Supporting Information

Cleavage of Carbon Dioxide by an Iridium supported Fischer Carbene. A DFT Investigation

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1. Structural Validation and Reduced Model Structure

The size reduced model predicted almost identical bond lengths and angles to the full ligand optimisations and x-ray crystal data. The only exception being the reduced model's absence of benzyl group canting and the accompanying distortion to the ^{i}Pr ligand positions.

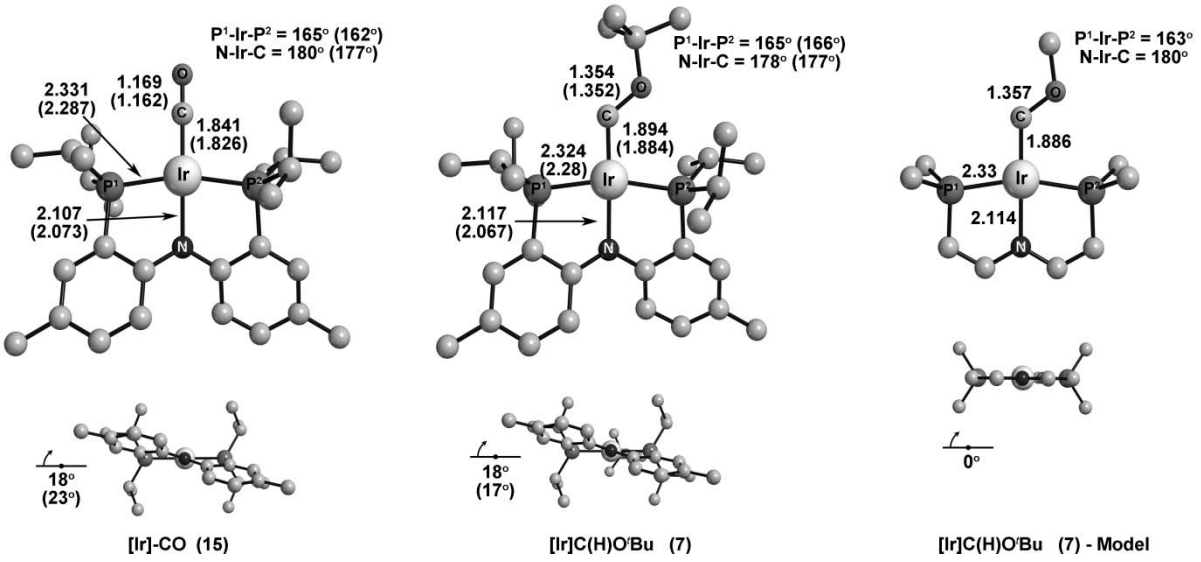
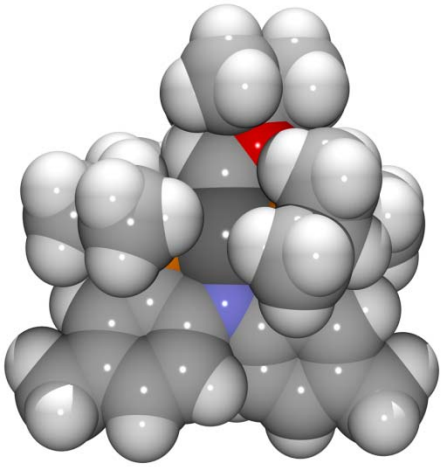
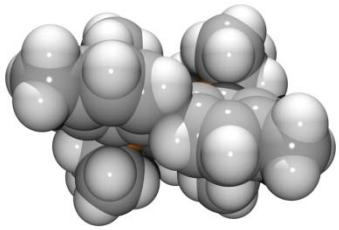


Figure sup1 Real-opt structures for[Ir]-CO, [Ir]=C(H)O^{t}Bu and reduced model structure for [Ir]=C(H)O^{t}Bu. Selected bond lengths and angles indicated, values in parentheses are from x-ray diffraction measurements[1]. Hydrogen atoms removed for clarity.

The canting is due to the close proximity of the hydrogen atoms of the adjacent benzyl groups and plays no role in the activity of the species. This is easily seen in the axial view of the Ortep[2] space filled diagram Figure sup2, which also shows that the ^{i}Pr ligands provide little or no hindrance to binding to the metal centre from above the (PNP)Ir plane.



Planar View

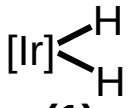
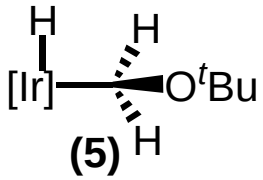
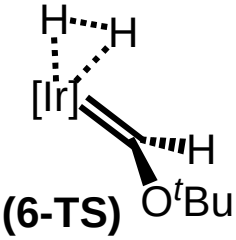
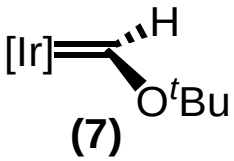
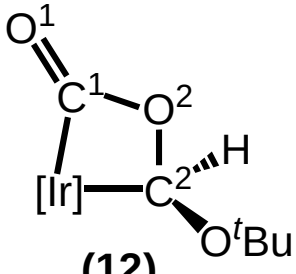
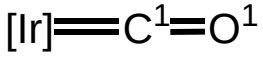


Axial View

Figure sup2. Ortep space filling diagram of [Ir]=C(H)O^{t}Bu highlighting the access to metal centre from above the plane (in planar view) and the canting present in the benzyl groups (in the axial view).

Additional comparison can be made between calculations using the model optimised geometries and those using the full ligand optimised geometries. Table sup1 outlines a comparison between the two.

Table sup1. Table outlining **relative** reaction energies and differences between geometries of model and full ligand system. Absolute energies, corrections and Cartesian geometries are available in other sections of the Supporting Information. Energies in kJ mol^{-1} and measurements in Å.

Structure No	Optimised Full Ligand Structure			Optimised Model Structure		
	*ΔG_{298}	E (uncorr')	details	ΔG_{298}	E (uncorr')	details
 **(1)**	0	0	Ir-H = 1.597	0	0	Ir-H = 1.592
[Ir] **(2)**	+62.5	+42.9		+48.7	+28.1	
 **(5)**	+20.9	-52.1	Ir-C = 2.109 Ir-H = 1.567	-15.1	-79.2	Ir-C = 2.107 Ir-H = 1.551
 **(6-TS)**	+129.1	+75.8	Ir-C = 1.925 Ir-H1 = 1.781 Ir-H2 = 1.656	+76.2	+26.7	Ir-C = 1.908 Ir-H1 = 1.817 Ir-H2 = 1.693
 **(7)**	+15.1	-2.7	Ir-C = 1.894	-0.2	-10.6	Ir-C = 1.886
 **(12)**	+102.3	+40.2	Ir-C1 = 2.003 C1-O1 = 1.211 C1-O2 = 1.348 O2-C2 = 1.504 C2-Ir = 2.096	+81.5	+20.9	Ir-C1 = 2.003 C1-O1 = 1.206 C1-O2 = 1.346 O2-C2 = 1.511 C2-Ir = 2.066
 **(15)**	-132.3	-126.6	Ir-C1 = 1.841 C1-O1 = 1.170	-128.4	-126.6	Ir-C1 = 1.844 C1-O1 = 1.167

2. Structural Comparison Tables

Table sup2 – Selected bond lengths and selected atomic Mulliken charge

Structure		**7**	**7-TS**	**12**	**13**	**14**	**14-TS**	**15**
Bond Lengths (Å)	Ir-C2	1.886	1.979	2.066	2.092	2.019	2.182	-
	Ir-C1	-	2.116	2.003	2.006	2.080	1.980	1.845
	C1-O2	1.170*	1.271	1.346	1.369	1.437	1.729	-
	O2-C2	-	2.034	1.511	1.467	1.403	1.327	1.207**
	O1-C1		1.214	1.206	1.207	1.204	1.177	1.167
Mulliken Charge	Ir	-0.029	-0.275	-0.203	-0.242	-0.303	-0.341	-0.121
	C2	-0.111	+0.023	+0.138	+0.228	+0.291	+0.389	-
	C1	+0.720*	+0.528	+0.420	+0.410	+0.347	+0.279	+0.116
	O2	-0.360*	-0.479	-0.419	-0.424	-0.425	-0.495	-
	O1	-0.360*	-0.419	-0.423	-0.433	-0.445	-0.361	-0.312

* Taken from optimised linear CO_2, ** Taken from optimised formate $HC(O)CH_3$

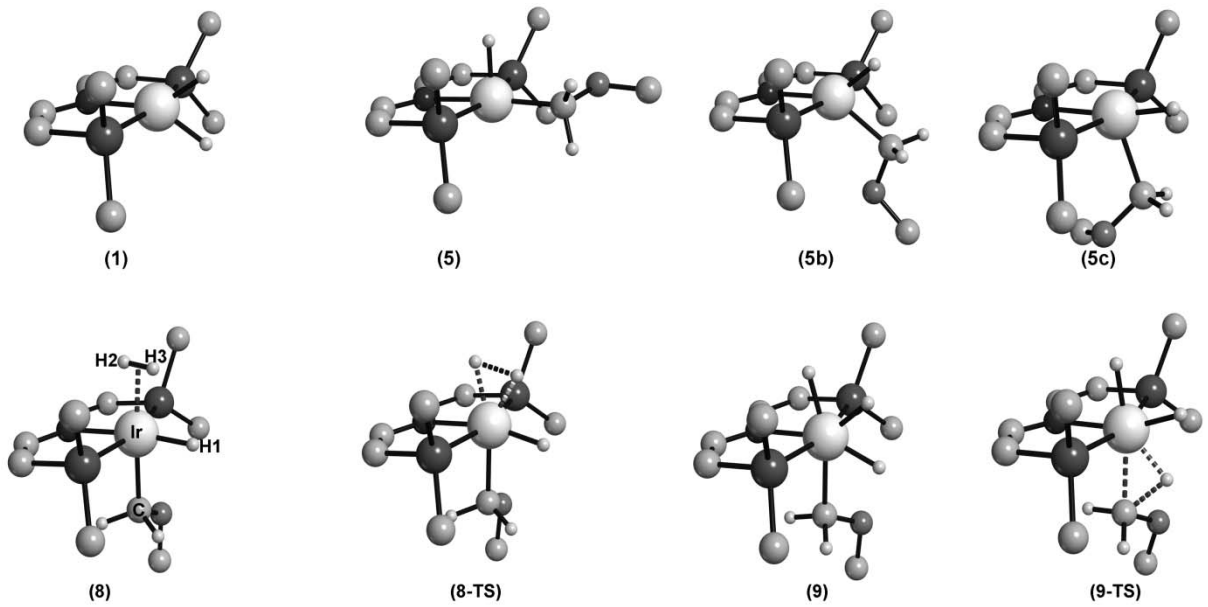


Figure sup3. Diagrams of structure **1, 5, 5b, 5c, 8, 8-TS, 9** and **9-TS.** See **Table sup3** for measurements**.**

Table sup3 (See figure sup3 for labelling)

Bond	**5**	**5b**	**5c**	**8**	**8-TS**	**9**	**9-TS**	**1**
Ir-C	2.071	2.079	2.087	2.085	2.147	2.194	2.300	-
Ir-H1	1.551	1.588	1.623	1.622	1.620	1.616	1.627	-
Ir-H2				1.871	1.691	1.664	1.634	1.593
Ir-H3				1.828	1.648	1.617	1.624	1.593
H2-H3	0.743*			0.835	1.252	1.746	2.030	1.700
H3-H1				2.132	1.859	1.664	1.812	
H1-C	2.600	2.225	2.406	2.539	2.476	2.263	1.648	1.093[#]

* Taken from an optimised H_2 molecule. [#] from the MTBE molecule

3. B3LYP, BMK and TPSS functional comparison diagrams.

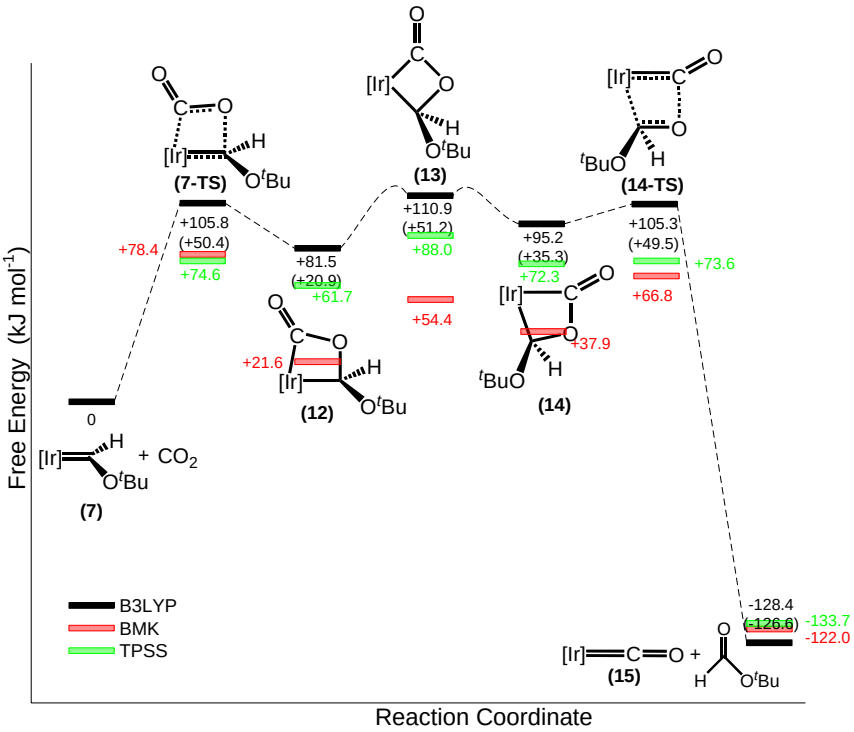


Figure sup4. From manuscript Figure 6 with BMK and TPSS functionals overlaid. All levels of theory agree with the findings outlined in the manuscript. The maximum barrier heights are 110.9 kJ mol^{-1} (B3LYP), 78.4 kJ mol^{-1} (BMK) and 88.0 kJ mol^{-1} (TPSS) .

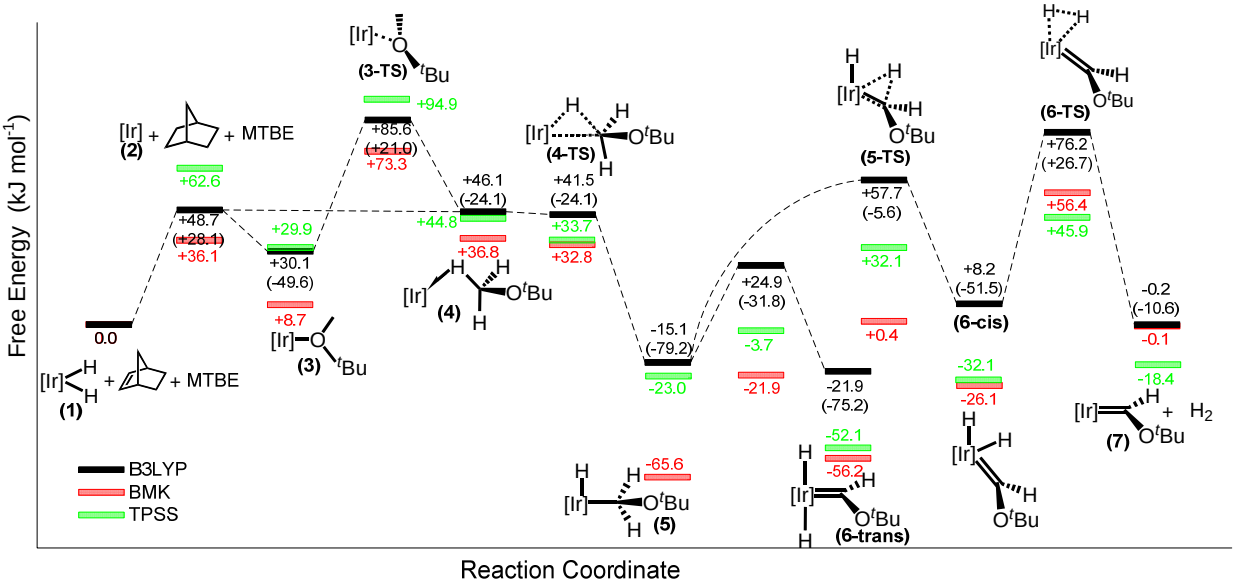


Figure sup5. Taken from manuscript Figures 1 and 3 (combined) with BMK and TPSS functionals overlaid. All functionals provide a similar reaction sequence. Maximum barrier height from **5** to **7** being

91.3 kJ mol^{-1} (B3LYP), 122.1 kJ mol^{-1} (BMK) and 68.9 kJ mol^{-1} (TPSS). Note that the BMK results suggest that intermediate **5** is very stable and perhaps isolable (which is not observed experimentally) and TPSS suggests **6-trans** to be stable (which is also not observed experimentally).

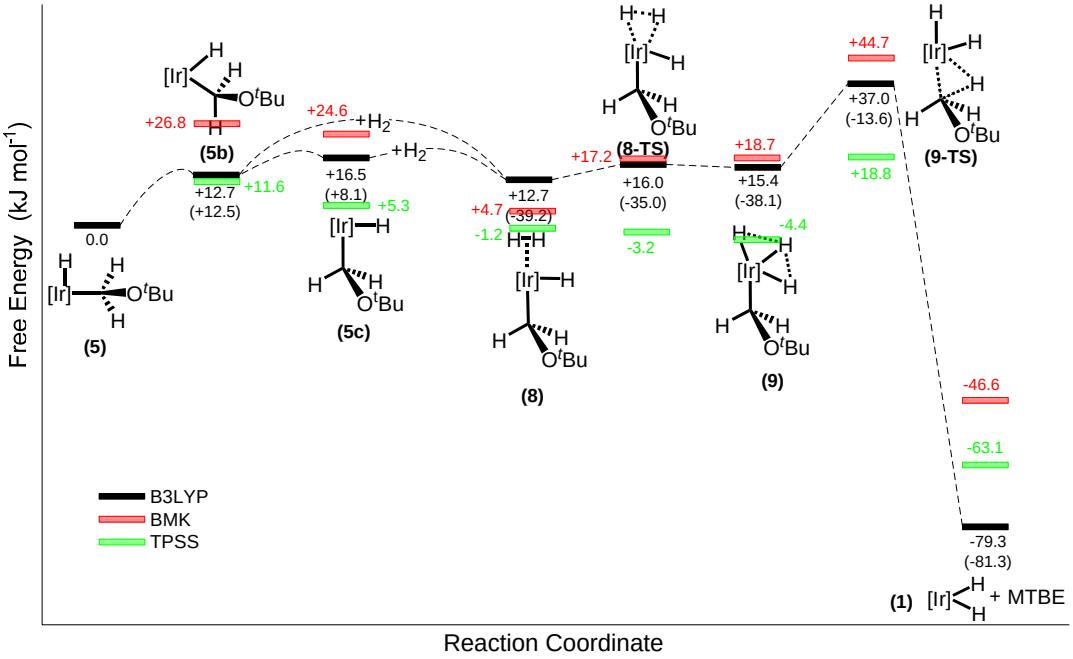


Figure sup6. Taken from manuscript Figure 4 with BMK and TPSS functionals overlaid. All levels of theory agree with the findings outlined in the manuscript. The maximum barrier heights are 37.0 kJ mol^{-1} (B3LYP), 44.7 kJ mol^{-1} (BMK) and 18.8 kJ mol^{-1} (TPSS) .

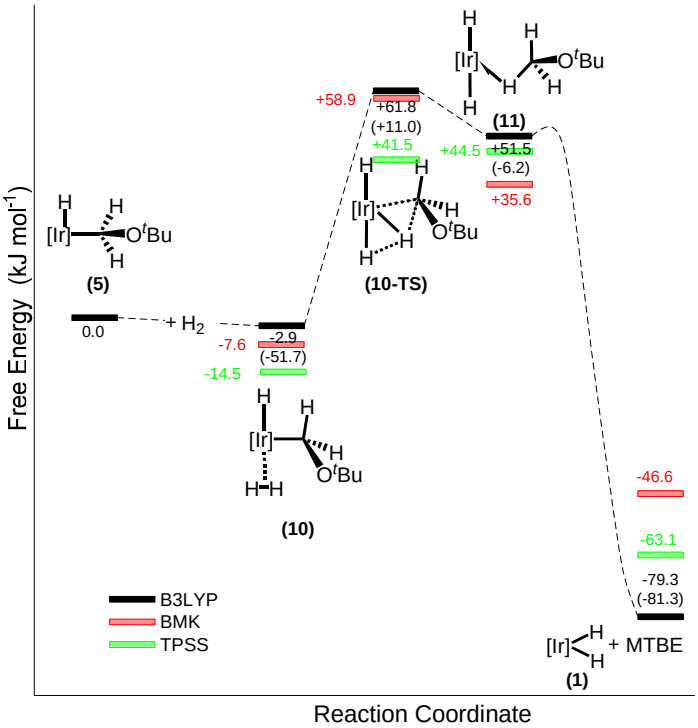


Figure sup7. Taken from manuscript Figure 5 with BMK and TPSS functionals overlaid. All levels of theory agree with the findings outlined in the manuscript. The maximum barrier heights are 64.7 kJ mol^{-1} (B3LYP), 66.5 kJ mol^{-1} (BMK) and 56.0 kJ mol^{-1} (TPSS) .

