3	6	0	-3.046591	1.091680	1.830105
4	6	0	-1.877433	1.426654	2.724308
5	6	0	-0.998080	2.194606	1.803179
6	6	0	-2.398389	-0.547167	0.969043
7	6	0	-1.042308	-0.400658	0.555445
8	6	0	-0.017506	-0.850692	1.363608
9	7	0	1.215564	-1.175800	0.993555
10	1	0	-0.816684	-0.087615	-0.455880
11	1	0	-2.521038	-1.117161	1.886910
12	1	0	-2.243641	2.126112	3.488858
13	1	0	-1.405864	0.601475	3.252022
14	1	0	0.026367	2.465061	2.014977
15	1	0	-3.988111	0.725306	2.218942
16	1	0	-0.228891	-1.045033	2.412666
17	1	0	-1.369334	3.267154	-0.059961

18	1	0	-3.785580	2.149891	0.048202
19	6	0	-3.444591	-0.874816	-0.038446
20	6	0	-3.403319	-0.370322	-1.339305
21	6	0	-4.497350	-1.708274	0.331058
22	6	0	-4.392525	-0.701834	-2.250543
23	1	0	-2.602007	0.295440	-1.642131
24	6	0	-5.487778	-2.044010	-0.583580
25	1	0	-4.539929	-2.105350	1.339451
26	6	0	-5.436691	-1.542210	-1.875247
27	1	0	-4.352801	-0.305762	-3.257013
28	1	0	-6.297025	-2.697396	-0.285022
29	1	0	-6.207050	-1.800927	-2.589688
30	6	0	2.144920	-1.840149	1.945647
31	1	0	1.546443	-2.187894	2.788584
32	6	0	1.553304	-1.454026	-0.410068
33	1	0	0.658638	-1.852347	-0.893137
34	6	0	2.660071	-3.020111	1.117093
35	1	0	3.646176	-3.359275	1.429043
36	1	0	1.962660	-3.856717	1.178783
37	6	0	2.687023	-2.500808	-0.311184
38	1	0	2.598995	-3.291632	-1.054410
39	6	0	2.184664	-0.333775	-1.267641
40	6	0	3.683277	-0.526366	-0.992142
41	8	0	3.901366	-1.789765	-0.550568
42	8	0	4.563266	0.252892	-1.154880
43	6	0	2.006762	-0.746803	-2.741699
44	1	0	0.949544	-0.780305	-3.007769
45	1	0	2.519077	-0.039246	-3.392077
46	1	0	2.426995	-1.737808	-2.919894
47	6	0	1.764500	1.097846	-1.000338
48	6	0	0.985992	1.814497	-1.907785
49	6	0	2.252468	1.764960	0.123667
50	6	0	0.727180	3.166312	-1.712108
51	1	0	0.611266	1.340942	-2.805384
52	6	0	1.994767	3.113480	0.322089
53	1	0	2.894493	1.243859	0.821823
54	6	0	1.236750	3.822962	-0.601193
55	1	0	0.150277	3.711407	-2.449041
56	1	0	2.420278	3.620672	1.179409
57	1	0	1.064331	4.883327	-0.465650
58	6	0	3.233595	-0.911690	2.466118
59	1	0	2.794690	-0.029102	2.933880
60	1	0	3.819300	-1.440052	3.219292
61	1	0	3.919816	-0.597964	1.679765

TS4-*Z-exo*





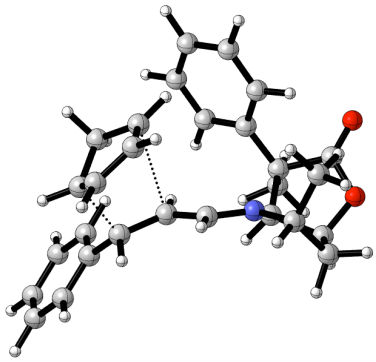
E(RM062X) = -1289.84457716

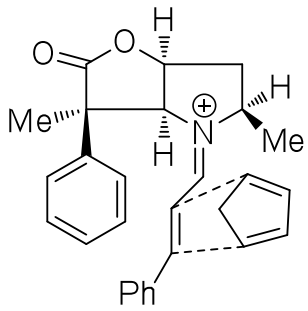
Zero-point correction=	0.520633 (Hartree/Particle)
Thermal correction to Energy=	0.546621
Thermal correction to Enthalpy=	0.547565
Thermal correction to Gibbs Free Energy=	0.465077
Sum of electronic and zero-point Energies=	-1289.323944
Sum of electronic and thermal Energies=	-1289.297956
Sum of electronic and thermal Enthalpies=	-1289.297012
Sum of electronic and thermal Free Energies=	-1289.379500

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.679698	3.238566	-1.472888
2	6	0	2.882463	2.766586	-0.926969
3	6	0	2.764492	2.669027	0.472412
4	6	0	1.591074	3.550083	0.838017
5	6	0	0.828256	3.559990	-0.440458
6	6	0	1.976733	0.926476	0.741956
7	6	0	0.685643	0.914016	0.144531
8	6	0	-0.462217	1.198025	0.867521
9	7	0	-1.710892	1.054618	0.461679
10	1	0	0.585257	0.523455	-0.858311
11	1	0	1.962134	1.010401	1.826513
12	1	0	1.986232	4.563841	0.991068
13	1	0	1.034540	3.279904	1.730963
14	1	0	-0.179807	3.938263	-0.546611
15	1	0	3.641448	2.593373	1.103255
16	1	0	-0.362738	1.572146	1.883778
17	1	0	1.447279	3.295562	-2.526376
18	1	0	3.739165	2.433400	-1.495885
19	6	0	-2.860686	1.635923	1.205374
20	1	0	-2.505252	2.549606	1.684149

21	6	0	-3.833589	1.960763	0.066971
22	1	0	-4.873685	1.946570	0.387482
23	1	0	-3.610555	2.941412	-0.356490
24	6	0	-2.074702	0.537295	-0.857938
25	1	0	-1.460343	1.026335	-1.618272
26	6	0	-3.569071	0.894318	-0.985563
27	1	0	-3.849391	1.206781	-1.990370
28	6	0	-2.052592	-1.008749	-1.015798
29	6	0	-1.998879	-1.324622	-2.520543
30	1	0	-1.075920	-0.948628	-2.963100
31	1	0	-2.054586	-2.401512	-2.673848
32	1	0	-2.835550	-0.860143	-3.045831
33	6	0	-3.475169	-1.385364	-0.580635
34	8	0	-4.284822	-0.297116	-0.666663
35	8	0	-3.878285	-2.449582	-0.246940
36	6	0	-1.004110	-1.743407	-0.204731
37	6	0	0.171455	-2.216262	-0.783228
38	6	0	-1.189575	-1.927519	1.165726
39	6	0	1.149764	-2.826921	-0.007722
40	1	0	0.341344	-2.117699	-1.847934
41	6	0	-0.212558	-2.530446	1.943283
42	1	0	-2.116898	-1.621118	1.631341
43	6	0	0.966652	-2.975609	1.358266
44	1	0	2.060816	-3.180118	-0.474465
45	1	0	-0.382705	-2.673933	3.002801
46	1	0	1.729412	-3.453231	1.959762
47	6	0	3.003639	-0.042876	0.262391
48	6	0	3.804850	-0.695202	1.193991
49	6	0	3.161029	-0.339212	-1.091374
50	6	0	4.737877	-1.640644	0.784172
51	1	0	3.687024	-0.478428	2.249826
52	6	0	4.096351	-1.274245	-1.503331
53	1	0	2.548681	0.162179	-1.833864
54	6	0	4.885265	-1.932186	-0.563856
55	1	0	5.350437	-2.145542	1.519777
56	1	0	4.211601	-1.494882	-2.556818
57	1	0	5.614941	-2.663755	-0.885476
58	6	0	-3.423901	0.702763	2.268640
59	1	0	-2.643909	0.396156	2.967398
60	1	0	-4.194446	1.231857	2.830534
61	1	0	-3.882577	-0.184401	1.832780

TS4-*Z-endo*-top





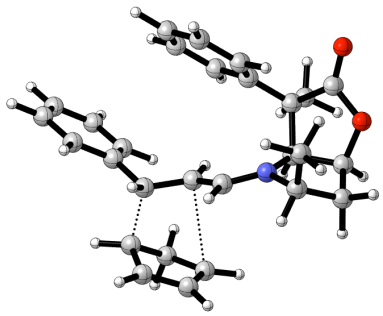
E(RM062X) = -1289.84265945

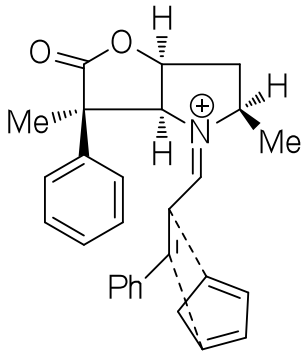
Zero-point correction=	0.521168 (Hartree/Particle)
Thermal correction to Energy=	0.547128
Thermal correction to Enthalpy=	0.548072
Thermal correction to Gibbs Free Energy=	0.465756
Sum of electronic and zero-point Energies=	-1289.321492
Sum of electronic and thermal Energies=	-1289.295532
Sum of electronic and thermal Enthalpies=	-1289.294588
Sum of electronic and thermal Free Energies=	-1289.376903

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.791208	2.032547	1.480903
2	6	0	-2.054085	2.092168	0.701020
3	6	0	-2.964554	1.229863	1.545004
4	6	0	-2.410738	1.258620	2.842621
5	6	0	-1.080267	1.686089	2.784753
6	6	0	-2.459373	-0.527375	0.935410
7	6	0	-1.093852	-0.471878	0.514832
8	6	0	-0.054851	-0.808139	1.361952
9	7	0	1.188826	-1.115157	1.017336
10	1	0	-1.967404	1.842336	-0.351606
11	1	0	-2.426390	3.124746	0.766686
12	1	0	-2.630175	-1.093641	1.843861
13	1	0	-0.867908	-0.264281	-0.522041
14	1	0	-4.035870	1.215562	1.394805
15	1	0	0.170014	2.350410	1.102212
16	1	0	-0.261487	-0.889090	2.426332
17	1	0	-0.381492	1.688225	3.609088
18	1	0	-2.917240	0.908399	3.732950
19	6	0	2.161897	-1.623136	2.014755

20	1	0	1.597481	-1.896569	2.906967
21	6	0	2.713352	-2.865862	1.309200
22	1	0	3.716700	-3.132012	1.636749
23	1	0	2.050474	-3.716106	1.474904
24	6	0	2.701817	-2.504742	-0.169844
25	1	0	2.606258	-3.373055	-0.819677
26	6	0	1.551093	-1.485684	-0.356162
27	1	0	0.672467	-1.937235	-0.820373
28	6	0	2.167260	-0.410414	-1.282717
29	6	0	3.674342	-0.604539	-1.065910
30	6	0	1.942619	-0.881151	-2.736152
31	1	0	0.878926	-0.946945	-2.964859
32	1	0	2.417060	-0.185845	-3.427011
33	1	0	2.375764	-1.871193	-2.891943
34	8	0	3.904014	-1.820202	-0.517783
35	8	0	4.555002	0.135409	-1.361362
36	6	0	1.744266	1.035801	-1.078623
37	6	0	0.680486	1.578593	-1.801305
38	6	0	2.464191	1.884204	-0.235072
39	6	0	0.358094	2.926960	-1.701825
40	1	0	0.116971	0.961981	-2.491095
41	6	0	2.152899	3.235166	-0.143695
42	1	0	3.317176	1.510991	0.313981
43	6	0	1.101998	3.764525	-0.881387
44	1	0	-0.453561	3.328639	-2.295931
45	1	0	2.751895	3.878517	0.488040
46	1	0	0.875867	4.821789	-0.830230
47	6	0	-3.519361	-0.796873	-0.081698
48	6	0	-3.418330	-0.364648	-1.404424
49	6	0	-4.664830	-1.485797	0.316048
50	6	0	-4.438455	-0.623443	-2.307755
51	1	0	-2.541653	0.173288	-1.746072
52	6	0	-5.683466	-1.748347	-0.588355
53	1	0	-4.756008	-1.825713	1.341791
54	6	0	-5.573270	-1.315659	-1.902803
55	1	0	-4.347521	-0.285957	-3.332055
56	1	0	-6.562279	-2.291584	-0.266457
57	1	0	-6.366678	-1.517750	-2.610180
58	6	0	3.213678	-0.588248	2.390161
59	1	0	2.739258	0.333656	2.730013
60	1	0	3.828757	-0.979706	3.201239
61	1	0	3.878572	-0.359016	1.558145

TS4-*Z-endo*





E(RM062X) = -1289.84427321

Zero-point correction=	0.520742 (Hartree/Particle)
Thermal correction to Energy=	0.546708
Thermal correction to Enthalpy=	0.547652
Thermal correction to Gibbs Free Energy=	0.465197
Sum of electronic and zero-point Energies=	-1289.323532
Sum of electronic and thermal Energies=	-1289.297565
Sum of electronic and thermal Enthalpies=	-1289.296621
Sum of electronic and thermal Free Energies=	-1289.379076

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.846915	3.381195	-0.903885
2	6	0	2.177255	2.837906	-1.289491
3	6	0	2.785298	2.588152	0.074149
4	6	0	2.136354	3.502673	0.939593
5	6	0	0.940986	3.929487	0.364887
6	6	0	1.984120	0.922932	0.516926
7	6	0	0.693553	0.889645	-0.097301
8	6	0	-0.453431	1.273020	0.585233
9	7	0	-1.703873	1.071099	0.217717
10	1	0	2.174995	2.004167	-1.983518
11	1	0	2.743701	3.658761	-1.751518
12	1	0	1.960970	0.996290	1.598856
13	1	0	0.585430	0.391769	-1.050849
14	1	0	3.839906	2.372219	0.186191
15	1	0	0.021421	3.517639	-1.589791
16	1	0	-0.338337	1.801663	1.528889
17	1	0	0.186670	4.532484	0.850316
18	1	0	2.472738	3.746624	1.938686
19	6	0	-2.842900	1.772797	0.868527
20	1	0	-2.483466	2.758037	1.169782

21	6	0	-2.087061	0.336457	-0.989742
22	1	0	-1.495266	0.693553	-1.836036
23	6	0	-3.840517	1.888149	-0.288468
24	1	0	-4.873984	1.925125	0.051138
25	1	0	-3.634231	2.780476	-0.881630
26	6	0	-3.587245	0.655641	-1.143683
27	1	0	-3.892202	0.785037	-2.181063
28	6	0	-2.051759	-1.213166	-0.883557
29	6	0	-3.458986	-1.519025	-0.353668
30	6	0	-2.030982	-1.780844	-2.313464
31	1	0	-2.887283	-1.421883	-2.887515
32	1	0	-1.125302	-1.476539	-2.838944
33	1	0	-2.074226	-2.868595	-2.279222
34	8	0	-4.282228	-0.466891	-0.604349
35	8	0	-3.842079	-2.512494	0.168479
36	6	0	-0.973842	-1.788710	0.012297
37	6	0	0.200580	-2.326212	-0.509611
38	6	0	-1.126465	-1.747056	1.398474
39	6	0	1.210325	-2.778393	0.331191
40	1	0	0.346074	-2.400070	-1.579881
41	6	0	-0.118663	-2.193369	2.240116
42	1	0	-2.050642	-1.385356	1.829890
43	6	0	1.058977	-2.703868	1.707253
44	1	0	2.121487	-3.181604	-0.093786
45	1	0	-0.263214	-2.164286	3.312711
46	1	0	1.845754	-3.059493	2.360206
47	6	0	3.021893	-0.053461	0.062983
48	6	0	3.923717	-0.547596	1.003398
49	6	0	3.116791	-0.495481	-1.256025
50	6	0	4.888002	-1.477687	0.641364
51	1	0	3.857082	-0.216012	2.033685
52	6	0	4.085763	-1.418498	-1.621908
53	1	0	2.423214	-0.145581	-2.011113
54	6	0	4.971867	-1.915623	-0.673758
55	1	0	5.573451	-1.860072	1.386521
56	1	0	4.146162	-1.755476	-2.648762
57	1	0	5.724366	-2.638676	-0.959866
58	6	0	-3.375774	1.038500	2.091224
59	1	0	-2.578776	0.863784	2.815845
60	1	0	-4.140306	1.652476	2.568518
61	1	0	-3.833251	0.085541	1.826882

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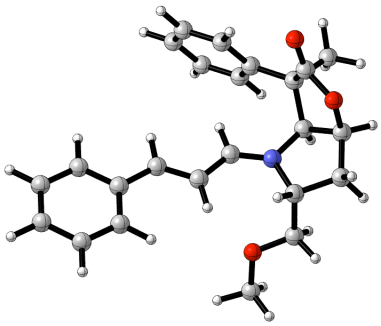
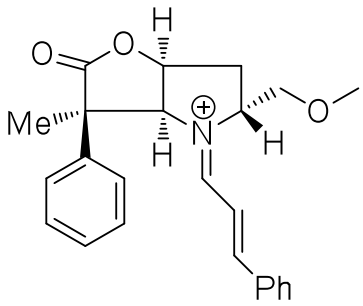
5 - *E*-iminium ion





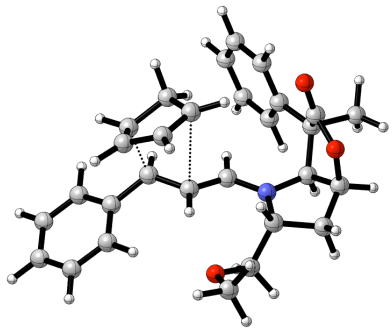
E(RM062X) = -1210.29432051

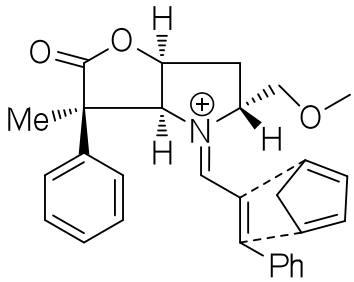
Zero-point correction=	0.458154 (Hartree/Particle)
Thermal correction to Energy=	0.482771
Thermal correction to Enthalpy=	0.483715
Thermal correction to Gibbs Free Energy=	0.402246
Sum of electronic and zero-point Energies=	-1209.836166
Sum of electronic and thermal Energies=	-1209.811549
Sum of electronic and thermal Enthalpies=	-1209.810605
Sum of electronic and thermal Free Energies=	-1209.892075

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.282242	2.203453	0.048369
2	6	0	2.650197	2.675241	0.539691
3	6	0	3.478539	1.413496	0.613618
4	6	0	2.506069	0.312773	1.059000
5	6	0	3.572329	-0.237845	-1.010208
6	6	0	2.949022	-0.914468	0.216391
7	1	0	1.287328	2.048154	-1.034494
8	1	0	3.090702	3.412568	-0.128300
9	8	0	3.890435	1.048492	-0.703017
10	7	0	1.174437	0.866597	0.708898
11	1	0	2.537545	0.104824	2.128235
12	1	0	4.355643	1.498829	1.252712
13	6	0	1.838060	-1.879937	-0.129362
14	6	0	1.512346	-2.922243	0.739595
15	6	0	1.047253	-1.682093	-1.261794
16	6	0	0.409323	-3.730308	0.495124
17	1	0	2.115381	-3.115829	1.617255
18	6	0	-0.050950	-2.494506	-1.510848
19	1	0	1.294373	-0.899261	-1.968457
20	6	0	-0.379476	-3.514851	-0.628799
21	1	0	0.176387	-4.538492	1.176633
22	1	0	-0.645436	-2.332097	-2.400609
23	1	0	-1.231442	-4.152676	-0.826559
24	1	0	2.556091	3.109841	1.538403
25	6	0	0.094066	0.174180	0.934983

26	1	0	0.245749	-0.739487	1.502750
27	6	0	-1.219709	0.460061	0.501185
28	1	0	-1.402834	1.325901	-0.119844
29	6	0	-2.189852	-0.439775	0.806634
30	1	0	-1.912447	-1.299097	1.414592
31	6	0	-3.571615	-0.393229	0.390744
32	6	0	-4.075703	0.626466	-0.432395
33	6	0	-4.432694	-1.412025	0.820833
34	6	0	-5.405355	0.623517	-0.803960
35	1	0	-3.424034	1.417079	-0.783537
36	6	0	-5.765656	-1.410948	0.447263
37	1	0	-4.046871	-2.202748	1.453843
38	6	0	-6.251335	-0.393844	-0.364796
39	1	0	-5.791737	1.408945	-1.439823
40	1	0	-6.424972	-2.199118	0.785167
41	1	0	-7.292699	-0.390958	-0.660088
42	8	0	3.809486	-0.717042	-2.067887
43	6	0	4.133311	-1.584021	0.941582
44	1	0	3.841107	-1.939113	1.928919
45	1	0	4.488293	-2.426067	0.349265
46	1	0	4.960836	-0.884061	1.069291
47	6	0	0.187712	3.207936	0.395977
48	1	0	-0.249393	2.976325	1.378335
49	1	0	0.655377	4.196963	0.468441
50	8	0	-0.790320	3.227706	-0.610789
51	6	0	-1.758437	4.241720	-0.399238
52	1	0	-2.314703	4.065253	0.527757
53	1	0	-1.284389	5.226143	-0.350553
54	1	0	-2.439858	4.216245	-1.245616

TS5-*E-exo*-top





E(RM062X) = -1404.35582216

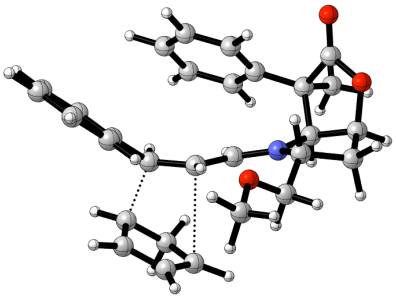
Zero-point correction=	0.554612 (Hartree/Particle)
Thermal correction to Energy=	0.583152
Thermal correction to Enthalpy=	0.584096
Thermal correction to Gibbs Free Energy=	0.495238
Sum of electronic and zero-point Energies=	-1403.801210

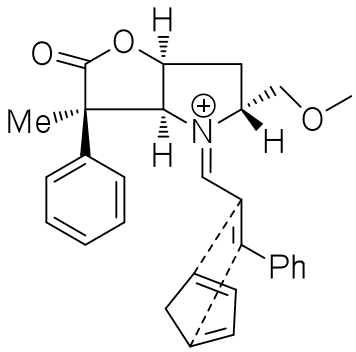
Sum of electronic and thermal Energies= -1403.772670
Sum of electronic and thermal Enthalpies= -1403.771726
Sum of electronic and thermal Free Energies= -1403.860585

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.154781	-0.549975	2.691697
2	6	0	2.271164	-1.245503	2.193064
3	6	0	1.879646	-2.090583	1.142519
4	6	0	0.378727	-2.208554	1.240085
5	6	0	0.031275	-1.014059	2.053116
6	6	0	2.062327	-0.935429	-0.413480
7	6	0	1.179466	0.168352	-0.238765
8	6	0	-0.078699	0.169983	-0.792855
9	7	0	-0.927252	1.200525	-0.811403
10	1	0	1.525673	1.036908	0.301790
11	1	0	1.695800	-1.697189	-1.099362
12	1	0	0.153142	-3.096970	1.847084
13	1	0	-0.172884	-2.319944	0.308568
14	1	0	-0.979577	-0.648737	2.191911
15	1	0	2.503342	-2.916206	0.824957
16	1	0	-0.425403	-0.722046	-1.298504
17	1	0	1.185600	0.245932	3.421083
18	1	0	3.296191	-1.084152	2.499817
19	6	0	-0.565695	2.539767	-0.283053
20	6	0	-1.750685	3.394491	-0.716671
21	1	0	-1.915415	4.244394	-0.056472
22	1	0	-1.597374	3.762447	-1.734321
23	6	0	-2.347677	1.098405	-1.223533
24	1	0	-2.436383	0.983887	-2.304908
25	6	0	-2.909304	2.433533	-0.711437
26	1	0	-3.781486	2.785943	-1.257010
27	6	0	-3.219285	0.086071	-0.438555
28	6	0	-4.653784	0.106499	-1.033296
29	1	0	-4.623777	-0.241106	-2.066478
30	1	0	-5.280113	-0.577163	-0.462041
31	1	0	-5.110253	1.095194	-1.002377
32	6	0	-3.311121	0.827433	0.898360
33	8	0	-3.269606	2.158862	0.650320
34	8	0	-3.422320	0.404328	2.006677
35	6	0	-2.792503	-1.370792	-0.406107
36	6	0	-2.397915	-1.975625	-1.603617
37	6	0	-2.956463	-2.177212	0.719655
38	6	0	-2.119337	-3.332752	-1.665998
39	1	0	-2.315645	-1.381503	-2.508477
40	6	0	-2.693364	-3.542686	0.651845

41	1	0	-3.311187	-1.747900	1.645098
42	6	0	-2.265540	-4.124216	-0.531379
43	1	0	-1.814427	-3.776563	-2.605132
44	1	0	-2.839619	-4.153501	1.533941
45	1	0	-2.069114	-5.187385	-0.580106
46	6	0	3.532073	-0.723051	-0.533128
47	6	0	4.318332	-1.757598	-1.040962
48	6	0	4.145084	0.472105	-0.154016
49	6	0	5.692207	-1.610810	-1.160844
50	1	0	3.848534	-2.684914	-1.352465
51	6	0	5.520104	0.615975	-0.273293
52	1	0	3.556520	1.305470	0.211475
53	6	0	6.297086	-0.423093	-0.771424
54	1	0	6.288756	-2.420310	-1.560783
55	1	0	5.986757	1.549091	0.014873
56	1	0	7.368583	-0.303499	-0.864265
57	1	0	-0.514407	2.472392	0.810666
58	6	0	0.780049	3.091971	-0.803475
59	1	0	1.158866	2.460577	-1.608266
60	1	0	0.618395	4.095227	-1.212041
61	8	0	1.773596	3.146084	0.192023
62	6	0	1.646153	4.270505	1.043946
63	1	0	2.442650	4.209058	1.781216
64	1	0	1.751683	5.198825	0.474850
65	1	0	0.681369	4.276970	1.562963

