

Supporting Information

1,3-Dipolar Cycloaddition Reactions of Low-Valent Rhodium and Iridium with Arylnitrile *N*-Oxides

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Table S1. Intramolecular distances of the metalocycle product **1d-2a** (in Å) calculated with different methods and basis sets. See Figure 4 in the main text for atom labelling.

distance	B3LYP/ 6-31G(d)+SDD(Rh,Ir)	B3LYP-D3/ 6-31G(d)+SDD(Rh,Ir)	B3LYP-D3/ 6-31+G(d)+SDD(Rh,Ir)	SMD_{THF}/B3LYP-D3/ 6-31G(d)+SDD(Rh,Ir)	X-ray
R(1,2)	2.415	2.368	2.375	2.391	2.346
R(1,3)	2.408	2.365	2.264	2.265	2.330
R(1,4)	2.311	2.279	2.348	2.369	2.234
R(1,5)	2.287	2.271	2.268	2.275	2.260
R(1,11)	2.381	2.344	2.279	2.296	2.282
R(1,13)	2.272	2.254	2.367	2.389	2.232
R(1,25)	1.998	2.003	1.997	1.984	1.989
R(1,29)	2.035	2.028	2.040	2.027	2.016
R(2,41)	1.853	1.842	1.851	1.845	1.834
R(2,52)	1.862	1.854	1.847	1.843	1.841
R(2,63)	1.855	1.846	1.846	1.839	1.839
R(3,4)	1.699	1.711	1.703	1.700	1.690
R(3,5)	1.685	1.693	1.829	1.820	1.681
R(3,7)	1.695	1.696	1.777	1.781	1.706
R(3,9)	1.691	1.691	1.800	1.800	1.706
R(4,9)	1.793	1.788	1.695	1.691	1.791
R(4,11)	1.685	1.687	1.716	1.707	1.692
R(4,19)	1.792	1.786	1.692	1.688	1.802
R(4,24)	1.189	1.189	1.087	1.086	1.120
R(5,7)	1.807	1.800	1.793	1.791	1.802
R(5,13)	1.836	1.839	1.703	1.698	1.829
R(5,15)	1.786	1.785	1.805	1.803	1.801
R(7,9)	1.764	1.766	1.778	1.775	1.756
R(7,15)	1.775	1.775	1.777	1.774	1.756
R(7,17)	1.761	1.762	1.800	1.797	1.742
R(9,17)	1.783	1.785	1.764	1.764	1.775

R(9,19)	1.776	1.778	1.767	1.765	1.757
R(11,13)	1.698	1.710	1.685	1.684	1.702
R(11,19)	1.688	1.690	1.787	1.789	1.686
R(11,21)	1.693	1.693	1.786	1.789	1.684
R(13,15)	1.788	1.789	1.695	1.689	1.779
R(13,21)	1.804	1.801	1.689	1.686	1.788
R(15,17)	1.801	1.802	1.766	1.766	1.772
R(15,21)	1.777	1.779	1.764	1.762	1.761
R(17,19)	1.782	1.782	1.785	1.783	1.755
R(17,21)	1.762	1.765	1.782	1.781	1.746
R(19,21)	1.764	1.765	1.779	1.776	1.754
R(25,26)	1.213	1.214	1.213	1.213	1.198
R(25,27)	1.392	1.393	1.403	1.398	1.390
R(27,28)	1.409	1.411	1.412	1.422	1.426
R(28,29)	1.289	1.289	1.288	1.288	1.273
R(29,30)	1.491	1.487	1.492	1.491	1.476
R(30,32)	1.409	1.408	1.407	1.406	1.393
R(30,33)	1.402	1.402	1.410	1.407	1.364
R(31,34)	1.388	1.389	1.390	1.389	1.367
R(31,35)	1.399	1.399	1.400	1.398	1.349
R(32,35)	1.392	1.393	1.396	1.396	1.386
R(33,34)	1.389	1.388	1.386	1.387	1.374
R(34,40)	1.357	1.357	1.369	1.358	1.364

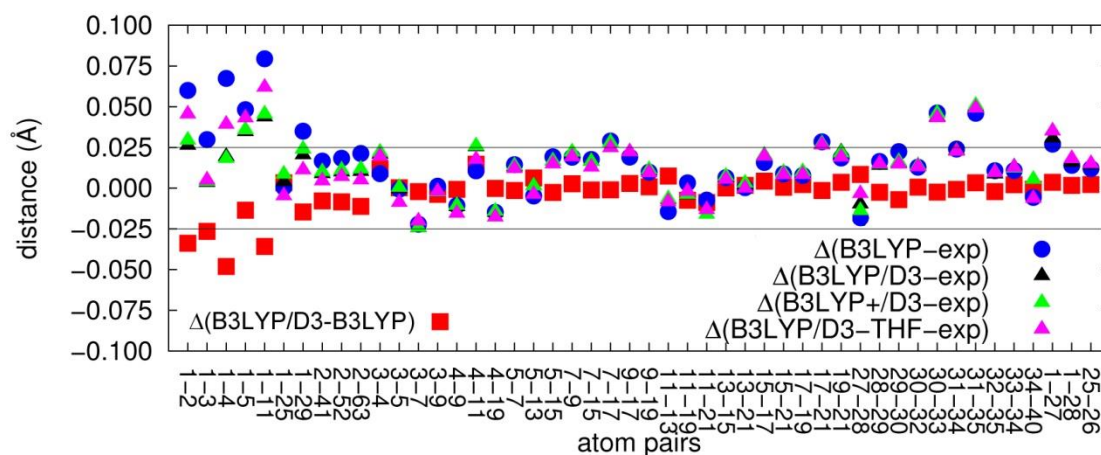


Figure S1. Differences between the calculated and the experimentally measured distances in **1d-2a**. See Figure 4 in the main text for atom labelling.

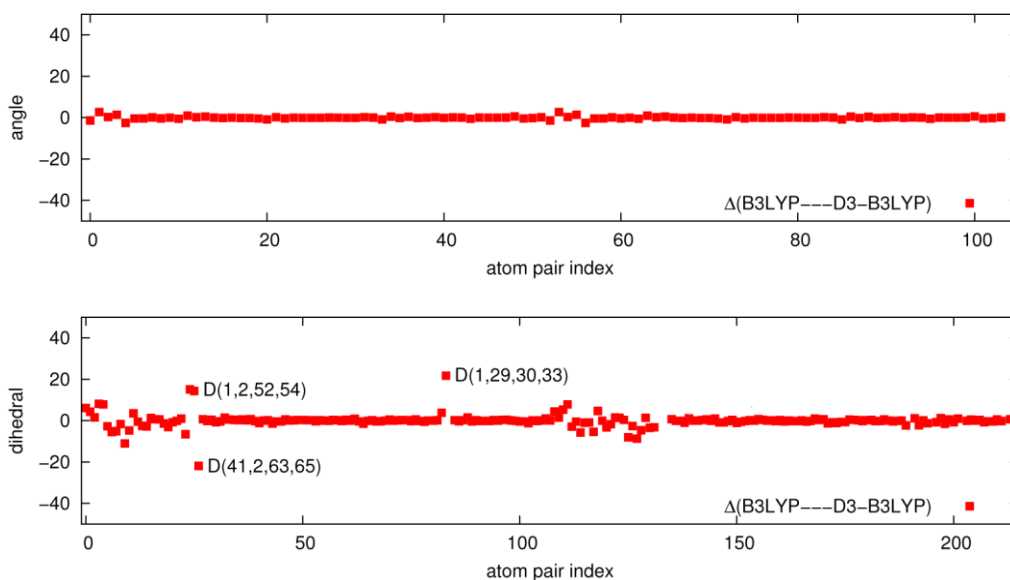


Figure S2. Differences between the calculated angles and dihedrals (B3LYP-D3 minus B3LYP) of the metalocycle product **1d-2a**. The numbering is given in Figure S1, only most relevant atom pairs are labeled. D(1,29,30,33) corresponds to the dihedral around the aryl group (see main text). D(1,2,52,54) or D(41,2,63,54) correspond to the rotation around the phenyl ligands. The values are given in degrees.

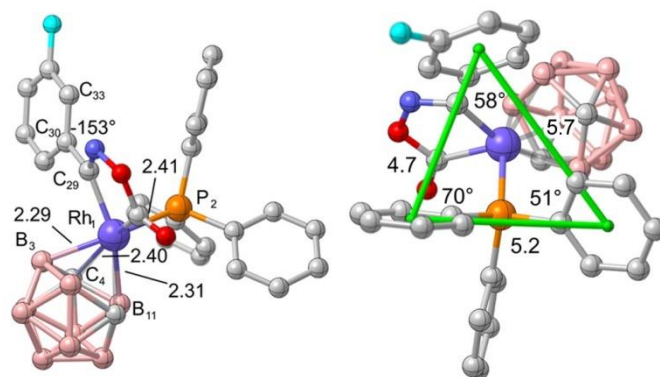


Figure S3. B3LYP/6-31G(d)+SDD(Rh,Ir) optimized structures of the metallocycle product **1d-2a**. C is in gray, O in red, H in white, P in orange, B in pink and Rh in purple. The side view representation is given in the right-hand side of the figure.

Table S2. Gibbs free activation ($\Delta G^\ddagger$) and reaction (ΔG_r) energies for all the studied reactions calculated with different functionals and basis sets. N/A: not available.

Reaction	B3LYP/6-31G(d) +SDD(Rh,Ir)		B3LYP-D3/6-31G(d) +SDD(Rh,Ir)		M06-D3/6-31G(d) +SDD(Rh,Ir)// B3LYP-D3/6-31G(d) +SDD(Rh,Ir)	
	$\Delta G^\ddagger$	ΔG_n	$\Delta G^\ddagger$	ΔG_r	$\Delta G^\ddagger$	ΔG_{rxn}
2a + 1a	26.1	−5.5	8.0	−22.5	8.4	−20.9
2a + 1b	23.1	−8.3	5.5	−25.8	5.9	−24.8
2a + 1c	24.3	−6.4	7.3	−24.0	7.6	−22.1
2a + 1d	24.9	−7.3	7.1	−24.7	7.4	−22.2
2b + 1a	25.3	−13.3	7.7	−30.0	8.8	−29.1
2b + 1b	22.6	−15.5	4.7	−33.3	7.1	−32.2
2b + 1c	N/A	N/A	6.0	−31.3	7.6	−30.6
2b + 1d	23.9	−14.7	5.3	−32.7	6.7	−30.9
2c + 1a	26.9	−4.3	10.5	−19.4	11.5	−15.7
2c + 1b	26.0	−5.1	9.5	−20.6	12.0	−16.6
2c + 1c	26.5	−4.6	10.2	−20.1	11.4	−15.9
2c + 1d	25.8	−4.7	10.0	−20.6	12.1	−16.4
2d + 1a	28.3	−8.8	11.4	−24.2	10.8	−23.2
2d + 1b	27.1	−9.7	10.0	−25.0	11.5	−27.7
2d + 1c	27.4	−9.9	10.7	−24.7	11.8	−23.4
2d + 1d	27.6	−8.9	10.6	−25.8	12.6	−24.5

Table S3. Gibbs free activation ($\Delta G^\ddagger$) and reaction (ΔG_r) energies for reactions **2a** + **1a** and **2b** + **1a** calculated with different functionals and basis sets.

Reaction	M06/6-31G(d) +SDD(Rh,Ir)// B3LYP-D3/6-31G(d) +SDD(Rh,Ir)		M06/6-31+G(d) +SDD(Rh,Ir)// B3LYP-D3/6-31+G(d) +SDD(Rh,Ir)		SMD _{THF} /M06/6-31G(d) +SDD(Rh,Ir)// B3LYP-D3/6-31G(d) +SDD(Rh,Ir)	
	$\Delta G^\ddagger$	ΔG_r	$\Delta G^\ddagger$	ΔG_r	$\Delta G^\ddagger$	ΔG_r
2a + 1a	13.7	−15.5	22.3	−6.5	25.6	−4.2
2b + 1a	14.1	−23.7	21.3	−15.3	26.3	−12.8

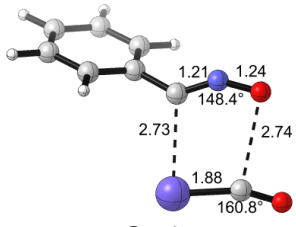
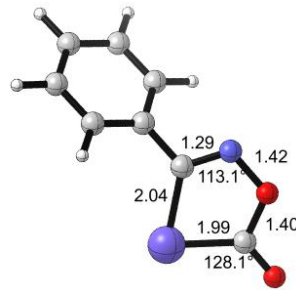
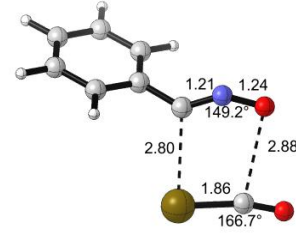
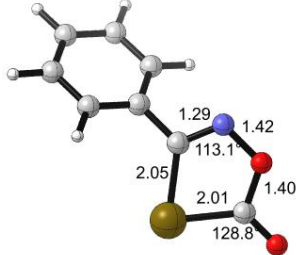
Table S4. Bond distances (Å) and angles (degrees) for transition states (**ts-2a-1a** and **ts-2b-1a**) and products (**2a-1a** and **2b-1a**) for the reaction **2a** + **1a**, calculated with:

M06/6-31G(d)+SDD(Rh,Ir)//B3LYP-D3/6-31G(d)+SDD(Rh,Ir) (shown in the figures).