4. Solvent Comparison Diagrams.

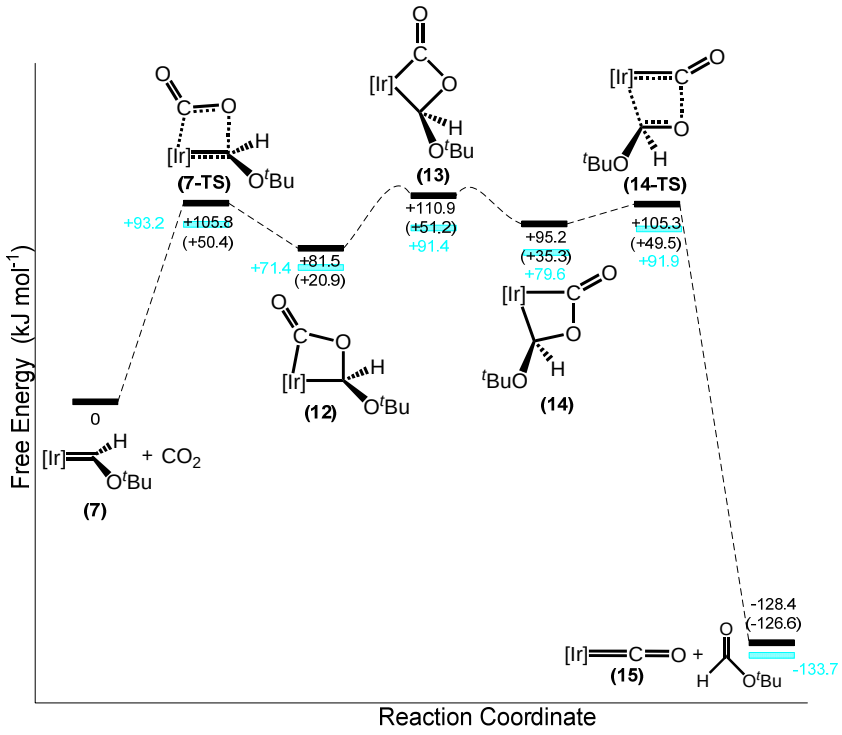


Figure sup8. From manuscript Figure 6 with IEFPCM B3LYP/GBS1 benzene solvent corrections overlaid.

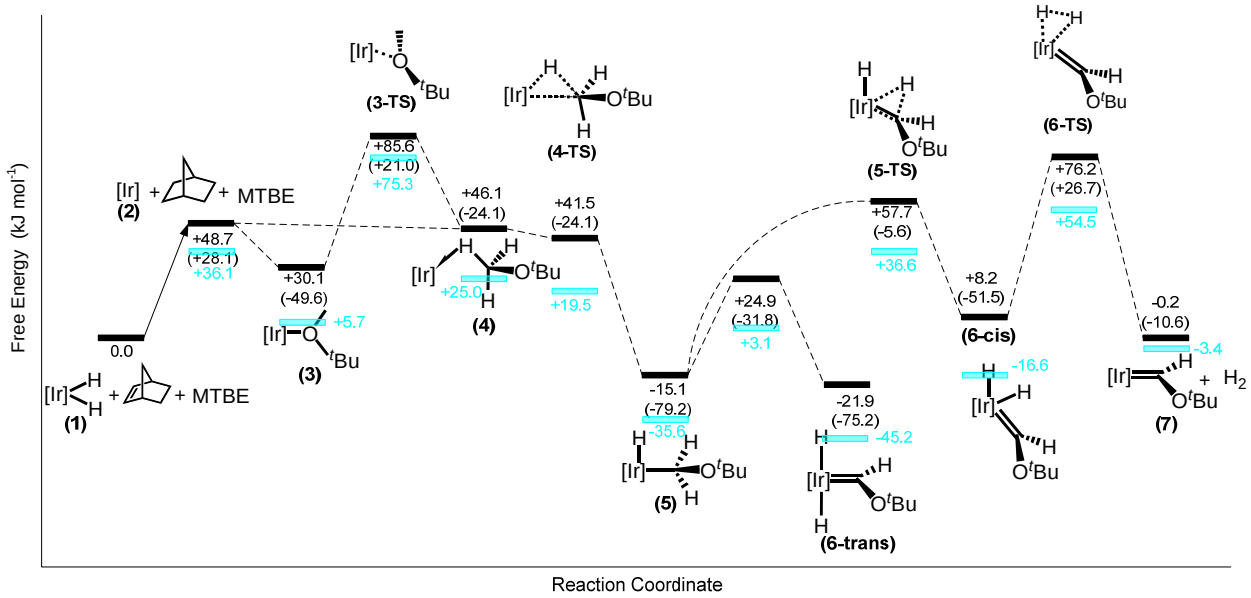


Figure sup9. Taken from manuscript Figures 1 and 3 (combined) with IEFPCM B3LYP/GBS1 MTBE solvent corrections overlaid.

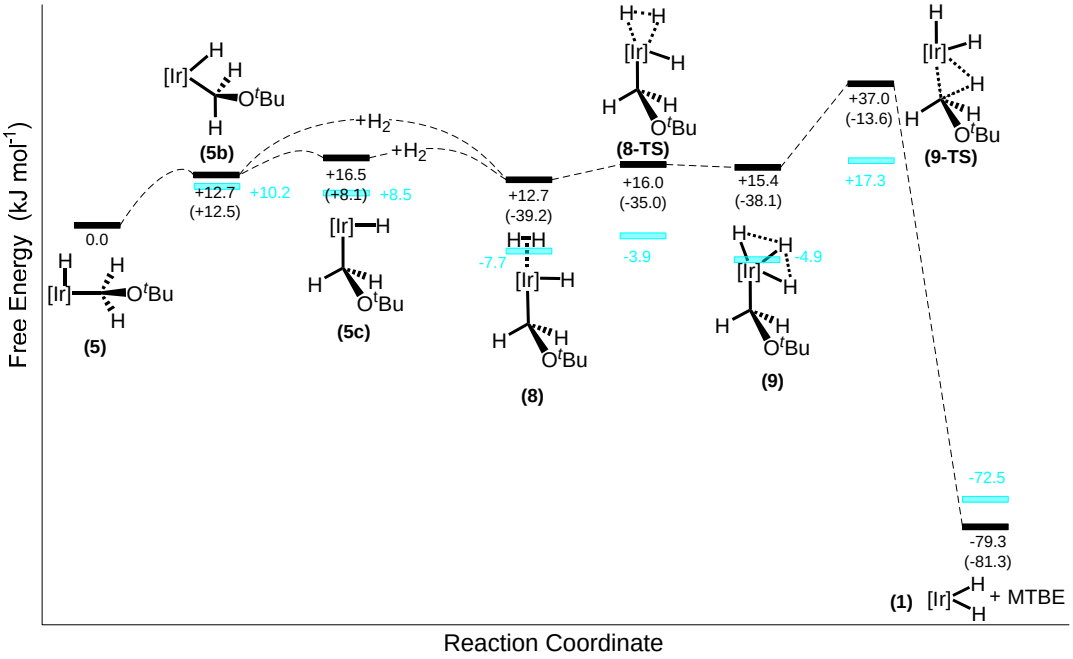


Figure sup10. Taken from manuscript Figure 4 with IEFPCM B3LYP/GBS1 MTBE solvent corrections overlaid.

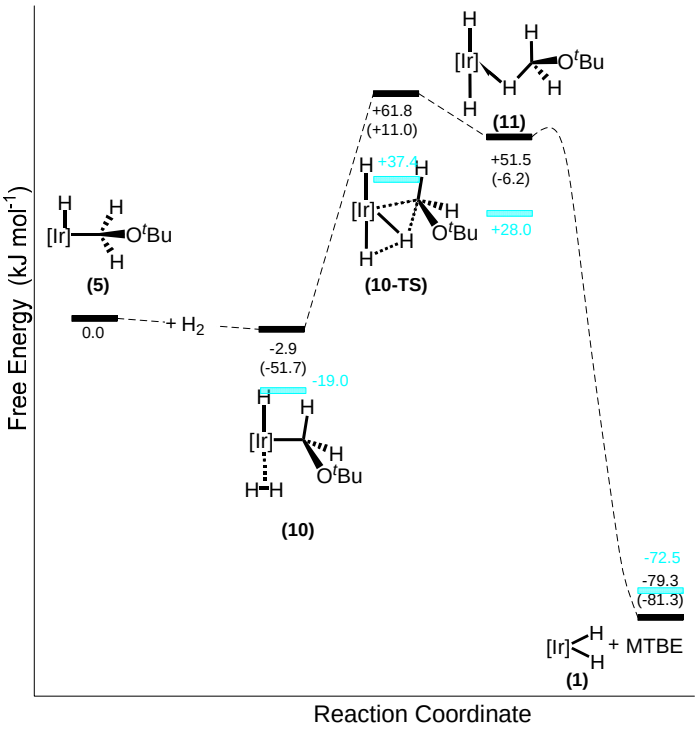


Figure sup11. Taken from manuscript Figure 5 with IEFPCM B3LYP/GBS1 MTBE solvent corrections overlaid.

5. Geometric details of Model-Opt structures

CO_2
B3LYP/GBS(1) = -188.577570 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -188.650304 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -188.562181 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -188.675365 a.u.
Enthalpy Correction = 0.015204
Gibbs Free Energy Correction = -0.009752
B3LYP/GBS(1) IEFPCM corrections = 0.001895

Atomic No	x-coord	y-coord	z-coord
8	0.000000	0.000000	1.169591
6	0.000000	0.000000	0.000000
8	0.000000	0.000000	-1.169591

Formate
B3LYP/GBS(1) = -229.058902a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -229.143923a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -229.014938a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -229.173488 a.u.
Enthalpy Correction = 0.067993
Gibbs Free Energy Correction = 0.035657
B3LYP/GBS(1) IEFPCM corrections = 0.002532

Atomic No	x-coord	y-coord	z-coord
6	-0.828940	0.435915	0.000043
8	-1.304407	-0.673100	-0.000013
8	0.480470	0.730967	-0.000012
1	-1.406157	1.373145	-0.000077
6	1.365874	-0.404550	0.000001
1	2.373675	0.010426	-0.000046
1	1.201214	-1.017317	0.890174
1	1.201159	-1.017381	-0.890118

Norbornane
B3LYP/GBS(1) = -273.963973 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -274.046026a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -273.847900 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -274.092664a.u.
Enthalpy Correction = 0.184582
Gibbs Free Energy Correction = 0.149043
B3LYP/GBS(1) IEFPCM corrections = 0.018648

Atomic No	x-coord	y-coord	z-coord
6	-1.255680	-0.782709	-0.493750
6	0.000011	-1.133596	0.340249
6	-0.000010	1.133596	0.340249
6	-1.255702	0.782686	-0.493737
1	-1.208925	-1.206174	-1.503414
1	-2.161351	-1.177057	-0.018444
1	-1.208983	1.206172	-1.503393
1	-2.161372	1.177000	-0.018401
6	-0.000002	0.000000	1.389182
1	0.891277	0.000008	2.028350
1	-0.891283	-0.000009	2.028348
6	1.255702	-0.782689	-0.493735

1	2.161375	-1.176999	-0.018402
1	1.208983	-1.206169	-1.503393
6	1.255680	0.782711	-0.493747
1	2.161353	1.177055	-0.018442
1	1.208928	1.206175	-1.503412
1	0.000017	-2.155722	0.731168
1	-0.000020	2.155723	0.731166

Norbornylene
B3LYP/GBS(1) = -272.722693 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -272.805319 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -272.611798 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -272.855129 a.u.
Enthalpy Correction = 0.159859
Gibbs Free Energy Correction = 0.125197
B3LYP/GBS(1) IEFPCM corrections = 0.017140

Atomic No	x-coord	y-coord	z-coord
6	1.191072	0.781215	-0.516488
6	-0.088270	1.128551	0.322933
6	-0.087690	-1.128566	0.323018
6	1.191573	-0.780702	-0.516270
1	1.146187	1.206946	-1.523336
1	2.088508	1.178211	-0.027995
1	1.147098	-1.206730	-1.523010
1	2.089177	-1.177017	-0.027528
6	-0.041153	0.000052	1.380753
1	-0.912375	-0.000148	2.043397
1	0.878469	0.000315	1.979534
6	-1.279351	0.670027	-0.507648
1	-1.921211	1.328259	-1.085475
6	-1.278851	-0.670674	-0.507820
1	-1.920234	-1.329254	-1.085780
1	-0.120316	2.157640	0.689572
1	-0.119286	-2.157637	0.689750

Structure 1
B3LYP/GBS(1) = --1157.898649a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1158.11644a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1157.0636295 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1158.14678051 a.u.
Enthalpy Correction = 0.261248
Gibbs Free Energy Correction = 0.199716
B3LYP/GBS(1) IEFPCM corrections = 0.044525

Atomic No	x-coord	y-coord	z-coord
7	-0.000031	1.638003	-0.000224
6	-1.203018	2.307354	0.000140
6	-2.400183	1.663281	0.000295
1	-1.156235	3.400176	0.000281
1	-3.334112	2.217345	0.000371
6	1.202978	2.307329	0.000209
6	2.400129	1.663251	0.000361
1	1.156221	3.400152	0.000375
1	3.334058	2.217321	0.000497
15	-2.305480	-0.141519	0.000126

15	2.305532	-0.141566	0.000178
6	-3.312480	-0.724116	-1.437636
1	-3.340456	-1.818448	-1.446718
1	-4.337087	-0.338767	-1.385262
1	-2.845295	-0.380527	-2.364246
6	-3.311164	-0.724583	1.438601
1	-4.335905	-0.339469	1.387303
1	-3.338846	-1.818931	1.447330
1	-2.843188	-0.381231	2.364900
6	3.312261	-0.724052	-1.437830
1	4.336750	-0.338334	-1.385869
1	3.340621	-1.818378	-1.446734
1	2.844637	-0.380794	-2.364340
6	3.311669	-0.724507	1.438372
1	3.339547	-1.818851	1.447070
1	4.336328	-0.339214	1.386763
1	2.843925	-0.381252	2.364824
77	-0.000032	-0.454062	-0.000317
1	0.000120	-1.800885	-0.850197
1	-0.000327	-1.800600	0.850012

Structure 2
B3LYP/GBS(1) = -1156.658443a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1156.865021a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1155.821627a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1156.893255a.u.
Enthalpy Correction = 0.244383
Gibbs Free Energy Correction = 0.18372
B3LYP/GBS(1) IEFPCM corrections = 0.038216

Atomic No	x-coord	y-coord	z-coord
7	1.386923	1.601318	-0.089570
6	2.754828	1.495233	-0.137330
6	3.406748	0.303219	-0.106026
1	3.294758	2.441034	-0.202999
1	4.490263	0.254224	-0.145585
6	0.786574	2.835505	-0.124199
6	-0.561042	3.005011	-0.079588
1	1.468183	3.684828	-0.190730
1	-1.004059	3.995390	-0.108954
15	2.323946	-1.120527	0.003455
15	-1.488059	1.475124	0.028628
6	2.888957	-2.115278	1.463313
1	2.301862	-3.037237	1.539333
1	3.949788	-2.378851	1.378201
1	2.734957	-1.529456	2.373283
6	2.780015	-2.251975	-1.393589
1	3.845202	-2.510054	-1.364499
1	2.192228	-3.174857	-1.336517
1	2.555279	-1.755089	-2.340981
6	-2.607719	1.627219	1.499409
1	-3.242314	2.518229	1.425457
1	-3.249809	0.742686	1.575421
1	-1.998258	1.692842	2.404498
6	-2.720356	1.493655	-1.357415
1	-3.363541	0.608536	-1.299684
1	-3.350064	2.390280	-1.317369
1	-2.184235	1.471956	-2.309802
77	0.267231	-0.044205	0.031515

Structure 3
B3LYP/GBS(1) = -1311.714494a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.975469a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.828050 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.027319a.u.
Enthalpy Correction = 0.332446
Gibbs Free Energy Correction = 0.261186
B3LYP/GBS(1) IEFPCM corrections = 0.050351

Atomic No	x-coord	y-coord	z-coord
7	2.380827	0.278910	-5.315239
6	1.392476	0.276663	-6.260284
6	0.125044	0.696483	-5.994210
1	1.673917	-0.083318	-7.252279
1	-0.647161	0.687726	-6.757333
6	3.634335	-0.157045	-5.651147
6	4.666133	-0.182649	-4.762236
1	3.767552	-0.488293	-6.683360
1	5.652373	-0.532600	-5.050997
15	-0.127138	1.247095	-4.308217
15	4.230586	0.402938	-3.127278
8	1.688992	1.604132	-1.336398
6	1.441081	3.000376	-1.159835
1	1.566931	3.261922	-0.100487
1	2.169209	3.529209	-1.774092
1	0.426405	3.258863	-1.488665
6	-1.598545	0.295955	-3.677970
1	-1.898181	0.657864	-2.687227
1	-2.454066	0.396305	-4.356740
1	-1.331142	-0.761228	-3.597149
6	-0.880428	2.945098	-4.435709
1	-1.765179	2.937171	-5.083679
1	-1.179027	3.311517	-3.446309
1	-0.140016	3.632690	-4.853658
6	4.739161	-0.925053	-1.930572
1	5.802456	-1.171583	-2.036581
1	4.556698	-0.595701	-0.901280
1	4.144236	-1.822250	-2.121784
6	5.457969	1.728014	-2.689034
1	5.282147	2.082091	-1.666818
1	6.487615	1.357223	-2.759466
1	5.333763	2.568680	-3.377011
77	1.999652	0.922707	-3.425132
6	0.841212	0.786436	-0.527219
1	1.145720	-0.245985	-0.696075
1	0.971080	1.059550	0.528734
1	-0.209927	0.911389	-0.817032

Structure 3-TS
B3LYP/GBS(1) = -1311.68656a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.948576a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.797696 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1311.996619 a.u.
Enthalpy Correction = 0.330693
Gibbs Free Energy Correction = 0.255447
Imaginary Freq = -99.1i
B3LYP/GBS(1) IEFPCM corrections = 0.0557069

Atomic No	x-coord	y-coord	z-coord
7	1.035035	-1.799555	-0.041855
6	2.404038	-1.882969	-0.031339
6	3.210098	-0.788925	0.012544
1	2.813041	-2.894240	-0.059762
1	4.291145	-0.886138	0.021051
6	0.274100	-2.942424	-0.071276
6	-1.085449	-2.929674	-0.063368
1	0.836469	-3.877244	-0.100775
1	-1.654973	-3.853411	-0.085972
15	2.325980	0.769578	0.060078
15	-1.796036	-1.284750	0.001640
8	-2.363892	2.232619	0.056561
6	-3.160997	3.256247	0.615069
1	-3.806663	3.725418	-0.145107
1	-3.789179	2.796909	1.382483
1	-2.544507	4.041973	1.079973
6	3.019233	1.811132	-1.311560
1	2.573257	2.811954	-1.288705
1	4.107795	1.910248	-1.224990
1	2.776784	1.343147	-2.269442
6	2.949718	1.691245	1.545638
1	4.040651	1.798357	1.520707
1	2.498651	2.689020	1.588030
1	2.662661	1.142480	2.446498
6	-3.020328	-1.146175	-1.382227
1	-3.795515	-1.918637	-1.314041
1	-3.492968	-0.159220	-1.340309
1	-2.495665	-1.245777	-2.336293
6	-2.917149	-1.220491	1.474916
1	-3.388866	-0.233661	1.523082
1	-3.696648	-1.989997	1.423610
1	-2.321884	-1.367910	2.379834
77	0.140574	-0.015183	0.005168
6	-1.497032	2.709438	-0.954615
1	-0.892801	1.848851	-1.291739
1	-2.055807	3.106429	-1.818030
1	-0.829837	3.499626	-0.576021

Structure 4

B3LYP/GBS(1) = -1311.698564a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.965768a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.813743a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.018031 a.u.
Enthalpy Correction = 0.330598
Gibbs Free Energy Correction = 0.257572
B3LYP/GBS(1) IEFPCM corrections = 0.051629

Atomic No	x-coord	y-coord	z-coord
7	-0.880181	-1.841077	-0.186740
6	-2.235080	-2.026659	-0.259427
6	-3.124263	-0.999382	-0.182684
1	-2.570163	-3.058706	-0.381055
1	-4.194146	-1.171742	-0.244066
6	-0.037615	-2.922391	-0.238205
6	1.314476	-2.810143	-0.142421
1	-0.518928	-3.894932	-0.360007
1	1.956831	-3.683974	-0.187165
15	-2.366095	0.610733	0.020970

15	1.896937	-1.125598	0.052988
8	2.297976	2.390430	0.317645
6	2.920496	3.389396	-0.467114
1	2.508545	4.388525	-0.253511
1	3.983083	3.382380	-0.211290
1	2.806415	3.188942	-1.544370
6	-3.142730	1.390053	1.514933
1	-2.771557	2.413151	1.643580
1	-4.234941	1.420832	1.424956
1	-2.871418	0.807796	2.399479
6	-3.045248	1.691475	-1.327767
1	-4.141516	1.704634	-1.312911
1	-2.681345	2.718671	-1.210806
1	-2.705253	1.308921	-2.293953
6	2.971103	-1.069515	1.560044
1	3.804984	-1.777394	1.484560
1	3.367784	-0.056206	1.680295
1	2.366623	-1.316745	2.436733
6	3.140467	-0.817205	-1.285689
1	3.550309	0.191085	-1.168360
1	3.959725	-1.544662	-1.245931
1	2.644567	-0.887379	-2.257593
77	-0.117790	0.021247	0.046454
6	0.910911	2.312330	0.071028
1	0.513648	1.568036	0.863006
1	0.392918	3.245162	0.342042
1	0.683396	2.076896	-0.980086

Structure 4-TS

B3LYP/GBS(1) = -1311.695215a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.965735a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.813499 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.020468a.u.
Enthalpy Correction = 0.326746
Gibbs Free Energy Correction = 0.255809
Imaginary Freq = -587.1i
B3LYP/GBS(1) IEFPCM corrections = 0.051236

Atomic No	x-coord	y-coord	z-coord
7	-0.769920	-1.876050	-0.244258
6	-2.113896	-2.124186	-0.335215
6	-3.051865	-1.143739	-0.229232
1	-2.404417	-3.165480	-0.494558
1	-4.111824	-1.365261	-0.305196
6	0.132118	-2.909374	-0.297504
6	1.472867	-2.724699	-0.163044
1	-0.286585	-3.906858	-0.451929
1	2.163427	-3.560854	-0.212891
15	-2.383493	0.499462	0.045399
15	1.969226	-1.013890	0.075491
8	2.067821	2.348514	0.213775
6	2.604179	3.508771	-0.388778
1	2.069311	4.417611	-0.068783
1	3.648680	3.583761	-0.073778
1	2.562054	3.452970	-1.488799
6	-3.193207	1.165050	1.573862
1	-2.875693	2.199183	1.747887
1	-4.285725	1.140166	1.487362
1	-2.886265	0.558439	2.429826
6	-3.122147	1.596350	-1.256441