TS5-*E-exo*





E(RM062X) = -1404.35509326

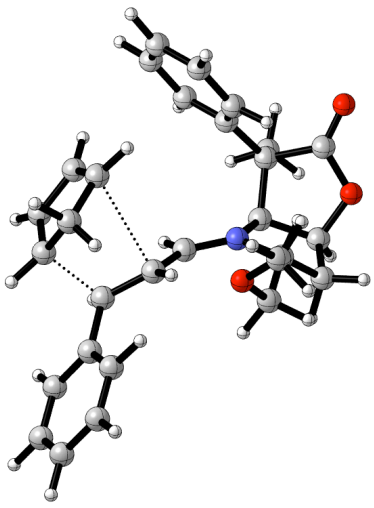
Zero-point correction=	0.553755 (Hartree/Particle)
Thermal correction to Energy=	0.582641
Thermal correction to Enthalpy=	0.583585
Thermal correction to Gibbs Free Energy=	0.492520
Sum of electronic and zero-point Energies=	-1403.801338

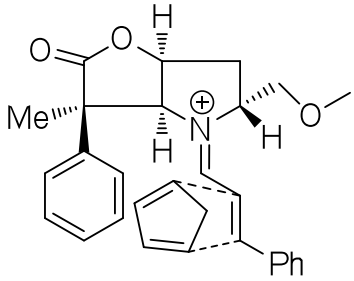
Sum of electronic and thermal Energies= -1403.772452
Sum of electronic and thermal Enthalpies= -1403.771508
Sum of electronic and thermal Free Energies= -1403.862573

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.662599	2.604649	1.599107
2	6	0	-3.540046	1.512004	1.515628
3	6	0	-2.963523	0.391698	2.138943
4	6	0	-1.865582	0.934507	3.023708
5	6	0	-1.579790	2.237026	2.362620
6	6	0	-1.903511	-0.373147	0.723458
7	6	0	-0.901852	0.566612	0.344788
8	6	0	0.391919	0.391548	0.795143
9	7	0	1.503141	0.971997	0.358715
10	1	0	-1.087995	1.264360	-0.457694
11	1	0	-1.530776	-1.195470	1.333196
12	1	0	-2.312724	1.152384	4.003483
13	1	0	-1.008065	0.287143	3.188512
14	1	0	-0.727161	2.859579	2.597343
15	1	0	-3.564080	-0.461577	2.427877
16	1	0	0.564016	-0.351786	1.569046
17	1	0	-2.796803	3.554571	1.103394
18	1	0	-4.468146	1.496289	0.960741
19	6	0	-2.901280	-0.839503	-0.281565
20	6	0	-3.276131	-0.064012	-1.378706
21	6	0	-3.481402	-2.095448	-0.111853
22	6	0	-4.208709	-0.542124	-2.287159
23	1	0	-2.836454	0.914375	-1.535638
24	6	0	-4.414082	-2.574714	-1.021541
25	1	0	-3.192712	-2.705019	0.737986
26	6	0	-4.779481	-1.797995	-2.112275
27	1	0	-4.488125	0.063966	-3.139269
28	1	0	-4.854035	-3.553211	-0.878863
29	1	0	-5.504412	-2.168415	-2.825108
30	6	0	1.620805	2.032868	-0.673243
31	6	0	2.820379	0.457103	0.782342
32	1	0	2.915039	0.539684	1.865928
33	6	0	3.030340	2.562628	-0.403031
34	1	0	3.465992	3.043607	-1.276520
35	1	0	3.000348	3.280225	0.421495
36	6	0	3.817095	1.343545	0.017512
37	1	0	4.717139	1.573192	0.585350
38	6	0	3.185210	-0.973887	0.295750
39	6	0	3.795645	-0.694771	-1.081847
40	8	0	4.180896	0.605672	-1.149105

41	8	0	3.976949	-1.459213	-1.970492
42	6	0	4.363937	-1.477112	1.151403
43	1	0	4.087181	-1.538021	2.203411
44	1	0	4.671813	-2.462530	0.804611
45	1	0	5.219696	-0.804435	1.070785
46	6	0	2.033806	-1.953439	0.234513
47	6	0	1.736266	-2.775379	1.320793
48	6	0	1.195352	-1.991606	-0.880702
49	6	0	0.621229	-3.605254	1.298482
50	1	0	2.375419	-2.785411	2.194018
51	6	0	0.082566	-2.819897	-0.905959
52	1	0	1.414802	-1.378149	-1.746267
53	6	0	-0.209277	-3.628069	0.185467
54	1	0	0.415228	-4.247642	2.145265
55	1	0	-0.555452	-2.836706	-1.780527
56	1	0	-1.068106	-4.286768	0.158575
57	1	0	1.555882	1.575205	-1.665897
58	6	0	0.611288	3.175704	-0.602159
59	1	0	0.275291	3.325862	0.433560
60	1	0	1.135260	4.086409	-0.915812
61	8	0	-0.477916	2.953864	-1.462185
62	6	0	-1.210968	4.135600	-1.723115
63	1	0	-2.048279	3.863213	-2.360772
64	1	0	-1.588031	4.582335	-0.796897
65	1	0	-0.588782	4.871382	-2.241070

TS5-*E-endo*-top





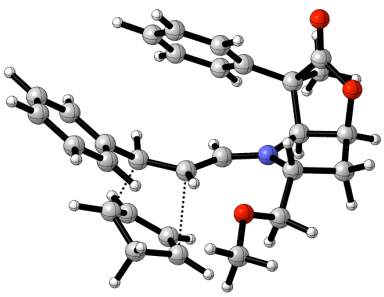
E(RM062X) = -1404.34993057

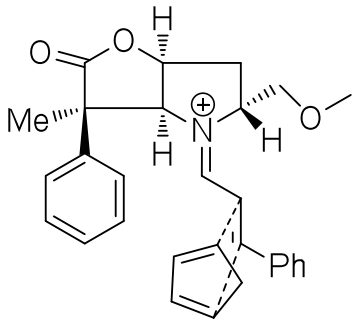
Zero-point correction= 0.554906 (Hartree/Particle)
Thermal correction to Energy= 0.583437
Thermal correction to Enthalpy= 0.584381
Thermal correction to Gibbs Free Energy= 0.495022
Sum of electronic and zero-point Energies= -1403.795024
Sum of electronic and thermal Energies= -1403.766493
Sum of electronic and thermal Enthalpies= -1403.765549
Sum of electronic and thermal Free Energies= -1403.854909

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.802977	1.964795	1.335558
2	6	0	-2.284868	1.948594	1.462290
3	6	0	-2.697169	2.357867	0.068226
4	6	0	-1.599432	3.055523	-0.465861
5	6	0	-0.443543	2.756893	0.266031
6	6	0	-2.511494	0.622275	-0.826102
7	6	0	-1.463784	-0.077393	-0.160229
8	6	0	-0.215972	-0.185105	-0.750788
9	7	0	0.777352	-1.035272	-0.521048
10	1	0	-2.723507	1.035361	1.855755
11	1	0	-2.565278	2.769531	2.137313
12	1	0	-2.278863	0.956286	-1.831828
13	1	0	-1.687068	-0.646263	0.724649
14	1	0	-3.717477	2.625027	-0.171051
15	1	0	-0.122975	1.545201	2.062992
16	1	0	-0.003644	0.496396	-1.574134
17	1	0	0.566438	3.036965	0.005042
18	1	0	-1.630416	3.649038	-1.370299
19	6	0	0.796595	-2.260886	0.322854
20	6	0	1.945834	-1.035085	-1.425209
21	1	0	1.604117	-0.770542	-2.425445
22	6	0	1.401240	-3.277558	-0.644225
23	1	0	1.816582	-4.146700	-0.137634
24	1	0	0.640557	-3.603032	-1.358473
25	6	0	2.481504	-2.483775	-1.349003
26	1	0	2.771697	-2.888948	-2.316478
27	6	0	3.178039	-0.184218	-1.033071
28	6	0	4.010550	-1.173188	-0.204568
29	6	0	4.002205	0.021435	-2.319223
30	1	0	4.233601	-0.936984	-2.787039
31	1	0	3.448182	0.621728	-3.041213
32	1	0	4.941887	0.519056	-2.083619
33	8	0	3.630947	-2.440757	-0.505170
34	8	0	4.888864	-0.933434	0.555455
35	6	0	2.949698	1.100228	-0.262374

36	6	0	3.184483	2.350773	-0.831108
37	6	0	2.617509	1.042195	1.092821
38	6	0	3.121527	3.507665	-0.060883
39	1	0	3.462219	2.438001	-1.872542
40	6	0	2.561629	2.192621	1.864594
41	1	0	2.464073	0.079808	1.569455
42	6	0	2.823427	3.431652	1.291460
43	1	0	3.334424	4.465515	-0.517847
44	1	0	2.347008	2.120355	2.923682
45	1	0	2.805446	4.327701	1.898123
46	6	0	-3.912500	0.119781	-0.718346
47	6	0	-4.830451	0.492971	-1.701614
48	6	0	-4.341808	-0.697207	0.328671
49	6	0	-6.146680	0.062389	-1.643986
50	1	0	-4.506776	1.125065	-2.521697
51	6	0	-5.661099	-1.124555	0.387205
52	1	0	-3.652827	-1.024508	1.098701
53	6	0	-6.566680	-0.746117	-0.595357
54	1	0	-6.844071	0.355918	-2.417708
55	1	0	-5.981216	-1.761626	1.201493
56	1	0	-7.593455	-1.084048	-0.546873
57	1	0	1.497445	-2.081254	1.145643
58	6	0	-0.524756	-2.748700	0.896260
59	1	0	-1.308057	-2.705171	0.136792
60	1	0	-0.386057	-3.802364	1.162730
61	8	0	-0.961879	-2.019990	2.019426
62	6	0	-0.407395	-2.466446	3.245910
63	1	0	-0.818023	-1.835465	4.029953
64	1	0	-0.683948	-3.506601	3.438494
65	1	0	0.683264	-2.377631	3.253105

TS5-*E-endo*





E(RM062X) = -1404.35433136

Zero-point correction=	0.554152 (Hartree/Particle)
Thermal correction to Energy=	0.582975
Thermal correction to Enthalpy=	0.583919
Thermal correction to Gibbs Free Energy=	0.492545
Sum of electronic and zero-point Energies=	-1403.800180
Sum of electronic and thermal Energies=	-1403.771356
Sum of electronic and thermal Enthalpies=	-1403.770412
Sum of electronic and thermal Free Energies=	-1403.861786

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.554656	2.413286	1.968807
2	6	0	-2.858999	2.074530	1.337953
3	6	0	-3.053883	0.660723	1.838591
4	6	0	-2.306194	0.576520	3.032351
5	6	0	-1.359413	1.603158	3.070574
6	6	0	-1.925803	-0.283665	0.601470
7	6	0	-0.894457	0.618441	0.199889
8	6	0	0.387640	0.448126	0.686275
9	7	0	1.516417	0.983006	0.234763
10	1	0	-2.921171	2.226601	0.263940
11	1	0	-3.627537	2.698269	1.815896
12	1	0	-1.583907	-1.110490	1.216954
13	1	0	-1.045473	1.282485	-0.635499
14	1	0	-4.001008	0.149282	1.731569
15	1	0	-0.970573	3.286232	1.714848
16	1	0	0.526938	-0.251682	1.505578
17	1	0	-0.571009	1.708791	3.801617
18	1	0	-2.384432	-0.229025	3.750446
19	6	0	1.643451	2.035356	-0.804876
20	6	0	3.121257	2.425417	-0.685674
21	1	0	3.527823	2.797212	-1.623903
22	1	0	3.231780	3.200893	0.077276
23	6	0	3.830114	1.175185	-0.227829
24	1	0	4.774357	1.370577	0.278141
25	6	0	2.818839	0.416579	0.645480
26	1	0	2.970425	0.576561	1.714089
27	6	0	3.083835	-1.067498	0.257767
28	6	0	3.644641	-0.931391	-1.162824
29	6	0	4.274472	-1.564587	1.101698
30	1	0	4.042105	-1.531256	2.165586
31	1	0	4.517690	-2.588142	0.820330
32	1	0	5.158014	-0.946062	0.934414
33	8	0	4.075508	0.340443	-1.358557
34	8	0	3.756304	-1.775459	-1.988657
35	6	0	1.894164	-2.002579	0.313616

36	6	0	1.609639	-2.731303	1.467823
37	6	0	1.023821	-2.107853	-0.772537
38	6	0	0.480526	-3.539153	1.537161
39	1	0	2.271098	-2.686948	2.323165
40	6	0	-0.101726	-2.916748	-0.707448
41	1	0	1.229412	-1.566821	-1.688151
42	6	0	-0.377005	-3.635174	0.448858
43	1	0	0.285371	-4.109685	2.436285
44	1	0	-0.762121	-2.988364	-1.562431
45	1	0	-1.244932	-4.280979	0.493584
46	6	0	-2.929582	-0.738339	-0.407105
47	6	0	-3.249706	0.003411	-1.543659
48	6	0	-3.578759	-1.955033	-0.191334
49	6	0	-4.196278	-0.466948	-2.443873
50	1	0	-2.752323	0.943588	-1.750269
51	6	0	-4.521815	-2.425860	-1.091780
52	1	0	-3.334854	-2.537446	0.690884
53	6	0	-4.834071	-1.680333	-2.221974
54	1	0	-4.431154	0.113963	-3.326352
55	1	0	-5.012521	-3.373904	-0.913318
56	1	0	-5.568475	-2.044952	-2.928029
57	1	0	1.413527	1.608256	-1.786034
58	6	0	0.816854	3.302147	-0.594357
59	1	0	0.807780	3.552507	0.476460
60	1	0	1.352113	4.108057	-1.112546
61	8	0	-0.484272	3.214426	-1.113628
62	6	0	-1.120787	4.476953	-1.187147
63	1	0	-2.112735	4.316148	-1.602546
64	1	0	-1.212043	4.933209	-0.194949
65	1	0	-0.564122	5.156568	-1.839026

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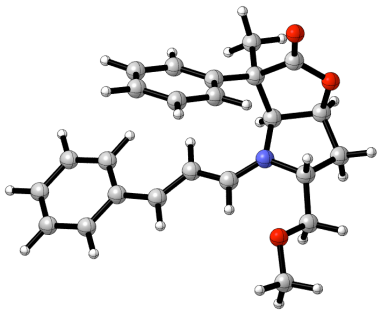
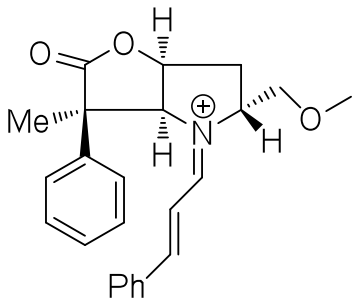
5 - *Z*-iminium ion





E(RM062X) = -1210.29973075

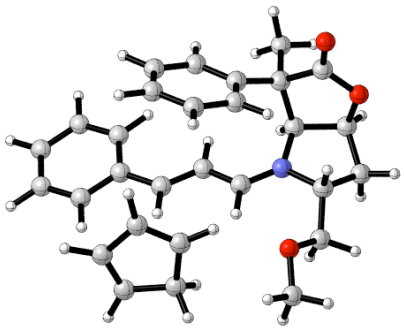
Zero-point correction= 0.458120 (Hartree/Particle)

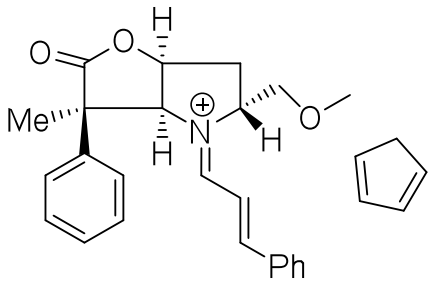
Thermal correction to Energy=	0.482663
Thermal correction to Enthalpy=	0.483607
Thermal correction to Gibbs Free Energy=	0.402665
Sum of electronic and zero-point Energies=	-1209.841611
Sum of electronic and thermal Energies=	-1209.817068
Sum of electronic and thermal Enthalpies=	-1209.816124
Sum of electronic and thermal Free Energies=	-1209.897066

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.794530	1.326510	-0.337289
2	6	0	-3.691029	0.741059	-1.422264
3	6	0	-3.216145	-0.697524	-1.519984
4	6	0	-1.695131	-0.653079	-1.261868
5	6	0	-2.828843	-2.047931	0.326855
6	6	0	-1.449620	-1.867816	-0.321350
7	1	0	-3.112149	0.979275	0.650932
8	1	0	-4.746779	0.792839	-1.164874
9	8	0	-3.774267	-1.436492	-0.436475
10	7	0	-1.491976	0.673282	-0.647928
11	1	0	-1.105850	-0.718773	-2.175567
12	1	0	-3.479138	-1.186320	-2.456163
13	6	0	-0.356875	-1.683826	0.708140
14	6	0	0.907624	-2.244007	0.537675
15	6	0	-0.585617	-0.879759	1.825908
16	6	0	1.933122	-1.964229	1.431578
17	1	0	1.108366	-2.905661	-0.295225
18	6	0	0.437943	-0.594338	2.716876
19	1	0	-1.575846	-0.479556	2.014820
20	6	0	1.706356	-1.125329	2.513571
21	1	0	2.910402	-2.405084	1.281527
22	1	0	0.240010	0.027576	3.580369
23	1	0	2.505364	-0.908725	3.210785
24	1	0	-3.523350	1.257308	-2.370688
25	6	0	-0.330849	1.204094	-0.402312
26	1	0	-0.360476	2.151103	0.130477
27	6	0	0.923408	0.656354	-0.766232
28	1	0	0.966361	-0.248199	-1.355231
29	6	0	2.046641	1.249450	-0.293676
30	1	0	1.923531	2.142568	0.315156
31	6	0	3.411075	0.814546	-0.489185
32	6	0	4.439725	1.578052	0.077816
33	6	0	3.739754	-0.345042	-1.207875
34	6	0	5.763433	1.200726	-0.074039
35	1	0	4.192001	2.472335	0.637707
36	6	0	5.060616	-0.718253	-1.359306
37	1	0	2.960990	-0.956321	-1.646027
38	6	0	6.073809	0.053332	-0.792238
39	1	0	6.551430	1.797546	0.365269
40	1	0	5.310567	-1.610941	-1.917228
41	1	0	7.107440	-0.244196	-0.913443
42	6	0	-1.262470	-3.108746	-1.212278
43	1	0	-1.156701	-3.994781	-0.587738

44	1	0	-2.124939	-3.252729	-1.865493
45	1	0	-0.378893	-3.007010	-1.842725
46	8	0	-3.095664	-2.651412	1.310453
47	6	0	-2.744571	2.837972	-0.334029
48	1	0	-3.779147	3.202237	-0.317372
49	1	0	-2.274126	3.204604	-1.258658
50	8	0	-2.045392	3.280562	0.800622
51	6	0	-2.140079	4.684783	0.986062
52	1	0	-1.577608	4.928496	1.883017
53	1	0	-1.718427	5.222144	0.131094
54	1	0	-3.183096	4.984041	1.120636

5-*Z* and Cyclopentadiene Adduct





E(RM062X) = -1404.38091048

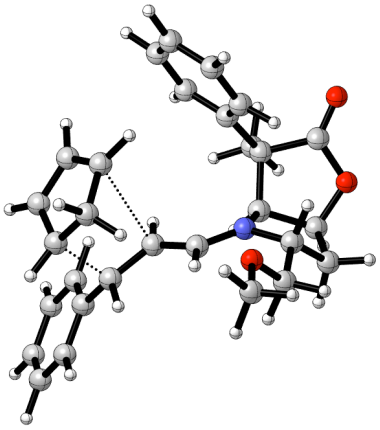
Zero-point correction=	0.552446 (Hartree/Particle)
Thermal correction to Energy=	0.583113
Thermal correction to Enthalpy=	0.584057
Thermal correction to Gibbs Free Energy=	0.486186
Sum of electronic and zero-point Energies=	-1403.828464
Sum of electronic and thermal Energies=	-1403.797797
Sum of electronic and thermal Enthalpies=	-1403.796853
Sum of electronic and thermal Free Energies=	-1403.894724

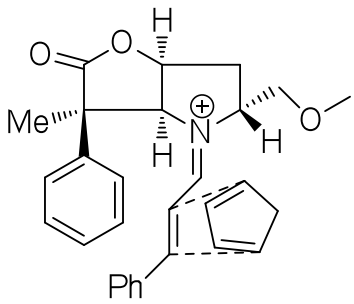
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.418587	-2.333098	1.917546
2	6	0	-3.680352	-2.573608	1.207443
3	6	0	-3.435270	-3.296213	0.103694
4	6	0	-1.968489	-3.606699	0.033256
5	6	0	-1.412523	-2.914875	1.246234
6	6	0	-1.856123	0.083139	-0.815041
7	6	0	-0.556991	0.391100	-1.053518

8	6	0	0.440542	-0.584867	-0.821873
9	7	0	1.723365	-0.378582	-0.912261
10	1	0	-0.268301	1.379791	-1.379790
11	1	0	-2.092189	-0.921005	-0.466741
12	1	0	-1.805895	-4.689507	0.084285
13	1	0	-1.507631	-3.278901	-0.907771
14	1	0	-0.366968	-2.922784	1.521588
15	1	0	-4.160666	-3.650945	-0.614006
16	1	0	0.142892	-1.594891	-0.548183
17	1	0	-2.335291	-1.782920	2.844016
18	1	0	-4.647969	-2.231006	1.546921
19	6	0	-2.983109	0.978794	-0.961069
20	6	0	-2.831694	2.347872	-1.231511
21	6	0	-4.273461	0.451103	-0.823601
22	6	0	-3.942082	3.156904	-1.370669
23	1	0	-1.843848	2.782670	-1.316663
24	6	0	-5.385347	1.264722	-0.968489
25	1	0	-4.388315	-0.604190	-0.607311
26	6	0	-5.220518	2.616143	-1.241427
27	1	0	-3.821171	4.212122	-1.577228
28	1	0	-6.378764	0.848355	-0.867544
29	1	0	-6.087590	3.254570	-1.352344
30	6	0	2.762931	-1.434845	-0.781815
31	6	0	2.338430	0.941608	-1.147147
32	1	0	1.866144	1.410000	-2.009452
33	6	0	3.869432	-0.881193	-1.672780
34	1	0	4.844846	-1.302027	-1.438137
35	1	0	3.637003	-1.068022	-2.724108
36	6	0	3.825920	0.608611	-1.385497
37	1	0	4.284847	1.220830	-2.159512
38	6	0	2.368777	1.889735	0.086818
39	6	0	3.694877	1.498925	0.753011
40	8	0	4.486042	0.854632	-0.146505
41	8	0	4.047614	1.732886	1.859382
42	6	0	2.587533	3.320102	-0.435316
43	1	0	1.752561	3.638840	-1.059891
44	1	0	2.688780	4.005842	0.404844
45	1	0	3.496839	3.379828	-1.036164
46	6	0	1.198719	1.755000	1.035721
47	6	0	0.154549	2.676414	1.046289
48	6	0	1.116284	0.642995	1.875962
49	6	0	-0.971961	2.461419	1.830496
50	1	0	0.205181	3.572061	0.440365
51	6	0	-0.008485	0.423392	2.655150
52	1	0	1.942279	-0.057738	1.933214
53	6	0	-1.065330	1.325550	2.621556
54	1	0	-1.777252	3.184838	1.821771
55	1	0	-0.051963	-0.444896	3.300223

56	1	0	-1.944340	1.158744	3.230858
57	1	0	3.089584	-1.456151	0.262756
58	6	0	2.299997	-2.819046	-1.174864
59	1	0	3.193412	-3.447125	-1.276948
60	1	0	1.794389	-2.791127	-2.151413
61	8	0	1.451173	-3.329019	-0.178234
62	6	0	1.212236	-4.720064	-0.320870
63	1	0	2.153505	-5.275788	-0.290460
64	1	0	0.589500	-5.025302	0.516346
65	1	0	0.694781	-4.936219	-1.260955

TS5-*Z*-*exo*-top





E(RM062X) = -1404.35675237

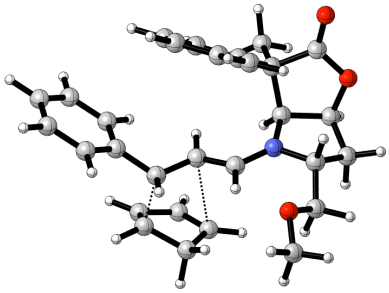
Zero-point correction=	0.554540 (Hartree/Particle)
Thermal correction to Energy=	0.583154
Thermal correction to Enthalpy=	0.584098
Thermal correction to Gibbs Free Energy=	0.494849
Sum of electronic and zero-point Energies=	-1403.802212
Sum of electronic and thermal Energies=	-1403.773598
Sum of electronic and thermal Enthalpies=	-1403.772654
Sum of electronic and thermal Free Energies=	-1403.861904

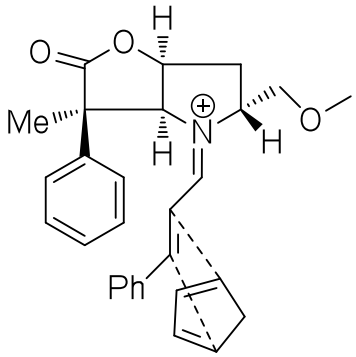
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.659106	-2.118154	1.696532
2	6	0	2.959600	-1.580400	1.664350
3	6	0	2.929078	-0.241232	2.065821
4	6	0	1.607488	-0.047200	2.767736

5	6	0	0.809143	-1.177509	2.220320
6	6	0	2.518632	0.646710	0.333821
7	6	0	1.208276	0.283776	-0.080624
8	6	0	0.149464	1.133074	0.201193
9	7	0	-1.037772	1.156562	-0.382277
10	1	0	1.064548	-0.551907	-0.752047
11	1	0	2.582797	1.631656	0.789804
12	1	0	1.776374	-0.253345	3.834012
13	1	0	1.143730	0.934022	2.701197
14	1	0	-0.260806	-1.281061	2.332827
15	1	0	3.826750	0.293741	2.347989
16	1	0	0.292682	1.905263	0.948221
17	1	0	1.368815	-3.089076	1.325356
18	1	0	3.837549	-2.088920	1.289731
19	6	0	3.695062	0.345214	-0.524920
20	6	0	3.751519	-0.788892	-1.336581
21	6	0	4.778891	1.220358	-0.512751
22	6	0	4.865926	-1.035159	-2.121781
23	1	0	2.927666	-1.493651	-1.349795
24	6	0	5.895576	0.975886	-1.301968
25	1	0	4.747302	2.104556	0.114595
26	6	0	5.941130	-0.151779	-2.107992
27	1	0	4.899224	-1.917402	-2.747870
28	1	0	6.727914	1.667256	-1.285842
29	1	0	6.809647	-0.345524	-2.723578
30	6	0	-2.029221	2.243450	-0.202197
31	6	0	-1.339352	0.385196	-1.591424
32	1	0	-0.408452	0.239743	-2.139306
33	6	0	-2.326937	2.625631	-1.650378
34	1	0	-3.278714	3.139160	-1.771276
35	1	0	-1.523319	3.255106	-2.040030
36	6	0	-2.333010	1.286462	-2.369482
37	1	0	-2.099273	1.360289	-3.430123
38	6	0	-2.100953	-0.954686	-1.431254
39	6	0	-3.563859	-0.550726	-1.682496
40	8	0	-3.617082	0.687984	-2.230631
41	8	0	-4.534319	-1.201361	-1.480466
42	6	0	-1.725428	-1.843495	-2.628315
43	1	0	-0.670073	-2.117136	-2.589968
44	1	0	-2.333136	-2.747307	-2.630208
45	1	0	-1.899249	-1.313394	-3.567040
46	6	0	-2.005626	-1.668360	-0.093810
47	6	0	-1.359338	-2.893307	0.045375
48	6	0	-2.693413	-1.155187	1.008614
49	6	0	-1.418746	-3.597298	1.244534
50	1	0	-0.838173	-3.337402	-0.792590
51	6	0	-2.755102	-1.852761	2.204739
52	1	0	-3.245528	-0.227241	0.918795