M06/6-31+G(d)+SDD(Rh,Ir)//B3LYP-D3/6-31+G(d)+SDD(Rh,Ir) (shown in red).

SMD_{THF}/M06/6-31G(d)+SDD(Rh,Ir)//B3LYP-D3/6-31G(d)+SDD(Rh,Ir) (shown in blue).

Carboranyl ligands have been omitted for clarity.

	Rh-C ₁	C ₁ -N ₁	N ₁ -O ₁	Rh-C ₂	C ₂ -O ₁	Rh-C ₂ -O ₂	C ₁ -N ₁ -O ₁
 ts-2a-1a	2.74 2.72	1.21 1.21	1.24 1.24	2.79 2.67	1.88 1.87	161.9 159.8	148.1 147.2
 2a-1a	2.04 2.03	1.29 1.29	1.42 1.42	1.40 1.40	2.00 1.98	128.4 128.6	113.4 113.0
 ts-2b-1a	2.82 2.78	1.21 1.21	1.24 1.24	2.92 2.83	1.86 1.85	167.5 166.1	149.3 147.9
 2b-1a	2.04 2.05	1.29 1.29	1.42 1.41	1.40 1.40	2.00 2.01	129.2 129.8	113.3 113.1

Coordinates and energies of the structures optimized with B3LYP3-D3/6-31G(d)+SDD(Rh,Ir)

Dipole **1a**

Energy = -399.639144182

1	2.154895	-0.107466	0.000000
6	1.220123	-0.659042	0.000000
6	-1.201465	-2.061276	0.000000
6	0.000000	0.045103	0.000000
6	1.218318	-2.051554	0.000000
6	0.011241	-2.756158	0.000000
6	-1.214427	-0.668829	0.000000
1	2.162753	-2.588232	0.000000
1	0.015611	-3.842392	0.000000
1	-2.153591	-0.124767	0.000000
1	-2.141561	-2.605516	0.000000
6	-0.005775	1.472343	0.000000
7	-0.010941	2.641132	0.000000
8	-0.016202	3.857116	0.000000

Dipole **1b**

Energy = -859.232487166

1	2.155035	0.807394	0.000000
6	1.215343	0.264838	0.000000
6	-1.216280	-1.126200	0.000000
6	0.000000	0.976967	0.000000
6	1.216265	-1.126210	0.000000
6	-0.000010	-1.812705	0.000000
6	-1.215351	0.264846	0.000000
1	2.150332	-1.677318	0.000000
1	-2.155038	0.807409	0.000000
1	-2.150351	-1.677302	0.000000
6	-0.000001	2.402510	0.000000
7	-0.000085	3.571500	0.000000
8	0.000141	4.786145	0.000000
17	-0.000018	-3.565536	0.000000

Dipole **1c**

Energy = -498.871738852

1	2.155328	0.347297	0.000000
6	1.216827	-0.197206	0.000000
6	-1.217702	-1.588662	0.000000
6	0.000000	0.514299	0.000000
6	1.218317	-1.588304	0.000000
6	0.000413	-2.262451	0.000000
6	-1.216626	-0.197575	0.000000
1	2.143265	-2.154639	0.000000
1	-2.155282	0.346662	0.000000
1	-2.142471	-2.155289	0.000000
6	-0.000231	1.940327	0.000000
7	-0.000620	3.109201	0.000000
8	-0.000992	4.324826	0.000000
9	0.000605	-3.607735	0.000000

Dipole **1d**

Energy = -498.871048738

8	-4.157905	-0.403458	-0.000074
7	-2.957851	-0.217241	0.000018
6	-1.802174	-0.042566	0.000072
6	-0.396384	0.199397	0.000034
6	2.370676	0.678536	-0.000023
6	0.095634	1.519816	0.000014
6	0.501758	-0.884442	0.000021
6	1.863241	-0.617452	-0.000006
6	1.470359	1.746100	-0.000012
1	-0.601805	2.350446	0.000022
1	0.151383	-1.909954	0.000034
1	1.846991	2.764482	-0.000025
1	3.444455	0.830902	-0.000044
9	2.723167	-1.653762	-0.000013

Dipolarophile **2a**

Energy = -1567.08821118

45	-1.087497	0.948262	-0.105503
15	0.994664	-0.024624	-0.025838
6	-2.730807	-0.067528	-1.554267
5	-2.163169	-1.071361	-0.310615
5	-3.149081	1.420680	-0.893775
1	-3.118894	2.433694	-1.526221
5	-4.390014	0.248421	-1.477626
1	-4.991530	0.485313	-2.481174
5	-3.728815	-1.355956	-1.163049
1	-3.850757	-2.268433	-1.923013
6	-2.589219	-0.395538	1.190634
1	-2.057573	-0.709839	2.082827
5	-3.063965	1.194279	0.964805
1	-2.953527	2.029971	1.811638
5	-4.614400	1.076586	0.083299
1	-5.476287	1.894456	0.222118
5	-5.004685	-0.681803	-0.115430
1	-6.116318	-1.121382	-0.114394
5	-3.633790	-1.569823	0.605243
1	-3.683304	-2.638739	1.133128
5	-4.249603	-0.100465	1.364238
1	-4.745508	-0.128325	2.449824
1	-2.315505	-0.132500	-2.555007
1	-1.354733	-1.938528	-0.443178
6	-0.478615	2.682056	-0.003901
8	-0.116731	3.790990	0.061730
6	2.463712	1.057829	0.296098
6	4.666904	2.775094	0.632878
6	2.673363	2.135922	-0.579739
6	3.374041	0.852882	1.342327
6	4.466049	1.709638	1.510846
6	3.766298	2.984278	-0.415620
1	1.967410	2.313727	-1.386098
1	3.232704	0.024188	2.029042

1	5.160353	1.539089	2.330541	6	3.472283	-0.642148	-1.452179
1	3.907442	3.817283	-1.099667	6	4.566432	-1.473306	-1.709927
1	5.515453	3.441879	0.766407	6	3.889922	-2.926284	0.094584
6	1.637101	-0.977914	-1.486964	1	2.099792	-2.356384	1.142951
6	2.537626	-2.412504	-3.731663	1	3.322358	0.245874	-2.057740
6	0.745955	-1.340513	-2.505863	1	5.252562	-1.222507	-2.515750
6	2.990238	-1.334944	-1.612752	1	4.040939	-3.818848	0.696355
6	3.437047	-2.048086	-2.725828	1	5.629524	-3.262692	-1.140845
6	1.192550	-2.056694	-3.618865	6	1.754222	0.882508	1.569792
1	-0.296138	-1.056482	-2.422087	6	2.669643	2.039387	3.961653
1	3.697620	-1.048602	-0.839256	6	0.884618	1.059191	2.652991
1	4.488048	-2.315367	-2.809687	6	3.094759	1.280666	1.703737
1	0.486416	-2.331647	-4.398329	6	3.549037	1.857092	2.890376
1	2.886122	-2.965982	-4.600556	6	1.338197	1.638079	3.840562
6	1.104937	-1.256670	1.354863	1	-0.143951	0.732485	2.556685
6	1.130408	-3.009398	3.554693	1	3.786475	1.132918	0.878572
6	0.632126	-0.838208	2.611373	1	4.590066	2.158903	2.980860
6	1.578611	-2.567121	1.214989	1	0.649164	1.770103	4.671016
6	1.586450	-3.438513	2.308208	1	3.024163	2.485722	4.887887
6	0.654334	-1.703299	3.704043	6	1.208657	1.471848	-1.225106
1	0.226622	0.165297	2.715009	6	1.195520	3.457533	-3.216741
1	1.933578	-2.916684	0.251245	6	0.769400	1.177713	-2.528305
1	1.946283	-4.456743	2.179962	6	1.628309	2.775232	-0.932644
1	0.282631	-1.363197	4.667389	6	1.615919	3.762692	-1.922409
1	1.133613	-3.690195	4.402534	6	0.774175	2.158694	-3.518444
Dipolarophile 2b				1	0.399142	0.178420	-2.744676
Energy = -1560.90446336				1	1.953472	3.030159	0.070350
77	-0.975167	-0.859547	0.008437	1	1.931198	4.773690	-1.675185
15	1.108458	0.097043	0.012935	1	0.429528	1.914269	-4.520105
6	-2.613276	0.053223	1.557661	1	1.183003	4.228089	-3.983820
5	-2.001362	1.185934	0.448674	Dipolarophile 2c			
5	-3.075496	-1.354959	0.721873	Energy = -1453.85300491			
1	-3.103490	-2.425960	1.249438	45	-1.710194	-0.792200	0.025091
5	-4.276991	-0.205454	1.422954	15	0.408175	0.020689	-0.003031
1	-4.895814	-0.536304	2.388240	6	-3.953964	-0.854399	0.528380
5	-3.571995	1.407816	1.299353	6	-3.384378	0.060351	1.457173
1	-3.680100	2.230737	2.156686	6	-3.856470	-0.285516	-0.799126
6	-2.415620	0.676299	-1.129915	6	-2.812725	1.118736	0.693647
1	-1.869596	1.073487	-1.978789	6	-3.159811	0.930635	-0.696006
5	-2.958701	-0.930811	-1.097951	6	-1.182580	-2.525851	-0.281493
1	-2.885174	-1.657426	-2.043128	8	-0.872655	-3.630151	-0.479963
5	-4.517594	-0.841155	-0.221660	6	1.767279	-1.039206	-0.659102
1	-5.408753	-1.602552	-0.458833	6	3.813862	-2.740772	-1.551359
5	-4.848015	0.892164	0.168226	6	2.535644	-0.696224	-1.779265
1	-5.944637	1.366017	0.202658	6	2.039827	-2.241346	0.014678
5	-3.438876	1.811256	-0.428898	6	3.056136	-3.084700	-0.428064
1	-3.448782	2.930863	-0.840306	6	3.551765	-1.546990	-2.223483
5	-4.083473	0.452090	-1.354970	1	2.348645	0.233408	-2.306339
1	-4.554294	0.620125	-2.438702	1	1.454008	-2.517742	0.886731
1	-2.216196	-0.010759	2.564913	1	3.252244	-4.013523	0.100392
1	-1.172076	2.007475	0.691067	1	4.139156	-1.270560	-3.095138
6	-0.346973	-2.572232	-0.213159	1	4.603315	-3.401349	-1.899538
8	0.031846	-3.674578	-0.355242	6	0.502477	1.556822	-1.028941
6	2.573143	-0.949087	-0.421627	6	0.529118	3.825820	-2.686979
6	4.779462	-2.615590	-0.938000	6	-0.051691	1.506149	-2.320554
6	2.795536	-2.102212	0.348845	6	1.062529	2.759324	-0.577881

6	1.068789	3.888525	-1.402331
6	-0.028036	2.628413	-3.146907
1	-0.513214	0.584467	-2.665092
1	1.489590	2.823745	0.417125
1	1.498257	4.817185	-1.035824
1	-0.453765	2.571908	-4.145248
1	0.537059	4.704616	-3.326159
6	1.113210	0.533977	1.627971
6	2.138299	1.354092	4.108849
6	2.487579	0.781397	1.783797
6	0.263397	0.689802	2.730830
6	0.773095	1.101654	3.964175
6	2.995387	1.190866	3.016687
1	3.160658	0.649306	0.941337
1	-0.793172	0.466040	2.619043
1	0.104278	1.215167	4.813294
1	4.060421	1.377516	3.126181
1	2.536124	1.668435	5.070094
1	-2.887331	1.593258	-1.506497
1	-2.287845	1.979037	1.090925
1	-3.343955	-0.057488	2.531419
1	-4.459243	-1.779180	0.777394
1	-4.240320	-0.733751	-1.706186

Dipolarophile **2d**

Energy = -1447.66595673

77	-1.563761	-0.547611	-0.008452
15	0.617333	0.064646	-0.003216
6	-3.817634	-0.423452	0.498420
6	-3.164926	0.399148	1.465802
6	-3.665615	0.187942	-0.803136
6	-2.508897	1.442198	0.745616
6	-2.863006	1.339322	-0.649406
6	-1.159506	-2.303616	-0.370496
8	-0.925118	-3.425443	-0.600772
6	1.859779	-1.093984	-0.716677
6	3.715165	-2.948467	-1.711322
6	2.610964	-0.798309	-1.861357
6	2.051307	-2.326150	-0.070275
6	2.972674	-3.246280	-0.565044
6	3.532899	-1.724944	-2.355978
1	2.484287	0.152765	-2.367876
1	1.476455	-2.565049	0.819802
1	3.106557	-4.198099	-0.058615
1	4.109661	-1.484798	-3.245277
1	4.431479	-3.667967	-2.098736
6	0.869946	1.636715	-0.947475
6	1.150522	3.966964	-2.493185
6	0.284779	1.724037	-2.223369
6	1.589967	2.733177	-0.454727
6	1.722932	3.893488	-1.223250
6	0.433260	2.876057	-2.994219
1	-0.297545	0.885284	-2.595674
1	2.044987	2.691603	0.529049
1	2.276284	4.739716	-0.824651
1	-0.018234	2.926115	-3.981569
1	1.257372	4.869601	-3.088824