1	-4.217566	1.557183	-1.236178
1	-2.804922	2.633561	-1.099870
1	-2.771256	1.269114	-2.238994
6	3.012058	-0.930940	1.600280
1	3.881256	-1.594830	1.526792
1	3.353164	0.099410	1.740925
1	2.406770	-1.221670	2.462800
6	3.207983	-0.622596	-1.243396
1	3.551773	0.407342	-1.108872
1	4.066698	-1.302542	-1.200739
1	2.728517	-0.711122	-2.222139
77	-0.099329	0.042558	0.055489
6	0.701205	2.157111	-0.125423
1	0.345273	1.378932	0.924804
1	0.105308	3.025157	0.200713
1	0.575473	2.059001	-1.215411

Structure 5

B3LYP/GBS(1) = -1311.718135a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.986776a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.850442 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.041535a.u.
Enthalpy Correction = 0.327101
Gibbs Free Energy Correction = 0.255275
B3LYP/GBS(1) IEFPCM corrections = 0.051829

Atomic No	x-coord	y-coord	z-coord
7	0.460955	-1.969064	-0.495782
6	1.748456	-2.347300	-0.715066
6	2.806165	-1.501643	-0.524835
1	1.918210	-3.374272	-1.054205
1	3.824119	-1.829804	-0.713507
6	-0.584930	-2.836421	-0.613062
6	-1.870438	-2.481633	-0.319168
1	-0.355071	-3.850350	-0.955703
1	-2.682131	-3.195153	-0.426800
15	2.407061	0.153735	0.045886
15	-2.117656	-0.792119	0.250229
8	-1.717051	2.198535	1.163201
6	-1.984709	3.544665	1.477263
1	-1.827223	4.208537	0.609134
1	-3.032569	3.615317	1.788965
1	-1.345351	3.908851	2.299622
6	3.180971	1.341915	-1.149148
1	3.018185	2.371291	-0.811715
1	4.258540	1.164293	-1.242521
1	2.718067	1.218861	-2.132684
6	3.392379	0.476194	1.577322
1	4.463708	0.333687	1.396003
1	3.220976	1.502135	1.920098
1	3.067314	-0.212477	2.361557
6	-3.360316	0.008980	-0.859488
1	-4.317295	-0.524758	-0.839305
1	-3.501185	1.039284	-0.520900
1	-2.981578	0.018109	-1.885870
6	-3.008189	-0.841723	1.864161
1	-3.129866	0.186583	2.215122
1	-3.987685	-1.322773	1.764090
1	-2.407032	-1.397177	2.588895
6	-0.354660	1.987364	0.740581

1	0.309444	2.386580	1.529425
1	-0.176964	2.629705	-0.153928
77	0.065168	0.031647	0.205562
1	0.201372	-0.364898	1.698575

Structure 5b
B3LYP/GBS(1) = -1311.71467a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.982018a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.840275 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.037177 a.u.
Enthalpy Correction = 0.328091
Gibbs Free Energy Correction = 0.255347
B3LYP/GBS(1) IEFPCM corrections = 0.058854

Atomic No	x-coord	y-coord	z-coord
7	0.000526	-1.644240	1.008702
6	-1.200170	-2.150570	1.447944
6	-2.398509	-1.665295	1.027633
1	-1.153643	-2.977618	2.162564
1	-3.331578	-2.087919	1.388212
6	1.201527	-2.149508	1.448333
6	2.399572	-1.663176	1.028407
1	1.155500	-2.976593	2.162942
1	3.332898	-2.084977	1.389287
15	-2.312738	-0.299983	-0.151284
15	2.312979	-0.297955	-0.150556
8	-0.001088	2.451164	0.890615
6	-0.001709	3.855841	1.039901
1	-0.893789	4.315666	0.582351
1	-0.001843	4.072641	2.112636
1	0.890001	4.316447	0.582415
6	-3.286573	1.098467	0.564796
1	-3.388018	1.894059	-0.181320
1	-4.284851	0.774920	0.878889
1	-2.736894	1.497871	1.420552
6	-3.335236	-0.801049	-1.608621
1	-4.355824	-1.061572	-1.306046
1	-3.374745	0.019247	-2.332659
1	-2.870453	-1.666388	-2.088484
6	3.285381	1.101353	0.565791
1	4.283855	0.778687	0.880170
1	3.386337	1.897025	-0.180306
1	2.735103	1.500284	1.421382
6	3.336354	-0.798165	-1.607571
1	3.375407	0.022165	-2.331596
1	4.357063	-1.057838	-1.304674
1	2.872444	-1.663890	-2.087583
6	-0.000842	2.036589	-0.476892
1	0.887135	2.450022	-0.981195
1	-0.889137	2.449239	-0.981275
77	0.000038	-0.039213	-0.354523
1	0.000119	0.326214	-1.899496

Structure 5c
B3LYP/GBS(1) = -1311.719272a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.983678a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.844216 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.042694 a.u.
Enthalpy Correction = 0.32875

Gibbs Free Energy Correction = 0.258447
B3LYP/GBS(1) IEFPCM corrections = 0.051351

Atomic No	x-coord	y-coord	z-coord
7	0.762625	-1.675038	-0.578243
6	2.119304	-1.790380	-0.723993
6	2.961544	-0.728626	-0.582075
1	2.512039	-2.784168	-0.961260
1	4.033250	-0.846644	-0.714291
6	-0.073585	-2.753292	-0.654040
6	-1.422719	-2.653948	-0.465471
1	0.383646	-3.723229	-0.874790
1	-2.060064	-3.530398	-0.540129
15	2.196169	0.835826	-0.108277
15	-2.042682	-1.016248	-0.039296
8	0.369179	0.964646	-2.913559
6	0.021426	-0.229845	-3.591176
1	-1.032927	-0.207993	-3.909346
1	0.657131	-0.285812	-4.478976
1	0.189525	-1.110968	-2.962762
6	2.886715	2.143978	-1.212749
1	2.557269	3.129930	-0.867500
1	3.982150	2.115345	-1.213359
1	2.510349	1.976283	-2.223935
6	2.932842	1.289707	1.530919
1	4.026917	1.326387	1.477971
1	2.554379	2.267764	1.845266
1	2.638492	0.546883	2.277833
6	-3.489668	-0.679981	-1.143573
1	-4.231997	-1.481885	-1.063361
1	-3.958528	0.269263	-0.863962
1	-3.154997	-0.614385	-2.182281
6	-2.872087	-1.179713	1.609832
1	-3.337821	-0.227669	1.884234
1	-3.635450	-1.965973	1.596102
1	-2.120929	-1.428215	2.365026
6	-0.450955	1.317600	-1.833551
1	-1.509453	1.177895	-2.092491
1	-0.246827	2.371045	-1.639979
77	-0.068070	0.240911	-0.087577
1	-0.672244	1.607703	0.544857

Structure 5-TS
B3LYP/GBS(1) = -1311.682592a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.958725a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.824995a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.020205 a.u.
Enthalpy Correction = 0.323893
Gibbs Free Energy Correction = 0.254947
Imaginary Freq = -112.8i

B3LYP/GBS(1) IEFPCM corrections = 0.051609

Atomic No	x-coord	y-coord	z-coord
7	0.449701	-1.849163	-0.544425
6	1.732549	-2.217489	-0.818943
6	2.800045	-1.397389	-0.610132
1	1.864691	-3.222105	-1.225226
1	3.810505	-1.720665	-0.839332
6	-0.585792	-2.719803	-0.732534

6	-1.877308	-2.397666	-0.457099
1	-0.317497	-3.702234	-1.125638
1	-2.681140	-3.106633	-0.629385
15	2.406958	0.206742	0.074323
15	-2.144982	-0.727558	0.136842
8	-1.525757	2.491579	-0.661346
6	-1.641910	3.866941	-0.328777
1	-0.843532	4.461072	-0.797647
1	-2.610554	4.211522	-0.701465
1	-1.598641	4.017859	0.761082
6	3.223111	1.481850	-0.992598
1	3.065046	2.483111	-0.575954
1	4.301672	1.301271	-1.066254
1	2.780729	1.445137	-1.991361
6	3.350767	0.401181	1.654888
1	4.425919	0.258687	1.495726
1	3.183700	1.400552	2.071723
1	2.987537	-0.340525	2.370276
6	-3.421622	0.018469	-0.971334
1	-4.325597	-0.601662	-0.988687
1	-3.668032	1.025751	-0.628033
1	-3.010998	0.093830	-1.981187
6	-3.057702	-0.825402	1.742504
1	-3.286675	0.185095	2.098023
1	-3.994629	-1.383567	1.632636
1	-2.421694	-1.320744	2.479993
6	-0.287309	1.925384	-0.405422
1	0.506648	2.671898	-0.552985
77	0.071379	0.038423	0.197463
1	-0.200816	1.730312	0.865491
1	0.256738	-0.839239	1.574531

Transition state prior to Structure 6-trans

B3LYP/GBS(1) = -1311.69505841 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.968692a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.830904 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.031332a.u.
Enthalpy Correction = 0.322488
Gibbs Free Energy Correction = 0.252416
Imaginary Freq = -797.4i
B3LYP/GBS(1) IEFPCM corrections = 0.051351

Atomic No	x-coord	y-coord	z-coord
77	0.049902	0.139005	-0.201710
7	0.536512	-1.924902	0.197065
6	-0.470538	-2.834279	0.259751
6	-1.779663	-2.491571	0.084336
1	-0.189290	-3.873458	0.455731
1	-2.565978	-3.238323	0.143986
6	1.839755	-2.277836	0.319663
6	2.862035	-1.380028	0.189620
1	2.052363	-3.331158	0.526859
1	3.897392	-1.691792	0.289624
15	-2.113754	-0.756823	-0.233221
15	2.390512	0.304537	-0.194926
8	-1.605661	2.539289	0.160332
6	-1.744706	3.780067	0.856492
1	-0.951977	4.482906	0.570608
1	-2.716386	4.192937	0.578405
1	-1.711885	3.614864	1.940767

6	-0.371499	1.990700	0.123302
1	0.389798	2.753030	0.349760
6	-3.353505	-0.212921	1.027269
1	-3.627610	0.830145	0.844262
1	-4.253231	-0.838054	0.990783
1	-2.902596	-0.290457	2.020177
6	-3.100886	-0.647489	-1.792219
1	-4.007818	-1.260150	-1.731008
1	-3.383810	0.394414	-1.975132
1	-2.483577	-0.994118	-2.624487
6	3.228789	1.408988	1.034269
1	4.315662	1.268516	1.018650
1	3.010460	2.459938	0.810790
1	2.851700	1.176694	2.033660
6	3.251464	0.788349	-1.759746
1	3.037693	1.836431	-1.996181
1	4.336295	0.655603	-1.674893
1	2.872200	0.164632	-2.572808
1	0.177710	-0.422114	-1.722460
1	-0.129496	0.994774	1.379623

Structure 6-trans
B3LYP/GBS(1) = -1311.712578a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.98524a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.842723 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.048508a.u.
Enthalpy Correction = 0.323767
Gibbs Free Energy Correction = 0.251151
B3LYP/GBS(1) IEFPCM corrections = 0.050723

Atomic No	x-coord	y-coord	z-coord
77	0.041829	0.091038	-0.004169
7	0.561625	-2.003459	-0.008117
6	-0.441166	-2.919736	-0.009671
6	-1.759652	-2.568543	-0.008742
1	-0.148481	-3.974079	-0.011731
1	-2.539238	-3.324530	-0.010029
6	1.870746	-2.357274	-0.009089
6	2.880430	-1.437926	-0.007519
1	2.096959	-3.427920	-0.011241
1	3.921333	-1.746898	-0.008334
15	-2.117327	-0.809382	-0.005465
15	2.386690	0.284392	-0.004054
8	-1.642508	2.442971	0.000577
6	-1.774710	3.873457	-0.000341
1	-1.325648	4.300867	-0.903486
1	-2.844952	4.084522	0.011608
1	-1.304902	4.304369	0.890499
6	-0.405188	1.932423	-0.001174
1	0.338050	2.749211	-0.000567
6	-3.232820	-0.468088	1.428007
1	-3.499536	0.593829	1.436207
1	-4.148211	-1.068752	1.373168
1	-2.696841	-0.702787	2.350721
6	-3.233206	-0.463070	-1.437454
1	-4.148412	-1.064196	-1.384586
1	-3.500264	0.598788	-1.441741
1	-2.697375	-0.694278	-2.361133

6	3.232172	1.098300	1.428089
1	4.319088	0.964476	1.377485
1	3.010851	2.171726	1.437668
1	2.853671	0.656300	2.352796
6	3.231930	1.103906	-1.433140
1	3.010501	2.177339	-1.438601
1	4.318868	0.970028	-1.383130
1	2.853426	0.665388	-2.359502
1	0.072075	-0.081148	-1.676328
1	0.072467	-0.087261	1.667330

Structure 6-cis

B3LYP/GBS(1) = -1311.703595a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.976207a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.833732 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.040674 a.u.
Enthalpy Correction = 0.32474
Gibbs Free Energy Correction = 0.253605
B3LYP/GBS(1) IEFPCM corrections = 0.050185

Atomic No	x-coord	y-coord	z-coord
7	0.714131	-2.102198	0.041914
6	2.043912	-2.341841	0.185718
6	2.986092	-1.355669	0.117141
1	2.340512	-3.378928	0.370141
1	4.042125	-1.584192	0.227838
6	-0.226253	-3.060800	0.268450
6	-1.562242	-2.792646	0.279113
1	0.139984	-4.075117	0.453580
1	-2.288518	-3.582027	0.450362
15	2.368619	0.314882	-0.110301
15	-2.035596	-1.076144	0.019017
8	-1.032398	0.069915	-3.042606
6	-1.026953	0.684092	-4.339717
1	-0.013579	0.993759	-4.619569
1	-1.404337	-0.050895	-5.054399
1	-1.689579	1.555269	-4.324652
6	3.328458	1.046500	-1.519654
1	3.048967	2.095804	-1.666013
1	4.404949	0.995730	-1.320827
1	3.119165	0.491478	-2.438631
6	2.978328	1.343769	1.297319
1	4.070513	1.299611	1.379847
1	2.669257	2.384714	1.154855
1	2.524543	0.970260	2.217893
6	-3.349624	-1.095969	-1.285157
1	-4.180295	-1.743597	-0.981059
1	-3.729703	-0.081604	-1.445898
1	-2.924888	-1.459732	-2.221965
6	-3.017526	-0.543284	1.491741
1	-3.372278	0.482375	1.344540
1	-3.878640	-1.201833	1.654703
1	-2.366999	-0.563221	2.368631
6	-0.013472	0.257619	-2.207821
1	0.776887	0.824714	-2.733753
77	0.066728	-0.083487	-0.279241
1	-0.422919	1.454660	-0.089570
1	0.077944	0.019699	1.396644

Structure 6-TS
B3LYP/GBS(1) = -1311.67083a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1311.946428a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1310.798478a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1312.009827 a.u.
Enthalpy Correction = 0.320772
Gibbs Free Energy Correction = 0.249815
Imaginary Freq = -760.3
B3LYP/GBS(1) IEFPCM corrections = 0.051252

Atomic No	x-coord	y-coord	z-coord
7	0.328523	-1.807406	-0.791995
6	1.580370	-2.164290	-1.171324
6	2.683866	-1.418062	-0.869118
1	1.680036	-3.092528	-1.742887
1	3.674915	-1.732996	-1.182563
6	-0.767409	-2.546114	-1.106423
6	-2.028859	-2.171841	-0.749764
1	-0.598318	-3.469674	-1.668962
1	-2.888378	-2.779756	-1.017604
15	2.399562	0.084070	0.068474
15	-2.189490	-0.614170	0.133462
8	-1.334993	2.545486	-0.358763
6	-1.241238	3.888069	-0.835717
1	-0.847349	3.914464	-1.859675
1	-2.253618	4.297831	-0.828061
1	-0.599254	4.493560	-0.183449
6	3.231068	1.459464	-0.854757
1	3.159580	2.398014	-0.293718
1	4.290200	1.230206	-1.017113
1	2.743478	1.587988	-1.824802
6	3.458950	-0.009409	1.584684
1	4.507428	-0.194619	1.324046
1	3.391666	0.926511	2.149781
1	3.098491	-0.826059	2.215620
6	-3.435146	0.376954	-0.807977
1	-4.342280	-0.216065	-0.973206
1	-3.686967	1.286356	-0.256545
1	-3.008211	0.663905	-1.771711
6	-3.124294	-0.967495	1.692294
1	-3.319524	-0.031949	2.227264
1	-4.079183	-1.461168	1.477530
1	-2.520767	-1.618376	2.330248
6	-0.171750	1.863433	-0.210788
1	0.669812	2.543381	-0.424569
77	0.061129	0.046476	0.323437
1	0.078096	-0.077816	2.011495
1	0.259085	-1.044627	1.762571

Structure 7
B3LYP/GBS(1) = -1310.519668a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1310.781042a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1309.636783 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1310.839782 a.u.
Enthalpy Correction = 0.307627
Gibbs Free Energy Correction = 0.236166
B3LYP/GBS(1) IEFPCM corrections = 0.051652(MTBE)/0.051652(Benzene)

Atomic No	x-coord	y-coord	z-coord
77	-0.033402	-0.512482	-0.410026
7	-1.973888	-0.002145	0.255836
6	-2.273961	1.316205	0.488946
6	-1.368617	2.316570	0.308313
1	-3.288845	1.538396	0.832513
1	-1.632614	3.352296	0.500342
6	-2.905561	-0.987685	0.446426
6	-2.632952	-2.303132	0.222381
1	-3.895834	-0.675260	0.791700
1	-3.386156	-3.069250	0.379657
15	0.259716	1.790438	-0.260672
15	-0.960794	-2.657887	-0.342476
8	2.710431	-0.095392	-1.231737
6	3.957826	-0.633889	-1.682486
1	3.837082	-1.147935	-2.643577
1	4.638432	0.210804	-1.806151
1	4.372466	-1.330520	-0.944048
6	1.697496	-0.968648	-1.003999
1	2.056767	-1.991077	-1.224704
6	1.494340	2.477317	0.934228
1	2.501732	2.210540	0.599513
1	1.413538	3.567816	1.011072
1	1.323537	2.032961	1.918342
6	0.635154	2.763458	-1.789125
1	0.589650	3.841989	-1.598542
1	1.636479	2.499292	-2.143540
1	-0.090295	2.503493	-2.564526
6	-0.272603	-3.931409	0.816566
1	-0.920218	-4.814369	0.869119
1	0.723217	-4.243652	0.483024
1	-0.182515	-3.491914	1.813479
6	-1.130569	-3.646342	-1.902274
1	-0.142372	-3.955819	-2.260170
1	-1.744304	-4.540625	-1.742985
1	-1.597236	-3.022032	-2.668803

Structure 7-TS

B3LYP/GBS(1) = -1499.081764a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1499.412155a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1498.190172 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1499.507826 a.u.
Enthalpy Correction = 0.323255
Gibbs Free Energy Correction = 0.247514
Imaginary Freq = -295.6i
B3LYP/GBS(1) IEFPCM corrections = 0.014540

Atomic No	x-coord	y-coord	z-coord
6	-1.915952	-2.516910	-0.296618
6	-0.622213	-2.944676	-0.304605
15	-2.153108	-0.737078	-0.311702
7	0.440962	-2.086143	-0.338861
6	1.725937	-2.545994	-0.333443
6	2.806171	-1.714241	-0.353776
77	0.079611	0.007805	-0.346073
15	2.440030	0.041103	-0.356033
8	-1.467104	2.483539	-0.587316
6	-0.268924	1.955436	-0.351284
1	0.513543	2.723358	-0.338228

6	-1.629499	3.882257	-0.296374
1	-0.815204	4.465679	-0.741678
1	-2.584120	4.184632	-0.729699
1	-1.638385	4.021086	0.788174
1	-2.739346	-3.223720	-0.266547
1	-0.392248	-4.013669	-0.286842
1	1.863304	-3.630812	-0.315361
1	3.818315	-2.106421	-0.345501
6	0.006915	0.634483	1.674086
8	-0.178858	1.891697	1.679415
8	0.141519	-0.200689	2.545233
6	3.310924	0.798437	1.085801
1	4.385666	0.589364	1.047072
1	3.155428	1.882289	1.095246
1	2.890326	0.378700	2.003096
6	-3.194680	-0.288138	1.142805
1	-3.387305	0.789144	1.134061
1	-4.147150	-0.829234	1.126425
1	-2.647325	-0.539060	2.054943
6	-3.249729	-0.328511	-1.742170
1	-4.208725	-0.853692	-1.667323
1	-3.426248	0.751058	-1.762605
1	-2.754737	-0.622042	-2.672193
6	3.326663	0.790174	-1.798592
1	3.187777	1.876770	-1.802012
1	4.399699	0.571369	-1.757456
1	2.916551	0.381902	-2.726621

Structure 8
B3LYP/GBS(1) = -1312.901516a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1313.181281a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1312.036616 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1313.241302a.u.
Enthalpy Correction = 0.345483
Gibbs Free Energy Correction = 0.273707
B3LYP/GBS(1) IEFPCM corrections = 0.050797

Atomic No	x-coord	y-coord	z-coord
7	-0.142472	-0.981091	1.431775
6	-1.339225	-1.093600	2.057069
6	-2.520878	-0.719060	1.474048
1	-1.335209	-1.501433	3.073136
1	-3.459476	-0.821570	2.011014
6	1.038599	-1.326945	2.015008
6	2.239422	-1.195047	1.381559
1	0.990359	-1.728124	3.032264
1	3.162043	-1.481275	1.878205
15	-2.424118	-0.036326	-0.182799
15	2.207810	-0.543812	-0.295952
8	1.297687	2.279232	0.625877
6	1.281357	3.504675	1.320674
1	0.826039	3.403600	2.320550
1	2.319065	3.833909	1.437312
1	0.723077	4.280016	0.769138
6	-3.364455	1.554757	-0.181564
1	-3.409679	1.958987	-1.198202
1	-4.384157	1.401949	0.189579
1	-2.857708	2.278441	0.461405
6	-3.480290	-1.078035	-1.290906
1	-4.507170	-1.137310	-0.913049