53	6	0	-2.122434	-3.085633	2.324144
54	1	0	-0.937975	-4.564758	1.320836
55	1	0	-3.321989	-1.448561	3.033340
56	1	0	-2.191947	-3.647478	3.246549
57	1	0	-2.920300	1.816532	0.266341
58	6	0	-1.562008	3.405572	0.642308
59	1	0	-2.337587	4.179657	0.593245
60	1	0	-0.638680	3.838027	0.227629
61	8	0	-1.368483	2.979520	1.967744
62	6	0	-1.159642	4.061818	2.858911
63	1	0	-2.026627	4.728492	2.867201
64	1	0	-1.022063	3.640858	3.851387
65	1	0	-0.270555	4.636538	2.578837

TS5-*Z-exo*





E(RM062X) = -1404.36105298

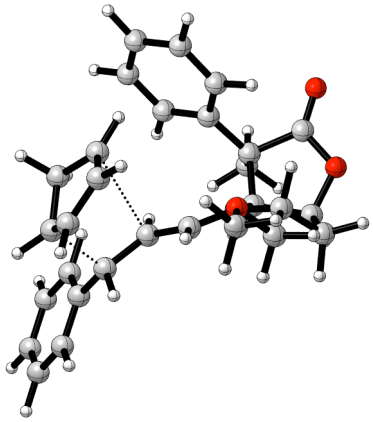
Zero-point correction=	0.553989 (Hartree/Particle)
Thermal correction to Energy=	0.582627
Thermal correction to Enthalpy=	0.583571
Thermal correction to Gibbs Free Energy=	0.494415
Sum of electronic and zero-point Energies=	-1403.807064
Sum of electronic and thermal Energies=	-1403.778426
Sum of electronic and thermal Enthalpies=	-1403.777482
Sum of electronic and thermal Free Energies=	-1403.866638

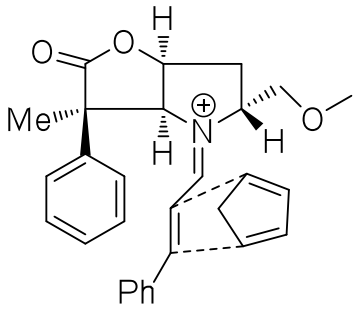
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.486356	2.537712	-2.556637
2	6	0	2.677722	2.519339	-1.818956
3	6	0	2.407602	2.838467	-0.475715
4	6	0	1.062296	3.528176	-0.486462

5	6	0	0.468344	2.967067	-1.732988
6	6	0	1.876163	1.126062	0.280178
7	6	0	0.675765	0.718767	-0.361886
8	6	0	-0.563742	0.993006	0.204655
9	7	0	-1.727170	0.511701	-0.190376
10	1	0	0.735362	0.030029	-1.192807
11	1	0	1.727900	1.526886	1.280380
12	1	0	1.249929	4.596023	-0.663689
13	1	0	0.461301	3.443387	0.415488
14	1	0	-0.570143	3.074728	-2.016819
15	1	0	3.197633	3.129598	0.205070
16	1	0	-0.623151	1.648108	1.068340
17	1	0	1.376671	2.212894	-3.581161
18	1	0	3.640882	2.202657	-2.193998
19	6	0	-3.039164	0.947883	0.339455
20	6	0	-3.935499	0.771114	-0.884119
21	1	0	-4.986593	0.659003	-0.626229
22	1	0	-3.819422	1.624294	-1.557854
23	6	0	-1.873941	-0.479145	-1.258515
24	1	0	-1.284294	-0.166154	-2.122458
25	6	0	-3.391142	-0.483688	-1.543893
26	1	0	-3.629797	-0.559453	-2.603470
27	6	0	-1.567226	-1.952013	-0.861384
28	6	0	-1.235198	-2.728828	-2.145010
29	1	0	-0.325750	-2.343157	-2.607180
30	1	0	-1.098666	-3.784388	-1.913655
31	1	0	-2.044777	-2.639578	-2.872332
32	6	0	-2.946727	-2.464125	-0.423634
33	8	0	-3.917214	-1.624666	-0.873484
34	8	0	-3.193390	-3.454044	0.179349
35	6	0	-0.547239	-2.128941	0.244491
36	6	0	0.757272	-2.538705	-0.016059
37	6	0	-0.901969	-1.829879	1.560581
38	6	0	1.694257	-2.615151	1.007256
39	1	0	1.063195	-2.802163	-1.020490
40	6	0	0.031288	-1.900925	2.583159
41	1	0	-1.924118	-1.556941	1.799144
42	6	0	1.337682	-2.286993	2.306106
43	1	0	2.708582	-2.922396	0.782897
44	1	0	-0.266362	-1.672760	3.598540
45	1	0	2.068866	-2.348647	3.101985
46	6	0	3.088086	0.264563	0.188744
47	6	0	3.897840	0.118880	1.310936
48	6	0	3.415661	-0.429126	-0.976122
49	6	0	5.006687	-0.718297	1.279213
50	1	0	3.648725	0.647693	2.224230
51	6	0	4.523622	-1.260490	-1.012247
52	1	0	2.803008	-0.321885	-1.865243

53	6	0	5.320144	-1.411717	0.119240
54	1	0	5.624035	-0.827402	2.161429
55	1	0	4.768718	-1.794098	-1.921624
56	1	0	6.184193	-2.062606	0.091102
57	1	0	-3.341617	0.264498	1.139300
58	6	0	-3.054109	2.362413	0.877402
59	1	0	-4.101841	2.651909	1.025817
60	1	0	-2.618278	3.050912	0.135884
61	8	0	-2.350284	2.424491	2.091592
62	6	0	-2.527748	3.661088	2.760841
63	1	0	-1.953297	3.614434	3.682047
64	1	0	-2.169601	4.495132	2.147842
65	1	0	-3.582502	3.822221	3.000697

TS5-*Z-endo*-top





E(RM062X) = -1404.35847007

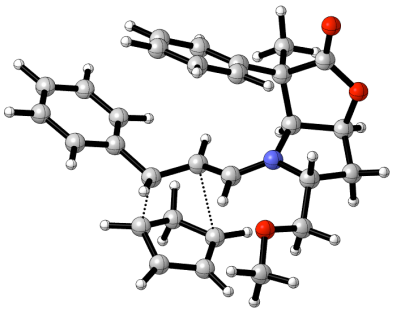
Zero-point correction=	0.554803 (Hartree/Particle)
Thermal correction to Energy=	0.583365
Thermal correction to Enthalpy=	0.584309
Thermal correction to Gibbs Free Energy=	0.495267
Sum of electronic and zero-point Energies=	-1403.803667
Sum of electronic and thermal Energies=	-1403.775105
Sum of electronic and thermal Enthalpies=	-1403.774161
Sum of electronic and thermal Free Energies=	-1403.863204

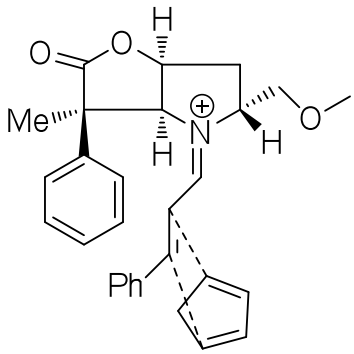
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.725969	0.742000	2.256934

2	6	0	2.044718	0.059183	2.203892
3	6	0	2.900303	1.122363	1.553943
4	6	0	2.245863	2.343856	1.818198
5	6	0	0.916215	2.105887	2.180271
6	6	0	2.460722	0.849370	-0.311978
7	6	0	1.136035	0.321019	-0.376056
8	6	0	0.021974	1.132313	-0.514876
9	7	0	-1.179666	0.734455	-0.909147
10	1	0	2.044035	-0.925818	1.747045
11	1	0	2.395633	-0.055795	3.239371
12	1	0	2.561764	1.867399	-0.669418
13	1	0	1.000193	-0.752172	-0.408276
14	1	0	3.980013	1.055137	1.537562
15	1	0	-0.209427	0.243467	2.462323
16	1	0	0.116425	2.194141	-0.318816
17	1	0	0.143707	2.852095	2.294589
18	1	0	2.686940	3.319914	1.660871
19	6	0	-2.333518	1.631308	-1.134394
20	1	0	-3.099276	1.389636	-0.390727
21	6	0	-2.788556	1.205290	-2.528980
22	1	0	-3.827486	1.453440	-2.736789
23	1	0	-2.148741	1.669949	-3.283044
24	6	0	-2.576100	-0.299726	-2.528273
25	1	0	-2.408374	-0.714563	-3.520751
26	6	0	-1.397137	-0.562349	-1.557207
27	1	0	-0.481310	-0.824679	-2.088067
28	6	0	-1.886063	-1.750092	-0.691394
29	6	0	-3.405814	-1.748055	-0.924508
30	6	0	-1.389701	-3.045759	-1.357525
31	1	0	-0.299777	-3.089913	-1.358607
32	1	0	-1.786738	-3.912180	-0.830558
33	1	0	-1.722845	-3.092760	-2.396536
34	8	0	-3.717309	-0.936443	-1.962873
35	8	0	-4.224356	-2.374746	-0.337541
36	6	0	-1.595126	-1.700391	0.800027
37	6	0	-0.565580	-2.446114	1.371064
38	6	0	-2.435590	-0.977108	1.649223
39	6	0	-0.396225	-2.490394	2.751270
40	1	0	0.088663	-3.043720	0.748308
41	6	0	-2.277251	-1.027624	3.026841
42	1	0	-3.266781	-0.414363	1.240702
43	6	0	-1.260145	-1.793727	3.584519
44	1	0	0.392224	-3.100562	3.173991
45	1	0	-2.964547	-0.487798	3.665202
46	1	0	-1.150939	-1.856043	4.659480
47	6	0	3.604165	-0.001857	-0.756603
48	6	0	3.612332	-1.388578	-0.603175
49	6	0	4.717420	0.618799	-1.322574

50	6	0	4.706760	-2.134785	-1.014275
51	1	0	2.764190	-1.902139	-0.165622
52	6	0	5.810675	-0.127610	-1.737631
53	1	0	4.724384	1.696276	-1.445072
54	6	0	5.808529	-1.507122	-1.582729
55	1	0	4.700072	-3.210209	-0.892514
56	1	0	6.663416	0.368306	-2.182610
57	1	0	6.660183	-2.091948	-1.904261
58	6	0	-2.025792	3.107408	-1.039237
59	1	0	-2.922040	3.651596	-1.361558
60	1	0	-1.211714	3.375391	-1.729659
61	8	0	-1.693155	3.444589	0.284846
62	6	0	-1.603413	4.845975	0.474406
63	1	0	-2.557199	5.329941	0.245780
64	1	0	-1.359990	5.018513	1.519986
65	1	0	-0.822449	5.280188	-0.158782

TS5-*Z-endo*





E(RM062X) = -1404.36029336

Zero-point correction=	0.554384 (Hartree/Particle)
Thermal correction to Energy=	0.582896
Thermal correction to Enthalpy=	0.583840
Thermal correction to Gibbs Free Energy=	0.495255
Sum of electronic and zero-point Energies=	-1403.805909
Sum of electronic and thermal Energies=	-1403.777397
Sum of electronic and thermal Enthalpies=	-1403.776453
Sum of electronic and thermal Free Energies=	-1403.865038

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.389127	2.837913	-1.817685

2	6	0	1.833806	2.546751	-2.038189
3	6	0	2.374625	2.760783	-0.642434
4	6	0	1.484542	3.674138	-0.032979
5	6	0	0.272388	3.675787	-0.719398
6	6	0	1.863242	1.081687	0.158146
7	6	0	0.663840	0.663603	-0.489888
8	6	0	-0.585220	0.934122	0.064992
9	7	0	-1.731364	0.382088	-0.282498
10	1	0	2.070851	1.598652	-2.510190
11	1	0	2.237864	3.349700	-2.670373
12	1	0	1.729807	1.396445	1.187100
13	1	0	0.731311	-0.040258	-1.307928
14	1	0	3.438264	2.794260	-0.446837
15	1	0	-0.392276	2.629211	-2.536388
16	1	0	-0.658189	1.663351	0.866348
17	1	0	-0.628604	4.180553	-0.401106
18	1	0	1.682367	4.203339	0.889606
19	6	0	-3.057137	0.829200	0.205631
20	6	0	-1.846862	-0.724969	-1.237500
21	1	0	-1.287817	-0.483702	-2.143195
22	6	0	-3.958057	0.468108	-0.973119
23	1	0	-4.999672	0.340887	-0.685491
24	1	0	-3.889908	1.239992	-1.744309
25	6	0	-3.365773	-0.829312	-1.491303
26	1	0	-3.614702	-1.040048	-2.530093
27	6	0	-1.469154	-2.132702	-0.692989
28	6	0	-2.815070	-2.646391	-0.162545
29	6	0	-1.139888	-3.029756	-1.896803
30	1	0	-1.971137	-3.049518	-2.604488
31	1	0	-0.259128	-2.662266	-2.424687
32	1	0	-0.954784	-4.048559	-1.558969
33	8	0	-3.829738	-1.904981	-0.681220
34	8	0	-3.005598	-3.568166	0.557438
35	6	0	-0.414572	-2.154273	0.393389
36	6	0	0.895532	-2.549033	0.138546
37	6	0	-0.744575	-1.726510	1.680238
38	6	0	1.862021	-2.484177	1.134807
39	1	0	1.183554	-2.909505	-0.840560
40	6	0	0.218318	-1.655721	2.674937
41	1	0	-1.769176	-1.462839	1.918808
42	6	0	1.529738	-2.027874	2.400916
43	1	0	2.880218	-2.780584	0.912529
44	1	0	-0.059606	-1.329959	3.669141
45	1	0	2.283750	-1.979691	3.176231
46	6	0	3.108969	0.276388	-0.010816
47	6	0	4.027700	0.251914	1.037485
48	6	0	3.383512	-0.462340	-1.160826
49	6	0	5.184588	-0.508668	0.950547

50	1	0	3.822810	0.818218	1.939366
51	6	0	4.542619	-1.219981	-1.251970
52	1	0	2.688480	-0.475812	-1.991862
53	6	0	5.444617	-1.249291	-0.195383
54	1	0	5.881815	-0.525077	1.778195
55	1	0	4.740506	-1.793068	-2.148658
56	1	0	6.345897	-1.843837	-0.266733
57	1	0	-3.323568	0.241685	1.089812
58	6	0	-3.132971	2.300476	0.552839
59	1	0	-4.191617	2.551749	0.693674
60	1	0	-2.755210	2.901689	-0.288930
61	8	0	-2.405395	2.566214	1.724738
62	6	0	-2.669710	3.855437	2.249083
63	1	0	-2.055913	3.974996	3.137820
64	1	0	-2.417755	4.636467	1.523339
65	1	0	-3.724200	3.952528	2.522295

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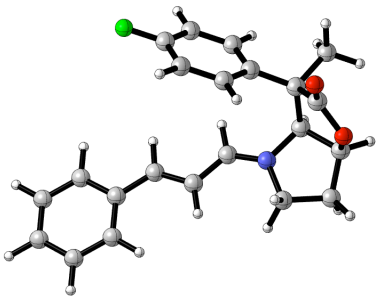
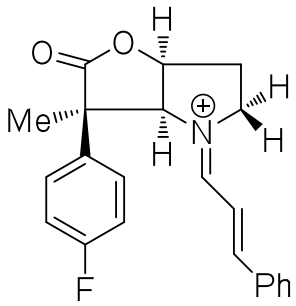
6 - *E*-iminium ion





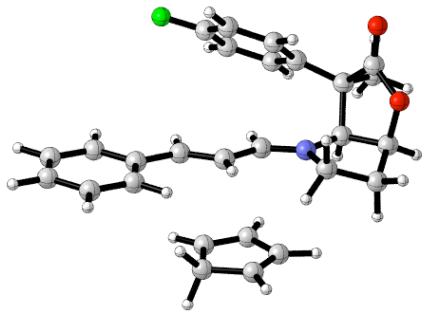
E(RM062X) = -1155.71957135

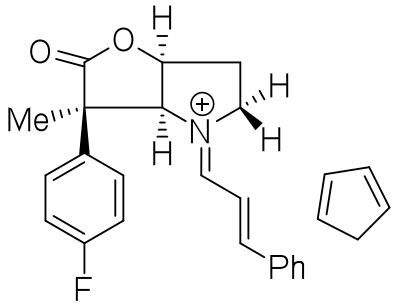
Zero-point correction=	0.387850 (Hartree/Particle)
Thermal correction to Energy=	0.409470
Thermal correction to Enthalpy=	0.410414
Thermal correction to Gibbs Free Energy=	0.335828
Sum of electronic and zero-point Energies=	-1155.331722
Sum of electronic and thermal Energies=	-1155.310101
Sum of electronic and thermal Enthalpies=	-1155.309157
Sum of electronic and thermal Free Energies=	-1155.383743

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.381101	-2.663241	0.149950
2	6	0	2.760919	-3.142617	-0.283991
3	6	0	3.537673	-1.848417	-0.445366
4	6	0	2.532240	-0.819744	-0.989296
5	6	0	3.526838	-0.073637	1.049606

6	1	0	1.342991	-2.446792	1.220392
7	1	0	3.227088	-3.799473	0.446620
8	8	0	3.904134	-1.363692	0.847632
9	7	0	1.224813	-1.400179	-0.602125
10	1	0	2.566563	-0.696740	-2.071323
11	1	0	4.431777	-1.945369	-1.058415
12	6	0	1.746723	1.418349	0.001073
13	6	0	1.369437	2.337125	-0.979272
14	6	0	0.941932	1.284329	1.133734
15	6	0	0.200552	3.076002	-0.858546
16	1	0	1.979995	2.484500	-1.860397
17	6	0	-0.227060	2.018035	1.274141
18	1	0	1.227804	0.606954	1.928537
19	6	0	-0.586419	2.890196	0.263977
20	1	0	-0.099972	3.791957	-1.611949
21	1	0	-0.854042	1.925782	2.150942
22	1	0	2.702961	-3.658071	-1.243455
23	1	0	0.581246	-3.351503	-0.112410
24	6	0	0.087955	-0.827021	-0.865980
25	1	0	0.140738	0.075670	-1.467346
26	6	0	-1.185063	-1.256654	-0.426533
27	1	0	-1.279767	-2.145775	0.181111
28	6	0	-2.253161	-0.465799	-0.714698
29	1	0	-2.059991	0.432905	-1.298015
30	6	0	-3.623485	-0.651637	-0.312109
31	6	0	-4.064021	-1.790216	0.382443
32	6	0	-4.545169	0.358870	-0.624276
33	6	0	-5.388947	-1.908112	0.749160
34	1	0	-3.372726	-2.586830	0.625908
35	6	0	-5.871949	0.239073	-0.250094
36	1	0	-4.208884	1.240841	-1.157043
37	6	0	-6.292984	-0.893603	0.435239
38	1	0	-5.727696	-2.787850	1.279738
39	1	0	-6.576792	1.023275	-0.491021
40	1	0	-7.330789	-0.991626	0.726892
41	8	0	3.709909	0.491845	2.075297
42	6	0	2.910505	0.484594	-0.238437
43	6	0	4.082534	1.147969	-0.987541
44	1	0	3.800428	1.414764	-2.005207
45	1	0	4.388102	2.046551	-0.453545
46	1	0	4.940982	0.476633	-1.044536
47	9	0	-1.727440	3.575908	0.374096

6-*E* and Cyclopentadiene Adduct





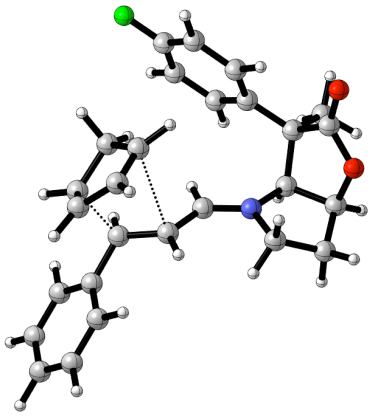
E(RM062X) = -1349.80679192

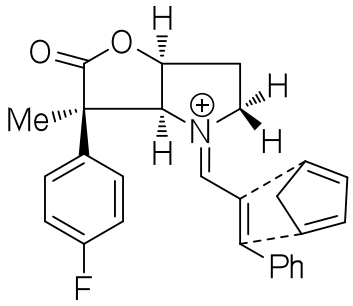
Zero-point correction=	0.482211 (Hartree/Particle)
Thermal correction to Energy=	0.509882
Thermal correction to Enthalpy=	0.510826
Thermal correction to Gibbs Free Energy=	0.419865
Sum of electronic and zero-point Energies=	-1349.324581
Sum of electronic and thermal Energies=	-1349.296910
Sum of electronic and thermal Enthalpies=	-1349.295966
Sum of electronic and thermal Free Energies=	-1349.386926

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.676461	2.386001	2.492967
2	6	0	-0.260140	3.315535	1.436385
3	6	0	-1.325471	3.637760	0.683503
4	6	0	-2.541573	2.958027	1.237472
5	6	0	-1.994710	2.155182	2.378212
6	6	0	-2.096721	-0.218975	-0.017403
7	6	0	-1.095216	0.497416	-0.585033
8	6	0	0.168401	0.469974	0.053200
9	7	0	1.245754	1.057067	-0.369311
10	1	0	-1.228251	1.048677	-1.505403
11	1	0	-1.859483	-0.767460	0.892238
12	1	0	-3.257587	3.703110	1.605603
13	1	0	-3.084336	2.355765	0.501980
14	1	0	-2.601271	1.539798	3.027180
15	1	0	-1.347029	4.335715	-0.141671
16	1	0	0.257883	-0.092826	0.976800
17	1	0	-0.024105	1.990046	3.259844
18	1	0	0.743155	3.705971	1.323469

19	6	0	-3.458662	-0.349450	-0.480851
20	6	0	-3.956325	0.369612	-1.579109
21	6	0	-4.312892	-1.220967	0.208294
22	6	0	-5.269383	0.210799	-1.975379
23	1	0	-3.317041	1.055781	-2.120579
24	6	0	-5.628009	-1.380920	-0.194429
25	1	0	-3.932502	-1.779328	1.055905
26	6	0	-6.105758	-0.665033	-1.284541
27	1	0	-5.650439	0.766815	-2.821588
28	1	0	-6.279662	-2.060126	0.338578
29	1	0	-7.133842	-0.786603	-1.600582
30	6	0	1.300827	1.952954	-1.542518
31	1	0	1.376087	1.350650	-2.450583
32	1	0	0.397350	2.559499	-1.569803
33	6	0	2.556120	0.930930	0.307190
34	1	0	2.465173	1.281118	1.335970
35	6	0	2.562235	2.770399	-1.290783
36	1	0	3.016058	3.137854	-2.208243
37	1	0	2.344258	3.616557	-0.637869
38	6	0	3.474293	1.795493	-0.569848
39	1	0	4.278401	2.274792	-0.014259
40	6	0	3.197277	-0.477664	0.214719
41	6	0	3.865733	-0.412277	-1.163612
42	8	0	4.034864	0.888557	-1.521577
43	8	0	4.236912	-1.313106	-1.839171
44	6	0	4.361931	-0.548542	1.221504
45	1	0	4.011187	-0.401093	2.242104
46	1	0	4.842782	-1.522745	1.146251
47	1	0	5.109924	0.217745	1.011720
48	6	0	2.211002	-1.613143	0.362137
49	6	0	1.854579	-2.069557	1.631654
50	6	0	1.531325	-2.123617	-0.744830
51	6	0	0.822410	-2.981376	1.802959
52	1	0	2.372893	-1.711410	2.511385
53	6	0	0.500461	-3.039714	-0.593278
54	1	0	1.808580	-1.814718	-1.744647
55	6	0	0.152287	-3.439618	0.682952
56	1	0	0.538837	-3.342279	2.782618
57	1	0	-0.028632	-3.445167	-1.445309
58	9	0	-0.859804	-4.297176	0.841206

TS6-*E-exo*-top





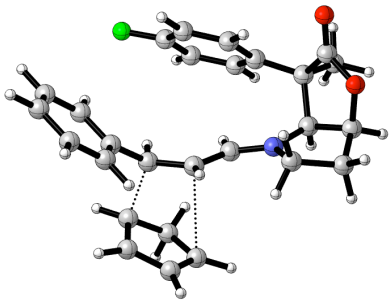
E(RM062X) = -1349.78331071

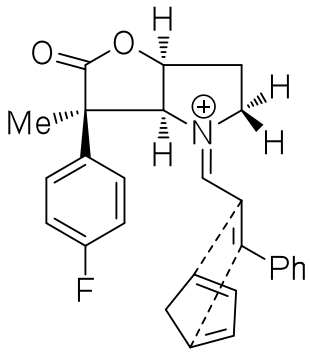
Zero-point correction=	0.484019 (Hartree/Particle)
Thermal correction to Energy=	0.509748
Thermal correction to Enthalpy=	0.510692
Thermal correction to Gibbs Free Energy=	0.427395
Sum of electronic and zero-point Energies=	-1349.299292
Sum of electronic and thermal Energies=	-1349.273563
Sum of electronic and thermal Enthalpies=	-1349.272619
Sum of electronic and thermal Free Energies=	-1349.355916