6	1.371546	0.418335	1.649587
6	2.479926	0.994246	4.162927
6	2.763480	0.529695	1.805194
6	0.545437	0.583698	2.768418
6	1.096725	0.874463	4.018247
6	3.313040	0.818304	3.054345
1	3.417058	0.385699	0.949368
1	-0.526946	0.457318	2.653618
1	0.445585	0.996363	4.879894
1	4.391260	0.899797	3.163638
1	2.909713	1.213962	5.136635
1	-2.534907	2.008982	-1.432151
1	-1.909583	2.233504	1.178190
1	-3.137751	0.235181	2.533876
1	-4.401384	-1.309609	0.711193
1	-4.082364	-0.186005	-1.728522

Transition state **ts-1a-2a**

Energy = -1966.74022767

45	-1.160281	0.298541	-0.795868
15	0.892798	0.797031	0.192086
5	-2.934392	-1.115169	-0.821953
6	-2.375164	-0.910025	0.755300
5	-3.367076	0.595329	-1.346036
1	-3.476518	1.033097	-2.449794
5	-4.619938	-0.571874	-0.775742
1	-5.434060	-1.033884	-1.518838
5	-3.970945	-1.495851	0.588343
1	-4.199782	-2.638455	0.850699
5	-2.315554	0.772273	1.145065
1	-1.551416	1.251699	1.920622
6	-3.144049	1.622841	-0.018422
1	-2.942737	2.677573	-0.177721
5	-4.724452	1.133920	-0.260773
1	-5.525228	1.915352	-0.674383
5	-5.032554	-0.140032	0.929097
1	-6.112764	-0.309263	1.410374
5	-3.515282	-0.352142	1.862756
1	-3.430564	-0.688502	3.003920
5	-4.038155	1.270018	1.355014
1	-4.327656	2.136908	2.121526
1	-2.685009	-2.055197	-1.509819
1	-1.679947	-1.593526	1.228795
6	-0.700594	1.051922	-2.452239
8	-0.546159	1.835710	-3.297824
8	0.272584	-1.051496	-3.921601
7	0.275424	-1.803798	-2.939101
6	0.006723	-1.975296	-1.769450
6	0.371562	-2.963549	-0.769109
6	1.150398	-4.745784	1.263951
6	-0.595657	-3.626332	0.006985
6	1.735739	-3.228554	-0.530112
6	2.117032	-4.110029	0.478725
6	-0.204431	-4.506917	1.015890
1	-1.645034	-3.437595	-0.181807
1	2.484216	-2.720838	-1.127801
1	-0.965254	-5.003263	1.612817

1	1.450188	-5.423847	2.059355	1	-0.750865	-3.439478	2.859554
6	2.454309	0.105965	-0.524606	5	-3.049732	-2.978944	1.663306
6	4.770595	-0.957910	-1.712576	1	-3.784935	-2.887000	2.597883
6	2.568587	0.028451	-1.920488	1	-0.105092	-3.131934	-1.861563
6	3.519080	-0.348916	0.268651	1	0.492571	-2.192711	0.882544
6	4.669225	-0.877457	-0.322039	6	-2.047411	0.144732	-2.196631
6	3.717587	-0.499903	-2.509080	8	-2.803158	0.717318	-2.870228
1	1.748269	0.336596	-2.558515	8	-0.058916	0.111255	-4.166306
1	3.444460	-0.308005	1.350456	7	0.768090	-0.322104	-3.358091
1	5.481030	-1.234633	0.307404	6	1.025632	-0.733457	-2.248709
1	3.771001	-0.573761	-3.591730	6	2.245043	-0.943704	-1.492074
1	5.660433	-1.381654	-2.172099	6	4.520450	-1.211667	0.108613
6	1.033303	0.300193	1.967288	6	2.499484	-2.144633	-0.806659
6	1.129594	-0.582581	4.634207	6	3.178299	0.107497	-1.385205
6	1.255136	1.210036	3.008906	6	4.311669	-0.020717	-0.587022
6	0.854852	-1.057483	2.278899	6	3.631712	-2.280459	-0.004891
6	0.909181	-1.496239	3.600053	1	1.798123	-2.964741	-0.892503
6	1.300207	0.769526	4.334309	1	2.991669	1.037483	-1.909998
1	1.384635	2.265016	2.791483	1	3.814510	-3.203516	0.534713
1	0.673924	-1.773373	1.487476	6	0.693396	2.299628	-0.632515
1	0.769418	-2.552527	3.813571	6	2.474298	3.909387	-2.099444
1	1.464601	1.489238	5.132730	6	0.525918	2.472530	-2.014850
1	1.161141	-0.921734	5.666793	6	1.760411	2.950880	0.006131
6	1.292135	2.606450	0.237848	6	2.645134	3.749291	-0.722665
6	1.790823	5.369344	0.344361	6	1.409427	3.271151	-2.741433
6	0.243915	3.525830	0.091652	1	-0.265116	1.954837	-2.545150
6	2.596525	3.088550	0.430684	1	1.914324	2.819639	1.072180
6	2.843637	4.460801	0.483714	1	3.472140	4.238016	-0.212912
6	0.491389	4.898871	0.148121	1	1.273059	3.369101	-3.814874
1	-0.761936	3.155804	-0.075809	1	3.169710	4.521084	-2.669216
1	3.421299	2.389548	0.534219	6	0.359752	0.945661	1.887178
1	3.859493	4.820652	0.629415	6	1.696541	0.368368	4.292116
1	-0.332323	5.598096	0.029793	6	-0.142792	1.412459	3.108648
1	1.985073	6.438621	0.381561	6	1.536595	0.179570	1.888011
1	3.174251	-4.288254	0.659773	6	2.204893	-0.100982	3.077973
				6	0.521945	1.121869	4.302824
				1	-1.057955	1.994574	3.133561
				1	1.933662	-0.195213	0.954365
				1	3.116945	-0.691447	3.050339
				1	0.114745	1.484030	5.243753
				1	2.209673	0.142346	5.223530
				6	-1.832720	2.418023	0.714424
				6	-3.910856	4.162304	1.440760
				6	-3.151506	1.952550	0.811901
				6	-1.567114	3.770502	0.980646
				6	-2.599985	4.636689	1.340637
				6	-4.183981	2.819151	1.176447
				1	-3.359082	0.910308	0.593810
				1	-0.552064	4.148538	0.901560
				1	-2.381565	5.683179	1.539987
				1	-5.201467	2.443201	1.245368
				1	-4.715551	4.839033	1.718100
				1	5.012123	0.801781	-0.488522
				17	5.929390	-1.362379	1.164194

Transition state **ts-1b-2a**
Energy = -2426.33821630

45	-1.280577	-0.742962	-0.735519
15	-0.500849	1.208624	0.271932
5	-0.898409	-2.962822	-0.988847
6	-0.511066	-2.466394	0.576995
5	-2.676170	-2.519644	-1.142045
1	-3.319611	-2.344003	-2.130516
5	-2.138771	-4.205322	-0.773730
1	-2.262274	-5.091950	-1.565423
5	-0.774381	-4.140479	0.352186
1	0.159421	-4.884652	0.389066
5	-1.867247	-1.666711	1.299135
1	-1.775788	-0.814614	2.124164
6	-3.207523	-1.934930	0.359390
1	-4.056115	-1.259651	0.405771
5	-3.562689	-3.542435	0.075764
1	-4.688774	-3.866306	-0.146965
5	-2.371297	-4.478797	0.995769
1	-2.631409	-5.543899	1.469668
5	-1.305272	-3.288308	1.814690

Transition state **ts-1c-2a**

Energy = -2065.97540900

45	-1.318674	-0.191250	-0.758915
15	0.250006	1.222605	0.233681
5	-2.076495	-2.322562	-0.922611
6	-1.562779	-2.002043	0.651608
5	-3.392262	-1.068711	-1.203082
1	-3.819234	-0.651918	-2.235394
5	-3.779441	-2.775210	-0.757015
1	-4.293041	-3.526625	-1.531512
5	-2.615557	-3.332920	0.454325
1	-2.179311	-4.438994	0.570498
5	-2.364989	-0.595682	1.259056
1	-1.899558	0.140238	2.069364
6	-3.621928	-0.215949	0.242085
1	-4.024730	0.791698	0.216703
5	-4.720403	-1.449400	-0.018127
1	-5.847596	-1.182735	-0.302706
5	-4.194640	-2.797969	1.001029
1	-4.971216	-3.565078	1.486096
5	-2.713479	-2.251564	1.855682
1	-2.355209	-2.598558	2.938915
5	-4.060767	-1.123060	1.581302
1	-4.690804	-0.625253	2.463257
1	-1.434067	-2.909467	-1.736683
1	-0.570546	-2.248982	1.010500
6	-1.481948	0.850539	-2.310479
8	-1.838527	1.671633	-3.053086
8	0.328534	-0.247916	-4.089679
7	0.805082	-0.980462	-3.214439
6	0.772319	-1.387552	-2.073722
6	1.684666	-2.118400	-1.213701
6	3.417382	-3.358084	0.579201
6	1.277407	-3.260087	-0.499964
6	2.997634	-1.636611	-1.033075
6	3.866681	-2.253413	-0.136282
6	2.141321	-3.880771	0.401391
1	0.276618	-3.646188	-0.645355
1	3.319937	-0.759469	-1.581836
1	1.832516	-4.751817	0.969940
9	4.247368	-3.939992	1.479954
6	1.870663	1.539084	-0.606224
6	4.284438	1.975100	-1.983120
6	1.881713	1.671525	-2.002890
6	3.084190	1.636918	0.092531
6	4.282673	1.852991	-0.591883
6	3.079199	1.887444	-2.685119
1	0.967088	1.563234	-2.574671
1	3.098969	1.523814	1.171622
1	5.215144	1.915622	-0.035711
1	3.064502	1.959769	-3.769075
1	5.219109	2.129605	-2.516963
6	0.795658	0.705006	1.922497
6	1.613655	-0.247133	4.438478
6	0.609774	1.484410	3.071268
6	1.390485	-0.560306	2.052391
6	1.804134	-1.030225	3.296835

6	1.013726	1.007345	4.321343
1	0.143194	2.461080	2.996814
1	1.533667	-1.178436	1.176271
1	2.269383	-2.010016	3.368004
1	0.854479	1.620514	5.205129
1	1.925478	-0.615255	5.412776
6	-0.355715	2.951648	0.510583
6	-1.370706	5.528573	0.983129
6	-1.738681	3.180598	0.528268
6	0.514422	4.032283	0.726131
6	0.009727	5.311908	0.960351
6	-2.243008	4.460569	0.766860
1	-2.412684	2.350622	0.345885
1	1.588742	3.874122	0.706999
1	0.695142	6.140690	1.121489
1	-3.317968	4.621067	0.774567
1	-1.762847	6.526910	1.161905
1	4.870698	-1.876408	0.028999

Transition state **ts-1d-2a**

Energy = -2065.97534341

45	-1.323305	-0.104112	-0.790121
15	0.393644	1.145105	0.175919
5	-2.389077	-2.108213	-0.810198
6	-1.918895	-1.709878	0.757431
5	-3.478357	-0.708993	-1.297549
1	-3.778608	-0.341323	-2.391539
5	-4.149680	-2.283203	-0.722034
1	-4.731168	-3.024591	-1.457259
5	-3.153514	-2.882032	0.612513
1	-2.901031	-4.022996	0.860618
5	-2.526923	-0.145399	1.178341
1	-1.995750	0.592291	1.945805
6	-3.651950	0.313034	0.044885
1	-3.890962	1.361567	-0.102627
5	-4.911360	-0.763322	-0.176614
1	-5.966784	-0.362780	-0.561844
5	-4.657764	-2.063994	0.998326
1	-5.568998	-2.653732	1.497156
5	-3.158024	-1.660783	1.897395
1	-2.916877	-1.945233	3.030301
5	-4.297970	-0.378333	1.428799
1	-4.890309	0.294679	2.215466
1	-1.802288	-2.865983	-1.518327
1	-0.998839	-2.065273	1.205822
6	-1.230060	0.791908	-2.433033
8	-1.397300	1.576063	-3.275680
8	0.476814	-0.779176	-3.990574
7	0.784444	-1.461892	-3.009041
6	0.633394	-1.737635	-1.840371
6	1.382051	-2.499806	-0.858600
6	2.850644	-3.819105	1.154895
6	0.776123	-3.493902	-0.068709
6	2.741340	-2.190628	-0.653187
6	3.437645	-2.850433	0.346767
6	1.509367	-4.140729	0.926051
1	-0.264589	-3.739968	-0.235123