1	-3.495396	-0.652524	-2.299952
1	-3.064332	-2.088130	-1.340488
6	3.587188	0.666418	-0.466825
1	4.534451	0.206329	-0.162712
1	3.662481	0.983082	-1.512246
1	3.364791	1.534947	0.150589
6	2.827327	-1.906917	-1.394650
1	2.851917	-1.562425	-2.434407
1	3.836072	-2.218488	-1.100781
1	2.158916	-2.769080	-1.323644
6	-0.015429	1.764741	0.419284
1	-0.585897	2.498072	-0.170637
1	-0.505079	1.662324	1.403239
77	-0.098467	-0.084915	-0.539628
1	-0.027087	0.770143	-1.916406
1	-0.278568	-1.835901	-1.173421
1	-0.240210	-1.349849	-1.851195

Structure 8 (Explicit dimethyl ether solvent included. H2 Excluded)
B3LYP/GBS(1) = -1466.750868 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1467.070461 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1465.837805 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1467.148112 a.u.
Enthalpy Correction = 0.416556
Gibbs Free Energy Correction = 0.333431

Atomic No	x-coord	y-coord	z-coord
7	-0.164476	-0.586769	1.750209
6	-1.366063	-0.542796	2.382244
6	-2.538829	-0.295901	1.720644
1	-1.371743	-0.719466	3.463488
1	-3.482141	-0.265531	2.258972
6	1.005651	-0.824910	2.408596
6	2.210145	-0.866632	1.768318
1	0.946445	-0.992419	3.489478
1	3.124275	-1.059913	2.323237
15	-2.414024	0.008518	-0.048157
15	2.197846	-0.576480	-0.013203
8	1.294445	2.438252	-0.496218
6	1.335163	3.830806	-0.286137
1	1.235353	4.090202	0.782310
1	2.302892	4.191961	-0.649063
1	0.534012	4.351220	-0.838052
6	-3.358730	1.567451	-0.375328
1	-3.370200	1.780450	-1.449520
1	-4.390759	1.472494	-0.018657
1	-2.883629	2.403864	0.142696
6	-3.510304	-1.224406	-0.895020
1	-4.522768	-1.203921	-0.476272
1	-3.562750	-0.999491	-1.965705
1	-3.092839	-2.225308	-0.767697
6	3.598004	0.577008	-0.355139
1	4.539380	0.145474	0.005378
1	3.668201	0.756293	-1.432289
1	3.400015	1.528190	0.136291
6	2.866042	-2.125167	-0.792368
1	2.993086	-1.969808	-1.869470
1	3.834507	-2.394518	-0.356188
1	2.161980	-2.944463	-0.637287
6	0.067849	1.866989	-0.046018
1	-0.748723	2.383124	-0.573598

1	-0.036167	2.065640	1.036973
77	-0.091295	-0.156277	-0.374753
1	-0.029270	0.188689	-1.959882
8	-0.383217	-2.526867	-0.875887
6	-0.567813	-3.563555	0.079328
1	0.206842	-4.336098	-0.032029
1	-0.494296	-3.104975	1.064960
1	-1.555186	-4.032592	-0.040856
6	-0.450602	-2.978441	-2.222837
1	-0.302224	-2.101697	-2.852021
1	0.334620	-3.722276	-2.420271
1	-1.431232	-3.429661	-2.432040

Structure 8-TS
B3LYP/GBS(1) = -1312.895886a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1313.179661a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1312.031499 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1313.24171 a.u.
Enthalpy Correction = 0.3433
Gibbs Free Energy Correction = 0.273354
Imaginary Freq = -732.6i
B3LYP/GBS(1) IEFPCM corrections = 0.050954

Atomic No	x-coord	y-coord	z-coord
7	-0.099533	-0.365414	1.654192
6	-1.279363	-0.228020	2.306932
6	-2.477799	-0.094101	1.659803
1	-1.241047	-0.222724	3.400368
1	-3.399695	0.021355	2.222238
6	1.099237	-0.506584	2.286512
6	2.274841	-0.661146	1.616344
1	1.080848	-0.497215	3.380181
1	3.211567	-0.763110	2.156419
15	-2.433584	-0.099461	-0.133942
15	2.191238	-0.671344	-0.181039
8	1.317585	2.303375	0.123031
6	1.317316	3.679680	0.420686
1	0.693667	3.906954	1.301927
1	2.350240	3.974455	0.634113
1	0.942476	4.282359	-0.424426
6	-3.350376	1.392700	-0.722283
1	-3.439026	1.364812	-1.813313
1	-4.353813	1.431991	-0.283443
1	-2.801499	2.293811	-0.438288
6	-3.528033	-1.464616	-0.729328
1	-4.544486	-1.353051	-0.335212
1	-3.567352	-1.460831	-1.823791
1	-3.117717	-2.420825	-0.394732
6	3.509514	0.428515	-0.848900
1	4.475051	0.200146	-0.383270
1	3.590345	0.275787	-1.930381
1	3.218733	1.459428	-0.649036
6	2.801724	-2.332076	-0.728854
1	2.793436	-2.388002	-1.822861
1	3.822888	-2.510457	-0.372997
1	2.143410	-3.108535	-0.331191
6	0.007239	1.815626	-0.170776
1	-0.385260	2.357027	-1.044105
1	-0.641821	2.057176	0.686988
77	-0.117327	-0.303474	-0.491338
1	-0.048814	0.185956	-2.034365

1	-0.301537	-1.976148	-0.326101
1	-0.259917	-1.586569	-1.515576

Structure 9
B3LYP/GBS(1) = -1312.898136a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1313.180873a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1312.031882 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1313.243143 a.u.
Enthalpy Correction = 0.345465
Gibbs Free Energy Correction = 0.274323
B3LYP/GBS(1) IEFPCM corrections = 0.050806

Atomic No	x-coord	y-coord	z-coord
7	-0.156788	-0.637517	1.624973
6	-1.361044	-0.636883	2.254856
6	-2.537955	-0.387739	1.609293
1	-1.352019	-0.849659	3.327430
1	-3.478629	-0.386081	2.151914
6	1.014371	-0.943436	2.252751
6	2.206613	-1.013130	1.598569
1	0.954885	-1.138741	3.326844
1	3.120118	-1.252620	2.134957
15	-2.433908	-0.066934	-0.154749
15	2.174676	-0.720365	-0.177111
8	1.323665	2.508637	-0.152533
6	1.411459	3.813899	0.372654
1	1.384329	3.816525	1.475840
1	2.362870	4.242302	0.039988
1	0.588908	4.454786	0.012227
6	-3.375591	1.490519	-0.481653
1	-3.395788	1.694520	-1.557328
1	-4.405125	1.399252	-0.117215
1	-2.893629	2.330317	0.024639
6	-3.482126	-1.313213	-1.026328
1	-4.513057	-1.292079	-0.655169
1	-3.485484	-1.106478	-2.101902
1	-3.056568	-2.305963	-0.862122
6	3.543338	0.442006	-0.582382
1	4.487230	0.086565	-0.153408
1	3.649025	0.514516	-1.669912
1	3.279928	1.424734	-0.191749
6	2.759229	-2.276037	-0.988626
1	2.783405	-2.137897	-2.074909
1	3.763422	-2.545561	-0.641960
1	2.063110	-3.084325	-0.753448
6	0.109652	1.861031	0.231690
1	-0.727167	2.470606	-0.136904
1	0.045236	1.831768	1.329795
77	-0.104199	-0.210513	-0.459259
1	0.054222	0.757663	-1.743791
1	-0.324514	-1.859378	-0.492480
1	-0.212361	-0.874391	-1.929982

Structure 9-TS
B3LYP/GBS(1) = -1312.890378a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1313.171524a.u.

BMK/GBS(2)//B3LYP/GBS(1) = -1312.020857 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1313.233179 a.u.
Enthalpy Correction = 0.3442
Gibbs Free Energy Correction = 0.2732
B3LYP/GBS(1) IEFPCM corrections = 0.051078
Imaginary Freq = -730.3

Atomic No	x-coord	y-coord	z-coord
7	-0.141461	-0.263716	1.741080
6	-1.330448	-0.082047	2.375346
6	-2.502875	0.129235	1.706708
1	-1.316538	-0.113343	3.469024
1	-3.430546	0.283623	2.250119
6	1.012678	-0.574710	2.397313
6	2.172770	-0.869634	1.745820
1	0.970821	-0.582522	3.490507
1	3.076606	-1.103965	2.300831
15	-2.418558	0.116711	-0.088711
15	2.100809	-0.910223	-0.053199
8	1.569407	2.505031	-0.576993
6	1.840085	3.793456	-0.064060
1	1.855146	3.797736	1.038180
1	2.824573	4.092125	-0.436540
1	1.092985	4.530731	-0.400527
6	-3.268642	1.651104	-0.680033
1	-3.296589	1.663729	-1.774676
1	-4.294998	1.694711	-0.297995
1	-2.727644	2.534953	-0.332742
6	-3.570698	-1.188946	-0.703818
1	-4.589878	-1.023950	-0.336086
1	-3.578865	-1.185614	-1.798852
1	-3.212043	-2.162264	-0.361119
6	3.553932	0.023050	-0.697716
1	4.478751	-0.334122	-0.230302
1	3.624344	-0.119670	-1.781267
1	3.406387	1.084424	-0.495437
6	2.514397	-2.637204	-0.567348
1	2.497198	-2.707899	-1.660037
1	3.505867	-2.931001	-0.204094
1	1.760673	-3.316080	-0.161968
6	0.308055	2.016920	-0.139639
1	-0.491198	2.660332	-0.531789
1	0.256813	2.029227	0.956303
77	-0.115779	-0.229135	-0.399227
1	0.200941	0.992268	-1.426399
1	-0.476130	-1.819061	-0.285604
1	-0.211593	-0.691924	-1.952545

Structure 10
B3LYP/GBS(1) = -1312.906496a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1313.186053a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1312.040077 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1313.245192 a.u.
Enthalpy Correction = 0.345119
Gibbs Free Energy Correction = 0.272511
B3LYP/GBS(1) IEFPCM corrections = 0.052449

Atomic No	x-coord	y-coord	z-coord
7	0.741642	-1.989297	-0.113443
6	2.074842	-2.240394	-0.083412

6	3.013513	-1.245779	-0.075015
1	2.384571	-3.290132	-0.060989
1	4.073609	-1.481750	-0.059933
6	-0.195129	-2.969106	-0.003037
6	-1.533261	-2.706332	0.080169
1	0.167231	-4.001742	0.020939
1	-2.253290	-3.516255	0.153181
15	2.395670	0.440040	-0.048950
15	-2.014041	-0.973275	0.068272
8	-1.869386	2.238051	-0.524420
6	-2.383679	3.538601	-0.347617
1	-1.692935	4.308442	-0.731613
1	-3.326325	3.604698	-0.901628
1	-2.578785	3.761455	0.715512
6	3.212921	1.349098	-1.440683
1	2.902739	2.399680	-1.433959
1	4.304840	1.301876	-1.357682
1	2.911277	0.900203	-2.391209
6	3.133216	1.286442	1.420302
1	4.228144	1.247566	1.394115
1	2.813979	2.333877	1.443892
1	2.776447	0.792734	2.327638
6	-3.238230	-0.731626	-1.293493
1	-4.139466	-1.334819	-1.134898
1	-3.499898	0.329292	-1.333684
1	-2.780789	-1.019567	-2.244346
6	-3.039708	-0.640013	1.565371
1	-3.346014	0.410942	1.553146
1	-3.931017	-1.277014	1.590443
1	-2.438225	-0.822697	2.459330
6	-0.620581	2.038943	0.170400
1	-0.782878	2.256535	1.238944
1	0.093065	2.796169	-0.200812
77	0.075522	0.069545	-0.088573
1	0.149386	-0.019996	1.494247
1	0.092999	-0.070824	-1.985788
1	-0.232629	0.657304	-1.847560

Structure 10 (Explicit dimethyl ether solvent included. H2 Excluded)
B3LYP/GBS(1) = -1466.76112361a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1467.08163304 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1465.84764612 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1467.15853102 a.u.
Enthalpy Correction = 0.345119
Gibbs Free Energy Correction = 0.272511

Atomic No	x-coord	y-coord	z-coord
7	-0.795245	-1.990194	-0.301848
6	-2.139571	-2.192752	-0.306255
6	-3.039127	-1.162456	-0.261650
1	-2.490742	-3.229431	-0.347594
1	-4.107782	-1.357917	-0.259466
6	0.096778	-3.007463	-0.474249
6	1.439303	-2.791788	-0.598505
1	-0.307361	-4.024583	-0.512892
1	2.125066	-3.625872	-0.718657
15	-2.348798	0.497388	-0.288605
15	1.981284	-1.073497	-0.558648
8	2.044691	2.118661	0.055074

6	2.537794	3.433838	-0.061587
1	1.969410	4.143623	0.564368
1	3.583048	3.433007	0.267388
1	2.492812	3.795177	-1.102899
6	-3.140541	1.444504	1.097485
1	-2.804983	2.487346	1.070422
1	-4.233871	1.422694	1.021143
1	-2.846880	1.009492	2.056385
6	-3.075481	1.367433	-1.752011
1	-4.170968	1.368926	-1.713909
1	-2.717350	2.402287	-1.783078
1	-2.747820	0.858092	-2.661760
6	3.268523	-0.939149	0.760497
1	4.092358	-1.641649	0.590466
1	3.648125	0.086318	0.771338
1	2.803305	-1.152676	1.726063
6	2.967837	-0.753888	-2.086154
1	3.316595	0.283407	-2.061556
1	3.829337	-1.427369	-2.159239
1	2.326957	-0.890592	-2.961039
6	0.659831	2.003929	-0.367407
1	0.591488	2.426222	-1.384864
1	0.071021	2.680296	0.284531
77	-0.052306	0.040710	-0.304849
1	-0.139798	0.107451	-1.870143
8	0.233807	-0.097619	2.103089
6	0.676234	1.048396	2.825515
1	1.211155	0.734140	3.733024
1	1.346129	1.591671	2.159025
1	-0.175347	1.681943	3.112680
6	-0.555098	-0.985261	2.883789
1	-0.833446	-1.813819	2.233454
1	0.028091	-1.354362	3.739383
1	-1.460238	-0.486425	3.259106

Structure 10-TS

B3LYP/GBS(1) = -1312.880666a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1313.162190 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1312.014444 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1313.22352 a.u.
Enthalpy Correction = 0.343605
Gibbs Free Energy Correction = 0.27218
Imaginary Freq = -758.8i
B3LYP/GBS(1) IEFPCM corrections = 0.050419

Atomic No	x-coord	y-coord	z-coord
7	-0.771055	-1.914812	-0.176086
6	-2.107467	-2.164552	-0.245695
6	-3.049835	-1.183913	-0.169166
1	-2.396318	-3.210870	-0.368497
1	-4.108261	-1.417277	-0.229429
6	0.153747	-2.915315	-0.248622
6	1.494893	-2.692668	-0.179222
1	-0.242080	-3.926408	-0.368194
1	2.201453	-3.514486	-0.240871
15	-2.418133	0.481663	0.026851
15	1.985267	-0.976881	0.009141
8	2.003128	2.366659	0.316302
6	2.595302	3.551684	-0.179445
1	2.022078	4.445708	0.113418
1	3.597731	3.616520	0.252444

1	2.674675	3.536659	-1.278523
6	-3.232147	1.217488	1.515596
1	-2.912776	2.258061	1.641265
1	-4.324331	1.191779	1.426276
1	-2.924644	0.649971	2.397173
6	-3.132411	1.511266	-1.334187
1	-4.227903	1.470500	-1.331418
1	-2.819756	2.555525	-1.220539
1	-2.755617	1.134685	-2.288143
6	3.073738	-0.839904	1.492058
1	3.971017	-1.461408	1.391024
1	3.365973	0.207428	1.615560
1	2.507413	-1.152877	2.372456
6	3.150781	-0.562476	-1.361521
1	3.458893	0.482676	-1.257628
1	4.038607	-1.204848	-1.339421
1	2.631993	-0.687702	-2.314936
6	0.693653	2.172730	-0.203968
1	0.718193	2.160430	-1.294818
1	0.027918	2.990043	0.111986
77	-0.114106	0.041910	0.061491
1	-0.114086	0.066669	-1.618329
1	-0.186723	-0.242153	1.723741
1	0.296644	1.350398	0.946953

Structure 11

B3LYP/GBS(1) = -1312.893691a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1313.16871a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1312.025904 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1313.224995 a.u.
Enthalpy Correction = 0.347759
Gibbs Free Energy Correction = 0.274781
B3LYP/GBS(1) IEFPCM corrections = 0.050770

Atomic No	x-coord	y-coord	z-coord
7	-0.782754	-1.938332	-0.196565
6	-2.117497	-2.207734	-0.283805
6	-3.076728	-1.246224	-0.216660
1	-2.376127	-3.259894	-0.412738
1	-4.129899	-1.497548	-0.290097
6	0.147669	-2.938022	-0.259536
6	1.485370	-2.717246	-0.171184
1	-0.255619	-3.943763	-0.387887
1	2.193155	-3.538078	-0.226727
15	-2.459245	0.419548	-0.004059
15	1.953649	-0.999736	0.030325
8	2.179316	2.519366	0.286087
6	2.752124	3.613118	-0.406386
1	2.380033	4.575547	-0.020938
1	3.832104	3.561755	-0.248090
1	2.541663	3.563346	-1.486107
6	-3.299880	1.140077	1.478864
1	-2.992113	2.183023	1.615048
1	-4.390745	1.105809	1.375739
1	-2.996441	0.569991	2.359992
6	-3.171253	1.451626	-1.366170
1	-4.266531	1.404639	-1.373061
1	-2.866108	2.497295	-1.244565
1	-2.782459	1.083228	-2.318382
6	3.027705	-0.864181	1.526591

1	3.919784	-1.495426	1.438289
1	3.335730	0.179177	1.650983
1	2.447728	-1.166855	2.401497
6	3.137459	-0.569883	-1.320839
1	3.430302	0.478720	-1.208978
1	4.032768	-1.201585	-1.287088
1	2.633141	-0.696203	-2.281613
6	0.777474	2.487201	0.150605
1	0.457128	2.421306	-0.892658
1	0.296620	3.360468	0.620318
77	-0.163031	-0.023445	0.049019
1	-0.085131	0.160258	-1.630170
1	-0.234176	-0.212874	1.730105
1	0.426581	1.640125	0.825834

Structure 12
B3LYP/GBS(1) = -1499.094184a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1499.423369a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1498.213799a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1499.514727 a.u.
Enthalpy Correction = 0.325048
Gibbs Free Energy Correction = 0.24949
B3LYP/GBS(1) IEFPCM corrections = 0.015489

Atomic No	x-coord	y-coord	z-coord
6	-1.665273	-2.681055	0.063427
6	-0.340140	-2.990231	0.043029
15	-2.071475	-0.936389	-0.113234
7	0.640688	-2.040243	-0.083947
6	1.967291	-2.373854	-0.050737
6	2.962399	-1.445296	-0.111218
77	0.084383	0.007875	-0.216453
15	2.432535	0.267676	-0.226584
8	-1.747525	2.193235	-1.032447
6	-0.483471	1.975133	-0.493946
1	0.229997	2.682117	-0.940852
6	-2.117016	3.568001	-1.114791
1	-1.372782	4.142626	-1.686178
1	-3.077652	3.609373	-1.634579
1	-2.221614	4.012760	-0.117792
1	-2.418680	-3.456089	0.165094
1	-0.010983	-4.029529	0.130762
1	2.207801	-3.437799	0.030236
1	4.006891	-1.738981	-0.075620
6	-0.155471	1.105813	1.441971
8	-0.496395	2.322026	0.976593
8	-0.023720	0.804462	2.602300
6	3.210329	1.195381	1.166435
1	4.293605	1.034880	1.186610
1	3.007869	2.266287	1.060224
1	2.769786	0.851390	2.105659
6	-3.173397	-0.453714	1.282453
1	-3.502408	0.580118	1.138336
1	-4.048559	-1.110150	1.335931
1	-2.610402	-0.515013	2.217268
6	-3.162989	-0.770647	-1.592180
1	-4.088809	-1.343667	-1.468165
1	-3.392547	0.288250	-1.736200
1	-2.630890	-1.137967	-2.474325
6	3.249411	1.001209	-1.715588

1	2.981762	2.059781	-1.800728
1	4.339837	0.913960	-1.652189
1	2.902228	0.479988	-2.612125

Structure 13
B3LYP/GBS(1) = -1499.083218a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1499.41211373a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1498.200944 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1499.504345 a.u.
Enthalpy Correction = 0.325343
Gibbs Free Energy Correction = 0.249132
B3LYP/GBS(1) IEFPCM corrections = 0.012194

Atomic No	x-coord	y-coord	z-coord
6	1.789326	2.680265	0.060872
6	0.489754	3.045220	-0.070498
15	2.118463	0.907852	0.084874
7	-0.529110	2.127753	-0.162439
6	-1.837060	2.537575	-0.221515
6	-2.882703	1.668620	-0.225587
77	-0.091052	0.046166	-0.064103
15	-2.443835	-0.069562	-0.119622
8	1.317445	-2.309412	-1.460011
6	0.168580	-1.899301	-0.786965
1	-0.655167	-2.185575	-1.447183
6	2.423368	-2.725410	-0.673912
1	2.225706	-3.679984	-0.175995
1	3.260212	-2.842804	-1.367456
1	2.687392	-1.987310	0.093808
1	2.579998	3.421822	0.122296
1	0.206385	4.100994	-0.103841
1	-2.012904	3.616372	-0.261299
1	-3.908832	2.019443	-0.269136
6	0.026231	-1.456513	1.259948
8	0.026539	-2.594018	0.497557
8	0.041749	-1.459812	2.466563
6	-3.297966	-0.778463	1.355504
1	-4.372469	-0.568409	1.320636
1	-3.142933	-1.861523	1.388007
1	-2.868283	-0.343848	2.261365
6	3.078036	0.576137	1.628096
1	3.480905	-0.441512	1.614873
1	3.904980	1.286588	1.734437
1	2.403811	0.665046	2.483824
6	3.359047	0.654566	-1.264202
1	4.217239	1.320955	-1.121766
1	3.708789	-0.379745	-1.287320
1	2.884720	0.883094	-2.222155
6	-3.277337	-0.936056	-1.523423
1	-3.076045	-2.011502	-1.471197
1	-4.361063	-0.778832	-1.490447
1	-2.888605	-0.550568	-2.469981

Structure 14
B3LYP/GBS(1) = -1499.089034a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1499.417912a.u.