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.710731	0.729830	2.696218
2	6	0	-2.828833	1.169710	1.962843
3	6	0	-2.416084	1.706221	0.732832
4	6	0	-0.936995	1.974304	0.875430
5	6	0	-0.577536	1.083253	2.009163
6	6	0	-2.396618	0.145846	-0.420710
7	6	0	-1.397217	-0.755639	0.047387
8	6	0	-0.139403	-0.770506	-0.521597
9	7	0	0.817649	-1.660294	-0.292924
10	1	0	-1.658438	-1.499828	0.785825
11	1	0	-2.091871	0.716813	-1.295408
12	1	0	-0.820572	3.013475	1.215878
13	1	0	-0.322623	1.861520	-0.014743
14	1	0	0.440465	0.851337	2.292090
15	1	0	-3.066671	2.353567	0.158270
16	1	0	0.107637	-0.015224	-1.260916
17	1	0	-1.746042	0.173948	3.621648

18	1	0	-3.860854	1.032828	2.256907
19	6	0	0.615771	-2.845405	0.555413
20	1	0	-0.414979	-3.185716	0.475068
21	1	0	0.832563	-2.599660	1.598310
22	6	0	1.608069	-3.852071	-0.013422
23	1	0	1.935713	-4.588725	0.716512
24	1	0	1.178355	-4.367277	-0.873501
25	6	0	2.114346	-1.678234	-0.997986
26	1	0	1.954816	-1.685576	-2.077576
27	6	0	2.753445	-2.974975	-0.471815
28	1	0	3.420544	-3.454703	-1.185278
29	6	0	3.139087	-0.605145	-0.567281
30	6	0	4.336038	-0.644363	-1.549737
31	1	0	4.017220	-0.355191	-2.550639
32	1	0	5.095844	0.058227	-1.210374
33	1	0	4.785506	-1.636779	-1.602738
34	6	0	3.689402	-1.224916	0.720554
35	8	0	3.505880	-2.566445	0.675775
36	8	0	4.255499	-0.697964	1.623986
37	6	0	2.626581	0.819838	-0.465959
38	6	0	2.170916	1.441058	-1.634301
39	6	0	2.668829	1.571755	0.706719
40	6	0	1.759061	2.764254	-1.641424
41	1	0	2.146123	0.889200	-2.567954
42	6	0	2.269843	2.904777	0.715204
43	1	0	3.059371	1.137433	1.615537
44	6	0	1.820777	3.477339	-0.456126
45	1	0	1.415036	3.250909	-2.544403
46	1	0	2.321855	3.501905	1.616492
47	6	0	-3.823427	-0.275412	-0.500370
48	6	0	-4.620340	0.247175	-1.516215
49	6	0	-4.387642	-1.169261	0.410428
50	6	0	-5.954834	-0.121642	-1.629364
51	1	0	-4.192786	0.943016	-2.229972
52	6	0	-5.718886	-1.536313	0.299605
53	1	0	-3.791448	-1.580063	1.217520
54	6	0	-6.506183	-1.013746	-0.722066
55	1	0	-6.560837	0.288283	-2.426658
56	1	0	-6.146263	-2.232515	1.009533
57	1	0	-7.545423	-1.302853	-0.806771
58	9	0	1.416508	4.751398	-0.446759

TS6-*E-exo*





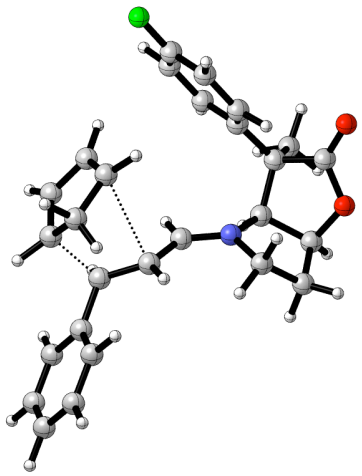
E(RM062X) = -1349.78421066

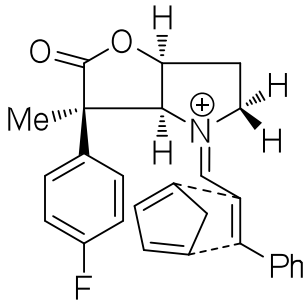
Zero-point correction=	0.483731 (Hartree/Particle)
Thermal correction to Energy=	0.509511
Thermal correction to Enthalpy=	0.510455
Thermal correction to Gibbs Free Energy=	0.426825
Sum of electronic and zero-point Energies=	-1349.300479
Sum of electronic and thermal Energies=	-1349.274700
Sum of electronic and thermal Enthalpies=	-1349.273756
Sum of electronic and thermal Free Energies=	-1349.357386

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.443369	3.587150	-0.551880
2	6	0	3.414205	2.582035	-0.714791
3	6	0	2.952573	1.613205	-1.619705
4	6	0	1.815259	2.265700	-2.371968
5	6	0	1.412768	3.340758	-1.424241
6	6	0	1.961434	0.402879	-0.475309
7	6	0	0.850490	1.102990	0.075275
8	6	0	-0.407811	0.924550	-0.468366
9	7	0	-1.551590	1.339988	0.051755
10	1	0	0.948470	1.590089	1.035807
11	1	0	1.690029	-0.265062	-1.291435
12	1	0	2.249830	2.752146	-3.256384
13	1	0	1.017203	1.612781	-2.715943
14	1	0	0.507963	3.926008	-1.518170
15	1	0	3.633194	0.917762	-2.094660
16	1	0	-0.502412	0.348243	-1.384550
17	1	0	2.486007	4.389183	0.170495
18	1	0	4.337736	2.510020	-0.156640
19	6	0	2.974764	-0.211761	0.426224
20	6	0	3.381095	0.397642	1.613929
21	6	0	3.515049	-1.447565	0.078192

22	6	0	4.305390	-0.222278	2.438750
23	1	0	2.979655	1.364183	1.898900
24	6	0	4.439048	-2.071640	0.907688
25	1	0	3.200740	-1.935377	-0.837851
26	6	0	4.835595	-1.460523	2.087803
27	1	0	4.613503	0.257026	3.358914
28	1	0	4.845488	-3.035055	0.629006
29	1	0	5.555807	-1.943730	2.734869
30	6	0	-1.638666	2.197478	1.239771
31	1	0	-1.506495	1.601118	2.147283
32	1	0	-0.858907	2.958454	1.198725
33	6	0	-2.871631	0.922006	-0.446189
34	1	0	-2.996294	1.225060	-1.486819
35	6	0	-3.047546	2.771961	1.135390
36	1	0	-3.459965	3.069844	2.096564
37	1	0	-3.061907	3.628270	0.459632
38	6	0	-3.837719	1.630016	0.521873
39	1	0	-4.771580	1.939887	0.056193
40	6	0	-3.207694	-0.579323	-0.243573
41	6	0	-3.727631	-0.585856	1.197618
42	8	0	-4.121989	0.667331	1.539964
43	8	0	-3.836627	-1.511607	1.931885
44	6	0	-4.434424	-0.924317	-1.109673
45	1	0	-4.229184	-0.759494	-2.166844
46	1	0	-4.705897	-1.967837	-0.956544
47	1	0	-5.291278	-0.305611	-0.837692
48	6	0	-2.040306	-1.514603	-0.465618
49	6	0	-1.756631	-1.994750	-1.744213
50	6	0	-1.153160	-1.814697	0.569539
51	6	0	-0.606303	-2.729937	-1.997012
52	1	0	-2.430735	-1.799080	-2.567650
53	6	0	-0.000290	-2.551152	0.338365
54	1	0	-1.358905	-1.477281	1.577375
55	6	0	0.255984	-2.987484	-0.947384
56	1	0	-0.381668	-3.114285	-2.983061
57	1	0	0.693831	-2.787761	1.134159
58	9	0	1.373617	-3.686678	-1.187080

TS6-*E*-*endo*-top





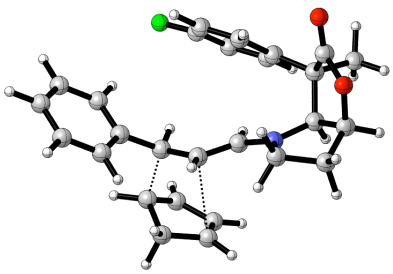
E(RM062X) = -1349.77708913

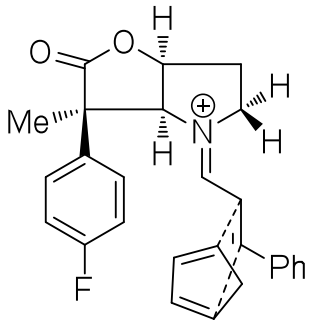
Zero-point correction=	0.484244 (Hartree/Particle)
Thermal correction to Energy=	0.509890
Thermal correction to Enthalpy=	0.510834
Thermal correction to Gibbs Free Energy=	0.428015
Sum of electronic and zero-point Energies=	-1349.292846
Sum of electronic and thermal Energies=	-1349.267199
Sum of electronic and thermal Enthalpies=	-1349.266255
Sum of electronic and thermal Free Energies=	-1349.349074

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.807944	1.984657	-1.040444
2	6	0	2.278976	2.042305	-1.242881
3	6	0	2.770011	2.054646	0.186282
4	6	0	1.692840	2.546311	0.950381
5	6	0	0.500556	2.427862	0.227574
6	6	0	2.694144	0.173494	0.599912
7	6	0	1.627225	-0.409080	-0.154313
8	6	0	0.403143	-0.673104	0.437180
9	7	0	-0.536209	-1.502059	0.009015
10	1	0	2.703288	1.289741	-1.901141
11	1	0	2.511527	3.026323	-1.674346
12	1	0	2.508912	0.224350	1.667197
13	1	0	1.835127	-0.806096	-1.137286
14	1	0	3.794789	2.299181	0.431760
15	1	0	0.090544	1.769708	-1.819588
16	1	0	0.178225	-0.197463	1.390173

17	1	0	-0.495213	2.590958	0.612340
18	1	0	1.768797	2.867908	1.981133
19	6	0	-0.355414	-2.452188	-1.099146
20	1	0	-0.920585	-2.120108	-1.973317
21	1	0	0.696333	-2.528882	-1.360915
22	6	0	-1.696410	-1.863635	0.841439
23	1	0	-1.385152	-1.888917	1.886002
24	6	0	-0.920340	-3.744139	-0.517392
25	1	0	-1.233189	-4.458009	-1.276019
26	1	0	-0.184034	-4.212894	0.136930
27	6	0	-2.100658	-3.256718	0.303511
28	1	0	-2.408666	-3.948275	1.085585
29	6	0	-2.989103	-1.033393	0.671156
30	6	0	-3.700803	-1.772059	-0.472285
31	6	0	-3.869556	-1.305409	1.907262
32	1	0	-4.056619	-2.374314	2.022351
33	1	0	-3.382972	-0.953199	2.816917
34	1	0	-4.829468	-0.803232	1.795205
35	8	0	-3.205108	-3.029534	-0.572031
36	8	0	-4.580027	-1.374386	-1.162278
37	6	0	-2.848336	0.443897	0.365526
38	6	0	-3.079865	1.418302	1.335686
39	6	0	-2.591756	0.863922	-0.941860
40	6	0	-3.079332	2.771021	1.016159
41	1	0	-3.303613	1.137106	2.355623
42	6	0	-2.597311	2.207036	-1.282948
43	1	0	-2.445205	0.130641	-1.726541
44	6	0	-2.850400	3.141260	-0.294362
45	1	0	-3.283537	3.529778	1.759725
46	1	0	-2.447016	2.537735	-2.302494
47	6	0	4.103654	-0.233119	0.317072
48	6	0	5.027021	-0.190580	1.362118
49	6	0	4.536884	-0.630470	-0.947814
50	6	0	6.351518	-0.544086	1.152773
51	1	0	4.703026	0.117178	2.350360
52	6	0	5.862582	-0.980788	-1.158257
53	1	0	3.847421	-0.682666	-1.781504
54	6	0	6.773269	-0.938178	-0.110081
55	1	0	7.053435	-0.513185	1.975810
56	1	0	6.184980	-1.291783	-2.143431
57	1	0	7.806104	-1.213934	-0.277124
58	9	0	-2.863954	4.436834	-0.617280

TS6-*E-endo*





E(RM062X) = -1349.78267440

Zero-point correction=	0.483994 (Hartree/Particle)
Thermal correction to Energy=	0.509723
Thermal correction to Enthalpy=	0.510668
Thermal correction to Gibbs Free Energy=	0.427247
Sum of electronic and zero-point Energies=	-1349.298680
Sum of electronic and thermal Energies=	-1349.272951
Sum of electronic and thermal Enthalpies=	-1349.272007
Sum of electronic and thermal Free Energies=	-1349.355427

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.298810	-3.313514	1.273710
2	6	0	2.640370	-3.011976	0.705265
3	6	0	2.965347	-1.712976	1.409521
4	6	0	2.206686	-1.736559	2.600966
5	6	0	1.162152	-2.656742	2.481043
6	6	0	1.979672	-0.469875	0.350411
7	6	0	0.854251	-1.161352	-0.199980
8	6	0	-0.403448	-0.961834	0.343797
9	7	0	-1.559588	-1.311111	-0.192208
10	1	0	2.716535	-3.014981	-0.377529
11	1	0	3.335505	-3.771457	1.090466
12	1	0	1.710143	0.269108	1.098577
13	1	0	0.942582	-1.636459	-1.167525
14	1	0	3.963897	-1.296753	1.390943
15	1	0	0.631671	-4.073857	0.890356
16	1	0	-0.474592	-0.431962	1.289585
17	1	0	0.355981	-2.792879	3.187238
18	1	0	2.353691	-1.062523	3.434746
19	6	0	-1.682068	-2.092133	-1.429585
20	1	0	-0.927538	-2.878508	-1.443993
21	1	0	-1.537841	-1.445015	-2.299546

22	6	0	-3.106632	-2.630328	-1.346775
23	1	0	-3.534879	-2.856550	-2.320479
24	1	0	-3.140926	-3.525805	-0.724695
25	6	0	-3.857997	-1.505901	-0.657042
26	1	0	-4.796114	-1.817322	-0.201093
27	6	0	-2.863570	-0.885957	0.342197
28	1	0	-2.988732	-1.247689	1.363692
29	6	0	-3.156343	0.634453	0.232953
30	6	0	-3.689908	0.742677	-1.199416
31	6	0	-4.363043	0.962231	1.132746
32	1	0	-4.151438	0.729035	2.175740
33	1	0	-4.606061	2.020217	1.044733
34	1	0	-5.240248	0.385247	0.835159
35	8	0	-4.123740	-0.475784	-1.612041
36	8	0	-3.777978	1.713921	-1.875194
37	6	0	-1.959379	1.521103	0.493415
38	6	0	-1.656522	1.936348	1.789871
39	6	0	-1.065172	1.835657	-0.531605
40	6	0	-0.479666	2.618345	2.069541
41	1	0	-2.335489	1.729985	2.606572
42	6	0	0.113818	2.520057	-0.273766
43	1	0	-1.285650	1.550458	-1.552513
44	6	0	0.389668	2.888389	1.029180
45	1	0	-0.238602	2.950782	3.070455
46	1	0	0.813229	2.766710	-1.061896
47	6	0	3.031304	0.063806	-0.566419
48	6	0	3.411450	-0.587935	-1.739696
49	6	0	3.657068	1.262882	-0.225134
50	6	0	4.396797	-0.048934	-2.553380
51	1	0	2.937696	-1.515173	-2.038896
52	6	0	4.638963	1.804355	-1.042922
53	1	0	3.363263	1.784108	0.679429
54	6	0	5.013499	1.147549	-2.207220
55	1	0	4.681473	-0.561421	-3.463095
56	1	0	5.109068	2.740098	-0.769939
57	1	0	5.780077	1.566705	-2.845538
58	9	0	1.537500	3.526396	1.295815

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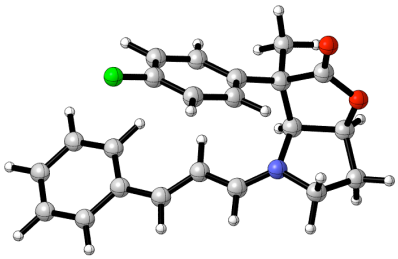
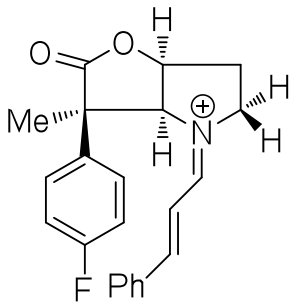
6 - *Z*-iminium ion





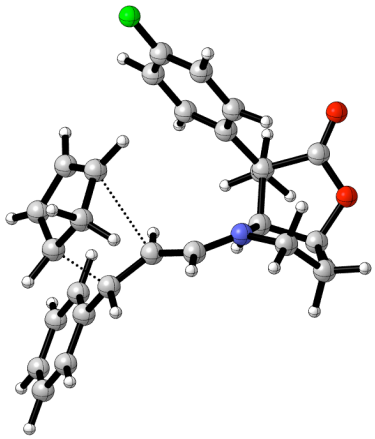
E(RM062X) = -1155.71860118

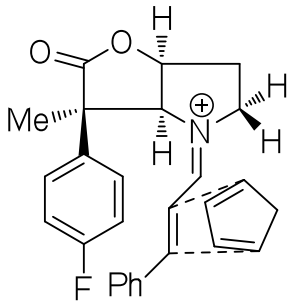
Zero-point correction=	0.388074 (Hartree/Particle)
Thermal correction to Energy=	0.409391
Thermal correction to Enthalpy=	0.410335
Thermal correction to Gibbs Free Energy=	0.337333
Sum of electronic and zero-point Energies=	-1155.330527
Sum of electronic and thermal Energies=	-1155.309211
Sum of electronic and thermal Enthalpies=	-1155.308266
Sum of electronic and thermal Free Energies=	-1155.381269

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.931882	-1.693390	-1.580992
2	6	0	-4.007217	-2.133534	-0.597561
3	6	0	-3.763150	-1.208713	0.585049
4	6	0	-2.233039	-1.005102	0.651215
5	6	0	-3.394258	1.073862	0.376423
6	6	0	-2.080050	0.516416	0.940068
7	1	0	-3.208747	-0.760106	-2.077366
8	1	0	-5.014246	-2.016140	-0.990771
9	8	0	-4.309102	0.073564	0.281437
10	7	0	-1.780631	-1.437653	-0.685840
11	1	0	-1.749918	-1.618579	1.410705
12	1	0	-4.190455	-1.565525	1.520174
13	6	0	-0.866461	1.173537	0.323804
14	6	0	0.287240	1.415982	1.068399
15	6	0	-0.853426	1.476033	-1.039200
16	6	0	1.446210	1.881523	0.465037
17	1	0	0.301891	1.236551	2.135529
18	6	0	0.295774	1.936181	-1.662002
19	1	0	-1.756366	1.366383	-1.629229
20	6	0	1.436281	2.110197	-0.897369
21	1	0	2.350050	2.062958	1.031447
22	1	0	0.315045	2.180988	-2.715678
23	1	0	-3.853840	-3.171262	-0.298668
24	1	0	-2.663328	-2.438461	-2.325445
25	6	0	-0.542505	-1.591553	-1.046553
26	1	0	-0.390294	-1.855640	-2.090050
27	6	0	0.593462	-1.445428	-0.219137
28	1	0	0.460974	-1.280996	0.840254

29	6	0	1.820273	-1.392987	-0.797325
30	1	0	1.873937	-1.510613	-1.877764
31	6	0	3.078622	-1.142395	-0.137349
32	6	0	4.213680	-0.931654	-0.931700
33	6	0	3.197480	-1.065894	1.259777
34	6	0	5.436379	-0.644014	-0.348775
35	1	0	4.127234	-0.987121	-2.010519
36	6	0	4.419934	-0.790043	1.837867
37	1	0	2.336324	-1.238410	1.893203
38	6	0	5.539342	-0.573146	1.034095
39	1	0	6.306486	-0.476280	-0.968972
40	1	0	4.512076	-0.743250	2.914862
41	1	0	6.494761	-0.353434	1.492931
42	8	0	-3.641163	2.196475	0.089850
43	6	0	-2.184145	0.709777	2.463652
44	1	0	-1.373009	0.196307	2.980207
45	1	0	-2.144412	1.772271	2.700137
46	1	0	-3.126575	0.311215	2.843055
47	9	0	2.556410	2.526495	-1.492444

TS6-*Z*-*exo*-top





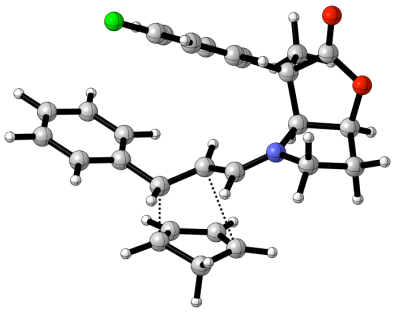
E(RM062X) = -1349.77688134

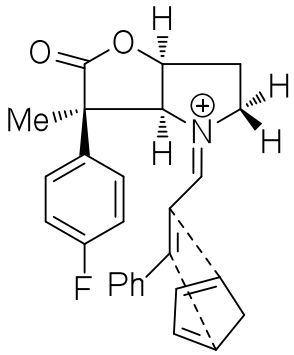
Zero-point correction=	0.483723 (Hartree/Particle)
Thermal correction to Energy=	0.509475
Thermal correction to Enthalpy=	0.510419
Thermal correction to Gibbs Free Energy=	0.426893
Sum of electronic and zero-point Energies=	-1349.293158
Sum of electronic and thermal Energies=	-1349.267407
Sum of electronic and thermal Enthalpies=	-1349.266463
Sum of electronic and thermal Free Energies=	-1349.349988

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.571371	2.629570	-0.459357
2	6	0	2.863341	2.065514	-0.497058
3	6	0	3.003242	1.256876	-1.630457
4	6	0	1.863209	1.628288	-2.547421
5	6	0	0.916527	2.290768	-1.612292
6	6	0	2.424693	-0.487762	-0.966585
7	6	0	1.045842	-0.476275	-0.600793
8	6	0	0.086520	-0.905343	-1.494161
9	7	0	-1.136057	-1.338770	-1.208725
10	1	0	0.761060	-0.286486	0.426285
11	1	0	2.618400	-0.953566	-1.929885
12	1	0	2.237443	2.399072	-3.235887
13	1	0	1.442524	0.835628	-3.161172
14	1	0	-0.103331	2.550132	-1.857803
15	1	0	3.979046	0.976231	-2.005911
16	1	0	0.344810	-0.974595	-2.548311
17	1	0	1.163843	3.211045	0.352581
18	1	0	3.613333	2.172382	0.275197
19	6	0	3.452760	-0.852896	0.047137
20	6	0	3.330434	-0.490460	1.389455
21	6	0	4.572325	-1.574402	-0.359843
22	6	0	4.306383	-0.851008	2.303929
23	1	0	2.475328	0.087196	1.724057
24	6	0	5.549720	-1.939529	0.557565
25	1	0	4.678365	-1.860601	-1.400644
26	6	0	5.418236	-1.579002	1.890081
27	1	0	4.203715	-0.565230	3.342770
28	1	0	6.411911	-2.504918	0.229125
29	1	0	6.178447	-1.860438	2.606796
30	6	0	-2.021971	-1.918549	-2.231295
31	1	0	-2.905565	-1.288273	-2.356255
32	1	0	-1.501451	-1.984681	-3.184419
33	6	0	-1.525315	-1.788472	0.134367
34	1	0	-0.628768	-2.144364	0.644579
35	6	0	-2.391212	-3.265410	-1.620487
36	1	0	-3.307812	-3.688955	-2.024723
37	1	0	-1.574784	-3.977184	-1.750942
38	6	0	-2.545165	-2.921924	-0.147383
39	1	0	-2.430891	-3.775922	0.517902
40	6	0	-2.321736	-0.807658	1.023657
41	6	0	-3.776157	-1.127174	0.646476
42	8	0	-3.835017	-2.347841	0.060051
43	8	0	-4.739633	-0.465303	0.847704
44	6	0	-2.178277	-1.283799	2.479833

45	1	0	-1.139918	-1.219552	2.807668
46	1	0	-2.802170	-0.676632	3.134512
47	1	0	-2.494169	-2.323863	2.578013
48	6	0	-2.031839	0.665339	0.840079
49	6	0	-1.352466	1.407661	1.802492
50	6	0	-2.518549	1.328117	-0.288298
51	6	0	-1.153031	2.773659	1.647297
52	1	0	-0.994501	0.937903	2.708657
53	6	0	-2.331937	2.689659	-0.461015
54	1	0	-3.099026	0.786450	-1.025893
55	6	0	-1.641166	3.388535	0.512635
56	1	0	-0.647395	3.362992	2.401236
57	1	0	-2.733364	3.217533	-1.316417
58	9	0	-1.432240	4.699923	0.344063

TS6-*Z-exo*





E(RM062X) = -1349.78255465

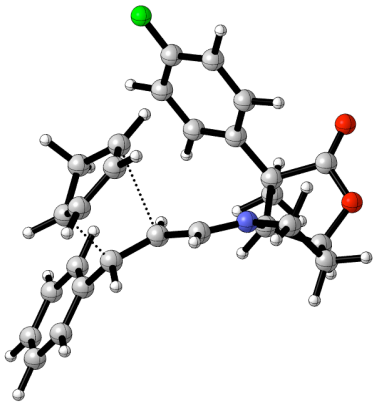
Zero-point correction=	0.483869 (Hartree/Particle)
Thermal correction to Energy=	0.509366
Thermal correction to Enthalpy=	0.510310
Thermal correction to Gibbs Free Energy=	0.428578
Sum of electronic and zero-point Energies=	-1349.298686
Sum of electronic and thermal Energies=	-1349.273189
Sum of electronic and thermal Enthalpies=	-1349.272244
Sum of electronic and thermal Free Energies=	-1349.353977

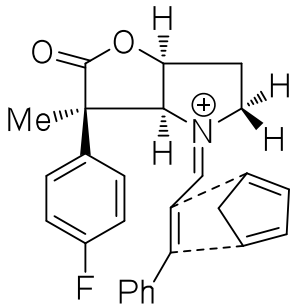
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.360427	3.636806	1.164574
2	6	0	-2.595816	3.108187	0.756052
3	6	0	-2.564036	2.831258	-0.622165