1	3.235772	-1.431086	-1.245130	1	5.943919	0.640761	1.590046
1	1.027616	-4.900056	1.535687	5	3.343734	0.498890	1.993047
1	3.437377	-4.299546	1.930994	1	3.215418	0.841738	3.127789
9	4.738363	-2.528879	0.553535	5	3.987160	-1.079234	1.504559
6	2.084877	1.122922	-0.578488	1	4.321428	-1.924031	2.277084
6	4.609112	1.027237	-1.814314	1	2.513562	2.175525	-1.410827
6	2.193871	1.117014	-1.977287	1	1.449288	1.627669	1.330641
6	3.257626	1.090056	0.192521	6	0.628941	-1.032986	-2.361575
6	4.511065	1.038949	-0.421573	8	0.462796	-1.734437	-3.279584
6	3.446669	1.070955	-2.589265	8	-0.439041	1.157653	-3.901415
1	1.306903	1.103259	-2.600363	7	-0.450643	1.877407	-2.894465
1	3.194319	1.080639	1.275652	6	-0.183536	2.032055	-1.723124
1	5.407764	0.991763	0.191096	6	-0.581129	2.985664	-0.702455
1	3.504797	1.041355	-3.673800	6	-1.424851	4.707333	1.358224
1	5.583985	0.972660	-2.292710	6	0.360841	3.652130	0.100938
6	0.755066	0.723622	1.939202	6	-1.953668	3.215397	-0.474465
6	1.235365	-0.076590	4.591135	6	-2.367203	4.067111	0.547350
6	0.630452	1.639846	2.991393	6	-0.062189	4.502225	1.123177
6	1.120909	-0.599938	2.233164	1	1.416619	3.491711	-0.077425
6	1.364974	-0.995492	3.546374	1	-2.682871	2.702331	-1.091284
6	0.867040	1.239344	4.309177	1	0.680290	5.001432	1.740510
1	0.340218	2.665353	2.788080	1	-1.749419	5.362208	2.163320
1	1.216033	-1.323317	1.433689	6	-2.535570	-0.153707	-0.489314
1	1.647311	-2.025584	3.746525	6	-4.873408	0.848081	-1.687200
1	0.757440	1.960191	5.115873	6	-2.637671	-0.061509	-1.884882
1	1.414429	-0.386374	5.617809	6	-3.622641	0.254636	0.298970
6	0.049025	2.963494	0.258212	6	-4.783787	0.752475	-0.296847
6	-0.583593	5.694072	0.442828	6	-3.797587	0.436441	-2.478433
6	-1.286992	3.388370	0.233302	1	-1.802463	-0.333988	-2.519335
6	1.066110	3.923898	0.373195	1	-3.558088	0.202643	1.380979
6	0.750979	5.280636	0.463088	1	-5.613139	1.074413	0.328690
6	-1.601324	4.745107	0.329198	1	-3.840639	0.524142	-3.560407
1	-2.073311	2.648047	0.132718	1	-5.772134	1.248332	-2.150499
1	2.106054	3.611208	0.389066	6	-1.116791	-0.322551	2.013373
1	1.548757	6.014997	0.546039	6	-1.210980	0.537202	4.687222
1	-2.641961	5.058162	0.306117	6	-1.235505	-1.252313	3.054381
1	-0.827742	6.751607	0.509514	6	-1.042656	1.043554	2.328495
				6	-1.094630	1.470463	3.653803
				6	-1.280407	-0.822941	4.383137
				1	-1.282800	-2.313419	2.833740
				1	-0.945941	1.774656	1.536902
				1	-1.035402	2.533708	3.870106
				1	-1.363432	-1.557222	5.180782
				1	-1.240901	0.868012	5.722546
				6	-1.322378	-2.630115	0.283774
				6	-1.763891	-5.401872	0.406989
				6	-0.256742	-3.528420	0.132503
				6	-2.614653	-3.137569	0.491533
				6	-2.833469	-4.514185	0.552719
				6	-0.476156	-4.906037	0.196778
				1	0.739626	-3.136680	-0.044944
				1	-3.452807	-2.455536	0.600044
				1	-3.840426	-4.893809	0.709451
				1	0.360346	-5.589152	0.073906
				1	-1.936122	-6.474689	0.450494
				1	-3.430326	4.217887	0.718823

Transition state **ts-1a-2b**
Energy = -1960.55783154

77	1.074817	-0.265130	-0.724802
15	-0.964697	-0.810721	0.237785
5	2.778399	1.234443	-0.731292
6	2.181304	0.980501	0.862190
5	3.326414	-0.447049	-1.227064
1	3.492176	-0.889893	-2.321997
5	4.492269	0.792308	-0.622193
1	5.296600	1.307954	-1.339646
5	3.739618	1.668520	0.717441
1	3.880182	2.824363	0.983065
5	2.240629	-0.708204	1.267801
1	1.495543	-1.239107	2.027078
6	3.142811	-1.493877	0.114980
1	3.003133	-2.556194	-0.054395
5	4.686492	-0.902136	-0.105124
1	5.542920	-1.630223	-0.503733
5	4.888373	0.394376	1.088276

Transition state **ts-1b-2b**

Energy = -2420.15622817

77	1.222966	0.632986	-0.632387
15	0.353775	-1.291889	0.326814
5	0.929970	2.857961	-0.936432
6	0.432629	2.373990	0.640834
5	2.704604	2.383533	-0.955601
1	3.416456	2.181725	-1.890893
5	2.177659	4.080543	-0.634352
1	2.363557	4.961531	-1.419494
5	0.740881	4.037564	0.398522
1	-0.185317	4.791017	0.365002
5	1.731220	1.573779	1.468080
1	1.578040	0.735073	2.296965
6	3.127964	1.807754	0.601150
1	3.953814	1.111708	0.703143
5	3.528754	3.399907	0.310594
1	4.672316	3.699290	0.153760
5	2.295989	4.372211	1.138154
1	2.538437	5.442075	1.610127
5	1.168091	3.212900	1.911645
1	0.545963	3.397164	2.911687
5	2.907918	2.876117	1.876158
1	3.584015	2.789006	2.854424
1	0.187634	3.064782	-1.845214
1	-0.594791	2.142403	0.894289
6	1.986599	-0.300217	-2.049256
8	2.666088	-0.895942	-2.787550
8	-0.036673	-0.174986	-4.174115
7	-0.839136	0.290818	-3.357553
6	-1.080309	0.705527	-2.246059
6	-2.292865	0.964908	-1.493752
6	-4.558255	1.330371	0.102761
6	-2.508615	2.183318	-0.826250
6	-3.262099	-0.051642	-1.374840
6	-4.390504	0.124775	-0.578550
6	-3.635033	2.367781	-0.025693
1	-1.782251	2.980102	-0.924818
1	-3.107908	-0.993079	-1.889534
1	-3.786821	3.303725	0.501243
6	-0.853994	-2.327948	-0.621462
6	-2.657906	-3.858736	-2.141653
6	-0.667484	-2.485064	-2.002863
6	-1.950927	-2.955021	-0.009924
6	-2.847217	-3.714782	-0.765478
6	-1.563337	-3.244088	-2.756094
1	0.147729	-1.985996	-2.513436
1	-2.118840	-2.834606	1.055363
1	-3.697580	-4.185036	-0.277259
1	-1.412201	-3.327321	-3.828683
1	-3.362477	-4.439273	-2.732411
6	-0.536781	-1.014985	1.921227
6	-1.916823	-0.427212	4.297157
6	-0.100544	-1.541891	3.143336
6	-1.670777	-0.187325	1.905023
6	-2.360462	0.099695	3.081087
6	-0.786870	-1.245606	4.323932

1	0.779310	-2.175628	3.179606
1	-2.017312	0.229900	0.969231
1	-3.238545	0.738839	3.041426
1	-0.431349	-1.654297	5.266734
1	-2.446546	-0.196818	5.218148
6	1.634082	-2.551059	0.787273
6	3.632722	-4.374316	1.543574
6	2.959774	-2.126115	0.953453
6	1.321419	-3.902594	1.000538
6	2.315061	-4.807998	1.375234
6	3.952344	-3.031749	1.332957
1	3.202651	-1.084054	0.772761
1	0.301333	-4.250780	0.868139
1	2.060438	-5.853619	1.531345
1	4.975988	-2.686885	1.454031
1	4.406908	-5.081615	1.831240
1	-5.118660	-0.672086	-0.470068
17	-5.959208	1.540685	1.159479

Transition state **ts-1c-2b**

Energy = -2059.79295694

77	-1.235457	-0.106418	-0.672671
15	0.403453	1.229669	0.283954
5	-2.045679	-2.218172	-0.830007
6	-1.481997	-1.885804	0.761446
5	-3.353975	-0.952306	-1.064284
1	-3.809964	-0.524435	-2.079679
5	-3.748372	-2.653428	-0.601097
1	-4.286893	-3.406630	-1.356050
5	-2.549953	-3.207673	0.576185
1	-2.111156	-4.313504	0.681422
5	-2.278129	-0.479046	1.403069
1	-1.793848	0.254624	2.203787
6	-3.548767	-0.095712	0.404523
1	-3.934741	0.918026	0.381486
5	-4.655622	-1.317945	0.156568
1	-5.785695	-1.041881	-0.105858
5	-4.116315	-2.676464	1.161455
1	-4.882749	-3.444709	1.660088
5	-2.619219	-2.135097	1.989332
1	-2.236712	-2.497127	3.058844
5	-3.965484	-1.006107	1.749644
1	-4.576884	-0.508509	2.644422
1	-1.444307	-2.843211	-1.645993
1	-0.492528	-2.158049	1.109413
6	-1.363756	0.952981	-2.198279
8	-1.633845	1.740326	-3.016254
8	0.453204	-0.285536	-4.100380
7	0.882390	-1.022716	-3.204174
6	0.830174	-1.413679	-2.059472
6	1.713850	-2.169525	-1.191503
6	3.401788	-3.450915	0.615785
6	1.261946	-3.279011	-0.454205
6	3.048565	-1.744450	-1.028190
6	3.895554	-2.382319	-0.124627
6	2.103131	-3.920083	0.454433
1	0.244421	-3.624149	-0.585210

1	3.404875	-0.891164	-1.593569	1	-5.372899	-2.710779	1.682593
1	1.758773	-4.764548	1.042361	5	-2.990163	-1.640582	2.032850
9	4.208536	-4.047362	1.529002	1	-2.712531	-1.931370	3.155309
6	2.016171	1.475655	-0.593612	5	-4.177067	-0.396874	1.598050
6	4.417291	1.811340	-2.018376	1	-4.772714	0.256380	2.398357
6	2.005668	1.590960	-1.991275	1	-1.708849	-2.848713	-1.428352
6	3.244526	1.541336	0.082588	1	-0.837280	-1.996974	1.299216
6	4.436980	1.707583	-0.625754	6	-1.130958	0.842826	-2.332271
6	3.197219	1.756255	-2.697584	8	-1.238201	1.566372	-3.241889
1	1.078391	1.509099	-2.546074	8	0.615491	-0.825623	-3.979956
1	3.275450	1.441409	1.162682	7	0.903803	-1.491158	-2.980323
1	5.381029	1.745031	-0.087149	6	0.747881	-1.750011	-1.809381
1	3.163780	1.813030	-3.781931	6	1.491656	-2.501648	-0.816511
1	5.346884	1.926067	-2.570818	6	2.960136	-3.808018	1.207213
6	0.956056	0.674380	1.957008	6	0.879786	-3.474135	-0.004468
6	1.773827	-0.331106	4.451178	6	2.856419	-2.207110	-0.625930
6	0.776502	1.432685	3.120655	6	3.552510	-2.859912	0.378835
6	1.545724	-0.595363	2.060168	6	1.612592	-4.114552	0.994750
6	1.959153	-1.092560	3.294140	1	-0.164971	-3.710797	-0.157487
6	1.180336	0.928702	4.360100	1	3.355386	-1.462930	-1.233411
1	0.315821	2.413450	3.065997	1	1.125469	-4.857133	1.620569
1	1.687244	-1.193499	1.170604	1	3.547123	-4.284140	1.985800
1	2.422255	-2.074727	3.343643	9	4.859052	-2.551526	0.570263
1	1.026097	1.525000	5.256154	6	2.185387	1.109142	-0.548924
1	2.085903	-0.719588	5.417449	6	4.695184	0.991633	-1.810274
6	-0.119609	2.982215	0.586408	6	2.278657	1.089276	-1.948419
6	-1.004347	5.597227	1.105653	6	3.365889	1.079103	0.210157
6	-1.489794	3.276224	0.622307	6	4.612523	1.017334	-0.416741
6	0.803866	4.015993	0.808440	6	3.524637	1.032022	-2.573096
6	0.363766	5.314797	1.065937	1	1.385929	1.074015	-2.562759
6	-1.929305	4.575647	0.883648	1	3.314565	1.080185	1.294004
1	-2.202610	2.479739	0.434902	1	5.515554	0.972134	0.186688
1	1.869169	3.807374	0.775414	1	3.569792	0.989980	-3.657744
1	1.089846	6.107281	1.231424	1	5.664614	0.928260	-2.298566
1	-2.995098	4.787854	0.904929	6	0.869825	0.724984	1.984850
1	-1.346022	6.610608	1.302489	6	1.334850	-0.089530	4.634331
1	4.915897	-2.046320	0.028886	6	0.698270	1.624459	3.044740
Transition state ts-1d-2b				6	1.275608	-0.588782	2.269116
Energy = -2059.79304658				6	1.511160	-0.991555	3.581818
77	-1.231701	-0.062825	-0.710148	6	0.928139	1.216979	4.361356
15	0.504343	1.157876	0.226505	1	0.375079	2.641228	2.848020
5	-2.276890	-2.078034	-0.719913	1	1.409342	-1.298080	1.462927
6	-1.766566	-1.650127	0.864066	1	1.824217	-2.014086	3.774604
5	-3.409524	-0.704569	-1.163009	1	0.781886	1.924245	5.174137
1	-3.755546	-0.335405	-2.243034	1	1.507892	-0.405223	5.660223
5	-4.030568	-2.292003	-0.563973	6	0.192250	2.982931	0.316593
1	-4.613912	-3.052841	-1.276816	6	-0.383959	5.724216	0.520080
5	-2.972599	-2.854272	0.737428	6	-1.133237	3.437078	0.268526
1	-2.676037	-3.985970	0.977539	6	1.227614	3.918939	0.463964
5	-2.423186	-0.104098	1.316761	6	0.940561	5.281026	0.563694
1	-1.897414	0.649347	2.071432	6	-1.419587	4.799593	0.373350
6	-3.581361	0.317428	0.201997	1	-1.931391	2.712997	0.140861
1	-3.840828	1.360539	0.055175	1	2.260049	3.583577	0.496535
5	-4.810088	-0.790711	-0.001232	1	1.752330	5.996538	0.671674
1	-5.883303	-0.417357	-0.363234	1	-2.452245	5.136240	0.331367
5	-4.493722	-2.090114	1.164668	1	-0.606009	6.786126	0.594171