BMK/GBS(2)//B3LYP/GBS(1) = -1498.207354 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1499.510419 a.u.
Enthalpy Correction = 0.324889
Gibbs Free Energy Correction = 0.249241
B3LYP/GBS(1) IEFPCM corrections = 0.013402

Atomic No	x-coord	y-coord	z-coord
6	-2.243326	2.114011	0.056679
6	-1.032733	2.684017	0.320408
15	-2.207096	0.409207	-0.523064
7	0.144177	1.990937	0.232067
6	1.352460	2.582993	0.467575
6	2.533593	1.906954	0.365593
77	0.082865	-0.091658	-0.266279
15	2.414883	0.189310	-0.153944
8	-1.115851	-1.158465	2.237635
6	-0.062763	-1.361101	1.374537
1	0.886186	-1.346410	1.931453
6	-0.876789	-0.153895	3.218050
1	-0.803260	0.836226	2.753587
1	-1.725736	-0.180240	3.903829
1	0.046446	-0.362807	3.777285
1	-3.159435	2.691933	0.132948
1	-0.967426	3.735539	0.615897
1	1.342117	3.641134	0.746040
1	3.480085	2.401627	0.561254
6	-0.062758	-2.064035	-0.671918
8	-0.242631	-2.558295	0.664881
8	-0.078349	-2.844794	-1.588803
6	3.262310	0.033826	-1.790906
1	4.304358	0.367553	-1.732925
1	3.231121	-1.009350	-2.121312
1	2.733954	0.646858	-2.526724
6	-2.724331	0.433003	-2.301652
1	-2.707668	-0.587019	-2.698833
1	-3.729951	0.852762	-2.416131
1	-2.019073	1.041707	-2.874998
6	-3.586405	-0.516316	0.270742
1	-4.535968	0.012937	0.133976
1	-3.658785	-1.509112	-0.184628
1	-3.372432	-0.642296	1.332613
6	3.516397	-0.804288	0.947472
1	3.510940	-1.852159	0.630210
1	4.543651	-0.425325	0.909653
1	3.160501	-0.747229	1.979982

Structure 14-TS
B3LYP/GBS(1) = -1499.083648a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1499.412498a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1498.194798 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1499.508389a.u.
Enthalpy Correction = 0.32301
Gibbs Free Energy Correction = 0.247673
Imaginary Freq = -415.4
B3LYP/GBS(1) IEFPCM corrections = 0.014235

Atomic No	x-coord	y-coord	z-coord
6	-2.265856	2.042382	-0.237243
6	-1.062013	2.639157	-0.012136
15	-2.212450	0.282719	-0.604399

7	0.116453	1.942514	0.010133
6	1.316108	2.578345	0.158678
6	2.509671	1.918403	0.115590
77	0.083223	-0.156939	-0.292413
15	2.410446	0.158439	-0.222985
8	-1.081120	-0.546619	2.477273
6	-0.112763	-1.093466	1.668431
1	0.888258	-0.934458	2.106360
6	-0.681719	0.611021	3.204725
1	-0.502633	1.453698	2.528187
1	-1.501830	0.847947	3.885069
1	0.226656	0.412813	3.790158
1	-3.183758	2.622310	-0.245173
1	-0.998009	3.717422	0.158549
1	1.284654	3.660607	0.312748
1	3.448554	2.449200	0.239719
6	-0.034277	-2.128152	-0.436782
8	-0.405162	-2.314911	1.241110
8	-0.019398	-3.154207	-1.013798
6	3.269834	-0.157773	-1.830781
1	4.304891	0.200836	-1.804034
1	3.264680	-1.231012	-2.047417
1	2.733488	0.361539	-2.629860
6	-2.805072	0.079598	-2.347042
1	-2.815804	-0.983102	-2.610684
1	-3.813329	0.490556	-2.470752
1	-2.122571	0.601257	-3.023887
6	-3.527672	-0.572285	0.359791
1	-4.500056	-0.092066	0.203366
1	-3.585066	-1.617173	0.038596
1	-3.258067	-0.553024	1.416736
6	3.519495	-0.708851	0.974837
1	3.526646	-1.783272	0.764072
1	4.543068	-0.324408	0.903372
1	3.157956	-0.554708	1.995378

Structure 15
B3LYP/GBS(1) = -1270.08568a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1270.33566a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1269.229795 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1270.386730 a.u.
Enthalpy Correction = 0.255652
Gibbs Free Energy Correction = 0.190077
B3LYP/GBS(1) IEFPCM corrections = 0.014795

Atomic No	x-coord	y-coord	z-coord
6	-2.387563	-1.769447	-0.000439
6	-1.178772	-2.394614	-0.000965
15	-2.313677	0.023418	0.000790
7	0.007900	-1.710953	-0.000564
6	1.200824	-2.383645	-0.001218
6	2.403799	-1.747360	-0.000955
77	-0.001783	0.389531	0.000933
15	2.313385	0.044747	0.000314
8	-0.015649	3.400995	0.003210
6	-0.010282	2.234290	0.002309
1	-3.315448	-2.332502	-0.000790
1	-1.114430	-3.485857	-0.001741
1	1.146544	-3.475435	-0.001982
1	3.336837	-2.301835	-0.001525

6	-3.309568	0.622335	1.439127
1	-3.333869	1.717040	1.443927
1	-4.336528	0.242367	1.392477
1	-2.840376	0.279884	2.365047
6	3.304001	0.652805	1.438463
1	4.334629	0.282982	1.391193
1	3.317524	1.747693	1.443740
1	2.838616	0.305343	2.364437
6	3.303403	0.654778	-1.437404
1	3.319017	1.749654	-1.439773
1	4.333380	0.282877	-1.392320
1	2.836271	0.310680	-2.363752
6	-3.309567	0.624275	-1.436739
1	-4.336271	0.243497	-1.391068
1	-3.334647	1.718972	-1.439547
1	-2.839870	0.283847	-2.363147

6. SCO Structures and Energies

Structure SCO7-TS
B3LYP/GBS(1) = -1822.035238a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1822.366895a.u.
Enthalpy Correction = 0.321295
Gibbs Free Energy Correction = 0.245094
Imaginary Freq = -282.4i

Atomic No	x-coord	y-coord	z-coord
6	-2.099426	-2.254388	-1.044126
6	-0.808096	-2.626619	-1.265561
15	-2.372219	-0.510810	-0.714336
7	0.233532	-1.741312	-1.241369
6	1.516359	-2.145543	-1.474073
6	2.574893	-1.287189	-1.458747
77	-0.153583	0.300014	-0.780380
15	2.192671	0.427250	-1.100090
8	-1.779607	2.734008	-0.531386
6	-0.548402	2.227750	-0.469487
1	0.215658	3.013948	-0.458440
6	-1.950560	4.077671	-0.049447
1	-1.201165	4.744239	-0.492307
1	-2.951418	4.392953	-0.348152
1	-1.857167	4.083313	1.040210
1	-2.903604	-2.983242	-1.063620
1	-0.561869	-3.670575	-1.477893
1	1.669745	-3.208128	-1.681533
1	3.586224	-1.638585	-1.637461
6	-0.035444	0.673249	1.240536
8	-0.258749	1.899056	1.444624
6	3.279697	0.977226	0.284208
1	4.332066	0.786258	0.047178
1	3.143318	2.047867	0.468948
1	3.000501	0.427023	1.186430
6	-3.343021	-0.358127	0.843416
1	-3.582312	0.694829	1.021723
1	-4.271539	-0.935908	0.779373
1	-2.735850	-0.727832	1.673596
6	-3.547484	0.120999	-1.993935
1	-4.493915	-0.430592	-1.964447
1	-3.738044	1.183162	-1.814376
1	-3.099126	0.005524	-2.984801

6	2.811749	1.439641	-2.521857
1	2.655211	2.505007	-2.321016
1	3.880342	1.265430	-2.690884
1	2.260354	1.168397	-3.426525
16	0.313099	-0.574447	2.292167

Structure SCO12
B3LYP/GBS(1) = -1822.043383a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1822.373731a.u.
Enthalpy Correction = 0.323036
Gibbs Free Energy Correction = 0.246222

Atomic No	x-coord	y-coord	z-coord
6	-1.497711	-2.842092	0.052306
6	-0.159844	-3.065333	-0.027919
15	-2.012286	-1.116597	0.013840
7	0.760005	-2.047303	-0.101143
6	2.104234	-2.309073	-0.159644
6	3.046537	-1.327926	-0.192866
77	0.092718	-0.036943	-0.009485
15	2.424332	0.357304	-0.152326
8	-1.840266	2.055017	-0.838210
6	-0.576658	1.895040	-0.295295
1	0.118744	2.624775	-0.733127
6	-2.269744	3.413770	-0.926189
1	-1.551280	4.016321	-1.500951
1	-3.231208	3.408637	-1.445229
1	-2.393237	3.855750	0.069425
1	-2.201080	-3.666857	0.110926
1	0.234844	-4.084996	-0.036968
1	2.400444	-3.361545	-0.178983
1	4.104974	-1.565744	-0.229342
6	-0.209172	1.061511	1.616578
6	3.290446	1.246466	1.209845
1	4.375978	1.136562	1.112936
1	3.033777	2.310490	1.184541
1	2.961147	0.834145	2.166834
6	-3.167559	-0.826193	1.416878
1	-3.569856	0.189248	1.347845
1	-3.992983	-1.545849	1.394162
1	-2.619970	-0.920892	2.357748
6	-3.089920	-0.912515	-1.470875
1	-3.969279	-1.563467	-1.409893
1	-3.399726	0.133185	-1.539071
1	-2.516615	-1.167085	-2.366573
6	3.053235	1.213632	-1.667108
1	2.718633	2.256693	-1.670490
1	4.147950	1.191792	-1.706945
1	2.653600	0.715222	-2.554553
16	0.000473	0.618019	3.189511
8	-0.613472	2.248201	1.179592

Structure SCO14
B3LYP/GBS(1) = -1822.039738a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1822.369187a.u.

Enthalpy Correction = 0.32324
Gibbs Free Energy Correction = 0.245786

Atomic No	x-coord	y-coord	z-coord
6	2.177386	-2.201294	-0.968169
6	0.951043	-2.784917	-1.046488
15	2.192814	-0.444597	-0.567715
7	-0.211699	-2.105114	-0.783919
6	-1.434467	-2.711156	-0.900883
6	-2.606479	-2.056558	-0.667871
77	-0.116401	-0.057321	-0.188737
15	-2.457187	-0.313481	-0.255006
8	1.038373	0.437168	2.519231
6	-0.018811	0.778681	1.705657
1	-0.970835	0.659106	2.241649
6	0.826109	-0.757218	3.261431
1	0.758820	-1.629385	2.599100
1	1.682695	-0.865250	3.929723
1	-0.092829	-0.690471	3.862218
1	3.080007	-2.765311	-1.182277
1	0.853275	-3.836781	-1.330146
1	-1.438005	-3.764605	-1.195520
1	-3.561502	-2.563398	-0.764091
6	0.014875	1.926857	-0.040706
8	0.139164	2.146639	1.300889
6	-3.275819	0.668524	-1.586733
1	-4.342399	0.429273	-1.661040
1	-3.147359	1.735938	-1.380930
1	-2.788858	0.446386	-2.539906
6	2.820008	0.456240	-2.053864
1	2.780061	1.533701	-1.865439
1	3.845455	0.157073	-2.297066
1	2.168542	0.237026	-2.904022
6	3.531042	-0.160274	0.667489
1	4.498897	-0.461684	0.251390
1	3.563268	0.900175	0.932849
1	3.329155	-0.735909	1.572267
6	-3.535916	0.012394	1.208780
1	-3.515838	1.079013	1.456312
1	-4.569999	-0.281325	0.997977
1	-3.176768	-0.559159	2.069192
16	0.020550	3.152115	-1.145790

Structure SCO14-TS
B3LYP/GBS(1) = -1822.014258a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1822.345181a.u.
Enthalpy Correction = 0.320687
Gibbs Free Energy Correction = 0.243378
Imaginary Freq = -521.1i

Atomic No	x-coord	y-coord	z-coord
6	2.128750	-2.475686	0.049481
6	0.911212	-2.963358	0.416791
15	2.147931	-0.782383	-0.552645
7	-0.226698	-2.203269	0.396530
6	-1.448490	-2.749374	0.665044
6	-2.610759	-2.040255	0.565739
77	-0.106059	-0.155926	-0.211991

15	-2.441146	-0.351881	-0.013161
8	1.187630	0.529020	2.477088
6	0.276441	1.081217	1.613679
1	-0.738805	1.077908	2.047042
6	0.666803	-0.450971	3.372219
1	0.339311	-1.341821	2.825157
1	1.479522	-0.710015	4.053008
1	-0.173452	-0.046066	3.952181
1	3.015304	-3.101489	0.082506
1	0.803055	-4.002377	0.740830
1	-1.465179	-3.800838	0.966055
1	-3.568862	-2.498051	0.791326
6	0.089553	1.686951	-0.713229
8	0.689844	2.147603	0.987277
6	-3.338423	-0.194268	-1.621751
1	-4.394285	-0.467581	-1.516146
1	-3.265220	0.836668	-1.983087
1	-2.869141	-0.854922	-2.355730
6	2.661525	-0.832454	-2.328597
1	2.686038	0.186524	-2.728556
1	3.651241	-1.288796	-2.442456
1	1.931365	-1.414269	-2.897800
6	3.542459	0.119463	0.241564
1	4.485089	-0.420076	0.095970
1	3.623255	1.117108	-0.200887
1	3.329942	0.232768	1.305664
6	-3.447668	0.732728	1.094605
1	-3.399128	1.768405	0.742889
1	-4.494486	0.409315	1.108726
1	-3.053979	0.689766	2.114122
16	0.086840	2.954916	-1.681773

Structure SCO16
B3LYP/GBS(1) = -1593.018958a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1593.271068a.u.
Enthalpy Correction = 0.253537
Gibbs Free Energy Correction = 0.186415

Atomic No	x-coord	y-coord	z-coord
6	-2.396016	1.881574	0.000036
6	-1.191554	2.515417	0.000022
15	-2.318017	0.088193	0.000062
7	-0.000002	1.839454	0.000020
6	1.191549	2.515419	0.000033
6	2.396011	1.881578	0.000058
77	0.000000	-0.280322	0.000022
15	2.318016	0.088197	0.000080
6	0.000002	-2.094220	-0.000016
1	-3.327488	2.438688	0.000035
1	-1.137289	3.607449	0.000013
1	1.137282	3.607451	0.000023
1	3.327483	2.438694	0.000067
6	-3.299371	-0.523522	-1.440281
1	-3.297439	-1.618265	-1.447709
1	-4.334211	-0.166019	-1.392036
1	-2.836635	-0.167590	-2.364276
6	3.299378	-0.523517	-1.440258
1	4.334234	-0.166063	-1.391977
1	3.297396	-1.618259	-1.447721
1	2.836681	-0.167534	-2.364252
6	3.299232	-0.523469	1.440538

1	3.297414	-1.618212	1.447930
1	4.334042	-0.165857	1.392448
1	2.836328	-0.167616	2.364479
6	-3.299241	-0.523474	1.440515
1	-4.334066	-0.165911	1.392391
1	-3.297371	-1.618217	1.447940
1	-2.836375	-0.167571	2.364455
16	0.000005	-3.677483	-0.000082

Structure OCS7-TS
B3LYP/GBS(1) = -1822.04307567a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1822.3740949 a.u.
Enthalpy Correction = 0.320916
Gibbs Free Energy Correction = 0.240048
Imaginary Freq = -135.9i

Atomic No	x-coord	y-coord	z-coord
6	-1.904452	-2.561299	0.346116
6	-0.606327	-2.941880	0.495799
15	-2.161590	-0.857417	-0.170506
7	0.444609	-2.091910	0.270313
6	1.737926	-2.528268	0.355517
6	2.801694	-1.730015	0.060936
77	0.046350	-0.086023	-0.292028
15	2.399494	-0.061801	-0.473777
8	-1.521559	2.204222	-1.105105
6	-0.306773	1.685062	-0.875311
1	0.462817	2.453862	-1.066369
6	-1.622799	3.605405	-1.404780
1	-0.813353	3.920420	-2.072678
1	-2.586345	3.754987	-1.895197
1	-1.584755	4.184550	-0.476643
1	-2.717944	-3.252251	0.544776
1	-0.358494	-3.962172	0.802071
1	1.891805	-3.565376	0.667355
1	3.819986	-2.098755	0.137174
6	-0.059690	0.757316	2.216306
8	-0.449108	-0.229001	2.736660
6	3.494464	1.082557	0.480781
1	4.546450	0.801182	0.356777
1	3.358070	2.111647	0.132241
1	3.229537	1.043810	1.539396
6	-3.388628	-0.110463	0.991330
1	-3.591571	0.921304	0.687591
1	-4.325511	-0.679043	0.990332
1	-2.969445	-0.108399	1.999789
6	-3.113659	-0.896705	-1.756132
1	-4.066323	-1.424528	-1.634211
1	-3.306380	0.129711	-2.083699
1	-2.518115	-1.403195	-2.520400
6	3.084250	0.129552	-2.186895
1	2.929845	1.154306	-2.542317
1	4.156643	-0.094872	-2.210974
1	2.559755	-0.554970	-2.858821
16	0.418927	2.310865	2.272972

Structure OCS12
B3LYP/GBS(1) = -1822.058896a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1822.393061a.u.
Enthalpy Correction = 0.322345
Gibbs Free Energy Correction = 0.245711

Atomic No	x-coord	y-coord	z-coord
6	-1.502971	-2.795297	0.086887
6	-0.159308	-3.028248	0.095694
15	-2.007252	-1.080515	-0.080580
7	0.765188	-2.028507	-0.005234
6	2.102694	-2.286837	-0.003120
6	3.045118	-1.304446	-0.103910
77	0.090224	-0.003789	-0.122853
15	2.427287	0.372905	-0.232966
8	-1.912807	2.102096	-0.736745
6	-0.616573	1.957563	-0.215385
1	0.031098	2.729780	-0.654028
6	-2.372446	3.442168	-0.805742
1	-1.686480	4.070333	-1.394507
1	-3.351537	3.425860	-1.292266
1	-2.477537	3.879716	0.198367
1	-2.211698	-3.613396	0.170482
1	0.224732	-4.048688	0.181761
1	2.405162	-3.334666	0.080113
1	4.104456	-1.541495	-0.093554
6	-0.026365	0.558449	1.794066
8	0.226202	-0.076975	2.780006
6	3.255856	1.379616	1.073424
1	4.345217	1.297754	0.990048
1	2.965386	2.431070	0.982626
1	2.941040	1.013902	2.054233
6	-3.198652	-0.689460	1.269218
1	-3.538015	0.344596	1.159632
1	-4.060284	-1.365034	1.233655
1	-2.695806	-0.796122	2.233827
6	-3.043291	-0.933599	-1.602084
1	-3.935063	-1.567048	-1.535594
1	-3.335864	0.112735	-1.723574
1	-2.454328	-1.240024	-2.471515
6	3.105103	1.106133	-1.791918
1	2.792282	2.152177	-1.878484
1	4.199840	1.059132	-1.805273
1	2.716952	0.552258	-2.651596
16	-0.570462	2.269748	1.685293

Structure OCS14
B3LYP/GBS(1) = -1822.05321a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1822.386354a.u.
Enthalpy Correction = 0.322259
Gibbs Free Energy Correction = 0.24418

Atomic No	x-coord	y-coord	z-coord
6	2.316243	-2.121081	-0.094865
6	1.132542	-2.723500	0.211524

15	2.221503	-0.408712	-0.639436
7	-0.063223	-2.058637	0.189079
6	-1.246882	-2.697247	0.419818
6	-2.455155	-2.068311	0.324700
77	-0.090747	0.015761	-0.343622
15	-2.410361	-0.353314	-0.205290
8	1.116522	0.507622	2.336574
6	0.052295	0.927923	1.564137
1	-0.888641	0.704598	2.080390
6	0.838746	-0.587247	3.207906
1	0.590317	-1.490668	2.640972
1	1.746091	-0.754891	3.791632
1	0.011480	-0.340879	3.887413
1	3.248605	-2.676530	-0.060193
1	1.103989	-3.781273	0.489501
1	-1.194989	-3.757407	0.685226
1	-3.379727	-2.602551	0.520814
6	-0.084523	1.958166	-0.808043
8	-0.169492	2.724926	-1.716129
6	-3.286908	-0.235764	-1.829866
1	-4.311405	-0.616766	-1.754278
1	-3.312400	0.807782	-2.160115
1	-2.743640	-0.824457	-2.574649
6	2.766080	-0.374900	-2.409099
1	2.734145	0.654105	-2.781894
1	3.783992	-0.765901	-2.516700
1	2.086456	-0.985653	-3.010494
6	3.538394	0.563611	0.200766
1	4.519438	0.098267	0.053706
1	3.552641	1.578199	-0.209446
1	3.301841	0.627538	1.263730
6	-3.519928	0.622037	0.902669
1	-3.534407	1.668103	0.581215
1	-4.539457	0.221901	0.875913
1	-3.154135	0.580089	1.932177
16	0.205812	2.667860	1.075625

7. PhNCO Structures and Energies

Structure NCO7-TS
B3LYP/GBS(1) = -1710.228987a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1710.616107a.u.
Enthalpy Correction = 0.420466
Gibbs Free Energy Correction = 0.331978
Imaginary Freq = -217.8i