4	6	0	-1.408399	3.639293	-1.168467
5	6	0	-0.574339	3.817499	0.051450
6	6	0	-1.803292	1.054927	-0.707725
7	6	0	-0.476191	1.095449	-0.195130
8	6	0	0.619653	1.228142	-1.031258
9	7	0	1.888680	1.071361	-0.701228
10	1	0	-0.314585	0.837074	0.842442
11	1	0	-1.855980	1.001721	-1.793094
12	1	0	-1.807020	4.626730	-1.439622
13	1	0	-0.902421	3.242229	-2.044068
14	1	0	0.438976	4.196133	0.046960
15	1	0	-3.477313	2.683839	-1.185037
16	1	0	0.454506	1.461031	-2.080021
17	1	0	-1.066197	3.828247	2.186223
18	1	0	-3.418352	2.862064	1.413059
19	6	0	3.016981	1.355110	-1.602950
20	1	0	2.717814	2.069276	-2.366984
21	1	0	3.350608	0.432633	-2.085457
22	6	0	4.072745	1.878705	-0.635742
23	1	0	5.087029	1.793438	-1.018887
24	1	0	3.871384	2.919577	-0.377806
25	6	0	2.351468	0.692884	0.634817
26	1	0	1.824482	1.288151	1.383072
27	6	0	3.867457	0.995132	0.586507
28	1	0	4.251544	1.425711	1.509628
29	6	0	2.287437	-0.826733	0.960287
30	6	0	2.298633	-0.985984	2.488746
31	1	0	1.408250	-0.538961	2.932427
32	1	0	2.337459	-2.042630	2.750524
33	1	0	3.171320	-0.493949	2.922709
34	6	0	3.666119	-1.314004	0.492732
35	8	0	4.509790	-0.257629	0.362955
36	8	0	4.009448	-2.431525	0.296582
37	6	0	1.174952	-1.588781	0.273048
38	6	0	0.017086	-1.968526	0.946708
39	6	0	1.275127	-1.877695	-1.088867
40	6	0	-1.034283	-2.581910	0.279222
41	1	0	-0.088902	-1.788578	2.008598
42	6	0	0.233803	-2.479866	-1.776054
43	1	0	2.189223	-1.651651	-1.626016
44	6	0	-0.913975	-2.807812	-1.076041
45	1	0	-1.944738	-2.865194	0.791526
46	1	0	0.305815	-2.716155	-2.829289
47	6	0	-2.799194	0.160725	-0.050645
48	6	0	-3.624906	-0.627532	-0.845973
49	6	0	-2.888275	0.050821	1.337414
50	6	0	-4.518726	-1.521452	-0.267284
51	1	0	-3.553742	-0.564923	-1.926084

52	6	0	-3.784832	-0.832106	1.916378
53	1	0	-2.253029	0.658075	1.974328
54	6	0	-4.601399	-1.624538	1.113003
55	1	0	-5.143704	-2.139125	-0.898643
56	1	0	-3.849576	-0.906978	2.994344
57	1	0	-5.299933	-2.315938	1.565867
58	9	0	-1.934200	-3.370682	-1.734914

TS6-*Z*-*endo*-top





E(RM062X) = -1349.77828397

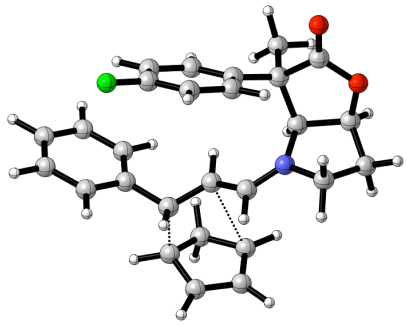
Zero-point correction=	0.484402 (Hartree/Particle)
Thermal correction to Energy=	0.509970
Thermal correction to Enthalpy=	0.510914
Thermal correction to Gibbs Free Energy=	0.428134
Sum of electronic and zero-point Energies=	-1349.293882
Sum of electronic and thermal Energies=	-1349.268314
Sum of electronic and thermal Enthalpies=	-1349.267370
Sum of electronic and thermal Free Energies=	-1349.350150

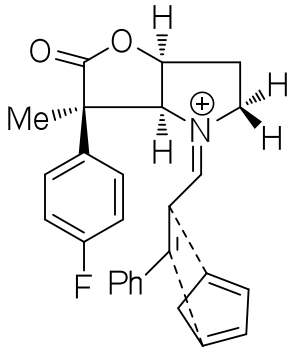
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.666454	2.003238	1.412810
2	6	0	-1.851947	2.107036	0.523754
3	6	0	-2.900574	1.391182	1.344630
4	6	0	-2.450653	1.471525	2.679333
5	6	0	-1.085787	1.779301	2.706617
6	6	0	-2.512345	-0.449418	0.922914
7	6	0	-1.127386	-0.540016	0.579405
8	6	0	-0.158574	-0.894281	1.498587

9	7	0	1.067423	-1.318439	1.220407
10	1	0	-1.704421	1.770461	-0.497868
11	1	0	-2.136178	3.168648	0.484856
12	1	0	-2.774865	-0.919661	1.863666
13	1	0	-0.834666	-0.430812	-0.456649
14	1	0	-3.953418	1.456882	1.104895
15	1	0	0.346948	2.204733	1.098438
16	1	0	-0.407913	-0.880521	2.556460
17	1	0	-0.456992	1.785824	3.585288
18	1	0	-3.056016	1.234553	3.544968
19	6	0	1.996153	-1.812823	2.247328
20	1	0	1.507209	-1.830322	3.219110
21	1	0	2.867581	-1.156151	2.302487
22	6	0	2.374246	-3.188163	1.707015
23	1	0	3.312838	-3.568895	2.103377
24	1	0	1.578246	-3.905209	1.912319
25	6	0	2.470670	-2.940897	0.208159
26	1	0	2.319835	-3.835744	-0.393089
27	6	0	1.446685	-1.818588	-0.105414
28	1	0	0.548881	-2.202264	-0.591486
29	6	0	2.222338	-0.863142	-1.041379
30	6	0	3.689362	-1.223465	-0.756604
31	6	0	1.984193	-1.332581	-2.489041
32	1	0	0.929596	-1.255098	-2.755763
33	1	0	2.576692	-0.731377	-3.177211
34	1	0	2.277419	-2.377859	-2.606230
35	8	0	3.755219	-2.402756	-0.096367
36	8	0	4.656656	-0.617585	-1.081289
37	6	0	1.991217	0.627070	-0.860456
38	6	0	1.110430	1.332554	-1.679340
39	6	0	2.734401	1.346958	0.078560
40	6	0	0.979186	2.712716	-1.582399
41	1	0	0.538672	0.817924	-2.441362
42	6	0	2.627434	2.725852	0.184099
43	1	0	3.455902	0.839531	0.706873
44	6	0	1.752767	3.388464	-0.658287
45	1	0	0.318668	3.268220	-2.235246
46	1	0	3.227805	3.290449	0.884895
47	6	0	-3.537917	-0.724606	-0.127547
48	6	0	-3.340123	-0.404921	-1.471088
49	6	0	-4.748771	-1.298988	0.257533
50	6	0	-4.330258	-0.662694	-2.407192
51	1	0	-2.411385	0.044243	-1.803079
52	6	0	-5.737714	-1.560920	-0.679564
53	1	0	-4.915499	-1.549740	1.299280
54	6	0	-5.531183	-1.241397	-2.014493
55	1	0	-4.164794	-0.412989	-3.447177
56	1	0	-6.668764	-2.015073	-0.366685

57	1	0	-6.301272	-1.442990	-2.747301
58	9	0	1.646285	4.716785	-0.570778

TS6-*Z-endo*





E(RM062X) = -1349.78187588

Zero-point correction=	0.484100 (Hartree/Particle)
Thermal correction to Energy=	0.509568
Thermal correction to Enthalpy=	0.510512
Thermal correction to Gibbs Free Energy=	0.428907
Sum of electronic and zero-point Energies=	-1349.297775
Sum of electronic and thermal Energies=	-1349.272308
Sum of electronic and thermal Enthalpies=	-1349.271364
Sum of electronic and thermal Free Energies=	-1349.352969

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.559568	3.697414	0.523805
2	6	0	-1.845043	3.212136	1.092993
3	6	0	-2.570398	2.783111	-0.164802
4	6	0	-2.002234	3.562524	-1.200804
5	6	0	-0.761430	4.056020	-0.796815
6	6	0	-1.803428	1.073420	-0.468574
7	6	0	-0.471947	1.090678	0.055286
8	6	0	0.622638	1.331749	-0.761027
9	7	0	1.892663	1.121044	-0.471863
10	1	0	-1.770722	2.481387	1.891108
11	1	0	-2.377530	4.088111	1.489839
12	1	0	-1.851866	1.020961	-1.550915
13	1	0	-0.304637	0.719638	1.057405
14	1	0	-3.629898	2.562626	-0.153750
15	1	0	0.321150	3.921201	1.110843

16	1	0	0.443832	1.723636	-1.759164
17	1	0	-0.054812	4.578982	-1.425412
18	1	0	-2.424705	3.667166	-2.191590
19	6	0	3.010303	1.550265	-1.329582
20	1	0	3.329038	0.722318	-1.968183
21	1	0	2.704147	2.386493	-1.954330
22	6	0	2.371036	0.532673	0.781614
23	1	0	1.866835	1.008741	1.624703
24	6	0	4.085029	1.896172	-0.305703
25	1	0	5.092460	1.870605	-0.714719
26	1	0	3.897200	2.879457	0.128395
27	6	0	3.889738	0.820508	0.752630
28	1	0	4.298453	1.082543	1.727010
29	6	0	2.292526	-1.017447	0.866501
30	6	0	3.647591	-1.437674	0.280367
31	6	0	2.353237	-1.415476	2.350029
32	1	0	3.251080	-1.013016	2.823010
33	1	0	1.489064	-1.029524	2.891782
34	1	0	2.377196	-2.500677	2.440850
35	8	0	4.505752	-0.384780	0.304540
36	8	0	3.965627	-2.510094	-0.111922
37	6	0	1.142802	-1.647205	0.111054
38	6	0	-0.003787	-2.097314	0.760634
39	6	0	1.192632	-1.729157	-1.281430
40	6	0	-1.093487	-2.576079	0.046371
41	1	0	-0.071460	-2.076812	1.840511
42	6	0	0.112675	-2.195269	-2.013754
43	1	0	2.094820	-1.443966	-1.810446
44	6	0	-1.021825	-2.597281	-1.330916
45	1	0	-1.996563	-2.908966	0.542282
46	1	0	0.144753	-2.271662	-3.092428
47	6	0	-2.803071	0.153862	0.157196
48	6	0	-3.705702	-0.507736	-0.672383
49	6	0	-2.845212	-0.089471	1.530167
50	6	0	-4.621095	-1.409471	-0.146781
51	1	0	-3.673547	-0.340981	-1.743206
52	6	0	-3.766059	-0.982106	2.057786
53	1	0	-2.148494	0.396515	2.202638
54	6	0	-4.654982	-1.647404	1.220180
55	1	0	-5.301276	-1.930003	-0.808025
56	1	0	-3.788625	-1.163321	3.124707
57	1	0	-5.369235	-2.347483	1.633313
58	9	0	-2.079107	-3.026771	-2.030932

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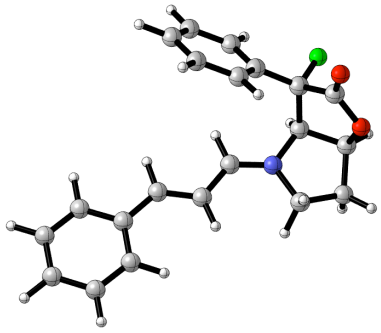
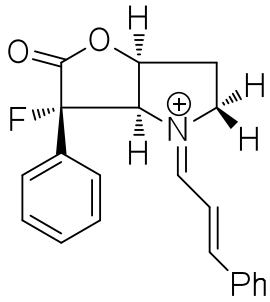
7 - *E*-iminium ion





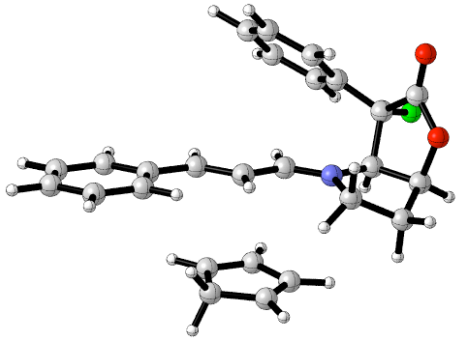
E(RM062X) = -1116.40144572

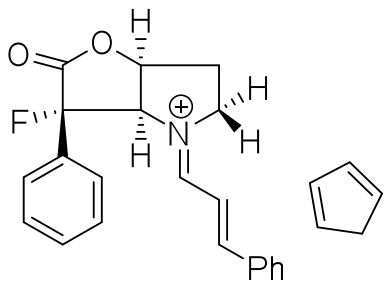
Zero-point correction=	0.359823 (Hartree/Particle)
Thermal correction to Energy=	0.380069
Thermal correction to Enthalpy=	0.381013
Thermal correction to Gibbs Free Energy=	0.309059
Sum of electronic and zero-point Energies=	-1116.041623
Sum of electronic and thermal Energies=	-1116.021377
Sum of electronic and thermal Enthalpies=	-1116.020432
Sum of electronic and thermal Free Energies=	-1116.092386

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.079538	-2.605795	0.039243
2	6	0	2.412837	-3.150830	-0.462104
3	6	0	3.282464	-1.910953	-0.550440
4	6	0	2.341319	-0.783598	-1.000375
5	6	0	3.449253	-0.245929	1.061392
6	6	0	2.846955	0.430295	-0.192376
7	1	0	1.069903	-2.484925	1.124793
8	1	0	2.840467	-3.892904	0.207957
9	8	0	3.696442	-1.544234	0.771894
10	7	0	1.009471	-1.269022	-0.594331
11	1	0	2.368009	-0.567305	-2.067584
12	1	0	4.160916	-2.015886	-1.182878
13	6	0	1.859014	1.525219	0.053580
14	6	0	1.686103	2.498823	-0.929045
15	6	0	1.036534	1.512898	1.176681
16	6	0	0.682398	3.447177	-0.792290
17	1	0	2.345526	2.521541	-1.787743
18	6	0	0.030753	2.463100	1.306266
19	1	0	1.189540	0.783171	1.962338
20	6	0	-0.151522	3.424768	0.321214
21	1	0	0.558681	4.211265	-1.548686
22	1	0	-0.597542	2.461156	2.187440
23	1	0	-0.926430	4.172491	0.431472
24	1	0	2.299905	-3.588681	-1.454592
25	1	0	0.225774	-3.204006	-0.270098
26	6	0	-0.083049	-0.584568	-0.779388

27	1	0	0.031350	0.359523	-1.305413
28	6	0	-1.374220	-0.963694	-0.351796
29	1	0	-1.513703	-1.884143	0.197580
30	6	0	-2.408290	-0.117532	-0.608801
31	1	0	-2.175632	0.798954	-1.147942
32	6	0	-3.790269	-0.280952	-0.240447
33	6	0	-4.260871	-1.398138	0.469776
34	6	0	-4.696305	0.724686	-0.610504
35	6	0	-5.598013	-1.500494	0.793732
36	1	0	-3.581808	-2.186500	0.767829
37	6	0	-6.036497	0.618269	-0.284020
38	1	0	-4.338254	1.588456	-1.158504
39	6	0	-6.486383	-0.493336	0.417699
40	1	0	-5.958331	-2.361638	1.340323
41	1	0	-6.729762	1.396289	-0.573731
42	1	0	-7.534303	-0.579779	0.674829
43	8	0	3.671787	0.249629	2.111805
44	9	0	3.924785	0.895157	-0.926073

7-*E* and Cyclopentadiene Adduct





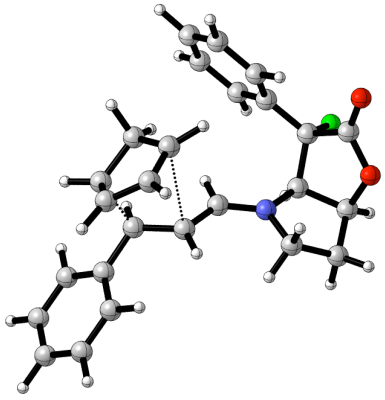
E(RM062X) = -1310.48922044

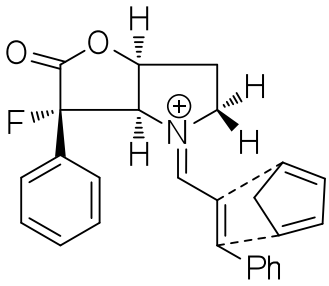
Zero-point correction=	0.454113 (Hartree/Particle)
Thermal correction to Energy=	0.480397
Thermal correction to Enthalpy=	0.481341
Thermal correction to Gibbs Free Energy=	0.392652
Sum of electronic and zero-point Energies=	-1310.035108
Sum of electronic and thermal Energies=	-1310.008824
Sum of electronic and thermal Enthalpies=	-1310.007879
Sum of electronic and thermal Free Energies=	-1310.096569

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.095797	2.031653	2.520235
2	6	0	-0.519677	2.978638	1.558819
3	6	0	-1.463620	3.343884	0.674301
4	6	0	-2.757162	2.676355	1.034012
5	6	0	-2.389436	1.834084	2.216976
6	6	0	-2.135935	-0.518764	-0.013944
7	6	0	-1.156609	0.199931	-0.619138
8	6	0	0.103063	0.253526	0.019686
9	7	0	1.135192	0.926089	-0.394539
10	1	0	-1.316258	0.724768	-1.550665
11	1	0	-1.879376	-1.019383	0.917118
12	1	0	-3.505070	3.426824	1.317964
13	1	0	-3.201309	2.102510	0.214166
14	1	0	-3.092397	1.216391	2.757617
15	1	0	-1.359244	4.068691	-0.121139
16	1	0	0.235925	-0.306910	0.940907
17	1	0	-0.562305	1.600788	3.356695
18	1	0	0.495701	3.352244	1.600056
19	6	0	-3.501449	-0.687027	-0.451273
20	6	0	-3.991800	-0.125674	-1.641151
21	6	0	-4.371611	-1.422900	0.365004
22	6	0	-5.313310	-0.303212	-1.999421
23	1	0	-3.337556	0.442107	-2.290733
24	6	0	-5.696920	-1.596674	0.004301
25	1	0	-3.997155	-1.858549	1.284174
26	6	0	-6.167153	-1.036873	-1.176797
27	1	0	-5.686908	0.126062	-2.919494
28	1	0	-6.362065	-2.166614	0.638999
29	1	0	-7.202220	-1.172540	-1.462919
30	6	0	1.132039	1.849088	-1.549141
31	1	0	1.282276	1.277523	-2.467332
32	1	0	0.176575	2.369234	-1.583989
33	6	0	2.425590	0.924228	0.313221
34	1	0	2.296418	1.220699	1.354103
35	6	0	2.305752	2.776290	-1.249290
36	1	0	2.742168	3.207208	-2.147349
37	1	0	1.992221	3.581366	-0.582959
38	6	0	3.289181	1.876713	-0.524641
39	1	0	4.041541	2.402648	0.058729
40	6	0	3.191110	-0.410537	0.219046
41	6	0	3.899753	-0.275678	-1.149546
42	8	0	3.942738	1.035210	-1.483810
43	8	0	4.343006	-1.142016	-1.821558
44	6	0	2.386962	-1.653036	0.432061

45	6	0	2.181350	-2.099184	1.736404
46	6	0	1.750667	-2.287618	-0.630964
47	6	0	1.329944	-3.168894	1.974105
48	1	0	2.699417	-1.620190	2.557867
49	6	0	0.896295	-3.355734	-0.386338
50	1	0	1.933651	-1.969427	-1.649968
51	6	0	0.680149	-3.792351	0.913960
52	1	0	1.182585	-3.523547	2.985938
53	1	0	0.413579	-3.856242	-1.215535
54	1	0	0.024331	-4.632965	1.100737
55	9	0	4.187214	-0.298029	1.174311

TS7-*E*-*exo*-top





E(RM062X) = -1310.46661994

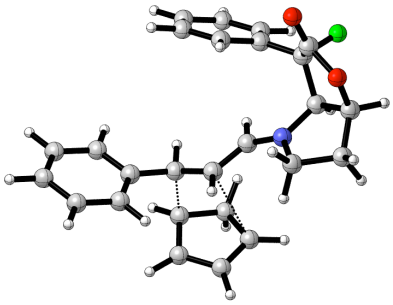
Zero-point correction=	0.455803 (Hartree/Particle)
Thermal correction to Energy=	0.480198
Thermal correction to Enthalpy=	0.481142
Thermal correction to Gibbs Free Energy=	0.400424
Sum of electronic and zero-point Energies=	-1310.010817
Sum of electronic and thermal Energies=	-1309.986422
Sum of electronic and thermal Enthalpies=	-1309.985478
Sum of electronic and thermal Free Energies=	-1310.066196

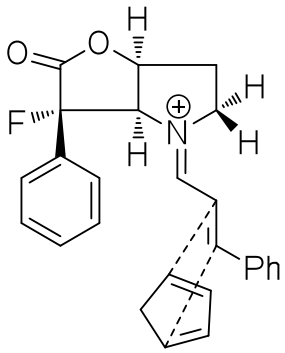
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.705777	1.009909	2.650189
2	6	0	-2.835489	1.364081	1.886631
3	6	0	-2.435164	1.850952	0.633712
4	6	0	-0.967433	2.178899	0.765547
5	6	0	-0.582970	1.372012	1.952730
6	6	0	-2.360439	0.221694	-0.433330
7	6	0	-1.335019	-0.621058	0.085949
8	6	0	-0.075524	-0.614694	-0.472344
9	7	0	0.912681	-1.462998	-0.207007
10	1	0	-1.575830	-1.340770	0.855473
11	1	0	-2.068151	0.758561	-1.333250
12	1	0	-0.891412	3.238638	1.048314
13	1	0	-0.339839	2.045843	-0.113445
14	1	0	0.440601	1.198520	2.255356
15	1	0	-3.106064	2.437439	0.018796
16	1	0	0.156148	0.119405	-1.239491
17	1	0	-1.726666	0.505766	3.605183
18	1	0	-3.863622	1.202462	2.181882
19	6	0	0.769256	-2.634513	0.672743
20	1	0	-0.249594	-3.014009	0.617944
21	1	0	0.993056	-2.355334	1.705342
22	6	0	1.791214	-3.619249	0.110634
23	1	0	2.163345	-4.319074	0.855287
24	1	0	1.362965	-4.178984	-0.721773
25	6	0	2.180110	-1.464954	-0.943055
26	1	0	2.016781	-1.480658	-2.021360
27	6	0	2.892402	-2.717081	-0.406670
28	1	0	3.561516	-3.177464	-1.129653
29	6	0	3.168554	-0.347372	-0.573338
30	6	0	3.825480	-0.911927	0.708241
31	8	0	3.664597	-2.249666	0.710223
32	8	0	4.401495	-0.321975	1.560599
33	6	0	2.672266	1.069876	-0.539767
34	6	0	2.314592	1.649850	-1.760052
35	6	0	2.615757	1.831227	0.623371
36	6	0	1.909374	2.974184	-1.815917
37	1	0	2.398296	1.072435	-2.674170
38	6	0	2.217848	3.163858	0.560774
39	1	0	2.937383	1.411785	1.566258
40	6	0	1.867996	3.737107	-0.652241
41	1	0	1.655922	3.420384	-2.768849
42	1	0	2.210158	3.759849	1.464932
43	1	0	1.580792	4.779922	-0.698690
44	6	0	-3.771414	-0.248543	-0.496851
45	6	0	-4.575557	0.188423	-1.547058
46	6	0	-4.313800	-1.107517	0.459804
47	6	0	-5.895673	-0.231584	-1.648968
48	1	0	-4.164518	0.855771	-2.296786

49	6	0	-5.630786	-1.525124	0.360189
50	1	0	-3.711637	-1.451077	1.293505
51	6	0	-6.425157	-1.088580	-0.695995
52	1	0	-6.507496	0.110951	-2.473127
53	1	0	-6.041561	-2.193644	1.105594
54	1	0	-7.453238	-1.417306	-0.771979
55	9	0	4.157476	-0.450506	-1.550931

TS7-*E-exo*





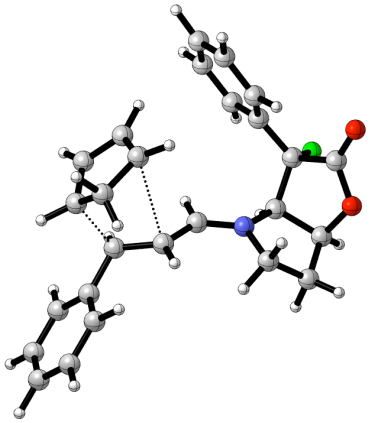
E(RM062X) = -1310.46638479

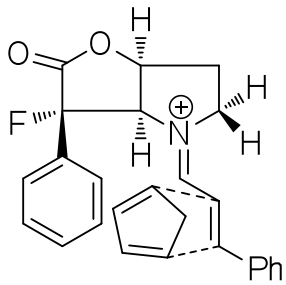
Zero-point correction=	0.455420 (Hartree/Particle)
Thermal correction to Energy=	0.479908
Thermal correction to Enthalpy=	0.480853
Thermal correction to Gibbs Free Energy=	0.399347
Sum of electronic and zero-point Energies=	-1310.010965
Sum of electronic and thermal Energies=	-1309.986476
Sum of electronic and thermal Enthalpies=	-1309.985532
Sum of electronic and thermal Free Energies=	-1310.067038

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.602590	-3.382575	0.454026
2	6	0	3.531617	-2.345583	0.658216
3	6	0	3.026968	-1.425696	1.591400
4	6	0	1.906350	-2.143743	2.308185
5	6	0	1.559802	-3.208426	1.328232
6	6	0	2.024274	-0.202305	0.481335
7	6	0	0.946094	-0.908247	-0.127586
8	6	0	-0.320555	-0.805865	0.407838
9	7	0	-1.444421	-1.250920	-0.139099
10	1	0	1.078818	-1.358378	-1.102048
11	1	0	1.709415	0.419854	1.317783