Transition state **ts-1a-2c**

Energy = -1853.50178525

45	-0.309492	-1.721050	-0.259156
15	-0.788645	0.486786	0.079639
6	1.053437	-3.403928	0.688464
6	0.726403	-2.457329	1.687169
6	-0.175910	-3.968469	0.213851
6	-0.704493	-2.507497	1.897288
6	-1.252015	-3.473508	1.025618
1	-2.295439	-3.744696	0.934347
1	2.033042	-3.627750	0.291563
6	-1.110138	-1.742879	-1.959832
8	-1.899078	-1.833321	-2.805091
8	0.968343	-1.477024	-3.484845
7	1.781827	-1.163665	-2.603343
6	1.936730	-1.040139	-1.396526
6	2.927622	-0.332436	-0.594489
6	4.717029	1.132927	1.014171
6	3.242871	1.006533	-0.904037
6	3.541139	-0.925772	0.521789
6	4.427407	-0.200207	1.317125
6	4.127343	1.728089	-0.105148
1	2.773632	1.474687	-1.761416
1	3.322810	-1.957882	0.762372
1	4.346940	2.762809	-0.354161
6	-0.041267	1.771170	-1.007083
6	1.054331	3.682811	-2.745662
6	0.063428	1.503574	-2.380518
6	0.402016	3.008066	-0.514555
6	0.950458	3.956396	-1.380427
6	0.605119	2.456430	-3.243201
1	-0.236817	0.542567	-2.782645
1	0.335679	3.229387	0.545648
1	1.299302	4.906555	-0.984680
1	0.692369	2.226752	-4.301216
1	1.487184	4.418849	-3.417849
6	-0.332220	0.992864	1.792975
6	0.439840	1.543750	4.436671
6	-1.298896	1.144055	2.797156
6	1.026753	1.121415	2.126830
6	1.407714	1.400434	3.438112
6	-0.911623	1.415216	4.112446
1	-2.353286	1.051891	2.556639
1	1.787361	1.008162	1.364660
1	2.463753	1.500551	3.673167
1	-1.670668	1.529566	4.881760
1	0.737587	1.755858	5.459990
6	-2.590809	0.880174	-0.011173
6	-5.338814	1.446507	-0.032570
6	-3.530299	-0.156401	0.081061
6	-3.042352	2.205419	-0.117357
6	-4.408372	2.485128	-0.127955
6	-4.897909	0.126490	0.071801
1	-3.183506	-1.183366	0.149804
1	-2.327779	3.018842	-0.198564
1	-4.746611	3.514158	-0.215151
1	-5.616275	-0.686167	0.137009

1	-6.402907	1.666538	-0.045856
1	-0.263680	-4.716074	-0.564469
1	-1.245500	-1.906430	2.616929
1	1.411615	-1.826006	2.236017
1	4.892858	-0.678352	2.174943
1	5.401098	1.700147	1.639531

Transition state **ts-1b-2c**

Energy = -2313.09741758

45	1.065234	-1.657685	-0.075288
15	0.949862	0.627518	-0.052175
6	-0.052423	-3.451623	-1.130751
6	-0.109210	-2.311172	-1.966753
6	1.330312	-3.773244	-0.939666
6	1.240935	-1.991988	-2.379026
6	2.120825	-2.919323	-1.783186
1	3.197665	-2.946379	-1.885321
1	-0.878275	-3.961942	-0.656929
6	2.151219	-1.726005	1.452775
8	3.069156	-1.738984	2.160960
8	0.354243	-2.243718	3.301058
7	-0.646058	-2.012550	2.609817
6	-1.038085	-1.754557	1.480312
6	-2.283397	-1.192125	0.976935
6	-4.561583	0.050903	-0.080229
6	-2.829491	-0.044759	1.587618
6	-2.931401	-1.715725	-0.154314
6	-4.064689	-1.103934	-0.685100
6	-3.960067	0.576864	1.064306
1	-2.343673	0.372911	2.461609
1	-2.544697	-2.607982	-0.627658
1	-4.358815	1.472416	1.528420
6	0.145099	1.495827	1.358020
6	-1.011107	2.775796	3.572974
6	0.362929	1.005306	2.654919
6	-0.650128	2.638947	1.183433
6	-1.227992	3.271794	2.285897
6	-0.210145	1.644830	3.754241
1	0.945935	0.105838	2.818627
1	-0.834442	3.029704	0.188146
1	-1.849802	4.150279	2.135441
1	-0.042490	1.243338	4.749445
1	-1.466102	3.265459	4.429753
6	0.077931	1.240936	-1.555968
6	-1.274498	1.943394	-3.915504
6	0.788467	1.727522	-2.662731
6	-1.318187	1.111095	-1.644337
6	-1.989573	1.465793	-2.813293
6	0.113228	2.072927	-3.836391
1	1.867023	1.839527	-2.611341
1	-1.882756	0.740623	-0.798715
1	-3.070823	1.366533	-2.857218
1	0.675497	2.448533	-4.687141
1	-1.796628	2.215655	-4.828671
6	2.596501	1.457063	-0.150154
6	5.094548	2.707311	-0.407500
6	3.724799	0.716983	-0.530031

6	2.731993	2.831751	0.101717
6	3.974230	3.451569	-0.026651
6	4.968030	1.340464	-0.658749
1	3.624475	-0.348792	-0.713647
1	1.869250	3.417035	0.405231
1	4.068924	4.515103	0.175215
1	5.836757	0.754731	-0.946652
1	6.062721	3.191622	-0.501850
1	1.707179	-4.588386	-0.334850
1	1.509889	-1.179061	-3.041127
1	-0.995399	-1.780468	-2.286090
1	-4.554611	-1.512388	-1.562489
17	-5.955852	0.863111	-0.780197

Transition state **ts-1c-2c**

Energy = -1952.73521172

45	0.721849	-1.705884	0.076976
15	0.857287	0.569423	-0.072632
6	-0.502361	-3.473664	-0.913132
6	-0.409063	-2.404369	-1.833970
6	0.833194	-3.899365	-0.613869
6	0.985657	-2.235323	-2.181160
6	1.743330	-3.188088	-1.467447
1	2.816987	-3.317418	-1.501515
1	-1.396651	-3.871419	-0.455583
6	1.696843	-1.768561	1.680363
8	2.572491	-1.825196	2.438487
8	-0.227085	-1.932213	3.425895
7	-1.164356	-1.668336	2.659548
6	-1.464802	-1.463482	1.492096
6	-2.618182	-0.836175	0.861461
6	-4.705655	0.493457	-0.426659
6	-3.074264	0.414140	1.328228
6	-3.258074	-1.408500	-0.251667
6	-4.301286	-0.750418	-0.900105
6	-4.115097	1.081460	0.687535
1	-2.591275	0.867620	2.185479
1	-2.936551	-2.375850	-0.613273
1	-4.460382	2.050943	1.030509
6	0.054130	1.626663	1.203105
6	-1.111670	3.190806	3.221678
6	0.137416	1.228902	2.546521
6	-0.612096	2.819322	0.882372
6	-1.194425	3.594457	1.887562
6	-0.440392	2.008986	3.548034
1	0.615428	0.295136	2.821041
1	-0.692405	3.139489	-0.151283
1	-1.715899	4.510931	1.624495
1	-0.379674	1.677982	4.580744
1	-1.571072	3.790979	4.002469
6	0.161317	1.152467	-1.677459
6	-0.947909	1.828648	-4.167716
6	0.988682	1.545503	-2.738934
6	-1.228668	1.102549	-1.876917
6	-1.778668	1.444534	-3.110877
6	0.433981	1.877670	-3.978176
1	2.064338	1.594869	-2.601988

1	-1.881639	0.800092	-1.068450
1	-2.856815	1.407137	-3.241752
1	1.086137	2.179666	-4.793332
1	-1.376023	2.090183	-5.131556
6	2.586710	1.212403	-0.100768
6	5.221355	2.163325	-0.254330
6	3.642486	0.335469	-0.386529
6	2.863920	2.572752	0.109216
6	4.174276	3.043494	0.033079
6	4.953568	0.809730	-0.464319
1	3.429750	-0.718999	-0.536127
1	2.057982	3.263240	0.338431
1	4.378544	4.097217	0.202758
1	5.764371	0.119078	-0.679396
1	6.242232	2.531786	-0.308034
1	1.099506	-4.694342	0.071293
1	1.364294	-1.503570	-2.883623
1	-1.225110	-1.830229	-2.250659
9	-5.697400	1.147518	-1.067757
1	-4.800279	-1.183862	-1.760460

Transition state **ts-1d-2c**

Energy = -1952.73559878

45	-0.824232	-1.650539	-0.331059
15	-0.788493	0.596146	0.093259
6	0.121880	-3.614465	0.585152
6	-0.040916	-2.652924	1.610473
6	-1.177254	-3.892369	0.049672
6	-1.458851	-2.417701	1.781531
6	-2.158712	-3.213772	0.851178
1	-3.231395	-3.259452	0.717105
1	1.048321	-4.023371	0.208893
6	-1.565797	-1.421857	-2.038257
8	-2.312640	-1.292175	-2.915689
8	0.601905	-1.612272	-3.523812
7	1.420044	-1.517061	-2.601068
6	1.556275	-1.477887	-1.386365
6	2.651606	-1.014691	-0.542622
6	4.652772	0.031028	1.155588
6	3.248343	0.229319	-0.825419
6	3.086627	-1.734147	0.584739
6	4.078645	-1.215653	1.416966
6	4.222406	0.724478	0.027949
1	2.937493	0.813886	-1.681409
1	2.647910	-2.697382	0.807358
9	4.760394	1.934347	-0.239400
6	0.275908	1.704573	-0.920862
6	1.865068	3.344969	-2.552700
6	0.335406	1.483351	-2.305827
6	1.012718	2.761429	-0.364469
6	1.810214	3.570602	-1.176282
6	1.120719	2.304199	-3.115283
1	-0.193884	0.652866	-2.760021
1	0.983460	2.945248	0.704340
1	2.394487	4.369711	-0.729066
1	1.165686	2.111033	-4.183203
1	2.491537	3.970399	-3.182701

6	-0.286903	0.906799	1.839869
6	0.488354	1.142244	4.528972
6	-1.235872	1.204384	2.828438
6	1.055886	0.728990	2.212661
6	1.439846	0.852164	3.546763
6	-0.848026	1.317603	4.166176
1	-2.277012	1.348997	2.557433
1	1.802363	0.500950	1.462621
1	2.484522	0.717202	3.813171
1	-1.593307	1.547988	4.922770
1	0.787746	1.233005	5.569568
6	-2.442651	1.405821	-0.023205
6	-4.974834	2.610187	-0.098449
6	-3.602890	0.618911	-0.026015
6	-2.562941	2.804226	-0.060613
6	-3.822356	3.401282	-0.097943
6	-4.863309	1.219564	-0.062417
1	-3.512276	-0.463370	-0.010522
1	-1.672740	3.425951	-0.067397
1	-3.904295	4.484329	-0.131350
1	-5.755289	0.599099	-0.071686
1	-5.955223	3.077626	-0.132953
1	-1.388281	-4.577498	-0.761729
1	-1.891077	-1.745877	2.511906
1	0.738916	-2.193775	2.202144
1	4.406976	-1.785317	2.281683
1	5.417069	0.461755	1.793503

Transition state **ts-1a-2d**

Energy = -1847.31481096

77	-0.343580	-1.559146	-0.181202
15	-0.758335	0.666723	0.083348
6	1.049268	-3.219151	0.781852
6	0.757717	-2.237603	1.767763
6	-0.194376	-3.807766	0.379514
6	-0.660397	-2.288431	2.039612
6	-1.240696	-3.281539	1.214604
1	-2.286797	-3.552573	1.171249
1	2.013051	-3.451300	0.353810
6	-1.150716	-1.580007	-1.862506
8	-1.880388	-1.634998	-2.767589
8	1.024339	-1.459181	-3.435207
7	1.833268	-1.120662	-2.557804
6	1.961229	-0.955222	-1.350386
6	2.959871	-0.234707	-0.567669
6	4.767638	1.258777	0.998637
6	3.291554	1.090976	-0.915122
6	3.572006	-0.801570	0.563315
6	4.465314	-0.062456	1.338482
6	4.184195	1.826409	-0.138104
1	2.828318	1.538968	-1.786182
1	3.352930	-1.827284	0.829866
1	4.414815	2.850859	-0.417861
6	0.025351	1.886487	-1.050650
6	1.154934	3.712952	-2.856311
6	0.133707	1.562217	-2.411475
6	0.483902	3.135230	-0.604155