Atomic No	x-coord	y-coord	z-coord
6	1.150570	-1.766491	-2.053101
6	1.468889	-0.451617	-2.214163
15	-0.225498	-2.112260	-0.954297
7	0.782684	0.557975	-1.598905
6	1.128478	1.865699	-1.780599
6	0.469613	2.894524	-1.175504
77	-0.834677	0.074497	-0.306935

15	-0.870310	2.428916	-0.079546
8	-2.926418	-1.579014	0.898943
6	-2.374164	-0.373620	0.842595
1	-2.959154	0.366336	1.401908
6	-3.843095	-1.827612	1.979676
1	-4.578841	-1.018712	2.054187
1	-4.345325	-2.769591	1.754955
1	-3.276445	-1.905326	2.911437
1	1.717668	-2.545540	-2.552942
1	2.300949	-0.159200	-2.860607
1	1.971213	2.066039	-2.448089
1	0.771500	3.925186	-1.333059
6	-0.064936	-0.155128	1.621830
8	-1.028112	-0.388799	2.427024
6	-0.521274	3.155087	1.579972
1	-0.409737	4.242687	1.512620
1	-1.331925	2.916854	2.275977
1	0.404165	2.714538	1.958353
6	0.356652	-3.278718	0.348157
1	-0.478268	-3.535590	1.007350
1	0.762216	-4.192583	-0.099569
1	1.131970	-2.782705	0.936803
6	-1.454920	-3.124579	-1.893323
1	-1.005252	-4.056527	-2.253941
1	-2.301094	-3.357335	-1.239934
1	-1.818681	-2.550653	-2.750392
6	-2.381639	3.352865	-0.617728
1	-3.210963	3.145368	0.067428
1	-2.198134	4.433116	-0.631983
1	-2.666988	3.028080	-1.622303
7	1.205269	-0.026612	1.719921
6	1.911210	-0.166401	2.930583
6	3.306424	0.015559	2.863487
6	1.338011	-0.470375	4.182934
6	4.102168	-0.099757	4.000027
1	3.741394	0.248843	1.895850
6	2.144211	-0.584382	5.316437
1	0.266144	-0.613266	4.253476
6	3.526488	-0.401282	5.237851
1	5.177140	0.046038	3.919868
1	1.682893	-0.819261	6.273554
1	4.145776	-0.491801	6.126558

Structure NCO12
B3LYP/GBS(1) = -1710.243962a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1710.627544a.u.
Enthalpy Correction = 0.422499
Gibbs Free Energy Correction = 0.335541

Atomic No	x-coord	y-coord	z-coord
6	-1.714522	-2.634980	0.684302
6	-0.384105	-2.926106	0.693940
15	-2.143732	-0.925782	0.301273
7	0.584540	-1.973643	0.498698
6	1.919435	-2.287941	0.551898
6	2.898535	-1.353260	0.418170
77	0.000320	0.046770	0.213160
15	2.342083	0.341111	0.171643
8	-1.883904	1.989055	-0.986210

6	-0.632100	1.926621	-0.366462
1	0.073903	2.563401	-0.920631
6	-2.310877	3.316424	-1.282265
1	-1.572987	3.837388	-1.910909
1	-3.252868	3.233742	-1.830822
1	-2.471047	3.897178	-0.365936
1	-2.456770	-3.411803	0.840660
1	-0.041215	-3.949732	0.869631
1	2.173620	-3.339343	0.712716
1	3.947433	-1.626259	0.479395
6	-0.290687	1.416436	1.676078
6	3.180299	1.392789	1.434672
1	4.267235	1.268780	1.375533
1	2.929358	2.445297	1.268914
1	2.834790	1.105632	2.430915
6	-3.368366	-0.322540	1.539016
1	-3.660341	0.696643	1.268848
1	-4.256504	-0.963601	1.557746
1	-2.913148	-0.302652	2.532160
6	-3.129326	-0.974994	-1.259576
1	-4.040849	-1.568397	-1.126338
1	-3.382283	0.048812	-1.544712
1	-2.524499	-1.423689	-2.052761
6	3.092783	0.933332	-1.412502
1	2.809620	1.976726	-1.587973
1	4.185685	0.860262	-1.383858
1	2.716832	0.325344	-2.240186
8	-0.716250	2.504526	0.995166
7	-0.130224	1.475738	2.932739
6	0.318668	0.493795	3.817020
6	1.114547	0.928510	4.896081
6	-0.026735	-0.869532	3.753225
6	1.570638	0.030733	5.858633
1	1.354869	1.985827	4.960015
6	0.423727	-1.760163	4.727901
1	-0.644408	-1.228213	2.939021
6	1.227453	-1.321906	5.782387
1	2.188052	0.391345	6.677876
1	0.140070	-2.808052	4.659731
1	1.574359	-2.021678	6.537919

Structure NCO14
B3LYP/GBS(1) = -1710.245005a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1710.627995a.u.
Enthalpy Correction = 0.422784
Gibbs Free Energy Correction = 0.336015

Atomic No	x-coord	y-coord	z-coord
6	-3.001542	-2.348906	-0.444753
6	-3.622198	-1.135595	-0.410957
15	-1.205088	-2.320010	-0.565990
7	-2.932035	0.045289	-0.381722
6	-3.572410	1.251856	-0.354200
6	-2.902643	2.439732	-0.309653
77	-0.794196	0.003464	-0.296802
15	-1.108268	2.333844	-0.335387
8	-0.518722	-1.117517	2.461532
6	-0.066654	-0.109027	1.644054
1	-0.212121	0.865917	2.133277

6	-1.753913	-0.830719	3.109809
1	-2.575276	-0.791954	2.385277
1	-1.925381	-1.639398	3.822650
1	-1.700123	0.124027	3.652062
1	-3.577663	-3.268922	-0.475582
1	-4.714345	-1.070611	-0.404930
1	-4.666195	1.232976	-0.371104
1	-3.438925	3.383643	-0.291635
6	1.220139	-0.085186	-0.074359
8	1.280036	-0.326847	1.312461
6	-0.515993	3.169103	-1.875074
1	-0.879900	4.201542	-1.924911
1	0.577998	3.164507	-1.902192
1	-0.881579	2.618316	-2.745630
6	-0.799693	-2.991722	-2.247064
1	0.285078	-3.009355	-2.392944
1	-1.194108	-4.007932	-2.358659
1	-1.246993	-2.356251	-3.016833
6	-0.518383	-3.638566	0.522228
1	-0.994009	-4.601258	0.304281
1	0.558869	-3.722420	0.346486
1	-0.674717	-3.366030	1.566020
6	-0.461579	3.455438	0.982232
1	0.633150	3.450900	0.967020
1	-0.816699	4.479545	0.822873
1	-0.802663	3.116268	1.964350
7	2.348519	0.006344	-0.662916
6	2.441257	0.274384	-2.034621
6	3.630747	0.881505	-2.483913
6	1.462326	-0.040192	-3.000436
6	3.821941	1.187160	-3.829160
1	4.394161	1.106353	-1.744905
6	1.659308	0.263225	-4.348276
1	0.553238	-0.542412	-2.683172
6	2.836834	0.881574	-4.773446
1	4.748427	1.661342	-4.144555
1	0.889484	0.004692	-5.072536
1	2.989643	1.111415	-5.824543

Structure NCO14-TS
B3LYP/GBS(1) = -1710.230981a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1710.615284a.u.
Enthalpy Correction = 0.420591
Gibbs Free Energy Correction = 0.332009
Imaginary Freq = -464.8i

Atomic No	x-coord	y-coord	z-coord
6	-3.131300	-1.953975	-0.130480
6	-3.699554	-0.723158	0.007266
15	-1.354178	-1.968362	-0.407369
7	-2.967582	0.434109	0.010417
6	-3.572534	1.657531	0.069004
6	-2.873974	2.827725	0.002373
77	-0.860027	0.325057	-0.187287
15	-1.101645	2.660715	-0.238295
8	-0.656391	-0.691976	2.656539
6	-0.019131	0.199308	1.817786
1	-0.149808	1.231050	2.190142
6	-1.829705	-0.194622	3.290192

1	-2.624575	-0.019484	2.557461
1	-2.144367	-0.957900	4.004614
1	-1.619520	0.739141	3.830482
1	-3.739786	-2.853248	-0.124190
1	-4.782439	-0.619281	0.119805
1	-4.661600	1.665424	0.169313
1	-3.380728	3.786506	0.055056
6	1.108821	0.128436	-0.271893
8	1.206408	-0.175412	1.489439
6	-0.673902	3.448715	-1.857514
1	-0.994162	4.496334	-1.886561
1	0.408401	3.397347	-2.015269
1	-1.169766	2.902017	-2.664375
6	-1.073502	-2.647981	-2.106330
1	0.001238	-2.677627	-2.313698
1	-1.488240	-3.657495	-2.204635
1	-1.552230	-1.992579	-2.839277
6	-0.592959	-3.258725	0.663873
1	-1.088240	-4.226013	0.523283
1	0.467416	-3.356196	0.410081
1	-0.669339	-2.939089	1.704168
6	-0.267162	3.798857	0.956762
1	0.816146	3.771945	0.800112
1	-0.621420	4.827184	0.823738
1	-0.480620	3.484698	1.982283
7	2.175459	0.073101	-0.881966
6	3.515873	-0.207709	-0.595403
6	4.442572	0.014272	-1.627800
6	3.968874	-0.712080	0.638536
6	5.796302	-0.252579	-1.435112
1	4.076465	0.395734	-2.576280
6	5.325668	-0.979877	0.817155
1	3.256427	-0.882814	1.435062
6	6.244878	-0.752625	-0.210492
1	6.500575	-0.073931	-2.243717
1	5.667241	-1.370620	1.772665
1	7.299889	-0.964968	-0.058651

Structure 16
B3LYP/GBS(1) = -229.0589028a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -229.1439237a.u.
Enthalpy Correction = 0.067993
Gibbs Free Energy Correction = 0.035657

Atomic No	x-coord	y-coord	z-coord
6	3.009770	2.393543	-0.095522
6	3.636802	1.185651	-0.132101
15	1.219042	2.316727	0.015080
7	2.955788	-0.000961	-0.086394
6	3.625059	-1.194373	-0.128333
6	2.986134	-2.395894	-0.087919
77	0.853658	0.009638	0.043895
15	1.196252	-2.301055	0.022390
6	-1.001173	0.019146	0.176570
1	3.570193	3.322489	-0.133001
1	4.726386	1.123967	-0.200175
1	4.715197	-1.143662	-0.196588
1	3.537365	-3.330437	-0.122435
6	0.535860	3.316258	-1.384125

1	-0.557167	3.340723	-1.321959
1	0.918741	4.343135	-1.361609
1	0.820247	2.846301	-2.329167
6	0.503207	-3.297823	-1.373941
1	0.875874	-4.328382	-1.348481
1	-0.590010	-3.311250	-1.311746
1	0.792251	-2.833404	-2.320306
6	0.683861	-3.301752	1.492512
1	-0.408725	-3.330589	1.560685
1	1.063840	-4.327647	1.424329
1	1.078324	-2.831306	2.396920
6	0.716536	3.326652	1.482303
1	1.106557	4.348573	1.411206
1	-0.375714	3.366384	1.550369
1	1.106364	2.854925	2.388050
7	-2.209064	0.025379	0.193494
6	-3.360609	0.032389	0.967247
6	-3.292437	0.033222	2.372402
6	-4.611990	0.038719	0.333342
6	-4.465800	0.040331	3.122659
1	-2.319426	0.028311	2.854432
6	-5.778882	0.045803	1.095665
1	-4.650007	0.037974	-0.751441
6	-5.712896	0.046648	2.490893
1	-4.405189	0.040938	4.207927
1	-6.743958	0.050677	0.596118
1	-6.624469	0.052177	3.081770

Structure OCN7-TS
B3LYP/GBS(1) = -1710.232838a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1710.618185 a.u.
Enthalpy Correction = 0.420167
Gibbs Free Energy Correction = 0.326755

Atomic No	x-coord	y-coord	z-coord
6	-2.864673	-1.320845	-1.956848
6	-2.686244	-0.018166	-2.306708
15	-2.089681	-1.825511	-0.412646
7	-1.958807	0.860273	-1.545358
6	-1.844859	2.177182	-1.899394
6	-1.178493	3.085727	-1.134517
77	-1.028608	0.165534	0.226334
15	-0.465390	2.445438	0.387458
8	-0.423998	-1.638259	2.407488
6	-0.241691	-0.433894	1.841954
1	0.464030	0.156631	2.451757
6	0.339394	-1.950905	3.583856
1	0.264060	-1.144098	4.321323
1	-0.084807	-2.867500	3.997130
1	1.389144	-2.115605	3.319573
1	-3.437690	-1.996559	-2.584464
1	-3.131072	0.376537	-3.224710
1	-2.324433	2.482582	-2.833957
1	-1.101725	4.126100	-1.435262
6	1.286207	-0.506150	-0.889314
8	0.870880	-0.963945	-1.912018
6	1.276259	3.059657	0.462876
1	1.303405	4.152384	0.382952
1	1.737763	2.758775	1.409060

1	1.853710	2.617998	-0.351126
6	-1.145795	-3.376150	-0.752177
1	-0.718154	-3.751023	0.183467
1	-1.796455	-4.144909	-1.184229
1	-0.335762	-3.148229	-1.448287
6	-3.439505	-2.429605	0.699946
1	-3.986725	-3.264443	0.247209
1	-3.003576	-2.753386	1.650308
1	-4.135323	-1.609105	0.895146
6	-1.245327	3.395283	1.777034
1	-0.798346	3.100624	2.732900
1	-1.111321	4.474616	1.642477
1	-2.314250	3.167997	1.807682
7	2.140611	-0.163618	-0.044784
6	3.531672	-0.300867	-0.281629
6	4.398931	0.089287	0.749804
6	4.073758	-0.797562	-1.479342
6	5.779446	-0.015998	0.589824
1	3.969363	0.473010	1.670526
6	5.456320	-0.898483	-1.630681
1	3.411361	-1.101539	-2.284353
6	6.317068	-0.510266	-0.601036
1	6.437584	0.290639	1.399065
1	5.862334	-1.283947	-2.562699
1	7.393292	-0.591015	-0.726069

Structure OCN12
B3LYP/GBS(1) = -1710.27348a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1710.657578a.u.
Enthalpy Correction = 0.423299
Gibbs Free Energy Correction = 0.336323

Atomic No	x-coord	y-coord	z-coord
6	-2.955613	-2.163507	-0.963479
6	-3.541558	-0.936247	-0.954023
15	-1.260960	-2.230755	-0.359049
7	-2.891152	0.191793	-0.520613
6	-3.481365	1.426003	-0.596537
6	-2.833360	2.574243	-0.257529
77	-0.874288	0.042087	0.135248
15	-1.131771	2.380941	0.290518
8	1.271047	-1.384665	1.783564
6	0.986018	-0.165527	1.106141
1	1.262131	0.663267	1.780177
6	0.807388	-1.377838	3.118571
1	-0.286681	-1.276482	3.172515
1	1.102761	-2.329700	3.567880
1	1.259328	-0.556021	3.698275
1	-3.494652	-3.039252	-1.311620
1	-4.570400	-0.808605	-1.302595
1	-4.515624	1.457462	-0.951225
1	-3.324790	3.539537	-0.329846
6	0.763791	0.129751	-1.039107
8	0.828201	0.344211	-2.236072
6	-0.074508	3.443422	-0.787652
1	-0.473942	4.461866	-0.842483
1	0.945497	3.481231	-0.390608
1	-0.040624	3.006136	-1.788606
6	-0.215581	-3.004268	-1.667434

1	0.798165	-3.148527	-1.279860
1	-0.626246	-3.972217	-1.974220
1	-0.166561	-2.334825	-2.529641
6	-1.219278	-3.500394	0.981332
1	-1.536999	-4.479253	0.604932
1	-0.198035	-3.565536	1.366254
1	-1.886518	-3.197282	1.793057
6	-0.995361	3.215948	1.936658
1	0.039429	3.167807	2.292193
1	-1.299991	4.266737	1.873647
1	-1.637285	2.701972	2.657528
7	1.767109	-0.097484	-0.129717
6	3.168881	0.018709	-0.278899
6	3.744442	0.327128	-1.523607
6	3.996881	-0.167792	0.840303
6	5.128368	0.457664	-1.629817
1	3.103144	0.462753	-2.385452
6	5.378410	-0.029085	0.714594
1	3.556937	-0.447205	1.790025
6	5.954892	0.285991	-0.517157
1	5.562109	0.698467	-2.597218
1	6.007207	-0.177553	1.589028
1	7.032367	0.389984	-0.610009

Structure OCN14- Flat surface and no minimum found. Structure reverts to 12.

Structure OCN14-TS
B3LYP/GBS(1) = -1710.240097a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1710.625348a.u.
Enthalpy Correction = 0.42058
Gibbs Free Energy Correction = 0.334002
Imaginary Freq = -419.2i

Atomic No	x-coord	y-coord	z-coord
6	3.712906	-0.192457	-1.090434
6	3.138713	0.942717	-1.580763
15	2.815498	-1.011684	0.232276
7	1.913053	1.390067	-1.169135
6	1.421329	2.593896	-1.593096
6	0.278946	3.141735	-1.091444
77	0.866363	0.305987	0.324299
15	-0.512774	2.229025	0.236922
8	0.211865	-1.818853	-1.658577
6	-0.503421	-0.947723	-0.854847
1	-1.072575	-0.240651	-1.477540
6	0.583006	-1.300273	-2.933159
1	1.314863	-0.492592	-2.840385
1	1.019860	-2.133335	-3.487873
1	-0.299945	-0.931736	-3.473638
1	4.681425	-0.528467	-1.447840
1	3.651067	1.543657	-2.336995
1	1.998524	3.117071	-2.360363
1	-0.091309	4.094954	-1.456179
6	-0.103493	-0.750449	1.646875
8	-0.388489	-1.147086	2.714505

6	-0.455890	3.290174	1.752544
1	-0.928839	4.261705	1.569756
1	-0.976984	2.787162	2.573801
1	0.585842	3.449468	2.044358
6	3.851070	-0.867006	1.760280
1	3.351050	-1.369372	2.594808
1	4.838734	-1.317124	1.609733
1	3.974779	0.190185	2.011017
6	2.818408	-2.829138	-0.069230
1	3.833547	-3.188241	-0.271893
1	2.427597	-3.340856	0.816344
1	2.160052	-3.050669	-0.910333
6	-2.323226	2.175255	-0.116496
1	-2.850328	1.683226	0.706445
1	-2.714695	3.191229	-0.241603
1	-2.514776	1.603697	-1.027506
7	-1.159931	-1.551842	0.203645
6	-2.551337	-1.497579	0.238811
6	-3.228102	-1.625572	1.476323
6	-3.347740	-1.378162	-0.928025
6	-4.617308	-1.584092	1.538218
1	-2.645763	-1.759800	2.379725
6	-4.739606	-1.337406	-0.848740
1	-2.874421	-1.371109	-1.905493
6	-5.390444	-1.428799	0.382133
1	-5.104683	-1.680854	2.506047
1	-5.319032	-1.252795	-1.765849
1	-6.475088	-1.404915	0.439062

8. MeNCS Structures and Energies

Structure SCN7-TS
B3LYP/GBS(1) = -1841.456271a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1841.79097862a.u.
Enthalpy Correction = 0.362762
Gibbs Free Energy Correction = 0.281002
Imaginary Freq = -210.4I

Atomic No	x-coord	y-coord	z-coord
6	-1.468894	-2.914982	0.365446
6	-0.124800	-3.126583	0.383038
15	-2.004253	-1.249721	-0.049149
7	0.784446	-2.138684	0.116886
6	2.128078	-2.382942	0.138364
6	3.057800	-1.419369	-0.113389
77	0.085352	-0.164386	-0.291809
15	2.417312	0.218783	-0.466121
8	-1.766310	1.708835	-1.545774
6	-0.531355	1.507420	-1.093898
1	0.146639	2.315641	-1.393156
6	-2.103816	3.042396	-1.951359
1	-1.336093	3.451313	-2.618572
1	-3.057911	2.980254	-2.477030
1	-2.198541	3.674283	-1.062777
1	-2.165227	-3.717994	0.586663
1	0.277310	-4.116730	0.614914
1	2.440893	-3.404932	0.370173
1	4.120089	-1.639798	-0.078245
6	-0.148365	1.116002	1.318113
6	3.231457	1.408773	0.682645

1	4.321807	1.320295	0.624234
1	2.939560	2.433281	0.429100
1	2.894862	1.189397	1.699286
6	-3.171675	-0.677985	1.256357
1	-3.595369	0.289643	0.968515
1	-3.983618	-1.400457	1.394807
1	-2.617705	-0.557253	2.190908
6	-3.097563	-1.396735	-1.533722
1	-3.954842	-2.047518	-1.327082
1	-3.453352	-0.403328	-1.821217
1	-2.522694	-1.817935	-2.363325
6	3.088274	0.728186	-2.115454
1	2.766181	1.748251	-2.352937
1	4.183582	0.694526	-2.124165
1	2.704271	0.051576	-2.883870
7	-0.512947	2.297306	0.948568
6	-0.725254	3.364251	1.914775
1	-0.211336	4.276247	1.584351
1	-1.795898	3.598163	1.999717
1	-0.351094	3.077671	2.907302
16	0.194197	0.365971	2.795828

Structure SCN12
B3LYP/GBS(1) = -1841.48880454 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1841.8214527 a.u.
Enthalpy Correction = 0.365326
Gibbs Free Energy Correction = 0.284061