12	1	0	2.347407	-2.635850	3.186404
13	1	0	1.077321	-1.533980	2.658327
14	1	0	0.676934	-3.830024	1.394121
15	1	0	3.680941	-0.728926	2.100688
16	1	0	-0.449596	-0.269546	1.344332
17	1	0	2.682715	-4.158567	-0.293104
18	1	0	4.456437	-2.220009	0.111513
19	6	0	3.042676	0.484938	-0.360137
20	6	0	3.483886	-0.037657	-1.575882
21	6	0	3.561542	1.699536	0.083302
22	6	0	4.419857	0.646939	-2.334228
23	1	0	3.100923	-0.986500	-1.935540
24	6	0	4.499132	2.387236	-0.676826
25	1	0	3.221672	2.113369	1.026769
26	6	0	4.929102	1.862291	-1.886513
27	1	0	4.754109	0.235215	-3.277648
28	1	0	4.892609	3.331249	-0.323082
29	1	0	5.659649	2.394853	-2.481050
30	6	0	-1.497774	-2.067369	-1.358584
31	1	0	-1.379015	-1.434745	-2.242760
32	1	0	-0.693967	-2.804004	-1.339106
33	6	0	-2.773740	-0.924807	0.380397
34	1	0	-2.898336	-1.253249	1.412869
35	6	0	-2.888927	-2.692126	-1.285996
36	1	0	-3.288347	-2.958028	-2.261890
37	1	0	-2.877155	-3.579696	-0.651951
38	6	0	-3.720221	-1.610258	-0.620544
39	1	0	-4.646315	-1.960941	-0.170960
40	6	0	-3.161477	0.563751	0.254017
41	6	0	-3.701934	0.640750	-1.191839
42	8	0	-4.030274	-0.605813	-1.595978
43	8	0	-3.827556	1.606430	-1.864842
44	6	0	-2.101049	1.558024	0.609629
45	6	0	-1.952400	1.931247	1.944011
46	6	0	-1.190138	2.004091	-0.343432
47	6	0	-0.883636	2.731498	2.323256
48	1	0	-2.679131	1.605838	2.677927
49	6	0	-0.118175	2.799581	0.041059
50	1	0	-1.315238	1.741664	-1.386719
51	6	0	0.039910	3.157616	1.373733
52	1	0	-0.778624	3.033158	3.357433
53	1	0	0.586799	3.146635	-0.703581
54	1	0	0.865833	3.792252	1.669890
55	9	0	-4.266102	0.708092	1.078802

TS7-*E-endo*-top





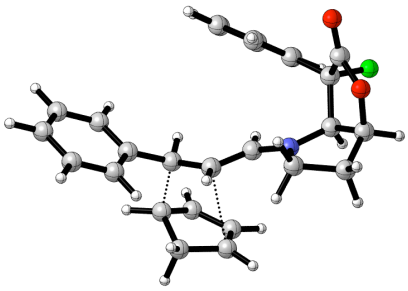
E(RM062X) = -1310.46217032

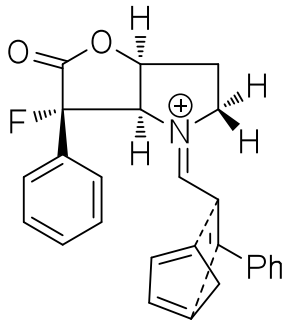
Zero-point correction=	0.455960 (Hartree/Particle)
Thermal correction to Energy=	0.480292
Thermal correction to Enthalpy=	0.481237
Thermal correction to Gibbs Free Energy=	0.400821
Sum of electronic and zero-point Energies=	-1310.006210
Sum of electronic and thermal Energies=	-1309.981878
Sum of electronic and thermal Enthalpies=	-1309.980934
Sum of electronic and thermal Free Energies=	-1310.061349

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.738934	1.989549	-1.242600
2	6	0	2.204855	1.930030	-1.479644
3	6	0	2.738631	2.050633	-0.070438
4	6	0	1.709417	2.663238	0.671081
5	6	0	0.490568	2.549972	-0.010688
6	6	0	2.595661	0.236844	0.554221
7	6	0	1.510409	-0.395348	-0.133416
8	6	0	0.265013	-0.518492	0.448272
9	7	0	-0.704827	-1.352761	0.085692
10	1	0	2.559176	1.089724	-2.069766
11	1	0	2.489647	2.847895	-2.013502
12	1	0	2.412352	0.411989	1.608402
13	1	0	1.711458	-0.912075	-1.061045
14	1	0	3.779868	2.269956	0.123951
15	1	0	-0.012178	1.746240	-1.981362
16	1	0	0.036298	0.079988	1.328177
17	1	0	-0.483476	2.805400	0.379980
18	1	0	1.831332	3.069285	1.667217

19	6	0	-0.518974	-2.465997	-0.861665
20	1	0	-0.977399	-2.224341	-1.823038
21	1	0	0.541519	-2.655568	-1.007023
22	6	0	-1.912200	-1.533008	0.895122
23	1	0	-1.683849	-1.440722	1.957116
24	6	0	-1.235860	-3.619121	-0.163869
25	1	0	-1.556655	-4.401890	-0.847454
26	1	0	-0.592431	-4.052789	0.602859
27	6	0	-2.419568	-2.934809	0.491969
28	1	0	-2.866668	-3.484580	1.316645
29	6	0	-3.115055	-0.636977	0.557239
30	6	0	-3.811807	-1.421513	-0.581331
31	8	0	-3.421801	-2.709439	-0.508034
32	8	0	-4.572906	-1.006506	-1.387970
33	6	0	-2.924470	0.826359	0.286109
34	6	0	-3.070586	1.733953	1.333909
35	6	0	-2.713562	1.296052	-1.008591
36	6	0	-3.037176	3.099517	1.081990
37	1	0	-3.269495	1.372621	2.334595
38	6	0	-2.683950	2.662370	-1.255937
39	1	0	-2.640192	0.601924	-1.836921
40	6	0	-2.858743	3.565679	-0.214915
41	1	0	-3.183735	3.798087	1.895527
42	1	0	-2.563067	3.021654	-2.270194
43	1	0	-2.867717	4.629269	-0.415662
44	6	0	3.988399	-0.251678	0.323939
45	6	0	4.903430	-0.165668	1.373197
46	6	0	4.412939	-0.766503	-0.901052
47	6	0	6.212105	-0.594584	1.207963
48	1	0	4.585608	0.233837	2.330000
49	6	0	5.722483	-1.191948	-1.067305
50	1	0	3.728571	-0.850598	-1.736460
51	6	0	6.625195	-1.107151	-0.014355
52	1	0	6.908122	-0.529782	2.033997
53	1	0	6.039088	-1.593867	-2.020922
54	1	0	7.645583	-1.441887	-0.146584
55	9	0	-3.952983	-0.800141	1.656049

TS7-*E-endo*





E(RM062X) = -1310.46494157

Zero-point correction=	0.455764 (Hartree/Particle)
Thermal correction to Energy=	0.480228
Thermal correction to Enthalpy=	0.481172
Thermal correction to Gibbs Free Energy=	0.399369
Sum of electronic and zero-point Energies=	-1310.009178
Sum of electronic and thermal Energies=	-1309.984714
Sum of electronic and thermal Enthalpies=	-1309.983769
Sum of electronic and thermal Free Energies=	-1310.065573

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.454029	-3.144100	1.183215
2	6	0	2.799792	-2.756035	0.684059
3	6	0	3.026376	-1.464044	1.439925
4	6	0	2.214280	-1.563901	2.594059
5	6	0	1.225619	-2.530679	2.399427
6	6	0	2.065354	-0.234514	0.372587
7	6	0	0.980266	-0.936615	-0.248507
8	6	0	-0.293470	-0.825529	0.273823
9	7	0	-1.422124	-1.217596	-0.299006
10	1	0	2.921040	-2.720326	-0.394236
11	1	0	3.516615	-3.491670	1.075895
12	1	0	1.739845	0.483448	1.119392
13	1	0	1.116412	-1.375512	-1.227449
14	1	0	4.008045	-1.011680	1.492374
15	1	0	0.841758	-3.920290	0.743766
16	1	0	-0.413354	-0.338360	1.237840
17	1	0	0.395736	-2.728604	3.062236
18	1	0	2.287993	-0.910703	3.453852
19	6	0	-1.490532	-1.954877	-1.567998
20	1	0	-0.699061	-2.703861	-1.599877
21	1	0	-1.363845	-1.268347	-2.409579

22	6	0	-2.889527	-2.565073	-1.530651
23	1	0	-3.295631	-2.760135	-2.520431
24	1	0	-2.886755	-3.493309	-0.957719
25	6	0	-3.704679	-1.520434	-0.790413
26	1	0	-4.632607	-1.889889	-0.360035
27	6	0	-2.745792	-0.914326	0.248907
28	1	0	-2.868750	-1.311469	1.257066
29	6	0	-3.118642	0.583056	0.225720
30	6	0	-3.664392	0.763230	-1.209295
31	8	0	-4.007642	-0.449767	-1.694968
32	8	0	-3.781831	1.773507	-1.814666
33	6	0	-2.049133	1.544139	0.640981
34	6	0	-1.903600	1.845495	1.993371
35	6	0	-1.131198	2.033739	-0.283873
36	6	0	-0.832331	2.619729	2.417925
37	1	0	-2.635268	1.486634	2.706351
38	6	0	-0.057384	2.803391	0.145709
39	1	0	-1.253705	1.828019	-1.340169
40	6	0	0.096228	3.091843	1.495847
41	6	0	3.144385	0.344969	-0.484720
42	6	0	3.562983	-0.247569	-1.675536
43	6	0	3.764339	1.520768	-0.061668
44	6	0	4.577262	0.327709	-2.427042
45	1	0	3.097212	-1.155819	-2.038264
46	6	0	4.776550	2.097880	-0.814585
47	1	0	3.444468	1.989572	0.862902
48	6	0	5.186822	1.500498	-1.998970
49	1	0	4.890119	-0.138521	-3.352216
50	1	0	5.243833	3.013935	-0.477436
51	1	0	5.976301	1.947742	-2.588377
52	1	0	0.923027	3.707179	1.828010
53	1	0	-0.730598	2.866779	3.466820
54	1	0	0.650500	3.187090	-0.577900
55	9	0	-4.218256	0.680983	1.063724

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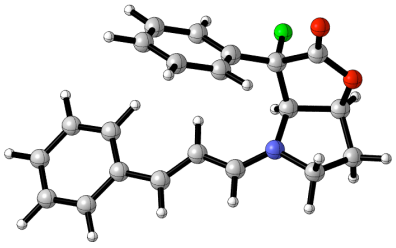
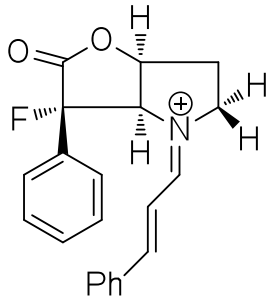
7 - *Z*-iminium ion





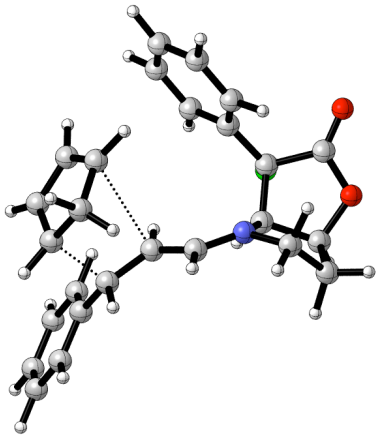
E(RM062X) = -1116.40059218

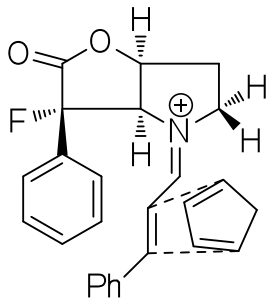
Zero-point correction=	0.359979 (Hartree/Particle)
Thermal correction to Energy=	0.379993
Thermal correction to Enthalpy=	0.380937
Thermal correction to Gibbs Free Energy=	0.310475
Sum of electronic and zero-point Energies=	-1116.040613
Sum of electronic and thermal Energies=	-1116.020599
Sum of electronic and thermal Enthalpies=	-1116.019655
Sum of electronic and thermal Free Energies=	-1116.090117

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.724049	-2.129819	1.077628
2	6	0	3.713744	-2.381940	-0.053176
3	6	0	3.522325	-1.159507	-0.937156
4	6	0	2.020045	-0.815821	-0.842938
5	6	0	3.418607	1.017954	-0.127376
6	6	0	2.014395	0.727360	-0.710098
7	1	0	3.112841	-1.397445	1.789068
8	1	0	4.740962	-2.463257	0.294290
9	8	0	4.210871	-0.056396	-0.341648
10	7	0	1.573308	-1.536810	0.356512
11	1	0	1.441909	-1.119901	-1.714169
12	1	0	3.870433	-1.281370	-1.960050
13	6	0	0.882775	1.348479	0.045830
14	6	0	-0.209822	1.864828	-0.645024
15	6	0	0.884872	1.335953	1.437852
16	6	0	-1.315897	2.322101	0.057500
17	1	0	-0.188045	1.914772	-1.726686
18	6	0	-0.226398	1.787552	2.135904
19	1	0	1.759544	0.997806	1.982761
20	6	0	-1.333268	2.267111	1.445803
21	1	0	-2.163534	2.728241	-0.479353
22	1	0	-0.218989	1.787289	3.218141
23	1	0	-2.196476	2.626759	1.990720
24	1	0	3.446106	-3.284526	-0.603945
25	1	0	2.405726	-3.022810	1.609259
26	6	0	0.332249	-1.688450	0.719272
27	1	0	0.185284	-2.225037	1.653011
28	6	0	-0.804707	-1.240147	0.015866
29	1	0	-0.685518	-0.765560	-0.946711
30	6	0	-2.024972	-1.353850	0.603815
31	1	0	-2.067879	-1.814703	1.588651
32	6	0	-3.288759	-0.910982	0.072893
33	6	0	-4.441696	-1.115947	0.844831
34	6	0	-3.405212	-0.277552	-1.175696
35	6	0	-5.679837	-0.705170	0.382637
36	1	0	-4.357483	-1.603035	1.809340
37	6	0	-4.641812	0.128548	-1.634278
38	1	0	-2.528509	-0.103034	-1.786402
39	6	0	-5.779457	-0.083395	-0.855727
40	1	0	-6.564854	-0.868406	0.982664

41	1	0	-4.730053	0.611946	-2.598139
42	1	0	-6.746563	0.237763	-1.220852
43	8	0	3.774155	2.003160	0.420128
44	9	0	2.047155	1.178247	-2.017243

TS7-*Z*-*exo*-top





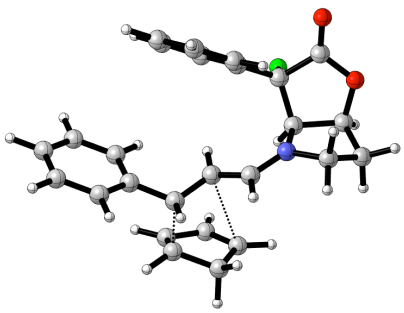
E(RM062X) = -1310.46115291

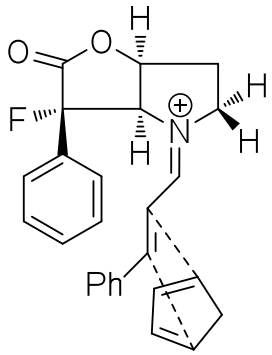
Zero-point correction=	0.455486 (Hartree/Particle)
Thermal correction to Energy=	0.479953
Thermal correction to Enthalpy=	0.480898
Thermal correction to Gibbs Free Energy=	0.399602
Sum of electronic and zero-point Energies=	-1310.005667
Sum of electronic and thermal Energies=	-1309.981199
Sum of electronic and thermal Enthalpies=	-1309.980255
Sum of electronic and thermal Free Energies=	-1310.061551

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.489375	2.671122	0.493226
2	6	0	-2.791968	2.125983	0.507069
3	6	0	-2.964997	1.322299	1.636696
4	6	0	-1.833125	1.666325	2.572702
5	6	0	-0.863212	2.325376	1.658539
6	6	0	-2.384410	-0.435034	0.947280
7	6	0	-1.007365	-0.399249	0.581429
8	6	0	-0.042887	-0.834047	1.461268
9	7	0	1.202699	-1.203052	1.165346
10	1	0	-0.726935	-0.162891	-0.437066
11	1	0	-2.573589	-0.905290	1.909338

12	1	0	-2.205844	2.431213	3.268410
13	1	0	-1.431227	0.858725	3.180442
14	1	0	0.156232	2.569739	1.920200
15	1	0	-3.947850	1.040006	1.991263
16	1	0	-0.305777	-0.967403	2.507722
17	1	0	-1.049740	3.234674	-0.314640
18	1	0	-3.524508	2.240588	-0.280759
19	6	0	-3.418148	-0.785796	-0.062299
20	6	0	-3.293736	-0.432747	-1.407146
21	6	0	-4.547639	-1.488528	0.352129
22	6	0	-4.277379	-0.784670	-2.316458
23	1	0	-2.430431	0.126874	-1.750090
24	6	0	-5.532692	-1.844239	-0.560116
25	1	0	-4.654502	-1.767857	1.394767
26	6	0	-5.398955	-1.493195	-1.895137
27	1	0	-4.171738	-0.508816	-3.357604
28	1	0	-6.401947	-2.395558	-0.226514
29	1	0	-6.164625	-1.768292	-2.608510
30	6	0	2.089623	-1.847447	2.150264
31	1	0	2.958625	-1.212324	2.336995
32	1	0	1.559151	-2.000354	3.087551
33	6	0	1.611983	-1.544137	-0.195414
34	1	0	0.742648	-1.854419	-0.776224
35	6	0	2.491687	-3.135132	1.438043
36	1	0	3.411345	-3.572994	1.819392
37	1	0	1.687780	-3.869899	1.501265
38	6	0	2.654041	-2.675246	-0.001715
39	1	0	2.567420	-3.467089	-0.742076
40	6	0	2.395358	-0.481850	-0.982740
41	6	0	3.870618	-0.802477	-0.631154
42	8	0	3.937219	-2.057750	-0.143170
43	8	0	4.807399	-0.091129	-0.759922
44	6	0	2.062994	0.970772	-0.817158
45	6	0	1.431574	1.663271	-1.845100
46	6	0	2.489450	1.653018	0.319409
47	6	0	1.238785	3.035167	-1.738244
48	1	0	1.140971	1.140537	-2.746744
49	6	0	2.293377	3.022480	0.422718
50	1	0	3.030049	1.129571	1.100196
51	6	0	1.671699	3.717049	-0.608614
52	1	0	0.777705	3.575721	-2.555377
53	1	0	2.661642	3.554841	1.290871
54	1	0	1.549630	4.790796	-0.541458
55	9	0	2.248652	-0.862456	-2.308990

TS7-*Z-exo*





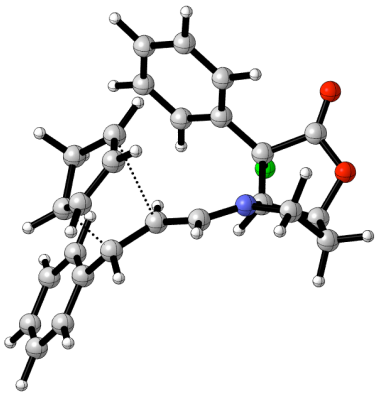
E(RM062X) = -1310.46474041

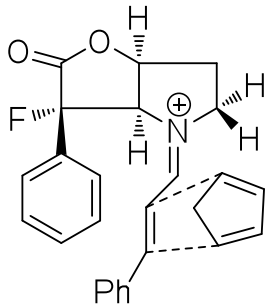
Zero-point correction=	0.455558 (Hartree/Particle)
Thermal correction to Energy=	0.479839
Thermal correction to Enthalpy=	0.480783
Thermal correction to Gibbs Free Energy=	0.400872
Sum of electronic and zero-point Energies=	-1310.009182
Sum of electronic and thermal Energies=	-1309.984901
Sum of electronic and thermal Enthalpies=	-1309.983957
Sum of electronic and thermal Free Energies=	-1310.063868

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.625331	3.289058	1.373908
2	6	0	-2.821861	2.719931	0.905333
3	6	0	-2.774035	2.587204	-0.493869
4	6	0	-1.672127	3.517577	-0.949137
5	6	0	-0.857984	3.639838	0.290254
6	6	0	-1.926281	0.874403	-0.755229
7	6	0	-0.604298	0.923815	-0.226818
8	6	0	0.487936	1.210120	-1.021888
9	7	0	1.762729	1.114603	-0.672301
10	1	0	-0.439585	0.574776	0.783178
11	1	0	-1.969579	0.931492	-1.840813
12	1	0	-2.134998	4.496781	-1.135108
13	1	0	-1.133644	3.237949	-1.850577
14	1	0	0.128297	4.082627	0.329619
15	1	0	-3.678794	2.445758	-1.071950
16	1	0	0.328175	1.524048	-2.049856
17	1	0	-1.344582	3.394908	2.411642
18	1	0	-3.624904	2.352824	1.529435
19	6	0	2.892910	1.551100	-1.508177
20	1	0	2.564906	2.305763	-2.219712

21	1	0	3.304531	0.698951	-2.055302
22	6	0	3.881984	2.064856	-0.466200
23	1	0	4.911110	2.074192	-0.817815
24	1	0	3.605149	3.068658	-0.140536
25	6	0	2.210341	0.674176	0.641824
26	1	0	1.610216	1.132398	1.429737
27	6	0	3.699424	1.085437	0.684373
28	1	0	4.011468	1.470734	1.652562
29	6	0	2.243974	-0.861052	0.839248
30	6	0	3.700989	-1.227670	0.462227
31	8	0	4.445512	-0.100653	0.406436
32	8	0	4.128496	-2.308944	0.247670
33	6	0	1.221708	-1.672213	0.101131
34	6	0	0.098433	-2.158020	0.760374
35	6	0	1.376269	-1.894354	-1.264447
36	6	0	-0.880335	-2.837901	0.046982
37	1	0	-0.005928	-2.012735	1.828300
38	6	0	0.392528	-2.565341	-1.975527
39	1	0	2.277139	-1.570239	-1.774313
40	6	0	-0.741683	-3.030654	-1.320270
41	1	0	-1.757564	-3.211183	0.560254
42	1	0	0.522382	-2.746228	-3.034678
43	1	0	-1.506946	-3.562221	-1.871207
44	6	0	-2.884245	-0.126460	-0.203884
45	6	0	-3.695915	-0.838095	-1.081762
46	6	0	-2.960822	-0.398153	1.162172
47	6	0	-4.560100	-1.817834	-0.606641
48	1	0	-3.640332	-0.640229	-2.146412
49	6	0	-3.827565	-1.367590	1.638863
50	1	0	-2.337892	0.147568	1.863479
51	6	0	-4.627498	-2.084260	0.752872
52	1	0	-5.181903	-2.368766	-1.300226
53	1	0	-3.880059	-1.569686	2.700960
54	1	0	-5.303574	-2.842693	1.125383
55	9	0	2.140806	-1.054267	2.205881

TS7-*Z-endo*-top





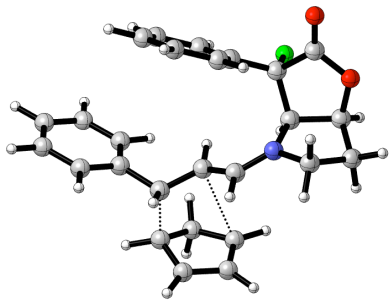
E(RM062X) = -1310.46262749

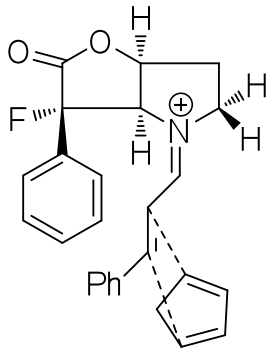
Zero-point correction=	0.455903 (Hartree/Particle)
Thermal correction to Energy=	0.480225
Thermal correction to Enthalpy=	0.481169
Thermal correction to Gibbs Free Energy=	0.400745
Sum of electronic and zero-point Energies=	-1310.006724
Sum of electronic and thermal Energies=	-1309.982403
Sum of electronic and thermal Enthalpies=	-1309.981458
Sum of electronic and thermal Free Energies=	-1310.061883

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.725246	0.599540	2.763332
2	6	0	-1.841383	1.145187	1.952627
3	6	0	-2.808210	-0.021760	1.941424
4	6	0	-2.447099	-0.812644	3.060313
5	6	0	-1.159521	-0.481743	3.495627
6	6	0	-2.237363	-1.089779	0.526592
7	6	0	-0.842606	-0.829428	0.274640
8	6	0	0.175323	-1.545070	0.848199
9	7	0	1.458553	-1.539348	0.460810
10	1	0	-1.547215	1.566104	0.994620
11	1	0	-2.306762	1.953242	2.535827
12	1	0	-2.441311	-2.085432	0.905166
13	1	0	-0.591678	-0.069362	-0.452601
14	1	0	-3.853306	0.126768	1.702677
15	1	0	0.249062	1.061960	2.828925
16	1	0	-0.045495	-2.228529	1.663651
17	1	0	-0.593276	-1.006204	4.251538
18	1	0	-3.051913	-1.618814	3.456863

19	6	0	2.458232	-2.437312	1.067761
20	1	0	1.967384	-3.140867	1.737415
21	1	0	3.184534	-1.855624	1.639175
22	6	0	3.110968	-3.089676	-0.146328
23	1	0	4.106712	-3.478542	0.054339
24	1	0	2.481318	-3.891495	-0.534892
25	6	0	3.150705	-1.947129	-1.143705
26	1	0	3.264532	-2.247717	-2.182462
27	6	0	1.866565	-1.125777	-0.882307
28	1	0	1.065105	-1.325969	-1.596337
29	6	0	2.368519	0.315685	-1.067279
30	6	0	3.854608	0.206347	-0.650847
31	8	0	4.237619	-1.077352	-0.793706
32	8	0	4.570458	1.074208	-0.279753
33	6	0	1.618057	1.462794	-0.459359
34	6	0	0.647055	2.114151	-1.220244
35	6	0	1.910763	1.919077	0.821325
36	6	0	-0.024254	3.212148	-0.701084
37	1	0	0.448778	1.784146	-2.232662
38	6	0	1.240543	3.024365	1.334521
39	1	0	2.697197	1.452304	1.401463
40	6	0	0.275067	3.672812	0.577059
41	6	0	-3.206596	-0.722374	-0.554957
42	6	0	-3.066840	0.447012	-1.303212
43	6	0	-4.292153	-1.560221	-0.800502
44	6	0	-3.992434	0.762165	-2.286024
45	1	0	-2.234810	1.120374	-1.127676
46	6	0	-5.215476	-1.246174	-1.788573
47	1	0	-4.411146	-2.470082	-0.222843
48	6	0	-5.067992	-0.083863	-2.532147
49	1	0	-3.874989	1.669399	-2.864439
50	1	0	-6.048586	-1.910552	-1.977085
51	1	0	-5.787221	0.163635	-3.301696
52	1	0	-0.224380	4.549723	0.968975
53	1	0	-0.757515	3.729520	-1.307056
54	1	0	1.501753	3.400728	2.316030
55	9	0	2.403704	0.469097	-2.450668