6	1.049235	4.041551	-1.503369
6	0.692228	2.473781	-3.307480
1	-0.176117	0.590333	-2.778639
1	0.416706	3.398389	0.446491
1	1.410132	5.001322	-1.143275
1	0.782338	2.200798	-4.354865
1	1.600533	4.416212	-3.554762
6	-0.273653	1.204008	1.778409
6	0.530165	1.792642	4.402959
6	-1.229031	1.379876	2.789187
6	1.089642	1.327265	2.094429
6	1.486469	1.624851	3.397136
6	-0.825956	1.669821	4.095615
1	-2.286401	1.292273	2.559959
1	1.840813	1.194374	1.326122
1	2.545656	1.720345	3.619276
1	-1.575670	1.803450	4.870921
1	0.840422	2.019809	5.419317
6	-2.545610	1.127061	-0.012194
6	-5.267456	1.809249	-0.043116
6	-3.528415	0.130706	0.068521
6	-2.940796	2.470838	-0.112277
6	-4.293442	2.808300	-0.126384
6	-4.882943	0.471346	0.053375
1	-3.225473	-0.910125	0.132564
1	-2.192815	3.254138	-0.187338
1	-4.587396	3.851257	-0.208290
1	-5.635005	-0.311024	0.108279
1	-6.321239	2.074161	-0.060051
1	-0.310195	-4.581758	-0.368048
1	-1.177066	-1.663617	2.756179
1	1.462873	-1.587842	2.266054
1	4.928337	-0.521725	2.207948
1	5.457778	1.836709	1.607334

Transition state **ts-1b-2d**

Energy = -2306.91059242

77	1.054399	-1.455134	-0.058362
15	0.831665	0.816846	-0.065007
6	-0.030330	-3.331251	-1.019880
6	-0.180290	-2.218244	-1.891583
6	1.373044	-3.596515	-0.899839
6	1.129215	-1.859603	-2.385404
6	2.081112	-2.730610	-1.804960
1	3.151269	-2.711310	-1.960226
1	-0.808880	-3.858970	-0.489499
6	2.138740	-1.409261	1.455477
8	3.003159	-1.347615	2.232103
8	0.316783	-2.049619	3.372194
7	-0.691576	-1.865146	2.677587
6	-1.081149	-1.634977	1.539912
6	-2.346559	-1.133080	1.022223
6	-4.665004	-0.001130	-0.075860
6	-2.928658	0.018363	1.589993
6	-2.984409	-1.721445	-0.083043
6	-4.136027	-1.164613	-0.635157
6	-4.078458	0.585232	1.046622

1	-2.456537	0.483110	2.447191	6	1.483585	-1.376254	-1.497464
1	-2.577403	-2.624365	-0.518244	6	2.662175	-0.794662	-0.867793
1	-4.503307	1.485334	1.477679	6	4.800370	0.453021	0.423630
6	-0.020383	1.655742	1.334612	6	3.161428	0.442192	-1.325948
6	-1.236480	2.909886	3.530608	6	3.290412	-1.398501	0.235422
6	0.209690	1.185039	2.636359	6	4.356889	-0.781216	0.886792
6	-0.860726	2.763302	1.144098	6	4.226843	1.068711	-0.684315
6	-1.468421	3.383627	2.237701	1	2.693297	0.917974	-2.178999
6	-0.392961	1.812704	3.726626	1	2.944826	-2.361863	0.585593
1	0.824298	0.309152	2.810667	1	4.604092	2.028199	-1.021804
1	-1.056760	3.135544	0.143805	6	0.087093	1.758886	-1.205764
1	-2.125242	4.234151	2.075867	6	1.316962	3.250805	-3.238919
1	-0.215391	1.426615	4.726149	6	-0.010915	1.348243	-2.543891
1	-1.714111	3.389728	4.380610	6	0.801111	2.926461	-0.896502
6	-0.071197	1.363198	-1.574883	6	1.415635	3.665975	-1.909354
6	-1.464669	1.978302	-3.932733	6	0.599143	2.093192	-3.553009
6	0.605822	1.905924	-2.675925	1	-0.525528	0.431312	-2.808077
6	-1.453697	1.132287	-1.666560	1	0.892944	3.254007	0.133969
6	-2.146463	1.444062	-2.835175	1	1.974488	4.562926	-1.655985
6	-0.090039	2.207053	-3.850026	1	0.526884	1.752387	-4.581722
1	1.673015	2.096150	-2.619507	1	1.800864	3.823048	-4.025875
1	-1.989272	0.713168	-0.824887	6	-0.036683	1.315668	1.680133
1	-3.217696	1.267953	-2.882539	6	1.121959	1.959408	4.154210
1	0.445246	2.626647	-4.697594	6	-0.835013	1.773093	2.737427
1	-2.003112	2.217533	-4.845695	6	1.348470	1.184587	1.873690
6	2.432356	1.733319	-0.164985	6	1.923917	1.510709	3.100305
6	4.859863	3.116677	-0.422087	6	-0.255527	2.088728	3.969779
6	3.599792	1.054956	-0.541943	1	-1.906058	1.885834	2.602035
6	2.493459	3.113783	0.084617	1	1.975902	0.831529	1.065665
6	3.700512	3.799741	-0.044006	1	2.998561	1.411505	3.227507
6	4.807459	1.744461	-0.670428	1	-0.884175	2.441324	4.783055
1	3.556532	-0.015342	-0.720404	1	1.569485	2.209246	5.112334
1	1.601275	3.652907	0.387912	6	-2.459320	1.506936	0.104765
1	3.737169	4.867037	0.156812	6	-5.029528	2.622894	0.244850
1	5.707079	1.205580	-0.954955	6	-3.567517	0.701771	0.403484
1	5.800644	3.652392	-0.515756	6	-2.651598	2.878603	-0.124897
1	1.814943	-4.377231	-0.294514	6	-3.929843	3.431567	-0.054920
1	1.331276	-1.053249	-3.078131	6	-4.846275	1.258374	0.474180
1	-1.104411	-1.738782	-2.180168	1	-3.420433	-0.361929	0.566762
1	-4.616859	-1.623510	-1.492480	1	-1.805431	3.514338	-0.366845
17	-6.082756	0.742630	-0.805107	1	-4.067906	4.493298	-0.240623
				1	-5.698453	0.622574	0.698335
				1	-6.025488	3.054897	0.292677
				1	-1.231514	-4.504670	-0.014206
				1	-1.254665	-1.317448	2.963693
				1	1.290410	-1.720198	2.205705
				9	5.815227	1.068355	1.067674
				1	4.845959	-1.240243	1.739616

Transition state **ts-1c-2d**

Energy = -1946.54818139

77	-0.749426	-1.514233	-0.048479
15	-0.770252	0.761807	0.082563
6	0.452488	-3.332935	0.890012
6	0.437285	-2.263791	1.826423
6	-0.907697	-3.722019	0.659494
6	-0.930135	-2.058657	2.244975
6	-1.753309	-2.981606	1.556986
1	-2.827838	-3.072722	1.639126
1	1.311060	-3.752125	0.386764
6	-1.730951	-1.497822	-1.633074
8	-2.553220	-1.485451	-2.456451
8	0.246469	-1.822077	-3.434199
7	1.192369	-1.583357	-2.668910

Transition state **ts-1d-2d**

Energy = -1946.54879239

77	-0.875558	-1.451170	-0.216562
15	-0.671608	0.802490	0.086433
6	-0.001937	-3.432507	0.745659
6	-0.058519	-2.422027	1.744265
6	-1.342682	-3.668849	0.298017
6	-1.448612	-2.108138	1.982058

6	-2.240863	-2.899810	1.118353
1	-3.319526	-2.886218	1.040396
1	0.880939	-3.902540	0.338612
6	-1.608992	-1.224722	-1.913495
8	-2.282377	-1.065963	-2.849223
8	0.602764	-1.698441	-3.444551
7	1.426674	-1.596260	-2.526678
6	1.552678	-1.490864	-1.313331
6	2.677434	-1.059996	-0.490877
6	4.743574	-0.072866	1.166880
6	3.342552	0.137941	-0.815639
6	3.081542	-1.766894	0.656012
6	4.103950	-1.277785	1.469033
6	4.346872	0.605686	0.018067
1	3.063215	0.709369	-1.690783
1	2.598145	-2.701673	0.906339
9	4.949551	1.774804	-0.290572
6	0.463576	1.766304	-0.994124
6	2.141088	3.205899	-2.722627
6	0.509278	1.452554	-2.361246
6	1.262411	2.810607	-0.503185
6	2.103157	3.520243	-1.363030
6	1.338929	2.174541	-3.219243
1	-0.063071	0.623456	-2.762026
1	1.248068	3.060972	0.552509
1	2.734363	4.310003	-0.965851
1	1.372611	1.909614	-4.272033
1	2.800620	3.753799	-3.389987
6	-0.126487	1.160510	1.810784
6	0.694685	1.477330	4.477534
6	-1.038133	1.584777	2.788020
6	1.202280	0.897857	2.183005
6	1.609537	1.061127	3.505987
6	-0.627771	1.738092	4.115071
1	-2.067448	1.797714	2.517144
1	1.920353	0.571138	1.442141
1	2.643471	0.858924	3.771607
1	-1.344085	2.067046	4.863142
1	1.011915	1.599934	5.509555
6	-2.255913	1.738649	-0.059521
6	-4.680123	3.145992	-0.164110
6	-3.477157	1.051895	-0.019437
6	-2.260229	3.139526	-0.156114
6	-3.466099	3.837462	-0.207065
6	-4.683674	1.753572	-0.070906
1	-3.473368	-0.032418	0.041262
1	-1.322503	3.685338	-0.198742
1	-3.458121	4.921218	-0.285898
1	-5.624044	1.209678	-0.046927
1	-5.618679	3.691819	-0.209528
1	-1.633710	-4.374200	-0.469489
1	-1.806949	-1.381706	2.699536
1	0.775690	-1.986170	2.274131
1	4.406704	-1.838479	2.348891
1	5.533582	0.335292	1.788072

Cycloadduct **1a-2a**

Energy = -1966.79663309

45	-1.104100	-0.203480	-0.768851
15	0.743104	0.860796	0.270455
5	-2.654133	-1.828899	-0.487937
6	-2.240749	-1.186294	1.034217
5	-3.244875	-0.413507	-1.483978
1	-3.328247	-0.313475	-2.665939
5	-4.393865	-1.509192	-0.649981
1	-5.101707	-2.246110	-1.268750
5	-3.741430	-1.968171	0.938728
1	-3.879751	-3.027760	1.469267
5	-2.374660	0.520939	0.977733
1	-1.731398	1.278245	1.625533
6	-3.154351	0.939543	-0.452531
1	-3.042770	1.930986	-0.877430
5	-4.686271	0.243808	-0.617890
1	-5.520849	0.813870	-1.249524
5	-4.961122	-0.696431	0.852070
1	-6.055969	-0.848672	1.303894
5	-3.524001	-0.496713	1.891539
1	-3.502759	-0.509757	3.083484
5	-4.123346	0.874535	0.928624
1	-4.547708	1.880803	1.406844
1	-2.259372	-2.875056	-0.891489
1	-1.504582	-1.651772	1.682889
6	-0.780227	0.559920	-2.580052
8	-1.124888	1.640786	-3.009249
8	-0.098775	-0.283851	-3.465390
7	0.469498	-1.434599	-2.861266
6	0.153258	-1.562447	-1.620002
6	0.921830	-2.606586	-0.882966
6	2.509030	-4.388971	0.629667
6	0.342497	-3.447987	0.081750
6	2.315381	-2.683381	-1.079024
6	3.098920	-3.559096	-0.327430
6	1.125865	-4.334860	0.820625
1	-0.723462	-3.401340	0.253852
1	2.776113	-2.024050	-1.805643
1	0.651398	-4.975486	1.560222
1	3.119713	-5.067250	1.221431
1	4.175095	-3.581400	-0.483161
6	2.436174	0.687333	-0.457502
6	4.958671	0.473512	-1.682783
6	2.567294	0.815295	-1.848867
6	3.588858	0.472980	0.312784
6	4.839822	0.361795	-0.296295
6	3.819192	0.708329	-2.455115
1	1.695311	0.976883	-2.470060
1	3.513637	0.375306	1.390406
1	5.720641	0.183786	0.316128
1	3.894975	0.792585	-3.535749
1	5.932045	0.377601	-2.157858
6	0.947889	0.247549	2.000507
6	1.021993	-0.891077	4.574082
6	0.463007	0.956135	3.110366
6	1.470710	-1.042083	2.200741