Atomic No	x-coord	y-coord	z-coord
6	-3.108920	-1.934363	-1.034413
6	-3.577006	-0.658595	-1.062041
15	-1.472556	-2.153054	-0.314531
7	-2.843960	0.410752	-0.608903
6	-3.334285	1.687881	-0.682077
6	-2.614722	2.776928	-0.296362
77	-0.868686	0.090602	0.087996
15	-0.959336	2.441277	0.318186
8	1.055937	-1.575551	1.683871
6	0.941966	-0.294479	1.082543
1	1.266311	0.466132	1.809527
6	2.042693	-1.677652	2.698418
1	1.873528	-0.940964	3.498384
1	1.961292	-2.682172	3.123568
1	3.063444	-1.542135	2.311504
1	-3.712006	-2.760431	-1.398405
1	-4.573575	-0.439294	-1.455153
1	-4.349071	1.804246	-1.072887
1	-3.025457	3.778789	-0.373873
6	0.783791	0.069991	-1.061061
6	0.212352	3.510846	-0.623314
1	-0.120886	4.554382	-0.611413
1	1.211979	3.450260	-0.179915
1	0.267742	3.150694	-1.653757
6	-0.466817	-3.186156	-1.460473
1	0.486809	-3.424202	-0.978809
1	-0.989148	-4.116699	-1.707950
1	-0.267607	-2.618222	-2.372753

6	-1.685951	-3.251747	1.155202
1	-2.087237	-4.228752	0.863064
1	-0.715539	-3.371451	1.642856
1	-2.376043	-2.777585	1.858793
6	-0.862614	3.152948	2.025521
1	0.145169	3.011131	2.430774
1	-1.095630	4.223724	2.021048
1	-1.575550	2.635862	2.673744
7	1.734537	-0.183783	-0.154304
16	0.879927	0.312026	-2.700826
6	3.162347	-0.354079	-0.358944
1	3.723516	0.293934	0.325977
1	3.460483	-1.395196	-0.185453
1	3.395400	-0.083240	-1.391114

Structure SCN14-TS
B3LYP/GBS(1) = -1841.42772537a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1841.76019618a.u.
Enthalpy Correction = 0.362464
Gibbs Free Energy Correction = 0.282776
Imaginary Freq = -542.8i

Atomic No	x-coord	y-coord	z-coord
6	2.673998	-1.835736	-0.181408
6	1.601234	-2.634811	0.081976
15	2.294309	-0.129852	-0.590344
7	0.321258	-2.158228	0.136918
6	-0.737956	-3.013321	0.224523
6	-2.028967	-2.597993	0.085849
77	-0.030188	-0.066267	-0.255096
15	-2.256904	-0.863404	-0.311361
8	1.083166	0.627211	2.478022
6	-0.100789	0.927588	1.852867
1	-0.956489	0.426350	2.335036
6	1.120686	-0.642788	3.124531
1	1.048027	-1.453311	2.394468
1	2.077186	-0.691862	3.648108
1	0.303841	-0.729492	3.854488
1	3.681996	-2.238782	-0.200442
1	1.736521	-3.705572	0.260599
1	-0.510062	-4.068659	0.401090
1	-2.856513	-3.295678	0.172401
6	-0.251741	1.789611	-0.596766
6	-3.043703	-0.762385	-1.983471
1	-3.991483	-1.312141	-2.011528
1	-3.226307	0.286013	-2.241951
1	-2.359797	-1.187938	-2.722633
6	2.776360	0.140037	-2.355769
1	2.540625	1.169561	-2.644717
1	3.846635	-0.041627	-2.506599
1	2.203289	-0.541912	-2.989639
6	3.464057	0.976529	0.305854
1	4.499852	0.653556	0.151852
1	3.347068	1.998999	-0.067076
1	3.216435	0.970122	1.368220
6	-3.634316	-0.261378	0.769592
1	-3.903814	0.765217	0.503450
1	-4.515940	-0.901321	0.647858
1	-3.326394	-0.285499	1.818386

7	-0.226973	2.191381	1.394481
6	-1.480316	2.854095	1.702857
1	-1.657556	3.636236	0.955726
1	-2.357088	2.183349	1.721081
1	-1.416291	3.346397	2.684618
16	-0.446057	3.133309	-1.443288

Structure NCS7-TS
B3LYP/GBS(1) = -1841.448678 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1841.78054023a.u.
Enthalpy Correction = 0.362784
Gibbs Free Energy Correction = 0.280407
Imaginary Freq = -167.4

Atomic No	x-coord	y-coord	z-coord
6	-1.619026	-2.783069	-0.149669
6	-0.282493	-3.050140	-0.196407
15	-2.075919	-1.042923	-0.248070
7	0.664320	-2.064358	-0.240585
6	1.992451	-2.361947	-0.370915
6	2.947618	-1.399619	-0.509000
77	0.030702	-0.029383	-0.353255
15	2.351609	0.298062	-0.571073
8	-1.814265	2.130160	-0.918438
6	-0.548026	1.764024	-0.711784
1	0.125840	2.621194	-0.862270
6	-2.103028	3.532640	-1.024054
1	-2.097884	3.973477	-0.022315
1	-1.363070	4.035083	-1.657245
1	-3.094736	3.617987	-1.471494
1	-2.347739	-3.586995	-0.103955
1	0.077317	-4.083551	-0.194751
1	2.268009	-3.420922	-0.361561
1	3.997651	-1.661816	-0.598100
6	0.080789	0.762953	2.031361
6	3.310394	1.255006	0.687126
1	4.386429	1.193496	0.488257
1	2.995575	2.303017	0.677463
1	3.102260	0.851415	1.680888
6	-3.211015	-0.672353	1.163098
1	-3.565545	0.359516	1.075586
1	-4.070401	-1.352361	1.170337
1	-2.665106	-0.766822	2.105141
6	-3.210029	-0.880274	-1.700276
1	-4.084465	-1.532445	-1.594155
1	-3.538444	0.159734	-1.784776
1	-2.667374	-1.152948	-2.609502
6	2.986648	1.023909	-2.153701
1	2.716571	2.084010	-2.214291
1	4.077008	0.935060	-2.219038
1	2.533013	0.497446	-2.997809
7	0.276162	-0.144813	2.833936
6	0.533175	-1.552602	2.861044
1	0.549518	-1.887306	3.903529

1	-0.240332	-2.111278	2.322416
1	1.503574	-1.781917	2.405767
16	-0.151941	2.420880	1.998922

Structure NCS12
B3LYP/GBS(1) = -1841.47139952a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1841.80597543a.u.
Enthalpy Correction = 0.364139
Gibbs Free Energy Correction = 0.284325

Atomic No	x-coord	y-coord	z-coord
6	1.200791	2.966376	-0.225154
6	-0.157412	3.056022	-0.317219
15	1.889323	1.303204	-0.251376
7	-0.967476	1.955992	-0.363420
6	-2.323795	2.064338	-0.459193
6	-3.147293	0.976296	-0.505337
77	-0.075672	0.011928	-0.306210
15	-2.342410	-0.630993	-0.478511
8	2.184622	-1.846800	-0.777363
6	0.847798	-1.857793	-0.318644
1	0.318740	-2.686945	-0.811146
6	2.800878	-3.122834	-0.799682
1	2.231628	-3.832255	-1.420659
1	3.799820	-2.995759	-1.226631
1	2.894746	-3.539293	0.214578
1	1.815733	3.860698	-0.189572
1	-0.647169	4.033701	-0.353548
1	-2.740892	3.075195	-0.496800
1	-4.224457	1.093626	-0.576646
6	0.051948	-0.529759	1.657046
6	-3.130210	-1.639359	0.851761
1	-4.218472	-1.663752	0.727725
1	-2.739524	-2.661292	0.823716
1	-2.883657	-1.206742	1.824519
6	3.062905	1.118048	1.156226
1	3.516107	0.124057	1.100495
1	3.845976	1.883337	1.120644
1	2.516615	1.197076	2.099320
6	2.998875	1.200398	-1.724582
1	3.804679	1.940725	-1.664430
1	3.417748	0.192215	-1.773798
1	2.413562	1.384934	-2.630210
6	-2.873199	-1.523639	-2.012120
1	-2.448606	-2.533200	-2.021360
1	-3.965332	-1.595859	-2.068050
1	-2.509306	-0.982640	-2.890450
7	-0.255228	0.037861	2.733146
6	-0.854096	1.356059	2.847017
1	-0.893428	1.634474	3.904871
1	-0.281929	2.117572	2.303941
1	-1.878932	1.362959	2.453453
16	0.731140	-2.173244	1.550412

Structure NCS14
B3LYP/GBS(1) = -1841.46785701a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1841.8020897a.u.
Enthalpy Correction = 0.364066
Gibbs Free Energy Correction = 0.283446

Atomic No	x-coord	y-coord	z-coord
6	2.381940	-1.849763	-1.008625
6	1.226057	-2.573674	-1.009509
15	2.219634	-0.082952	-0.699720
7	0.010851	-2.020016	-0.715709
6	-1.145709	-2.741437	-0.763020
6	-2.369601	-2.186558	-0.516856
77	-0.088363	0.070736	-0.209809
15	-2.387071	-0.417836	-0.197656
8	1.196080	-0.618417	2.401629
6	0.101204	0.046790	1.879661
1	-0.818753	-0.384138	2.293108
6	0.983631	-2.004966	2.656993
1	0.786476	-2.548449	1.727088
1	1.900042	-2.378362	3.118580
1	0.143667	-2.148328	3.351189
1	3.332487	-2.319737	-1.243198
1	1.240135	-3.641313	-1.250110
1	-1.060624	-3.803643	-1.013020
1	-3.272848	-2.787950	-0.557970
6	-0.127099	2.031244	0.359518
6	-3.355193	0.379837	-1.559794
1	-4.363519	-0.043996	-1.626525
1	-3.426740	1.457300	-1.380169
1	-2.839548	0.217041	-2.510534
6	2.707370	0.765444	-2.274691
1	2.661200	1.850841	-2.139036
1	3.723212	0.483807	-2.574006
1	2.013483	0.481262	-3.071258
6	3.561417	0.439920	0.447742
1	4.539509	0.119774	0.071417
1	3.549585	1.530280	0.542187
1	3.373395	0.006622	1.431062
6	-3.479928	-0.116005	1.261567
1	-3.544811	0.958754	1.458080
1	-4.485516	-0.510180	1.077878
1	-3.069414	-0.608060	2.147484
7	-0.279752	3.197791	-0.112804
6	-0.540647	3.327140	-1.535741
1	-1.436161	3.942716	-1.694655
1	0.291683	3.852317	-2.024359
1	-0.685115	2.359197	-2.050014
16	0.213544	1.848406	2.155990

Structure NCS14-TS
B3LYP/GBS(1) = -1841.46662547a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1841.8006926a.u.
Enthalpy Correction = 0.36293
Gibbs Free Energy Correction = 0.280888
Imaginary Freq = -255.5i

Atomic No	x-coord	y-coord	z-coord
6	2.431532	-2.027007	-0.560661
6	1.286783	-2.741114	-0.374217
15	2.236330	-0.243089	-0.698744
7	0.060591	-2.149336	-0.224422
6	-1.082556	-2.892028	-0.145444
6	-2.326654	-2.331374	-0.106443
77	-0.085207	-0.033237	-0.307285
15	-2.379778	-0.542899	-0.256108

8	1.136611	-0.187764	2.412167
6	0.039853	0.386981	1.795663
1	-0.880712	-0.044289	2.205639
6	0.908389	-1.467522	2.995681
1	0.631857	-2.205250	2.235661
1	1.846427	-1.761813	3.471173
1	0.119702	-1.410755	3.758439
1	3.389550	-2.527539	-0.664390
1	1.311771	-3.833984	-0.339654
1	-0.963709	-3.978999	-0.120029
1	-3.216096	-2.949869	-0.034685
6	-0.212138	1.939587	-0.406811
6	-3.293584	-0.124422	-1.809387
1	-4.305282	-0.545213	-1.801430
1	-3.354716	0.963781	-1.914535
1	-2.746975	-0.527150	-2.666727
6	2.761608	0.223232	-2.412054
1	2.662783	1.306031	-2.541581
1	3.800083	-0.069334	-2.604134
1	2.111940	-0.275266	-3.137200
6	3.511490	0.575525	0.345986
1	4.514908	0.214910	0.092870
1	3.463887	1.657739	0.190200
1	3.284283	0.370314	1.393187
6	-3.519613	0.112863	1.041320
1	-3.598355	1.200138	0.944812
1	-4.515813	-0.332620	0.943201
1	-3.128089	-0.116659	2.035849
7	-0.354917	2.975777	-1.048741
6	-0.353560	4.346865	-0.613863
1	0.461943	4.892713	-1.102192
1	-1.294232	4.830753	-0.900510
1	-0.230067	4.412707	0.477448
16	0.087855	2.174139	1.823657

Structure 18
B3LYP/GBS(1) = -1289.48306903a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1289.7346684a.u.
Enthalpy Correction = 0.297132
Gibbs Free Energy Correction = 0.223791

Atomic No	x-coord	y-coord	z-coord
6	-2.393477	-2.071843	-0.098631
6	-1.188444	-2.705357	-0.137110
15	-2.304437	-0.281544	0.012460
7	0.000835	-2.029837	-0.097225
6	1.190614	-2.704507	-0.137220
6	2.395160	-2.070087	-0.098826
77	0.000111	0.070361	0.028651
15	2.304724	-0.279862	0.012444
6	-0.000864	1.940586	0.134367
1	-3.325097	-2.628308	-0.131126
1	-1.132165	-3.795563	-0.202350
1	1.135110	-3.794750	-0.202484
1	3.327198	-2.625848	-0.131378
6	-3.307013	0.225972	1.484436
1	-3.324034	1.318301	1.562257
1	-4.336537	-0.143410	1.410696
1	-2.842965	-0.179081	2.387469
6	3.307009	0.228098	1.484472

1	4.336840	-0.140385	1.410550
1	3.323092	1.320413	1.562667
1	2.843355	-0.177650	2.387397
6	3.320421	0.403005	-1.377844
1	3.356803	1.495569	-1.310356
1	4.343786	0.011008	-1.350837
1	2.854616	0.127395	-2.327558
6	-3.320841	0.400360	-1.377802
1	-4.343859	0.007471	-1.350585
1	-3.358176	1.492897	-1.310401
1	-2.854980	0.125059	-2.327578
7	-0.001945	3.131368	0.274142
6	-0.002554	4.436712	-0.300815
1	-0.887785	4.993969	0.025947
1	0.881524	4.995277	0.026955
1	-0.001837	4.392572	-1.397574

9. Geometric and energetic details of selected CO_2 full ligand structures

Structure 1 (Full ligand)
B3LYP/GBS(1) = -1858.308996a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1858.721264a.u.
Enthalpy Correction = 0.660821
Gibbs Free Energy Correction = 0.555111

Atomic No	x-coord	y-coord	z-coord
1	-5.190014	4.358114	-1.326943
1	-5.939098	3.013545	-0.452540
6	-5.103116	3.721466	-0.438165
1	-5.243039	4.371834	0.436410
1	-2.612669	4.674928	-1.108283
6	-2.579615	3.649657	-0.743590
6	-3.773995	3.005168	-0.395505
1	-3.102969	-0.165254	-2.619928
1	-3.401024	-1.809830	-3.210497
1	-5.201607	-0.518741	-1.097938
1	-0.458602	3.562530	-0.950340
6	-1.343525	3.020588	-0.641025
6	-3.671911	1.661426	-0.024576
1	-4.583668	1.115181	0.203344
6	-2.877680	-1.223078	-2.445084
1	-5.349300	-2.190730	-1.639545
1	2.885383	-0.703361	-4.005625
6	-4.861972	-1.540577	-0.901783
1	-1.800805	-1.369318	-2.572972
1	2.378664	0.588181	-2.899789
1	1.339568	-0.826494	-3.140096
6	2.380032	-0.495306	-3.054047
6	-2.444576	0.991064	0.047772
6	-1.222288	1.691081	-0.173364
1	-5.224459	-1.839523	0.087246
6	-3.336687	-1.662300	-1.044857
1	0.458579	3.562536	0.950303
1	5.243037	4.371824	-0.436426

1	-3.060066	-2.717552	-0.916990
1	2.612640	4.674941	1.108256
6	1.343505	3.020595	0.640996
7	-0.000005	1.014477	-0.000014
6	2.579592	3.649668	0.743567
15	-2.282713	-0.821697	0.271314
6	1.222275	1.691085	0.173340
1	3.587468	-2.964033	-3.123535
6	3.093991	-1.232348	-1.910167
1	-4.127609	-0.864611	1.851522
1	4.127676	-0.864632	-1.851444
6	3.773977	3.005180	0.395497
6	5.103096	3.721482	0.438164
1	2.098234	-3.153814	-2.178337
6	2.444566	0.991071	-0.047783
1	5.189973	4.358155	1.326926
6	3.116194	-2.749710	-2.156223
6	3.671899	1.661436	0.024574
6	-3.093922	-1.232328	1.910209
1	5.939080	3.013563	0.452577
1	4.583661	1.115189	-0.203329
1	-2.378560	0.588222	2.899768
15	2.282714	-0.821691	-0.271312
1	-3.677855	-3.292345	1.388363
1	3.677908	-3.292353	-1.388256
6	-2.379913	-0.495263	3.054043
6	-3.116114	-2.749685	2.156297
1	-2.885218	-0.703306	4.005648
1	-3.587352	-2.963988	3.123631
1	-1.339443	-0.826443	3.140046
1	-2.098153	-3.153788	2.178384
1	5.224443	-1.839560	-0.087136
1	5.201568	-0.518714	1.097977
6	3.336645	-1.662267	1.044911
6	4.861933	-1.540559	0.901869
1	3.060019	-2.717521	0.917070
1	3.102908	-0.165168	2.619927
1	1.800729	-1.369215	2.572978
6	2.877609	-1.222994	2.445112
1	5.349239	-2.190675	1.639677
1	3.400926	-1.809728	3.210557
77	-0.000002	-1.067653	-0.000021
1	-0.069641	-2.413312	-0.856331
1	0.069640	-2.413321	0.856276

Structure 2 (Full Ligand)
B3LYP/GBS(1) = -1857.063574a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1857.464228a.u.
Enthalpy Correction = 0.64345
Gibbs Free Energy Correction = 0.538759

Atomic No	x-coord	y-coord	z-coord
1	-5.127007	4.197765	-1.677187
1	-5.886318	3.008416	-0.609072
6	-5.036654	3.692784	-0.707099
1	-5.148589	4.465429	0.065960
1	-2.510639	4.590242	-1.308015
6	-2.503961	3.577999	-0.907195
6	-3.722347	2.959454	-0.580312
1	-3.261974	-0.418834	-2.551981
1	-3.522383	-2.115870	-2.996529

1	-5.267122	-0.675427	-0.881813
1	-0.377256	3.451739	-1.040523
6	-1.284111	2.936711	-0.747563
6	-3.655575	1.632791	-0.153373
1	-4.582675	1.111902	0.071680
6	-2.993552	-1.451117	-2.301656
1	-5.412838	-2.377318	-1.320792
1	2.742713	-0.424130	-4.079050
6	-4.901009	-1.679496	-0.645585
1	-1.915596	-1.565657	-2.456771
1	2.372256	0.807905	-2.857391
1	1.239407	-0.524215	-3.133558
6	2.301677	-0.259708	-3.087535
6	-2.440746	0.946554	-0.012448
6	-1.205546	1.618352	-0.232819
1	-5.211155	-1.925918	0.375101
6	-3.381886	-1.786981	-0.852360
1	0.377246	3.451851	1.040134
1	5.148674	4.465322	-0.066339
1	-3.087967	-2.829509	-0.661231
1	2.510629	4.590363	1.307586
6	1.284105	2.936786	0.747253
7	0.000002	0.951221	-0.000073
6	2.503957	3.578081	0.906863
15	-2.274600	-0.831438	0.343292
6	1.205547	1.618380	0.232642
1	3.418453	-2.757154	-3.410581
6	3.030179	-1.114409	-2.039254
1	-4.077740	-0.786837	1.988905
1	4.077596	-0.786991	-1.988973
6	3.722347	2.959493	0.580086
6	5.036659	3.692818	0.706849
1	1.953320	-2.967798	-2.436525
6	2.440748	0.946553	0.012362
1	5.126943	4.197971	1.676854
6	2.987981	-2.604760	-2.412908
6	3.655578	1.632788	0.153269
77	0.000005	-1.057268	0.000116
6	-3.030331	-1.114264	2.039281
1	5.886317	3.008414	0.609014
1	4.582683	1.111868	-0.071693
1	-2.372422	0.808087	2.857344
15	2.274597	-0.831473	-0.343216
1	-3.551223	-3.230677	1.711876
1	3.551063	-3.230810	-1.711757
6	-2.301899	-0.259513	3.087571
6	-2.988178	-2.604595	2.413027
1	-2.743034	-0.423850	4.079055
1	-3.418718	-2.756922	3.410681
1	-1.239642	-0.524051	3.133714
1	-1.953524	-2.967646	2.436737
1	5.211134	-1.926009	-0.375256
1	5.267278	-0.675387	0.881520
6	3.382009	-1.786903	0.852398
6	4.901110	-1.679472	0.645439
1	3.088046	-2.829444	0.661410
1	3.262329	-0.418578	2.551895
1	1.915903	-1.565367	2.456948
6	2.993846	-1.450878	2.301704
1	5.412998	-2.377236	1.320662
1	3.522728	-2.115579	2.996587

Structure 5 (Full Ligand)
B3LYP/GBS(1) = -2130.067817a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2130.564582a.u.
Enthalpy Correction = 0.816059
Gibbs Free Energy Correction = 0.692504