TS7-*Z-endo*





E(RM062X) = -1310.46401033

Zero-point correction=	0.455812 (Hartree/Particle)
Thermal correction to Energy=	0.480092
Thermal correction to Enthalpy=	0.481037
Thermal correction to Gibbs Free Energy=	0.400710
Sum of electronic and zero-point Energies=	-1310.008198
Sum of electronic and thermal Energies=	-1309.983918
Sum of electronic and thermal Enthalpies=	-1309.982974
Sum of electronic and thermal Free Energies=	-1310.063300

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.875373	3.486975	0.720907
2	6	0	-2.131752	2.856605	1.204052
3	6	0	-2.798755	2.501880	-0.108684
4	6	0	-2.262147	3.413389	-1.051028
5	6	0	-1.068772	3.950207	-0.567553
6	6	0	-1.934231	0.883345	-0.547227
7	6	0	-0.610803	0.924281	0.000927
8	6	0	0.480175	1.313784	-0.754330
9	7	0	1.756959	1.168232	-0.435308
10	1	0	-2.019511	2.058021	1.929856
11	1	0	-2.734991	3.648852	1.669955
12	1	0	-1.964779	0.920616	-1.630966
13	1	0	-0.440862	0.472999	0.968602
14	1	0	-3.843890	2.223104	-0.146361
15	1	0	-0.024164	3.709425	1.350685
16	1	0	0.306029	1.776731	-1.722089
17	1	0	-0.386548	4.577147	-1.123730
18	1	0	-2.669384	3.583995	-2.039145
19	6	0	2.875353	1.746511	-1.199720
20	1	0	3.278313	1.002196	-1.891409

21	1	0	2.535541	2.611730	-1.764802
22	6	0	2.221655	0.523490	0.786429
23	1	0	1.640420	0.852901	1.648977
24	6	0	3.880400	2.076603	-0.100618
25	1	0	4.903930	2.147725	-0.461435
26	1	0	3.609639	3.009181	0.396731
27	6	0	3.714098	0.914622	0.867508
28	1	0	4.049345	1.124384	1.880805
29	6	0	2.249700	-1.022458	0.736387
30	6	0	3.688449	-1.324802	0.248736
31	8	0	4.442966	-0.209529	0.370495
32	8	0	4.096824	-2.352265	-0.170259
33	6	0	1.190374	-1.705913	-0.073981
34	6	0	0.086266	-2.275131	0.550459
35	6	0	1.289624	-1.722752	-1.462550
36	6	0	-0.928150	-2.833990	-0.215922
37	1	0	0.024884	-2.289172	1.631389
38	6	0	0.270440	-2.273931	-2.225048
39	1	0	2.174014	-1.331802	-1.953931
40	6	0	-0.843636	-2.823791	-1.601181
41	1	0	-1.790551	-3.271741	0.271407
42	1	0	0.357463	-2.297318	-3.303639
43	1	0	-1.635895	-3.262814	-2.193918
44	6	0	-2.887810	-0.141699	-0.018977
45	6	0	-3.785291	-0.733403	-0.905689
46	6	0	-2.903596	-0.535266	1.318646
47	6	0	-4.668460	-1.712195	-0.471664
48	1	0	-3.779546	-0.439680	-1.949499
49	6	0	-3.791788	-1.506846	1.755810
50	1	0	-2.210480	-0.108229	2.033339
51	6	0	-4.674483	-2.100907	0.861338
52	1	0	-5.352002	-2.170231	-1.174736
53	1	0	-3.791189	-1.805792	2.796069
54	1	0	-5.364027	-2.861553	1.203219
55	9	0	2.202477	-1.426177	2.059748

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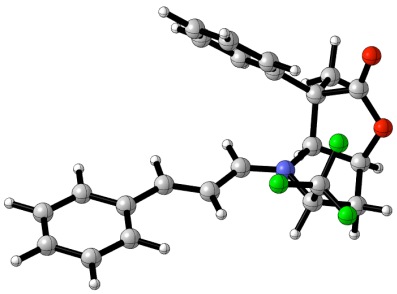
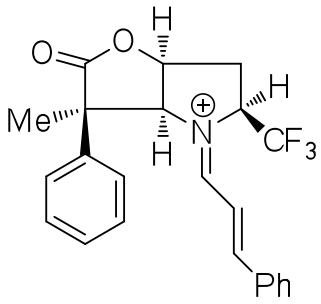
8 - *E*-iminium ion





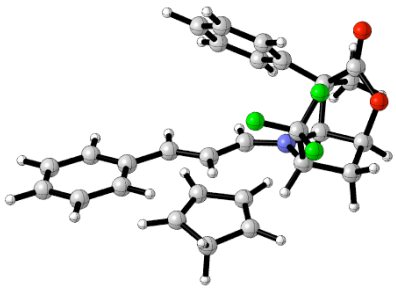
E(RM062X) = -1393.53885764

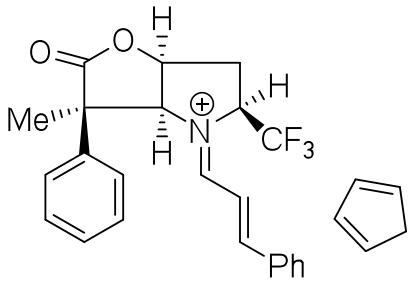
Zero-point correction=	0.401719 (Hartree/Particle)
Thermal correction to Energy=	0.425804
Thermal correction to Enthalpy=	0.426748
Thermal correction to Gibbs Free Energy=	0.346541
Sum of electronic and zero-point Energies=	-1393.137138
Sum of electronic and thermal Energies=	-1393.113054
Sum of electronic and thermal Enthalpies=	-1393.112109
Sum of electronic and thermal Free Energies=	-1393.192316

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.036980	-2.047355	-0.685175
2	6	0	2.390891	-2.378997	-1.322588
3	6	0	3.150434	-1.057451	-1.387797
4	6	0	2.088247	0.050205	-1.445409
5	6	0	3.562399	0.341143	0.413797
6	6	0	2.652470	1.152288	-0.516619
7	1	0	2.946996	-3.124901	-0.757186
8	8	0	3.886575	-0.835559	-0.192635
9	7	0	0.846146	-0.618684	-0.979135
10	1	0	1.911442	0.425439	-2.452920
11	1	0	3.837920	-1.024198	-2.231456
12	6	0	1.591038	1.957003	0.198942
13	6	0	1.068390	3.114514	-0.378690
14	6	0	1.028800	1.487709	1.386690
15	6	0	-0.009008	3.771946	0.203566
16	1	0	1.496704	3.519855	-1.286100
17	6	0	-0.046739	2.145344	1.968782
18	1	0	1.439905	0.613318	1.874607
19	6	0	-0.575577	3.283841	1.374265
20	1	0	-0.394397	4.674938	-0.252521
21	1	0	-0.462648	1.771942	2.895618
22	1	0	-1.407369	3.802068	1.833807
23	1	0	2.229945	-2.758566	-2.330786
24	1	0	0.222675	-2.623479	-1.127148
25	6	0	-0.305764	0.004552	-0.992489
26	1	0	-0.252262	1.047666	-1.291237
27	6	0	-1.574687	-0.522181	-0.691898

28	1	0	-1.690861	-1.553920	-0.396792
29	6	0	-2.636973	0.331046	-0.745322
30	1	0	-2.431208	1.362806	-1.024187
31	6	0	-4.013820	0.031410	-0.461876
32	6	0	-4.442127	-1.235089	-0.027774
33	6	0	-4.960658	1.055045	-0.626205
34	6	0	-5.778817	-1.464628	0.224144
35	1	0	-3.729270	-2.036107	0.119408
36	6	0	-6.299976	0.819877	-0.374233
37	1	0	-4.633835	2.034213	-0.956358
38	6	0	-6.707945	-0.439079	0.050275
39	1	0	-6.106954	-2.438995	0.560335
40	1	0	-7.025120	1.611626	-0.505117
41	1	0	-7.755258	-0.625930	0.250384
42	8	0	4.000901	0.660061	1.465909
43	6	0	3.622697	2.013997	-1.348784
44	1	0	3.109433	2.495060	-2.180391
45	1	0	4.063985	2.777624	-0.709952
46	1	0	4.429675	1.404990	-1.760251
47	6	0	0.994730	-2.343520	0.818132
48	9	0	1.960142	-1.728585	1.491245
49	9	0	1.118787	-3.653283	1.002475
50	9	0	-0.171399	-1.957064	1.350012

8-*E* and Cyclopentadiene Adduct





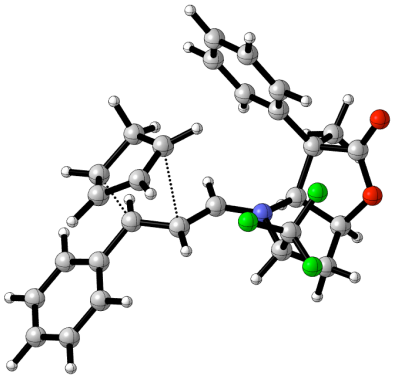
E(RM062X) = -1587.62698196

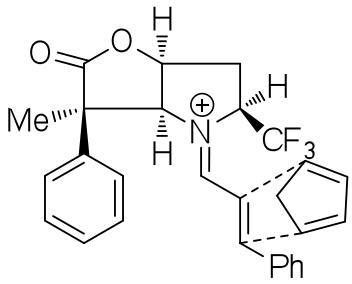
Zero-point correction=	0.496101 (Hartree/Particle)
Thermal correction to Energy=	0.526185
Thermal correction to Enthalpy=	0.527129
Thermal correction to Gibbs Free Energy=	0.430963
Sum of electronic and zero-point Energies=	-1587.130881
Sum of electronic and thermal Energies=	-1587.100797
Sum of electronic and thermal Enthalpies=	-1587.099853
Sum of electronic and thermal Free Energies=	-1587.196019

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.960955	-0.723075	3.340867
2	6	0	-2.393850	-0.311287	3.176873
3	6	0	-3.001183	-1.475882	2.457009
4	6	0	-2.069164	-2.427110	2.278716
5	6	0	-0.797444	-1.960051	2.837540
6	6	0	-2.384424	-0.149725	-0.303229
7	6	0	-1.325495	0.611454	0.087616
8	6	0	-0.113115	-0.055374	0.344925
9	7	0	1.038172	0.475218	0.678734
10	1	0	-2.519912	0.633723	2.637650
11	1	0	-2.867414	-0.171011	4.155799
12	1	0	-2.210494	-1.214926	-0.429029
13	1	0	-1.401651	1.684157	0.188224
14	1	0	-4.042730	-1.529633	2.174040
15	1	0	-0.217993	-0.133858	3.861198
16	1	0	-0.114332	-1.137400	0.270532
17	1	0	0.107082	-2.553878	2.871825
18	1	0	-2.221041	-3.397767	1.827375
19	6	0	1.274014	1.905797	0.911129
20	1	0	0.407113	2.346885	1.406332
21	6	0	2.522907	1.940834	1.799282
22	1	0	3.163976	2.794898	1.587311
23	1	0	2.219343	1.988179	2.844467
24	6	0	3.249130	0.625913	1.538460
25	1	0	3.807118	0.287779	2.410274
26	6	0	2.176653	-0.377627	1.094369
27	1	0	1.827447	-1.026224	1.898672
28	6	0	2.868452	-1.177655	-0.033391
29	6	0	3.908149	-0.168413	-0.535307
30	6	0	3.699877	-2.297123	0.622881
31	1	0	3.066580	-2.975902	1.193066
32	1	0	4.221648	-2.859431	-0.150162
33	1	0	4.444425	-1.882009	1.304477
34	8	0	4.147311	0.749695	0.443261
35	8	0	4.493176	-0.171823	-1.564583
36	6	0	1.919376	-1.676541	-1.099065
37	6	0	1.299786	-2.919599	-0.967429
38	6	0	1.544428	-0.848655	-2.157303
39	6	0	0.307980	-3.314310	-1.857629
40	1	0	1.583708	-3.595247	-0.171091
41	6	0	0.554465	-1.243854	-3.047538
42	1	0	2.033292	0.106701	-2.299564
43	6	0	-0.073807	-2.473274	-2.895217
44	1	0	-0.155012	-4.286597	-1.746630

45	1	0	0.282717	-0.591707	-3.867464
46	1	0	-0.838525	-2.784439	-3.595259
47	6	0	-3.725829	0.300317	-0.586542
48	6	0	-4.110924	1.646908	-0.494010
49	6	0	-4.681056	-0.659628	-0.951108
50	6	0	-5.414725	2.015714	-0.761483
51	1	0	-3.389584	2.407606	-0.223985
52	6	0	-5.986802	-0.287036	-1.217044
53	1	0	-4.386370	-1.700464	-1.022293
54	6	0	-6.353266	1.050295	-1.121326
55	1	0	-5.707491	3.054989	-0.694362
56	1	0	-6.718057	-1.032532	-1.499290
57	1	0	-7.373465	1.345474	-1.330470
58	6	0	1.450321	2.674943	-0.401963
59	9	0	0.361101	2.562111	-1.171378
60	9	0	1.631967	3.963629	-0.130810
61	9	0	2.485546	2.242859	-1.113668

TS8-*E-exo*-top





E(RM062X) = -1587.60963768

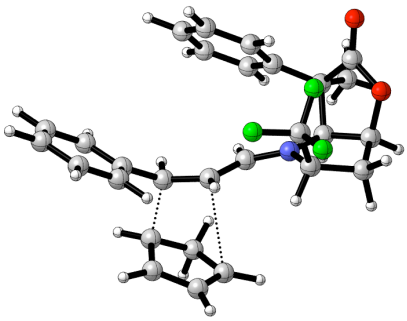
Zero-point correction=	0.497567 (Hartree/Particle)
Thermal correction to Energy=	0.525718
Thermal correction to Enthalpy=	0.526662
Thermal correction to Gibbs Free Energy=	0.438305
Sum of electronic and zero-point Energies=	-1587.112071
Sum of electronic and thermal Energies=	-1587.083920
Sum of electronic and thermal Enthalpies=	-1587.082976
Sum of electronic and thermal Free Energies=	-1587.171332

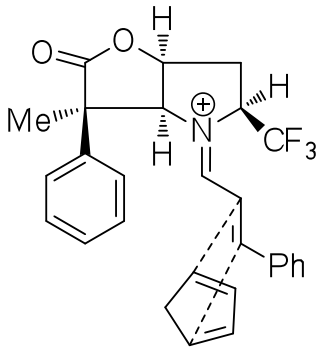
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.858560	0.338868	2.639006
2	6	0	-3.025673	0.849682	2.026525
3	6	0	-2.683271	1.750960	1.016886
4	6	0	-1.230686	2.091052	1.226754
5	6	0	-0.776479	0.985959	2.111018
6	6	0	-2.569438	0.510177	-0.561550
7	6	0	-1.490607	-0.387043	-0.333277
8	6	0	-0.250747	-0.123249	-0.861007
9	7	0	0.820361	-0.924006	-0.856120
10	1	0	-1.667397	-1.305063	0.207978
11	1	0	-2.330005	1.335435	-1.228127
12	1	0	-1.189312	3.023829	1.806974
13	1	0	-0.617873	2.254970	0.342144
14	1	0	0.261977	0.784969	2.337984
15	1	0	-3.398132	2.453008	0.608015
16	1	0	-0.095831	0.812151	-1.390441
17	1	0	-1.828480	-0.456651	3.368541
18	1	0	-4.035570	0.530629	2.248000
19	6	0	0.797278	-2.287808	-0.335340
20	1	0	-0.189232	-2.730213	-0.483934
21	6	0	1.856541	-3.014508	-1.166853
22	1	0	2.340510	-3.828635	-0.632928
23	1	0	1.383346	-3.413692	-2.063818
24	6	0	2.032575	-0.626211	-1.647843
25	1	0	1.740470	-0.385152	-2.671324
26	6	0	2.842574	-1.929442	-1.549462
27	1	0	3.397510	-2.159747	-2.457353
28	6	0	3.007189	0.423327	-1.073552
29	6	0	4.002416	0.813969	-2.194183
30	1	0	3.486277	1.296456	-3.022734
31	1	0	4.739845	1.504827	-1.788481
32	1	0	4.528855	-0.059792	-2.582219
33	6	0	3.860527	-0.420244	-0.121119
34	8	0	3.762445	-1.728236	-0.479202
35	8	0	4.578696	-0.056698	0.750172
36	6	0	2.389439	1.670508	-0.467173
37	6	0	1.821466	2.623552	-1.319973
38	6	0	2.427264	1.943724	0.898501
39	6	0	1.340163	3.829153	-0.829882
40	1	0	1.779583	2.441955	-2.388267
41	6	0	1.953660	3.158243	1.388454
42	1	0	2.880031	1.238876	1.581504
43	6	0	1.422620	4.108325	0.529859
44	1	0	0.928599	4.560961	-1.513346
45	1	0	2.028874	3.366896	2.448625
46	1	0	1.081805	5.062222	0.911958
47	6	0	-3.959984	0.023857	-0.732402

48	6	0	-4.831518	0.760284	-1.533012
49	6	0	-4.422926	-1.142917	-0.120896
50	6	0	-6.139184	0.336844	-1.730050
51	1	0	-4.482102	1.668133	-2.012814
52	6	0	-5.727583	-1.564236	-0.315426
53	1	0	-3.768522	-1.725519	0.517427
54	6	0	-6.589075	-0.825504	-1.121599
55	1	0	-6.803715	0.914807	-2.358699
56	1	0	-6.076861	-2.471265	0.160499
57	1	0	-7.607623	-1.158265	-1.272209
58	6	0	1.043140	-2.307374	1.185694
59	9	0	1.558627	-3.462458	1.582517
60	9	0	-0.120028	-2.143078	1.842980
61	9	0	1.849688	-1.322052	1.586008

TS8-*E-exo*





E(RM062X) = -1587.60445317

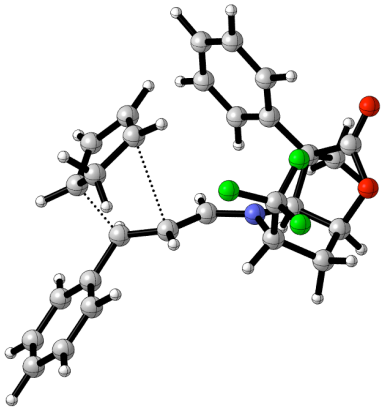
Zero-point correction=	0.497182 (Hartree/Particle)
Thermal correction to Energy=	0.525612
Thermal correction to Enthalpy=	0.526557
Thermal correction to Gibbs Free Energy=	0.436290
Sum of electronic and zero-point Energies=	-1587.107272
Sum of electronic and thermal Energies=	-1587.078841
Sum of electronic and thermal Enthalpies=	-1587.077897
Sum of electronic and thermal Free Energies=	-1587.168163

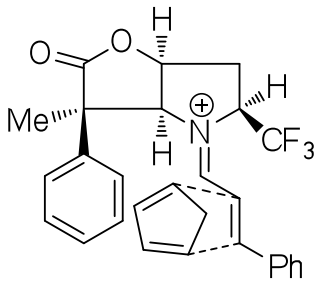
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.714249	-2.958347	1.767507
2	6	0	3.685236	-1.959520	1.551413
3	6	0	3.278276	-0.755139	2.144221
4	6	0	2.174648	-1.121876	3.108712

5	6	0	1.745189	-2.447912	2.589685
6	6	0	2.290764	0.088837	0.713656
7	6	0	1.158174	-0.719294	0.390646
8	6	0	-0.075507	-0.355015	0.865153
9	7	0	-1.275733	-0.838541	0.524295
10	1	0	1.250809	-1.490277	-0.358396
11	1	0	2.034236	0.967569	1.303792
12	1	0	2.641143	-1.285371	4.090424
13	1	0	1.380425	-0.391462	3.244511
14	1	0	0.852078	-2.965203	2.913648
15	1	0	3.989921	0.032170	2.358454
16	1	0	-0.124984	0.463102	1.578222
17	1	0	2.721780	-3.944808	1.327697
18	1	0	4.571509	-2.073291	0.941364
19	6	0	3.314200	0.404162	-0.320372
20	6	0	3.611428	-0.464235	-1.370888
21	6	0	3.990813	1.619584	-0.233052
22	6	0	4.564836	-0.118220	-2.315223
23	1	0	3.097503	-1.414036	-1.463566
24	6	0	4.945673	1.966897	-1.179326
25	1	0	3.761099	2.302627	0.577984
26	6	0	5.234418	1.097811	-2.221590
27	1	0	4.783946	-0.794968	-3.130794
28	1	0	5.461366	2.915185	-1.102707
29	1	0	5.976772	1.365310	-2.962007
30	6	0	-1.491733	-2.012280	-0.313693
31	1	0	-0.728043	-2.765295	-0.097696
32	6	0	-2.502058	-0.336244	1.169484
33	1	0	-2.389527	-0.398178	2.253234
34	6	0	-2.899181	-2.488068	0.072979
35	1	0	-3.447485	-2.914915	-0.764998
36	1	0	-2.821420	-3.243076	0.854491
37	6	0	-3.607046	-1.255113	0.626199
38	1	0	-4.352349	-1.513194	1.376975
39	6	0	-2.957891	1.078702	0.735103
40	6	0	-3.826731	0.764635	-0.487337
41	8	0	-4.248843	-0.528285	-0.414888
42	8	0	-4.169730	1.500908	-1.349799
43	6	0	-3.948272	1.608628	1.789010
44	1	0	-3.477777	1.683435	2.768872
45	1	0	-4.308193	2.591795	1.489004
46	1	0	-4.809065	0.943937	1.882276
47	6	0	-1.809557	2.021594	0.453586
48	6	0	-1.286047	2.824091	1.467072
49	6	0	-1.162657	1.998013	-0.782468
50	6	0	-0.122939	3.557778	1.261698
51	1	0	-1.778708	2.887590	2.428558
52	6	0	0.000927	2.726536	-0.987389

53	1	0	-1.567815	1.408374	-1.594756
54	6	0	0.530800	3.500985	0.037365
55	1	0	0.261664	4.184649	2.056364
56	1	0	0.490440	2.692426	-1.952298
57	1	0	1.432220	4.077550	-0.127734
58	6	0	-1.370005	-1.723462	-1.813967
59	9	0	-0.158389	-1.245560	-2.126981
60	9	0	-2.263958	-0.839708	-2.244099
61	9	0	-1.544641	-2.858510	-2.490319

TS8-*E-endo*-top





E(RM062X) = -1587.60475001

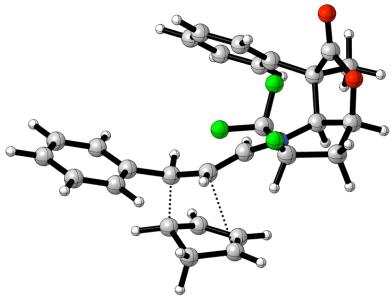
Zero-point correction=	0.497910 (Hartree/Particle)
Thermal correction to Energy=	0.526095
Thermal correction to Enthalpy=	0.527039
Thermal correction to Gibbs Free Energy=	0.438057
Sum of electronic and zero-point Energies=	-1587.106840
Sum of electronic and thermal Energies=	-1587.078655
Sum of electronic and thermal Enthalpies=	-1587.077711
Sum of electronic and thermal Free Energies=	-1587.166693

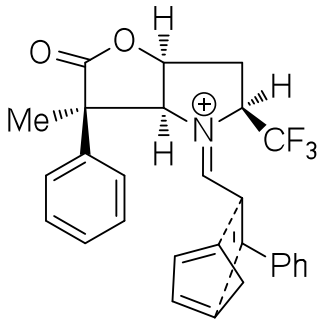
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.844540	1.017661	2.120461
2	6	0	-2.307893	0.776360	2.203444
3	6	0	-2.834553	1.695252	1.122834
4	6	0	-1.815295	2.636056	0.896212
5	6	0	-0.599033	2.175492	1.427820
6	6	0	-2.665190	0.623769	-0.488276

7	6	0	-1.602348	-0.310767	-0.275305
8	6	0	-0.341350	-0.086041	-0.762762
9	7	0	0.690355	-0.945911	-0.759265
10	1	0	-2.612181	-0.266153	2.165569
11	1	0	-2.655291	1.177204	3.166486
12	1	0	-2.443734	1.393801	-1.219626
13	1	0	-1.825199	-1.234530	0.236442
14	1	0	-3.878510	1.972884	1.074822
15	1	0	-0.098849	0.405228	2.609739
16	1	0	-0.126770	0.862458	-1.245066
17	1	0	0.366394	2.633557	1.283097
18	1	0	-1.934072	3.542182	0.315286
19	6	0	0.548414	-2.321856	-0.289753
20	1	0	-0.473077	-2.671610	-0.447725
21	6	0	1.906551	-0.737819	-1.578314
22	1	0	1.609778	-0.450757	-2.588598
23	6	0	1.528919	-3.118505	-1.150963
24	1	0	1.955068	-3.977572	-0.637943
25	1	0	1.008843	-3.465161	-2.043672
26	6	0	2.594316	-2.114296	-1.535786
27	1	0	3.100596	-2.368126	-2.465505
28	6	0	3.007866	0.192550	-1.025922
29	6	0	3.783485	-0.747272	-0.098729
30	6	0	4.011619	0.465513	-2.179123
31	1	0	4.411109	-0.459019	-2.598783
32	1	0	3.527358	1.031280	-2.974411
33	1	0	4.842237	1.052862	-1.790409
34	8	0	3.557068	-2.028876	-0.488752
35	8	0	4.546454	-0.484403	0.771737
36	6	0	2.585679	1.534464	-0.453020
37	6	0	1.908874	2.423907	-1.295312
38	6	0	2.986951	1.987322	0.802736
39	6	0	1.659823	3.732681	-0.909464
40	1	0	1.611680	2.106754	-2.290452
41	6	0	2.753984	3.307592	1.181593
42	1	0	3.531608	1.332680	1.466654
43	6	0	2.102129	4.186243	0.329181
44	1	0	1.156503	4.408048	-1.589930
45	1	0	3.104481	3.649330	2.147177
46	1	0	1.944821	5.216604	0.621036
47	6	0	-4.064370	0.126717	-0.623897
48	6	0	-4.942007	0.825587	-1.452699
49	6	0	-4.530119	-0.995969	0.061627
50	6	0	-6.255134	0.405553	-1.605815
51	1	0	-4.591342	1.700758	-1.988484
52	6	0	-5.843769	-1.412871	-0.088629
53	1	0	-3.874612	-1.560859	0.713311
54	6	0	-6.709367	-0.713824	-0.921782

55	1	0	-6.922523	0.951766	-2.259417
56	1	0	-6.193483	-2.287306	0.444450
57	1	0	-7.733581	-1.042903	-1.037801
58	6	0	0.790940	-2.413494	1.225010
59	9	0	1.096708	-3.650133	1.592987
60	9	0	1.750470	-1.591535	1.646016
61	9	0	-0.331113	-2.065645	1.891275