6	1.509764	-1.603496	3.476249	1	2.865550	0.546284	-2.206520
6	0.500991	0.389904	4.385862	1	3.611573	-3.335699	0.785913
1	0.043585	1.947333	2.981976	17	6.040161	-1.801133	0.671478
1	1.849060	-1.612674	1.362232	1	5.086794	0.211512	-1.149643
1	1.912069	-2.605369	3.599377	6	1.047140	2.216836	-0.495791
1	0.111152	0.951550	5.230928	6	2.973421	3.737571	-1.869754
1	1.042450	-1.332735	5.567357	6	0.874708	2.530571	-1.853209
6	0.643683	2.696515	0.429686	6	2.185967	2.695710	0.168711
6	0.511633	5.494191	0.566364	6	3.144075	3.446385	-0.515222
6	-0.290715	3.396901	-0.344547	6	1.831022	3.284356	-2.533409
6	1.527659	3.410861	1.254773	1	0.007533	2.170705	-2.393220
6	1.456716	4.800811	1.329270	1	2.340627	2.471362	1.218435
6	-0.352192	4.791512	-0.273863	1	4.026791	3.797962	0.013510
1	-0.942171	2.860277	-1.025524	1	1.686518	3.499007	-3.588673
1	2.269051	2.876538	1.842744	1	3.725183	4.312894	-2.404603
1	2.140245	5.343146	1.978281	6	0.475017	0.758230	1.952015
1	-1.078851	5.323899	-0.881820	6	1.565878	-0.211774	4.358692
1	0.456705	6.578761	0.623189	6	-0.199265	0.944727	3.167588
Cycloadduct 1b-2a				6	1.701455	0.071951	1.960922
Energy= -2426.39582214				6	2.245026	-0.403696	3.153160
45	-1.093927	-0.733905	-0.770033	6	0.343899	0.462586	4.360201
15	-0.269005	1.204615	0.322397	1	-1.155750	1.454740	3.186552
5	-1.162388	-2.992374	-0.644083	1	2.235538	-0.092665	1.034491
6	-1.074353	-2.353302	0.930365	1	3.194666	-0.931642	3.129311
5	-2.653079	-2.251109	-1.404559	1	-0.198566	0.608545	5.290778
1	-2.931656	-2.142992	-2.555613	1	1.982550	-0.590800	5.288466
5	-2.693507	-3.890597	-0.679508	6	-1.502719	2.519186	0.710442
1	-2.823126	-4.862484	-1.361650	6	-3.373632	4.549107	1.197845
5	-1.704511	-3.921155	0.797467	6	-2.766559	2.471842	0.108086
1	-1.051945	-4.843800	1.179612	6	-1.175412	3.603275	1.541703
5	-2.292577	-1.160978	1.119325	6	-2.107972	4.608461	1.790330
1	-2.217677	-0.219078	1.836228	6	-3.695968	3.486739	0.353383
6	-3.331435	-1.257897	-0.200448	1	-3.010170	1.669099	-0.578530
1	-3.945509	-0.412095	-0.488606	1	-0.189893	3.656603	1.996589
5	-4.049049	-2.777660	-0.388611	1	-1.847008	5.439523	2.441210
1	-5.125419	-2.856008	-0.893839	1	-4.671531	3.442283	-0.123321
5	-3.455290	-3.770097	0.946073	1	-4.100812	5.334507	1.389735
1	-4.118794	-4.640441	1.423512	Cycloadduct 1c-2a			
5	-2.375806	-2.748271	1.935189	Energy = -2066.03236354			
1	-2.199190	-2.832149	3.111032	45	-1.090238	-0.511803	-0.775678
5	-3.838794	-2.048454	1.202421	15	0.213946	1.154990	0.293292
1	-4.749518	-1.612177	1.835848	5	-1.809936	-2.647406	-0.574220
1	-0.241126	-3.485456	-1.211057	6	-1.612879	-1.982403	0.978386
1	-0.136736	-2.262852	1.471552	5	-2.987795	-1.553718	-1.444271
6	-1.575486	0.195095	-2.466213	1	-3.171257	-1.429608	-2.612610
8	-2.590475	0.806227	-2.723269	5	-3.531781	-3.074610	-0.664631
8	-0.624444	0.090164	-3.489980	1	-3.904653	-4.002536	-1.317725
7	0.620947	-0.447154	-3.082277	5	-2.660370	-3.310050	0.866017
6	0.619172	-0.858020	-1.862272	1	-2.317509	-4.359491	1.318232
6	1.965334	-1.195078	-1.317049	5	-2.443428	-0.483654	1.056111
6	4.473754	-1.581910	-0.122624	1	-2.138017	0.432046	1.745415
6	2.199756	-2.286897	-0.464419	6	-3.407432	-0.346945	-0.316474
6	3.034056	-0.312348	-1.567087	1	-3.738119	0.623268	-0.670100
6	4.281792	-0.493891	-0.971881	5	-4.520837	-1.607009	-0.492192
6	3.446389	-2.490680	0.125637	1	-5.550714	-1.400771	-1.055131
1	1.397544	-2.979294	-0.251942	5	-4.298560	-2.658299	0.909759

1	-5.204751	-3.278201	1.379200
5	-3.015539	-1.938408	1.921387
1	-2.922890	-2.009301	3.107723
5	-4.181972	-0.888520	1.081871
1	-4.956917	-0.180397	1.646854
1	-1.042741	-3.409323	-1.068646
1	-0.713984	-2.134685	1.568981
6	-1.211988	0.424577	-2.530641
8	-1.995701	1.286963	-2.866076
8	-0.292229	-0.005202	-3.495408
7	0.730970	-0.851450	-2.996980
6	0.564143	-1.173827	-1.761702
6	1.735745	-1.845130	-1.129252
6	3.976889	-2.874503	0.187567
6	1.613116	-2.907789	-0.217560
6	3.022340	-1.321331	-1.366660
6	4.144194	-1.825952	-0.708957
6	2.728413	-3.432271	0.435091
1	0.636966	-3.324993	-0.015002
1	3.129422	-0.488250	-2.051221
1	2.636882	-4.252017	1.140497
9	5.060196	-3.360271	0.846186
1	5.132675	-1.407673	-0.870499
6	1.784242	1.743717	-0.491185
6	4.098444	2.663567	-1.797878
6	1.773494	1.991347	-1.872563
6	2.963345	1.985818	0.229688
6	4.113242	2.436746	-0.420384
6	2.922502	2.447420	-2.519306
1	0.879758	1.808507	-2.455628
1	2.994721	1.807784	1.299163
1	5.021520	2.606918	0.152807
1	2.896719	2.615671	-3.592436
1	4.996886	3.006447	-2.305341
6	0.752612	0.578640	1.963191
6	1.438608	-0.582537	4.435324
6	0.080151	0.947879	3.138139
6	1.775399	-0.382046	2.048070
6	2.117018	-0.954391	3.272521
6	0.422073	0.370982	4.362760
1	-0.720803	1.677165	3.100044
1	2.310710	-0.685285	1.157805
1	2.908464	-1.698400	3.306477
1	-0.118268	0.663447	5.259421
1	1.696611	-1.035755	5.389202
6	-0.626330	2.768319	0.603040
6	-1.899851	5.237802	0.971838
6	-1.816018	3.055885	-0.078135
6	-0.066912	3.736262	1.452934
6	-0.704048	4.961254	1.642533
6	-2.447142	4.288952	0.107909
1	-2.226821	2.334531	-0.775537
1	0.865431	3.526638	1.970358
1	-0.267273	5.700723	2.309535
1	-3.367868	4.502702	-0.428367
1	-2.396910	6.193759	1.118786

Cycloadduct **1d-2a**

Energy = -2066.03244312

45	-1.121441	-0.443509	-0.769082
15	0.358945	1.087377	0.275928
5	-2.193788	-2.418158	-0.497954
6	-1.998886	-1.682086	1.023985
5	-3.114058	-1.216299	-1.523880
1	-3.191650	-1.149218	-2.708712
5	-3.952396	-2.569439	-0.700801
1	-4.426585	-3.471342	-1.324156
5	-3.239944	-2.829856	0.906962
1	-3.107135	-3.885289	1.447153
5	-2.574201	-0.068097	0.944334
1	-2.165265	0.835965	1.595587
6	-3.405709	0.120273	-0.509023
1	-3.550747	1.101838	-0.946162
5	-4.696441	-0.955215	-0.696696
1	-5.636863	-0.628597	-1.351790
5	-4.748157	-1.923886	0.778980
1	-5.774402	-2.355580	1.210571
5	-3.438343	-1.346365	1.845400
1	-3.442536	-1.345969	3.037471
5	-4.353770	-0.187649	0.853192
1	-5.038974	0.674700	1.309408
1	-1.530122	-3.326822	-0.881549
1	-1.181552	-1.937206	1.692584
6	-0.962706	0.369807	-2.581430
8	-1.566469	1.319962	-3.031033
8	-0.058858	-0.269612	-3.439767
7	0.774885	-1.224981	-2.808976
6	0.466908	-1.429617	-1.576310
6	1.465337	-2.225667	-0.805958
6	3.431441	-3.479017	0.799898
6	1.108244	-3.197771	0.145642
6	2.826950	-1.900852	-0.954425
6	3.770206	-2.520276	-0.148081
6	2.081589	-3.821478	0.925685
1	0.066617	-3.453576	0.274685
1	3.138447	-1.144272	-1.663129
1	1.784373	-4.571291	1.654313
1	4.205442	-3.930851	1.412052
9	5.073405	-2.162337	-0.276611
6	2.062850	1.295660	-0.413372
6	4.589201	1.563383	-1.617570
6	2.175470	1.508884	-1.796645
6	3.231490	1.244312	0.360302
6	4.485968	1.368587	-0.239711
6	3.429255	1.643224	-2.391952
1	1.289500	1.544025	-2.419701
1	3.171161	1.084640	1.431193
1	5.381810	1.300958	0.372115
1	3.494818	1.787013	-3.466906
1	5.566652	1.646095	-2.086143
6	0.643768	0.617745	2.038176
6	0.905795	-0.339908	4.672539
6	0.024983	1.284779	3.105629
6	1.390888	-0.541009	2.311031

6	1.525243	-1.011629	3.616177	1	2.861257	-2.020496	-1.790109
6	0.156592	0.808193	4.411532	1	0.756310	-4.983432	1.579131
1	-0.573594	2.169601	2.920629	1	3.218583	-5.098264	1.201097
1	1.870220	-1.080338	1.504824	1	4.263819	-3.606784	-0.503978
1	2.106935	-1.911769	3.796225	6	2.513689	0.693260	-0.440042
1	-0.339173	1.333589	5.223829	6	5.011292	0.477052	-1.713418
1	1.000298	-0.712014	5.689636	6	2.621253	0.847774	-1.830626
6	-0.188550	2.846818	0.349866	6	3.677005	0.452127	0.305712
6	-1.005500	5.527509	0.385262	6	4.915949	0.340384	-0.327480
6	-1.315867	3.248925	-0.376488	6	3.860954	0.738542	-2.460731
6	0.540821	3.802480	1.076551	1	1.740696	1.032833	-2.432680
6	0.130533	5.133901	1.100548	1	3.620370	0.335182	1.382348
6	-1.720001	4.586929	-0.356633	1	5.805427	0.141904	0.265811
1	-1.850383	2.528425	-0.983611	1	3.918391	0.842573	-3.540727
1	1.428854	3.499147	1.624787	1	5.975002	0.380160	-2.207654
1	0.697900	5.865043	1.671465	6	1.079010	0.266210	2.051090
1	-2.593376	4.888713	-0.928557	6	1.218959	-0.862989	4.625695
1	-1.324644	6.566932	0.401348	6	0.648290	0.989522	3.173040
				6	1.581000	-1.033429	2.239153
				6	1.652444	-1.590641	3.514971
				6	0.719088	0.427963	4.449516
				1	0.244625	1.988475	3.054494
				1	1.917145	-1.615246	1.390566
				1	2.037591	-2.600332	3.628738
				1	0.370799	1.001178	5.304913
				1	1.264679	-1.300804	5.619833
				6	0.744438	2.709128	0.469293
				6	0.631936	5.508237	0.582964
				6	-0.200145	3.407784	-0.293888
				6	1.650053	3.425257	1.268933
				6	1.588391	4.816171	1.332742
				6	-0.251688	4.803350	-0.234577
				1	-0.863897	2.868634	-0.960896
				1	2.401931	2.891967	1.844444
				1	2.288290	5.360202	1.962578
				1	-0.985539	5.334757	-0.834686
				1	0.584505	6.593590	0.631070

Cycloadduct 1a-2b

Energy = -1960.62405036

77	-1.023659	-0.183798	-0.676367
15	0.836452	0.872072	0.322141
5	-2.576238	-1.809852	-0.369161
6	-2.111831	-1.167645	1.164252
5	-3.187183	-0.386500	-1.343582
1	-3.312612	-0.272209	-2.520227
5	-4.319838	-1.470013	-0.471026
1	-5.054282	-2.198715	-1.067409
5	-3.619275	-1.937872	1.092751
1	-3.748029	-2.998522	1.622699
5	-2.240355	0.552111	1.126167
1	-1.590932	1.305224	1.771225
6	-3.050463	0.977446	-0.295928
1	-2.956308	1.971095	-0.718978
5	-4.588810	0.284622	-0.427011
1	-5.432629	0.866399	-1.034500
5	-4.836241	-0.660355	1.044830
1	-5.919415	-0.806688	1.525206
5	-3.375130	-0.471378	2.050203
1	-3.325929	-0.493704	3.240821
5	-3.988422	0.904401	1.111106
1	-4.397517	1.910535	1.601776
1	-2.208129	-2.863806	-0.777394
1	-1.370808	-1.647612	1.796106
6	-0.717188	0.593680	-2.504649
8	-1.089969	1.661641	-2.951649
8	-0.023579	-0.242109	-3.392748
7	0.553514	-1.394473	-2.801160
6	0.244562	-1.531457	-1.555101
6	1.016360	-2.592955	-0.844448
6	2.606116	-4.407702	0.625633
6	0.442531	-3.437257	0.120691
6	2.404979	-2.682961	-1.063450
6	3.190202	-3.574642	-0.332241
6	1.226567	-4.340521	0.838707
1	-0.619705	-3.377585	0.311576