Atomic No	x-coord	y-coord	z-coord
1	-1.567545	6.878857	-1.620473
1	-2.789065	6.284515	-0.485724
6	-1.710948	6.388378	-0.649802
1	-1.329903	7.077976	0.116078
1	0.787903	5.714726	-1.575733
6	0.287677	4.879163	-1.088960
6	-1.013181	5.049827	-0.593959
1	-2.465820	2.055194	-2.445737
1	-3.673801	0.834588	-2.883275
1	-4.243124	2.959795	-0.754303
1	1.959135	3.586736	-1.399006
6	0.963281	3.669406	-0.980087
6	-1.636168	3.915826	-0.066293
1	-2.662516	4.003104	0.280795
6	-2.840317	1.054243	-2.204069
1	-5.337854	1.636699	-1.154592
1	2.538795	-1.966081	-3.874135
6	-4.501152	1.925423	-0.505149
1	-2.041221	0.334013	-2.406696
1	2.730116	-0.520609	-2.863991
1	1.126130	-1.241261	-3.085131
6	2.191102	-1.468048	-2.960294
6	-0.993393	2.673318	0.016493
6	0.373639	2.543843	-0.356909
1	-4.867533	1.901744	0.526289
6	-3.321653	0.970847	-0.745407
1	2.818593	3.290070	0.540190
1	7.253167	1.238437	-0.602911
1	-3.644034	-0.059435	-0.557769
1	5.226527	3.047045	0.715833
6	3.254256	2.319158	0.341595
7	1.024498	1.313557	-0.164179
6	4.631592	2.173819	0.453010
15	-1.852660	1.106563	0.422835
6	2.413834	1.229235	0.004953
1	2.048737	-4.223716	-2.828109
6	2.421600	-2.381320	-1.745465
1	-3.181861	2.227692	2.108491
1	3.499892	-2.573964	-1.660324
6	5.271947	0.944896	0.239673
6	6.775946	0.815791	0.292044
1	0.613003	-3.573942	-2.023705
6	3.049037	-0.043756	-0.078548
1	7.196817	1.343508	1.156838
6	1.692376	-3.722775	-1.919279
6	4.444083	-0.153052	-0.004661
1	-5.233571	-2.114574	-0.369978
1	-3.796980	-2.863895	-2.334104
6	-2.562338	1.320639	2.142768
1	7.085268	-0.233011	0.359962
1	4.904061	-1.129961	-0.129941
1	-0.804457	2.403864	2.882545
15	1.927547	-1.486409	-0.166287

1	-4.323038	0.027027	1.899024
1	1.858165	-4.406028	-1.079746
8	-2.640923	-2.114923	-0.020757
6	-1.431112	1.549512	3.157842
6	-4.830005	-2.931544	0.238509
6	-3.444097	0.127205	2.543627
6	-3.460870	-3.707977	-1.721141
1	-4.803164	-2.600900	1.281912
1	-4.156577	-4.541130	-1.874453
1	-5.512461	-3.785678	0.162917
1	-1.856101	1.744359	4.150596
1	-3.797437	0.257735	3.574407
1	-2.477879	-4.023870	-2.084806
6	-3.421196	-3.310578	-0.235541
1	-0.786122	0.667468	3.228722
1	-2.886000	-0.812051	2.482529
1	3.772887	-3.989444	0.180611
1	4.558762	-2.779803	1.213097
6	2.373001	-2.652604	1.247474
6	3.688829	-3.437639	1.122138
1	1.541201	-3.370284	1.228700
1	3.133684	-1.170217	2.658944
1	1.372852	-1.356671	2.701694
6	2.317031	-1.896693	2.585938
6	-2.882977	-4.468776	0.625283
1	-2.838548	-4.165568	1.676916
1	3.751954	-4.169725	1.937316
1	-1.878977	-4.775741	0.314846
1	-3.535453	-5.346244	0.545214
1	2.417817	-2.604521	3.418181
6	-1.297821	-2.089069	-0.534020
1	-1.334446	-2.013110	-1.636345
1	-0.806716	-3.039470	-0.288742
77	-0.142696	-0.430223	0.065813
1	-0.555096	-1.235112	1.345980

Structure 6-TS (Full Ligand), - chosen since it is the highest energy transition structure in formation of **7**
B3LYP/GBS(1) = -2130.011181a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2130.515845a.u.
Enthalpy Correction = 0.808556
Gibbs Free Energy Correction = 0.684995
Imaginary Freq = -936.9i

Atomic No	x-coord	y-coord	z-coord
1	6.926965	2.148384	1.275350
1	7.022272	0.600792	0.423683
6	6.597574	1.609707	0.377397
1	7.054735	2.117240	-0.483248
1	4.802736	3.678380	0.609857
6	4.313334	2.730610	0.390196
6	5.091410	1.567310	0.271171
1	3.777106	-1.278562	2.407756
1	3.329852	-2.888420	3.003301
1	4.973427	-2.568517	0.429464
1	2.386240	3.638801	0.385638
6	2.933960	2.714643	0.249471
6	4.399143	0.373040	0.071214
1	4.970917	-0.548940	0.011273
6	3.012418	-2.060606	2.356951

1	4.363277	-4.088085	1.078874
1	-2.428468	2.097984	4.069336
6	4.116721	-3.249360	0.415228
1	2.084593	-1.649288	2.762321
1	-1.410440	2.754559	2.772656
1	-1.090572	1.136450	3.414022
6	-1.884079	1.843593	3.151059
6	3.001863	0.319177	-0.038378
6	2.221878	1.515170	-0.024815
1	4.020877	-3.651481	-0.597209
6	2.830813	-2.568404	0.917122
1	1.481616	3.703945	-1.563588
1	-2.201856	6.842620	-0.364537
1	2.035850	-3.328768	0.933779
1	0.035223	5.636263	-1.875565
6	0.480172	3.679223	-1.150434
7	0.852063	1.426043	-0.193164
6	-0.350386	4.772033	-1.336734
15	2.060188	-1.235712	-0.182364
6	0.045420	2.515079	-0.456748
1	-4.036083	0.204506	3.627537
6	-2.854175	1.240007	2.125433
1	3.508748	-1.925581	-1.992908
1	-3.623403	1.992435	1.907554
6	-1.671587	4.793108	-0.856216
6	-2.544537	6.016982	-1.003429
1	-2.798060	-0.810736	2.862709
6	-1.331933	2.482244	-0.093466
1	-2.546474	6.393283	-2.034647
6	-3.535872	-0.022083	2.677493
6	-2.136982	3.622657	-0.259394
1	-4.706093	-2.924313	-0.942071
77	-0.103840	-0.486224	0.403584
1	-2.811712	-3.375697	-2.561019
6	2.417723	-1.804403	-1.947132
1	-3.582824	5.801493	-0.728111
1	-3.166563	3.597738	0.088169
1	2.564083	0.216598	-2.777303
15	-2.002901	0.884563	0.486405
1	1.963158	-3.937787	-1.588646
1	-4.289441	-0.424318	1.992030
8	-2.286999	-2.403436	-0.128748
6	2.012329	-0.711746	-2.948234
6	-4.284098	-3.649383	-0.238477
6	-0.970589	-2.102179	-0.183096
6	1.754443	-3.141054	-2.311454
6	-2.431576	-4.136783	-1.871729
1	-4.522099	-3.322789	0.778937
1	-2.894519	-5.096531	-2.127062
1	-4.763584	-4.618526	-0.413144
1	2.220219	-1.049356	-3.971711
1	2.113941	-3.481459	-3.290688
1	-1.353276	-4.237085	-2.029059
6	-2.768715	-3.760640	-0.423816
1	0.943162	-0.488454	-2.867595
1	-0.399843	-2.994678	-0.466980
1	0.669238	-3.021133	-2.385204
1	-5.105369	1.353780	0.415069
1	-4.531579	2.314098	-0.963588
6	-3.418416	0.443562	-0.686782
6	-4.695240	1.295671	-0.598310
1	-3.663574	-0.578187	-0.383128
1	-2.624564	1.386965	-2.492040

1	-2.031515	-0.261259	-2.222008
6	-2.905424	0.389928	-2.134621
6	-2.176438	-4.754156	0.583399
1	-2.415276	-4.447705	1.607061
1	-5.469157	0.846917	-1.234761
1	-1.088073	-4.826794	0.492191
1	-2.592735	-5.753636	0.415191
1	-3.694507	0.005976	-2.794443
1	0.516908	0.095810	1.968296
1	-0.070431	-0.812955	2.026576

Structure 7 (Full Ligand)
B3LYP/GBS(1) = -2128.876221a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2129.366179a.u.
Enthalpy Correction = 0.795467
Gibbs Free Energy Correction = 0.672809

Atomic No	x-coord	y-coord	z-coord
1	-1.738908	6.880236	-1.515838
1	-3.069294	6.156033	-0.600226
6	-1.986563	6.324032	-0.603279
1	-1.758015	6.984528	0.244920
1	0.640593	5.821820	-1.243342
6	0.132060	4.939288	-0.858322
6	-1.226563	5.021135	-0.521225
1	-2.441523	1.871123	-2.600296
1	-3.603263	0.618338	-3.075327
1	-4.342811	2.772939	-1.038739
1	1.897857	3.751554	-1.016285
6	0.856156	3.761566	-0.719048
6	-1.842820	3.833428	-0.118624
1	-2.904841	3.854389	0.111431
6	-2.812493	0.869184	-2.356375
1	-5.384725	1.407350	-1.435602
1	2.585784	-1.326280	-4.042100
6	-4.582818	1.741119	-0.764014
1	-1.987166	0.161027	-2.482342
1	2.835642	-0.039765	-2.845518
1	1.206243	-0.670444	-3.131284
6	2.264220	-0.947240	-3.063568
6	-1.147959	2.621774	-0.011368
6	0.260038	2.574832	-0.225387
1	-4.989045	1.742062	0.252993
6	-3.367357	0.815339	-0.923397
1	2.609432	3.329446	0.974557
1	7.174201	1.555446	-0.219423
1	-3.685613	-0.215803	-0.729298
1	5.021889	3.164919	1.227330
6	3.098874	2.405714	0.690987
7	0.941437	1.370628	-0.014001
6	4.475645	2.304129	0.844697
15	-1.953379	1.007684	0.306661
6	2.321665	1.325715	0.202333
1	2.040571	-3.683290	-3.319608
6	2.476986	-2.022193	-1.986407
1	-3.417407	2.084779	1.919530
1	3.551056	-2.244834	-1.923069
6	5.177112	1.131723	0.526588
6	6.682437	1.058156	0.628370
1	0.640508	-3.124116	-2.387852
6	3.015661	0.096205	0.003432

1	7.049611	1.545483	1.540004
6	1.719178	-3.312504	-2.338131
6	4.410227	0.035280	0.125342
1	-4.818388	-2.794965	-0.870046
77	-0.159135	-0.437430	-0.004525
1	-2.871624	-3.762732	-2.155393
6	-2.764005	1.204140	1.991647
1	7.032483	0.019985	0.642348
1	4.918980	-0.900599	-0.091322
1	-1.113623	2.383876	2.820757
15	1.952296	-1.356195	-0.310077
1	-4.420601	-0.204285	1.655094
1	1.892747	-4.113943	-1.610925
8	-2.435284	-2.268201	0.023186
6	-1.691790	1.485105	3.056595
6	-4.521699	-3.370125	0.013149
6	-1.094217	-2.084553	0.013032
6	-3.615726	-0.015482	2.373344
6	-2.595298	-4.352171	-1.274945
1	-4.814882	-2.808577	0.905704
1	-3.101239	-5.322198	-1.335894
1	-5.067198	-4.320000	0.006153
1	-2.165297	1.631715	4.035922
1	-4.076274	0.145211	3.356587
1	-1.516981	-4.536312	-1.309118
6	-3.012131	-3.621481	0.007871
1	-0.991915	0.645877	3.134437
1	-0.593194	-3.065623	0.015780
1	-2.999361	-0.918353	2.428936
1	3.922432	-3.787137	-0.259107
1	4.600632	-2.721658	0.986368
6	2.412687	-2.701696	0.929280
6	3.771802	-3.396940	0.752807
1	1.628521	-3.454154	0.760484
1	2.993820	-1.399280	2.583507
1	1.253015	-1.718370	2.498125
6	2.242960	-2.165276	2.360507
6	-2.589732	-4.385165	1.269360
1	-2.872996	-3.826042	2.167180
1	3.842005	-4.245856	1.445314
1	-1.509480	-4.558583	1.299479
1	-3.085244	-5.361922	1.300395
1	2.365513	-2.980266	3.085294

Structure 12 (Full Ligand)
B3LYP/GBS(1) = -2317.444475a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2318.001155a.u.
Enthalpy Correction = 0.813274
Gibbs Free Energy Correction = 0.686687

Atomic No	x-coord	y-coord	z-coord
1	-1.284434	6.954645	-1.765804
1	-2.527106	6.441162	-0.614648
6	-1.446003	6.499947	-0.780575
1	-1.039002	7.197549	-0.035867
1	1.054474	5.725285	-1.618322
6	0.510099	4.914940	-1.136461
6	-0.798552	5.138773	-0.682846
1	-2.007654	1.928862	-2.604606
1	-3.281373	0.792608	-3.081033
1	-3.904577	3.137425	-1.214587

1	2.143891	3.561327	-1.373689
6	1.137706	3.684748	-0.991016
6	-1.475897	4.036713	-0.157237
1	-2.507387	4.167424	0.159190
6	-2.510808	0.995963	-2.326511
1	-5.049588	1.863766	-1.638133
1	2.147697	-1.146824	-4.130273
6	-4.272658	2.150384	-0.917605
1	-1.778744	0.182585	-2.362401
1	2.666938	-0.000197	-2.880422
1	0.952546	-0.412641	-3.045553
6	1.970518	-0.814451	-3.099733
6	-0.880214	2.772313	-0.038388
6	0.489526	2.589341	-0.369803
1	-4.755928	2.242257	0.060585
6	-3.156767	1.095988	-0.935026
1	2.925612	3.246358	0.644102
1	7.332283	1.156066	-0.507036
1	-3.584724	0.116878	-0.700445
1	5.329110	2.933139	0.833737
6	3.342712	2.275815	0.405997
7	1.093297	1.344568	-0.144065
6	4.714637	2.089674	0.523819
15	-1.818927	1.259135	0.378647
6	2.482445	1.222071	0.016445
1	1.469044	-3.519745	-3.523262
6	2.151241	-1.997975	-2.135587
1	-3.335501	2.499208	1.783932
1	3.192839	-2.339741	-2.203770
6	5.324896	0.853812	0.265489
6	6.823389	0.681071	0.342889
1	0.175425	-2.822802	-2.538430
6	3.085701	-0.056134	-0.136243
1	7.235025	1.132217	1.254077
6	1.217629	-3.156695	-2.518962
6	4.474986	-0.209754	-0.045480
1	-4.859876	-1.858942	-1.634011
77	-0.114855	-0.366741	0.153990
1	-2.908362	-3.022464	-2.754768
6	-2.712416	1.617218	1.987588
1	7.104497	-0.377657	0.340367
1	4.911273	-1.192670	-0.203235
1	-1.099210	2.842917	2.818973
15	1.919248	-1.443450	-0.352255
1	-4.388018	0.234823	1.635486
1	1.287512	-4.008777	-1.833937
8	-2.620169	-1.949506	-0.334150
6	-1.713955	1.981559	3.099347
6	-4.830233	-2.597197	-0.825349
6	-1.301278	-2.092839	0.071286
6	-3.634560	0.457250	2.398769
6	-2.913440	-3.769132	-1.953350
1	-5.176549	-2.117017	0.095790
1	-3.569679	-4.593929	-2.254135
1	-5.524213	-3.407366	-1.074695
1	-2.265951	2.243653	4.010841
1	-4.163619	0.722661	3.322411
1	-1.901971	-4.176535	-1.853263
6	-3.409946	-3.141144	-0.641935
1	-1.051230	1.143015	3.328973
1	-0.851707	-2.973859	-0.394810
1	-3.067996	-0.458473	2.587965
1	3.322963	-4.214228	-0.821808

1	4.530047	-3.270474	0.067671
6	2.469793	-2.888433	0.729154
6	3.573163	-3.795138	0.157111
1	1.550541	-3.484578	0.810229
1	3.768506	-1.826450	2.131947
1	2.056756	-1.785047	2.589978
6	2.838727	-2.403622	2.144177
6	-3.376416	-4.156499	0.508902
1	-3.698892	-3.690334	1.444018
1	3.731075	-4.636627	0.842999
1	-2.371932	-4.560168	0.666050
1	-4.046720	-4.994614	0.284062
1	2.989396	-3.275011	2.793200
6	-0.501715	-1.297588	1.885214
8	-0.166926	-1.026708	3.016877
8	-1.240832	-2.372875	1.548182

Structure 15 (Full Ligand)
B3LYP/GBS(1) = -1970.492543a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1970.936869a.u.
Enthalpy Correction = 0.655048
Gibbs Free Energy Correction = 0.545672

Atomic No	x-coord	y-coord	z-coord
1	5.165606	4.415437	1.542618
1	5.910018	3.172320	0.526529
6	5.067578	3.869030	0.596284
1	5.185269	4.605042	-0.210905
1	2.556882	4.795524	1.222172
6	2.536950	3.776823	0.838428
6	3.745308	3.144738	0.505296
1	3.159082	-0.180382	2.593229
1	3.460775	-1.860280	3.075468
1	5.231418	-0.444988	1.006457
1	0.412660	3.674950	0.998482
6	1.308751	3.144209	0.700964
6	3.660593	1.810363	0.105334
1	4.579859	1.276202	-0.120922
6	2.927702	-1.224964	2.357218
1	5.383628	-2.147415	1.441999
1	-2.763493	-0.348678	4.055184
6	4.883248	-1.451954	0.756443
1	1.851629	-1.374001	2.492329
1	-2.333510	0.899948	2.870456
1	-1.250757	-0.477016	3.131329
6	-2.302103	-0.174631	3.075010
6	2.436521	1.135235	-0.004322
6	1.205249	1.818257	0.209873
1	5.221809	-1.691547	-0.256907
6	3.360980	-1.578832	0.924884
1	-0.412757	3.674949	-0.998412
1	-5.184515	4.606586	0.209314
1	3.082091	-2.625486	0.739731
1	-2.556994	4.795489	-1.222112
6	-1.308847	3.144187	-0.700920
7	-0.000028	1.141839	0.000015
6	-2.537051	3.776780	-0.838389
15	2.288266	-0.653533	-0.315233
6	-1.205325	1.818227	-0.209842

1	-3.480085	-2.649029	3.317986
6	-3.044507	-0.981057	1.998024
1	4.082839	-0.624604	-1.949423
1	-4.082743	-0.624744	1.949543
6	-3.745401	3.144663	-0.505268
6	-5.067701	3.868879	-0.596446
1	-2.020271	-2.875850	2.338628
6	-2.436579	1.135187	0.004370
1	-5.166662	4.413325	-1.543824
6	-3.042616	-2.482513	2.325901
6	-3.660662	1.810302	-0.105284
77	-0.000001	-0.965304	-0.000031
6	3.044624	-0.980969	-1.997960
1	-5.910109	3.172367	-0.524406
1	-4.579921	1.276147	0.121013
1	2.333573	0.900003	-2.870419
15	-2.288263	-0.653582	0.315260
1	3.622055	-3.071659	-1.606823
1	-3.621862	-3.071771	1.606911
8	0.000297	-3.975991	-0.000175
6	2.302235	-0.174577	-3.074982
6	0.000112	-2.806615	-0.000119
6	3.042823	-2.482425	-2.325842
1	2.763688	-0.348591	-4.055132
1	3.480355	-2.648914	-3.317903
1	1.250908	-0.477019	-3.131363
1	2.020498	-2.875811	-2.338627
1	-5.221785	-1.691695	0.257110
1	-5.231526	-0.445123	-1.006239
6	-3.361041	-1.578895	-0.924808
6	-4.883300	-1.452077	-0.756259
1	-3.082100	-2.625540	-0.739689
1	-3.159306	-0.180414	-2.593144
1	-1.851797	-1.373978	-2.492343
6	-2.927868	-1.224988	-2.357161
1	-5.383702	-2.147550	-1.441789
1	-3.460956	-1.860316	-3.075391

10. GBS2 Basis set

This basis set is LANL2TZ+(3f).
It was obtained in the same way as described in Yates, B.F. J. Mol. Struct. (Theochem), 2000, 506, 223-232 for platinum.
a) The triple-zeta split was obtained by uncontracting the LANL2DZ basis set of Hay and Wadt to give: [341/321/21] -> [3311/3111/111]
b) The f-function exponent (0.9380) was taken from Frenking and co-workers (Chem. Phys. Lett., 1993, 208, 111-114) and then split according to the even scaling rule to give three exponents (3.752, 0.938, 0.2345).
c) Diffuse s, p and d functions were added using an even tempered extension of the two outermost exponents. This gave exponents of s=0.014304, p=0.008582 and d=0.05031.

```
-C -H -N -O -P -S 0
6-311+G(2d,p)
****
-Ir 0
 S   3 1.00       0.000000000000
      0.2350000000D+01 -0.1678464034D+01
      0.1582000000D+01  0.2095255043D+01
      0.5018000000D+00  0.4162934085D+00
 S   3 1.00       0.000000000000
      0.2350000000D+01  0.1646447056D+01
      0.1582000000D+01 -0.2274815077D+01
      0.5018000000D+00 -0.1049436036D+01
 S   1 1.00       0.000000000000
      0.2500000000D+00  0.1216779041D+01
 S   1 1.00       0.000000000000
      0.5980000000D-01  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.1430400000D-01  0.1000000000D+01
 P   3 1.00       0.000000000000
      0.2792000000D+01 -0.3889211885D+00
      0.1541000000D+01  0.9077515732D+00
      0.5285000000D+00  0.4691442862D+00
 P   1 1.00       0.000000000000
      0.5100000000D+00 -0.1170669243D+00
 P   1 1.00       0.000000000000
      0.9800000000D-01  0.1048900218D+01
 P   1 1.00       0.000000000000
      0.2900000000D-01  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.8582000000D-02  0.1000000000D+01
 D   1 1.00       0.000000000000
      0.1240000000D+01  0.5087021868D+00
 D   1 1.00       0.000000000000
      0.4647000000D+00  0.5862101848D+00
 D   1 1.00       0.000000000000
      0.1529000000D+00  0.1000000000D+01
 D   1 1.00       0.000000000000
      0.5031000000D-01  0.1000000000D+01
 F   1 1.00       0.000000000000
      3.7520000000D+00  0.1000000000D+01
 F   1 1.00       0.000000000000
      0.9380000000D+00  0.1000000000D+01
 F   1 1.00       0.000000000000
      0.2345000000D+00  0.1000000000D+01
 ****

Ir 0
lanl2dz
```

11. References, full Gaussian[3] citation and Arakawa[4] citation

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12. Parameters for MTBE solvation calculations

EPS = 2.6 (dielectric constant)
DENSITY = 0.00503 (solvent density in molecules/ $Å^3$)
RSOLVE = 2.95 (solvent radius in Å)