TS8-*E-endo*





E(RM062X) = -1587.60307147

Zero-point correction=	0.497658 (Hartree/Particle)
Thermal correction to Energy=	0.525982
Thermal correction to Enthalpy=	0.526926
Thermal correction to Gibbs Free Energy=	0.436718
Sum of electronic and zero-point Energies=	-1587.105413
Sum of electronic and thermal Energies=	-1587.077090
Sum of electronic and thermal Enthalpies=	-1587.076146
Sum of electronic and thermal Free Energies=	-1587.166353

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.604901	-0.871030	3.288989
2	6	0	2.942857	-1.076118	2.675375
3	6	0	3.247406	0.317647	2.166539
4	6	0	2.466122	1.182656	2.970615
5	6	0	1.435405	0.466664	3.583571
6	6	0	2.337381	0.346238	0.530008
7	6	0	1.203534	-0.533225	0.626744
8	6	0	-0.043358	-0.007038	0.862635
9	7	0	-1.234932	-0.602786	0.758975
10	1	0	3.023026	-1.887466	1.957916

11	1	0	3.646473	-1.285928	3.493682
12	1	0	2.058132	1.392877	0.451566
13	1	0	1.309683	-1.564914	0.327857
14	1	0	4.252848	0.597171	1.880040
15	1	0	0.949164	-1.673557	3.599929
16	1	0	-0.102598	1.040689	1.143696
17	1	0	0.620366	0.892057	4.150989
18	1	0	2.593146	2.256619	3.016159
19	6	0	-1.432083	-2.023050	0.488827
20	1	0	-0.664497	-2.609423	1.001880
21	6	0	-2.836794	-2.314469	1.033763
22	1	0	-3.374002	-3.055560	0.444481
23	1	0	-2.757453	-2.679980	2.056982
24	6	0	-3.561112	-0.972569	1.027820
25	1	0	-4.309737	-0.907057	1.815893
26	6	0	-2.470378	0.102954	1.146782
27	1	0	-2.359984	0.488637	2.161825
28	6	0	-2.945657	1.210268	0.174580
29	6	0	-3.797315	0.408862	-0.816266
30	6	0	-3.955595	2.101980	0.921332
31	1	0	-3.496301	2.576706	1.787887
32	1	0	-4.329169	2.872124	0.247901
33	1	0	-4.806059	1.515653	1.273882
34	8	0	-4.201126	-0.748524	-0.222902
35	8	0	-4.141480	0.722343	-1.905550
36	6	0	-1.815648	1.983307	-0.468084
37	6	0	-1.326839	3.149301	0.120503
38	6	0	-1.155756	1.470555	-1.585433
39	6	0	-0.186791	3.770966	-0.376639
40	1	0	-1.830777	3.589072	0.971212
41	6	0	-0.015497	2.088435	-2.080777
42	1	0	-1.533889	0.584618	-2.079102
43	6	0	0.478149	3.236118	-1.472708
44	1	0	0.169617	4.683438	0.084553
45	1	0	0.481287	1.675838	-2.949522
46	1	0	1.358806	3.726082	-1.868598
47	6	0	3.425262	0.014818	-0.442036
48	6	0	3.766924	-1.295140	-0.775144
49	6	0	4.133736	1.066890	-1.022406
50	6	0	4.794694	-1.544311	-1.673206
51	1	0	3.228111	-2.135763	-0.355182
52	6	0	5.159514	0.817762	-1.921907
53	1	0	3.872124	2.089368	-0.771800
54	6	0	5.493893	-0.490210	-2.247337
55	1	0	5.045905	-2.564949	-1.930635
56	1	0	5.695566	1.643862	-2.370583
57	1	0	6.293058	-0.688184	-2.949399
58	6	0	-1.295222	-2.377021	-0.995620

59	9	0	-0.077623	-2.070449	-1.460435
60	9	0	-1.470788	-3.688677	-1.149608
61	9	0	-2.180241	-1.744265	-1.759050

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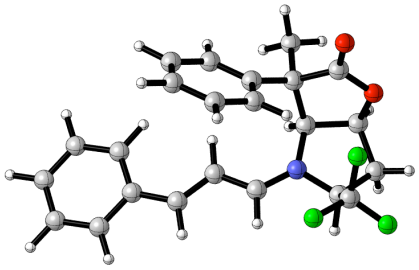
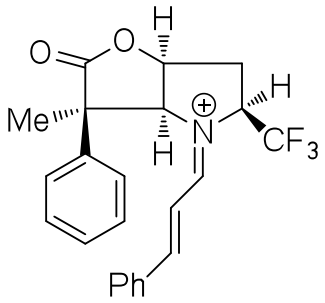
8 - *Z*-iminium ion





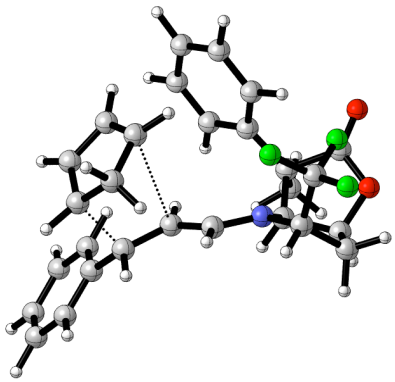
E(RM062X) = -1393.53799123

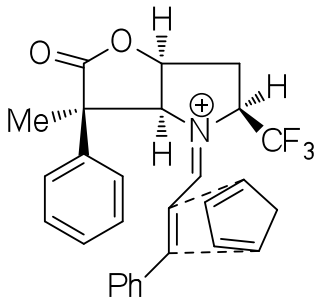
Zero-point correction=	0.401921 (Hartree/Particle)
Thermal correction to Energy=	0.425738
Thermal correction to Enthalpy=	0.426682
Thermal correction to Gibbs Free Energy=	0.348323
Sum of electronic and zero-point Energies=	-1393.136070
Sum of electronic and thermal Energies=	-1393.112254
Sum of electronic and thermal Enthalpies=	-1393.111309
Sum of electronic and thermal Free Energies=	-1393.189668

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.433454	-1.656472	-0.880803
2	6	0	3.402033	-0.889784	-1.782273
3	6	0	2.922110	0.557903	-1.762356
4	6	0	1.415103	0.521185	-1.435407
5	6	0	2.646808	1.834400	0.150572
6	6	0	1.235239	1.699804	-0.437094
7	1	0	4.434466	-0.961816	-1.443881
8	8	0	3.544500	1.270523	-0.703860
9	7	0	1.201891	-0.841583	-0.901181
10	1	0	0.788544	0.643537	-2.319315
11	1	0	3.133210	1.071039	-2.699152
12	6	0	0.173581	1.518918	0.625921
13	6	0	-1.079717	2.119565	0.509267
14	6	0	0.416537	0.690433	1.721884
15	6	0	-2.083610	1.850123	1.430021
16	1	0	-1.287897	2.807029	-0.300763
17	6	0	-0.587737	0.414460	2.638599
18	1	0	1.401607	0.271053	1.878466
19	6	0	-1.847239	0.980871	2.486330
20	1	0	-3.050144	2.326390	1.324628

21	1	0	-0.377864	-0.227479	3.484535
22	1	0	-2.629333	0.772223	3.204849
23	1	0	3.340734	-1.286263	-2.794833
24	1	0	2.210114	-2.649506	-1.271470
25	6	0	0.030553	-1.362642	-0.634487
26	1	0	0.053258	-2.373993	-0.238494
27	6	0	-1.219753	-0.755291	-0.837617
28	1	0	-1.277058	0.217362	-1.301991
29	6	0	-2.331861	-1.396960	-0.381905
30	1	0	-2.189327	-2.357826	0.108409
31	6	0	-3.692842	-0.939190	-0.460359
32	6	0	-4.699969	-1.758173	0.072691
33	6	0	-4.046055	0.291749	-1.039372
34	6	0	-6.025202	-1.363494	0.025296
35	1	0	-4.432133	-2.706985	0.522755
36	6	0	-5.368804	0.680639	-1.086840
37	1	0	-3.283645	0.943323	-1.446962
38	6	0	-6.358741	-0.145446	-0.554039
39	1	0	-6.796792	-2.000062	0.436753
40	1	0	-5.640326	1.626581	-1.536158
41	1	0	-7.394806	0.165674	-0.593838
42	6	0	1.047396	2.974285	-1.283080
43	1	0	0.982358	3.840422	-0.626037
44	1	0	1.891625	3.122095	-1.958647
45	1	0	0.141891	2.913934	-1.887216
46	8	0	2.969291	2.386298	1.146051
47	6	0	2.943471	-1.887887	0.541976
48	9	0	3.330427	-0.769123	1.144751
49	9	0	1.976757	-2.438483	1.290366
50	9	0	3.971641	-2.725083	0.505724

TS8-*Z*-*exo*-top





E(RM062X) = -1587.60140052

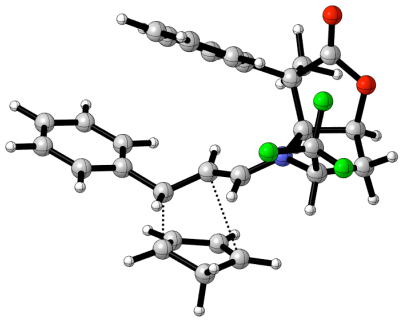
Zero-point correction=	0.497634 (Hartree/Particle)
Thermal correction to Energy=	0.525878
Thermal correction to Enthalpy=	0.526822

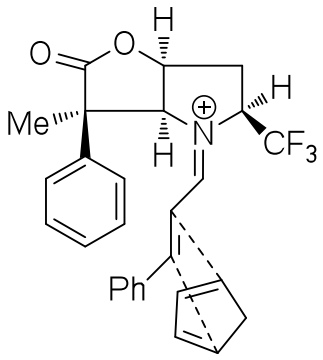
Thermal correction to Gibbs Free Energy= 0.438268
Sum of electronic and zero-point Energies= -1587.103766
Sum of electronic and thermal Energies= -1587.075522
Sum of electronic and thermal Enthalpies= -1587.074578
Sum of electronic and thermal Free Energies= -1587.163133

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.840630	0.877896	2.489707
2	6	0	-3.099740	0.349138	2.122633
3	6	0	-3.036217	-1.040646	2.057688
4	6	0	-1.758595	-1.438592	2.751781
5	6	0	-0.998434	-0.159800	2.770458
6	6	0	-2.541109	-1.266455	0.111511
7	6	0	-1.264006	-0.690638	-0.145508
8	6	0	-0.126329	-1.438530	0.004013
9	7	0	1.092524	-1.170884	-0.487599
10	1	0	-1.191570	0.314233	-0.541917
11	1	0	-2.530285	-2.344171	0.250320
12	1	0	-2.018876	-1.682862	3.791564
13	1	0	-1.224391	-2.301170	2.360769
14	1	0	0.044951	-0.073921	3.041648
15	1	0	-3.921449	-1.662754	2.054343
16	1	0	-0.193707	-2.398124	0.508409
17	1	0	-1.581340	1.923658	2.505944
18	1	0	-3.967318	0.936460	1.852911
19	6	0	-3.737326	-0.792943	-0.624070
20	6	0	-3.881951	0.537913	-1.023173
21	6	0	-4.746537	-1.705683	-0.925769
22	6	0	-5.009810	0.939853	-1.718284
23	1	0	-3.118224	1.268632	-0.778598
24	6	0	-5.875730	-1.303025	-1.626614
25	1	0	-4.644413	-2.740950	-0.618870
26	6	0	-6.008584	0.019184	-2.023904
27	1	0	-5.115408	1.972726	-2.023672
28	1	0	-6.649264	-2.022306	-1.861197
29	1	0	-6.888202	0.336345	-2.568496
30	6	0	2.141030	-2.186541	-0.380047
31	1	0	1.692096	-3.162067	-0.184890
32	6	0	1.291264	-0.252711	-1.622129
33	1	0	0.412256	-0.340367	-2.264879
34	6	0	2.861387	-2.156267	-1.728514
35	1	0	3.933540	-2.326787	-1.644368
36	1	0	2.438743	-2.923739	-2.375269
37	6	0	2.576975	-0.775345	-2.307609
38	1	0	2.488818	-0.797981	-3.392777

39	6	0	1.620546	1.235906	-1.361361
40	6	0	3.157824	1.232605	-1.323683
41	8	0	3.618431	0.126503	-1.961393
42	8	0	3.878033	2.064233	-0.884273
43	6	0	1.282877	1.983801	-2.668225
44	1	0	0.212718	1.938705	-2.874059
45	1	0	1.591360	3.025222	-2.590952
46	1	0	1.804776	1.537329	-3.516185
47	6	0	1.057656	1.927746	-0.132571
48	6	0	0.071639	2.909190	-0.236414
49	6	0	1.632767	1.699145	1.118300
50	6	0	-0.291797	3.675258	0.865549
51	1	0	-0.385221	3.132081	-1.191517
52	6	0	1.271699	2.462560	2.219556
53	1	0	2.426975	0.972577	1.223611
54	6	0	0.323289	3.469556	2.092196
55	1	0	-1.029065	4.459925	0.750780
56	1	0	1.768715	2.300827	3.168073
57	1	0	0.074196	4.095023	2.940387
58	6	0	3.038335	-1.921978	0.823004
59	9	0	3.744213	-0.799267	0.705153
60	9	0	2.290299	-1.815279	1.934284
61	9	0	3.886295	-2.930991	0.992373

TS8-*Z-exo*





E(RM062X) = -1587.60355224

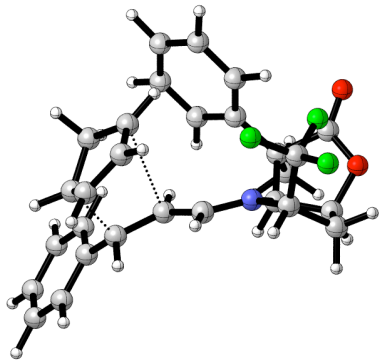
Zero-point correction=	0.497463 (Hartree/Particle)
Thermal correction to Energy=	0.525576
Thermal correction to Enthalpy=	0.526520
Thermal correction to Gibbs Free Energy=	0.438759
Sum of electronic and zero-point Energies=	-1587.106089
Sum of electronic and thermal Energies=	-1587.077977
Sum of electronic and thermal Enthalpies=	-1587.077033

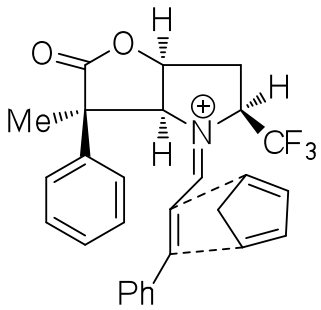
Sum of electronic and thermal Free Energies= -1587.164794

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.004558	3.181233	-1.821719
2	6	0	3.147034	2.764185	-1.115298
3	6	0	2.894666	2.788750	0.268167
4	6	0	1.672505	3.662881	0.439248
5	6	0	1.063236	3.598753	-0.915121
6	6	0	2.183202	1.042440	0.633915
7	6	0	0.970571	0.856327	-0.097374
8	6	0	-0.255075	1.162149	0.440805
9	7	0	-1.450195	0.884159	-0.093461
10	1	0	1.016816	0.352639	-1.053191
11	1	0	2.028646	1.243702	1.691779
12	1	0	2.032912	4.690812	0.587049
13	1	0	1.013650	3.432756	1.272188
14	1	0	0.070807	3.957611	-1.153790
15	1	0	3.710274	2.804534	0.980481
16	1	0	-0.303467	1.653217	1.408189
17	1	0	1.883675	3.150516	-2.894624
18	1	0	4.060065	2.398649	-1.564890
19	6	0	-2.668372	1.550899	0.372942
20	1	0	-2.434773	2.566401	0.698946
21	6	0	-3.594051	1.547125	-0.847445
22	1	0	-4.640812	1.404388	-0.583541
23	1	0	-3.498626	2.495210	-1.375291
24	6	0	-1.610580	0.196294	-1.377603
25	1	0	-0.937853	0.651105	-2.109933
26	6	0	-3.095137	0.410880	-1.734657
27	1	0	-3.246799	0.621784	-2.792364
28	6	0	-1.461620	-1.350024	-1.355888
29	6	0	-1.162331	-1.805127	-2.795025
30	1	0	-0.209301	-1.402338	-3.140031
31	1	0	-1.125780	-2.892810	-2.837382
32	1	0	-1.939195	-1.462028	-3.481109
33	6	0	-2.905207	-1.804582	-1.094667
34	8	0	-3.764806	-0.800229	-1.418489
35	8	0	-3.277455	-2.868145	-0.731000
36	6	0	-0.498334	-1.913601	-0.330303
37	6	0	0.775410	-2.353102	-0.685446
38	6	0	-0.868838	-1.964249	1.013419
39	6	0	1.668556	-2.796578	0.282097
40	1	0	1.089570	-2.359117	-1.721593
41	6	0	0.024495	-2.397169	1.981885
42	1	0	-1.871334	-1.688764	1.310352

43	6	0	1.301356	-2.807680	1.619166
44	1	0	2.656508	-3.128542	-0.012393
45	1	0	-0.287281	-2.434415	3.017873
46	1	0	1.998551	-3.154708	2.371122
47	6	0	3.319648	0.107578	0.397392
48	6	0	4.033154	-0.374696	1.490135
49	6	0	3.663196	-0.325917	-0.883011
50	6	0	5.063491	-1.290223	1.310555
51	1	0	3.769209	-0.051086	2.490754
52	6	0	4.695225	-1.231099	-1.065359
53	1	0	3.119523	0.041435	-1.747653
54	6	0	5.395943	-1.719578	0.034316
55	1	0	5.606088	-1.664448	2.168841
56	1	0	4.955159	-1.560844	-2.063015
57	1	0	6.201424	-2.428088	-0.108079
58	6	0	-3.268917	0.872427	1.601947
59	9	0	-4.277634	1.606686	2.064903
60	9	0	-2.347381	0.773870	2.571287
61	9	0	-3.725531	-0.350496	1.351478

TS8-*Z-endo*-top





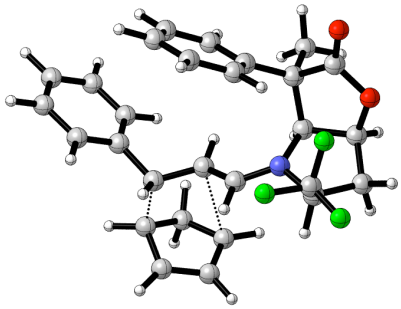
E(RM062X) = -1587.60606329

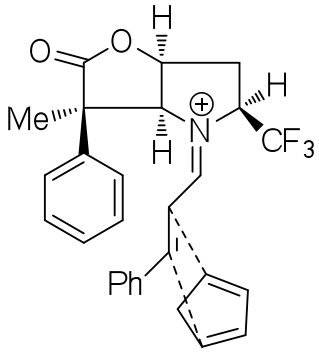
Zero-point correction=	0.497924 (Hartree/Particle)
Thermal correction to Energy=	0.526043
Thermal correction to Enthalpy=	0.526987
Thermal correction to Gibbs Free Energy=	0.439321
Sum of electronic and zero-point Energies=	-1587.108139
Sum of electronic and thermal Energies=	-1587.080021
Sum of electronic and thermal Enthalpies=	-1587.079077
Sum of electronic and thermal Free Energies=	-1587.166743

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.673985	1.773324	2.038601
2	6	0	1.931496	0.985871	2.042714
3	6	0	2.828928	1.820649	1.157277
4	6	0	2.237061	3.098888	1.113399
5	6	0	0.911946	3.043124	1.576838
6	6	0	2.467362	1.210381	-0.632356
7	6	0	1.184076	0.563920	-0.631027
8	6	0	0.013553	1.238698	-0.817434
9	7	0	-1.200605	0.685470	-1.025926
10	1	0	1.808145	-0.064631	1.789538
11	1	0	2.343627	1.022460	3.061819
12	1	0	2.502441	2.147806	-1.175094
13	1	0	1.151429	-0.506374	-0.478241
14	1	0	3.904614	1.712391	1.182024
15	1	0	-0.269552	1.404670	2.414385
16	1	0	0.024870	2.323412	-0.864144
17	1	0	0.195003	3.850670	1.547457
18	1	0	2.717928	3.980285	0.707060
19	6	0	-2.337148	1.550621	-1.325034
20	1	0	-1.986659	2.518620	-1.689191
21	6	0	-3.137385	0.802907	-2.392571
22	1	0	-4.214150	0.925698	-2.286819
23	1	0	-2.843065	1.165619	-3.376318
24	6	0	-2.741210	-0.660186	-2.239880
25	1	0	-2.734180	-1.184909	-3.193986
26	6	0	-1.361227	-0.683903	-1.539774
27	1	0	-0.541368	-0.871666	-2.237573
28	6	0	-1.505472	-1.867355	-0.549725
29	6	0	-3.024333	-1.929562	-0.330212
30	6	0	-1.195953	-3.147650	-1.355941
31	1	0	-0.167575	-3.139715	-1.718239
32	1	0	-1.350726	-4.025408	-0.730264
33	1	0	-1.852884	-3.228360	-2.223368
34	8	0	-3.649562	-1.323708	-1.369956
35	8	0	-3.614500	-2.465288	0.547271
36	6	0	-0.755989	-1.825680	0.769610
37	6	0	0.411006	-2.567658	0.964545
38	6	0	-1.275466	-1.118122	1.853238
39	6	0	1.032324	-2.612719	2.207039
40	1	0	0.831442	-3.151874	0.156072
41	6	0	-0.662076	-1.171789	3.099180
42	1	0	-2.200955	-0.567523	1.745166
43	6	0	0.490443	-1.923055	3.284003
44	1	0	1.920822	-3.217636	2.339551
45	1	0	-1.110419	-0.651881	3.937242

46	1	0	0.950393	-1.988194	4.261817
47	6	0	3.669986	0.372066	-0.903966
48	6	0	3.799409	-0.914742	-0.377929
49	6	0	4.698348	0.895902	-1.684784
50	6	0	4.933311	-1.665462	-0.643859
51	1	0	3.018603	-1.334417	0.247670
52	6	0	5.830705	0.139735	-1.955603
53	1	0	4.608258	1.896285	-2.092964
54	6	0	5.950265	-1.140986	-1.435052
55	1	0	5.027881	-2.662443	-0.233383
56	1	0	6.618474	0.551857	-2.572441
57	1	0	6.833621	-1.730558	-1.642296
58	6	0	-3.117606	1.867879	-0.055349
59	9	0	-3.654377	0.787407	0.507547
60	9	0	-4.091730	2.734509	-0.309785
61	9	0	-2.295154	2.425742	0.854659

TS8-*Z-endo*





E(RM062X) = -1587.60334725

Zero-point correction=	0.497651 (Hartree/Particle)
Thermal correction to Energy=	0.525748
Thermal correction to Enthalpy=	0.526693
Thermal correction to Gibbs Free Energy=	0.438760
Sum of electronic and zero-point Energies=	-1587.105697
Sum of electronic and thermal Energies=	-1587.077599
Sum of electronic and thermal Enthalpies=	-1587.076655
Sum of electronic and thermal Free Energies=	-1587.164587

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.010085	3.336319	-1.411463

2	6	0	2.381677	2.800616	-1.604811
3	6	0	2.868588	2.712626	-0.171545
4	6	0	2.084123	3.658631	0.538168
5	6	0	0.934274	3.971945	-0.187934
6	6	0	2.198341	1.076636	0.402559
7	6	0	0.980285	0.801910	-0.313392
8	6	0	-0.249697	1.171252	0.174423
9	7	0	-1.444216	0.790136	-0.293581
10	1	0	2.460120	1.901460	-2.207156
11	1	0	2.970224	3.585693	-2.100909
12	1	0	2.047307	1.264945	1.460313
13	1	0	1.032523	0.174213	-1.192147
14	1	0	3.924269	2.615385	0.047576
15	1	0	0.252212	3.359355	-2.183566
16	1	0	-0.294205	1.821387	1.043261
17	1	0	0.107733	4.571213	0.166454
18	1	0	2.304264	4.007242	1.539103
19	6	0	-2.663892	1.523063	0.053769
20	1	0	-2.437529	2.584035	0.178857
21	6	0	-1.608873	-0.120163	-1.431053
22	1	0	-0.955655	0.203152	-2.246173
23	6	0	-3.604933	1.280565	-1.130067
24	1	0	-4.646282	1.178604	-0.828534
25	1	0	-3.528986	2.113450	-1.828004
26	6	0	-3.101730	0.003805	-1.795225
27	1	0	-3.273167	0.007936	-2.870797
28	6	0	-1.434188	-1.634193	-1.133263
29	6	0	-2.863485	-2.049326	-0.755658
30	6	0	-1.162782	-2.341233	-2.473097
31	1	0	-1.964588	-2.143786	-3.187205
32	1	0	-0.228257	-1.993371	-2.914648
33	1	0	-1.103427	-3.417289	-2.315830
34	8	0	-3.745924	-1.134056	-1.241903
35	8	0	-3.210525	-3.029567	-0.189339
36	6	0	-0.435140	-1.987013	-0.050356
37	6	0	0.842210	-2.450671	-0.358929
38	6	0	-0.772086	-1.805376	1.290894
39	6	0	1.772520	-2.689276	0.644769
40	1	0	1.131304	-2.632827	-1.386246
41	6	0	0.157412	-2.036975	2.294174
42	1	0	-1.774690	-1.503941	1.562642
43	6	0	1.437586	-2.471697	1.972786
44	1	0	2.763973	-3.039770	0.384226
45	1	0	-0.128004	-1.898110	3.329165
46	1	0	2.162899	-2.660790	2.753964
47	6	0	3.357510	0.153315	0.187590
48	6	0	4.166463	-0.162834	1.276673
49	6	0	3.647746	-0.407810	-1.055102

50	6	0	5.232871	-1.039634	1.134289
51	1	0	3.946146	0.262168	2.249568
52	6	0	4.717882	-1.278071	-1.200802
53	1	0	3.032206	-0.192025	-1.920347
54	6	0	5.511161	-1.599527	-0.105509
55	1	0	5.845128	-1.285949	1.992015
56	1	0	4.930985	-1.710935	-2.169671
57	1	0	6.343141	-2.281934	-0.219735
58	6	0	-3.239669	1.080282	1.396904
59	9	0	-4.261610	1.867546	1.723790
60	9	0	-2.308697	1.188551	2.356780
61	9	0	-3.667925	-0.177704	1.390104