Cycloadduct 1b-2b

Energy = -2420.22319253

77	-1.023033	-0.665121	-0.672985
15	-0.160172	1.267107	0.376956
5	-1.130772	-2.927251	-0.530457
6	-0.987813	-2.266291	1.054040
5	-2.626659	-2.165413	-1.262710
1	-2.944824	-2.064134	-2.403673
5	-2.687621	-3.789733	-0.505427
1	-2.858903	-4.768489	-1.167573
5	-1.657582	-3.818934	0.941321
1	-1.014037	-4.750105	1.316899
5	-2.182719	-1.041239	1.271298
1	-2.084803	-0.104747	1.991475
6	-3.253164	-1.126852	-0.036937
1	-3.866143	-0.278022	-0.317120
5	-4.002242	-2.636597	-0.195952
1	-5.092387	-2.691110	-0.673230
5	-3.401598	-3.632150	1.133487

1	-4.071991	-4.482031	1.636881	Cycloadduct 1c-2b		
5	-2.279905	-2.626181	2.088230	Energy = -2059.85978956		
1	-2.075707	-2.707524	3.259420	77	-1.017847	-0.459284 -0.682226
5	-3.740714	-1.901828	1.386370	15	0.325185	1.187557 0.344395
1	-4.628467	-1.442173	2.034963	5	-1.774363	-2.585326 -0.443205
1	-0.233962	-3.456726	-1.103991	6	-1.522374	-1.896340 1.114799
1	-0.036645	-2.202619	1.573862	5	-2.951145	-1.480163 -1.300846
6	-1.513093	0.272793	-2.383638	1	-3.174890	-1.364431 -2.462722
8	-2.532700	0.874266	-2.660280	5	-3.511393	-2.971273 -0.474937
8	-0.558866	0.167516	-3.408343	1	-3.924435	-3.900866 -1.100242
7	0.683442	-0.384458	-3.012625	5	-2.601682	-3.199935 1.032747
6	0.685779	-0.797671	-1.789398	1	-2.268814	-4.249459 1.491141
6	2.035624	-1.167168	-1.272146	5	-2.327982	-0.370467 1.201120
6	4.554099	-1.620496	-0.125245	1	-2.003337	0.542942 1.883013
6	2.256267	-2.264004	-0.422732	6	-3.315759	-0.232173 -0.165484
6	3.121910	-0.314273	-1.544490	1	-3.644386	0.736465 -0.524119
6	4.375332	-0.528616	-0.972161	5	-4.454544	-1.476226 -0.302589
6	3.507772	-2.501394	0.144111	1	-5.491286	-1.250477 -0.844216
1	1.438477	-2.932466	-0.193117	5	-4.226281	-2.515915 1.107427
1	2.963779	0.547896	-2.181877	1	-5.133882	-3.109312 1.606819
1	3.663084	-3.350321	0.801825	5	-2.909264	-1.810475 2.082414
17	6.129530	-1.881568	0.638724	1	-2.791581	-1.872957 3.266655
1	5.195460	0.154944	-1.165510	5	-4.069811	-0.748716 1.258110
6	1.163226	2.243272	-0.472938	1	-4.819485	-0.019277 1.829169
6	3.099305	3.705802	-1.894691	1	-1.039006	-3.379394 -0.935551
6	0.965927	2.563407	-1.825353	1	-0.617726	-2.070285 1.689236
6	2.331720	2.687763	0.163231	6	-1.146977	0.481046 -2.454851
6	3.294335	3.410115	-0.544588	8	-1.938248	1.333153 -2.810312
6	1.927685	3.287279	-2.529546	8	-0.227121	0.045787 -3.421189
1	0.074750	2.231379	-2.343235	7	0.790106	-0.813126 -2.933312
1	2.506005	2.459653	1.208911	6	0.628967	-1.134377 -1.692963
1	4.199827	3.735135	-0.037878	6	1.798499	-1.835236 -1.086640
1	1.763736	3.505375	-3.581201	6	4.037104	-2.924368 0.184728
1	3.854700	4.258026	-2.448488	6	1.665630	-2.892691 -0.170933
6	0.597368	0.840727	2.006816	6	3.092841	-1.346425 -1.351139
6	1.717117	-0.089460	4.415390	6	4.213912	-1.880875 -0.715742
6	-0.037951	1.089727	3.231513	6	2.779233	-3.447519 0.459432
6	1.798755	0.111601	2.007011	1	0.682021	-3.280427 0.053382
6	2.357114	-0.344354	3.199983	1	3.207345	-0.516437 -2.038327
6	0.519464	0.626907	4.425535	1	2.680207	-4.264286 1.167342
1	-0.976003	1.632685	3.257693	9	5.120563	-3.439543 0.820814
1	2.301362	-0.101977	1.072944	1	5.209910	-1.489500 -0.897516
1	3.286932	-0.906123	3.169621	6	1.892939	1.739790 -0.470632
1	0.007004	0.821268	5.364249	6	4.200972	2.610597 -1.820211
1	2.144996	-0.452735	5.346368	6	1.860175	1.991784 -1.850691
6	-1.370013	2.608676	0.745378	6	3.090912	1.953036 0.227697
6	-3.197245	4.686118	1.194448	6	4.237577	2.380263 -0.443781
6	-2.634133	2.576659	0.142772	6	3.006507	2.422814 -2.518776
6	-1.018397	3.702352	1.553881	1	0.951144	1.831836 -2.416146
6	-1.929790	4.730973	1.784312	1	3.139657	1.772273 1.295894
6	-3.541740	3.615473	0.369407	1	5.160373	2.528552 0.112024
1	-2.891422	1.769907	-0.534330	1	2.963329	2.593675 -3.590904
1	-0.030369	3.745772	2.004357	1	5.096810	2.934414 -2.344599
1	-1.650531	5.569222	2.418143	6	0.882468	0.627030 2.015063
1	-4.517376	3.583544	-0.108130	6	1.600313	-0.503597 4.492060
1	-3.907717	5.490039	1.371696	6	0.252798	1.039533 3.198718
				6	1.879389	-0.361153 2.093147

6	3.406940	-1.037148	0.263375	8	2.881217	-1.676960	2.229151
6	4.498309	-0.445189	0.897743	8	0.820956	-1.569000	3.077534
6	4.248360	1.508553	-0.499024	7	-0.543801	-1.404818	2.740451
1	2.636460	1.437745	-1.930866	6	-0.754289	-1.374184	1.473898
1	3.070855	-2.019168	0.572449	6	-2.124421	-1.007403	1.036377
1	4.562606	2.506151	-0.794419	6	-4.597173	-0.104731	0.081060
6	-0.043553	1.939118	-0.788995	6	-2.763733	0.098213	1.625445
6	0.959836	4.026892	-2.369012	6	-2.765776	-1.657831	-0.028654
6	-0.174684	1.897342	-2.186143	6	-4.000911	-1.222885	-0.503701
6	0.578371	3.043545	-0.190378	6	-3.990657	0.556924	1.148714
6	1.078943	4.081071	-0.979730	1	-2.274169	0.618393	2.440675
6	0.326524	2.935177	-2.969575	1	-2.282616	-2.500295	-0.506851
1	-0.645562	1.048800	-2.669068	1	-4.464486	1.426361	1.591749
1	0.686169	3.096095	0.887341	6	0.102787	1.813383	1.029933
1	1.565907	4.928511	-0.504819	6	-1.035783	3.532914	2.932561
1	0.232405	2.881513	-4.050213	6	0.379074	1.643962	2.395888
1	1.357670	4.830892	-2.982265	6	-0.729730	2.867326	0.625649
6	-0.239648	0.853881	1.920467	6	-1.298813	3.718747	1.574491
6	0.614145	1.109096	4.583231	6	-0.189011	2.498709	3.339546
6	-1.176333	0.942471	2.959460	1	1.016813	0.836023	2.733737
6	1.132156	0.889484	2.229092	1	-0.949273	3.022581	-0.424870
6	1.553168	1.023876	3.550584	1	-1.950289	4.524956	1.248422
6	-0.748203	1.066983	4.284318	1	0.022587	2.344751	4.393622
1	-2.238775	0.912706	2.740545	1	-1.485643	4.191627	3.670397
1	1.870165	0.807147	1.439232	6	0.086512	0.987985	-1.779723
1	2.617026	1.054697	3.769213	6	-1.194675	1.200639	-4.270772
1	-1.484231	1.132327	5.081097	6	0.834696	1.194049	-2.947965
1	0.943571	1.206729	5.614059	6	-1.313025	0.889621	-1.873676
6	-2.537779	0.864086	0.113302	6	-1.947232	1.000431	-3.109847
6	-5.285862	1.393339	0.023132	6	0.195183	1.298094	-4.185814
6	-3.432640	-0.133888	-0.293603	1	1.915677	1.277047	-2.895139
6	-3.026497	2.137000	0.456465	1	-1.909838	0.727081	-0.984336
6	-4.394357	2.396745	0.418094	1	-3.030018	0.926145	-3.160485
6	-4.803669	0.135410	-0.337857	1	0.787120	1.457809	-5.082967
1	-3.059475	-1.098689	-0.616252	1	-1.689417	1.282533	-5.234634
1	-2.334654	2.921567	0.750943	6	2.590006	1.356750	-0.322217
1	-4.765161	3.381709	0.688457	6	5.158346	2.447387	-0.552180
1	-5.490188	-0.639592	-0.666978	6	3.715194	0.568292	-0.047720
1	-6.352322	1.599038	-0.012804	6	2.758291	2.701647	-0.695221
1	-0.489347	-4.513287	-0.993348	6	4.036671	3.241064	-0.815757
1	-1.397738	-1.929240	2.397229	6	4.995459	1.118050	-0.163007
1	1.266109	-2.287221	2.339742	1	3.593938	-0.453648	0.292853
1	5.018099	-0.981510	1.687571	1	1.888688	3.323200	-0.891006
1	5.756662	1.304723	1.033017	1	4.159247	4.280144	-1.108966
Cycloadduct 1b-2c				1	5.862810	0.503983	0.062580
Energy = -2313.14956569				1	6.155134	2.870837	-0.641593
45	0.802643	-1.610133	0.202255	1	1.682510	-4.457372	0.540180
15	0.897996	0.657807	-0.159582	1	2.025963	-1.433791	-2.579694
6	0.147735	-3.589343	-0.852044	1	-0.543363	-2.237629	-2.502029
6	0.252879	-2.608350	-1.870880	1	-4.489674	-1.731700	-1.327753
6	1.441402	-3.769456	-0.259368	17	-6.127592	0.489321	-0.553370
6	1.624524	-2.183384	-1.909792	Cycloadduct 1c-2c			
6	2.362645	-2.919522	-0.945704	Energy = -1952.78766247			
1	3.418582	-2.825639	-0.732743	45	0.428624	1.629488	-0.281242
1	-0.747081	-4.121156	-0.556213	15	0.831787	-0.582736	0.185418
6	1.699857	-1.593831	1.990142	6	-0.368378	3.620195	0.622205

6	-0.162426	2.739311	1.718215	1	-4.824795	1.398629	1.495504
6	0.897027	3.866929	-0.004635	Cycloadduct 1d-2c			
6	1.237661	2.437363	1.761156	Energy = -1952.78792996			
6	1.896264	3.153751	0.723099	45	-0.526484	-1.594318	-0.404445
1	2.954157	3.139787	0.500340	15	-0.761141	0.611938	0.195388
1	-1.310909	4.045906	0.303574	6	-0.033924	-3.739108	0.304098
6	1.225483	1.558646	-2.115682	6	-0.135680	-2.947089	1.484682
8	2.374395	1.757854	-2.431292	6	-1.316684	-3.763313	-0.334565
8	0.304931	1.322472	-3.137890	6	-1.477732	-2.465368	1.554617
7	-1.016760	1.058314	-2.706652	6	-2.216294	-2.986770	0.450364
6	-1.161877	1.124524	-1.431810	1	-3.262161	-2.815414	0.236739
6	-2.476607	0.683201	-0.899848	1	0.847298	-4.255884	-0.053124
6	-4.865264	-0.286192	0.167844	6	-1.141371	-1.304688	-2.286281
6	-3.068234	-0.489686	-1.404954	8	-2.270517	-1.350841	-2.712417
6	-3.119528	1.354645	0.152516	8	-0.109747	-1.099454	-3.206271
6	-4.317083	0.882132	0.687454	7	1.186435	-1.010528	-2.645251
6	-4.258785	-0.980416	-0.872862	6	1.204018	-1.188281	-1.374151
1	-2.572335	-1.025640	-2.205549	6	2.493914	-0.927734	-0.683755
1	-2.671628	2.250089	0.563898	6	4.814960	-0.237570	0.766587
1	-4.712267	-1.893091	-1.245035	6	3.177136	0.266387	-0.964868
6	-0.010583	-1.875150	-0.814732	6	2.998405	-1.780233	0.312667
6	-1.236598	-3.790237	-2.454687	6	4.151816	-1.441935	1.019677
6	0.188991	-1.851075	-2.204610	6	4.308446	0.590328	-0.228929
6	-0.819092	-2.872774	-0.253747	1	2.813235	0.947934	-1.722741
6	-1.429610	-3.825036	-1.073338	1	2.478750	-2.703008	0.536463
6	-0.422080	-2.803224	-3.017859	9	4.926619	1.766216	-0.478116
1	0.800891	-1.079142	-2.658148	6	0.282632	1.877027	-0.634087
1	-0.983835	-2.908890	0.817470	6	1.868841	3.724755	-2.022746
1	-2.059495	-4.590247	-0.627912	6	0.198130	1.973665	-2.032488
1	-0.270719	-2.763998	-4.092611	6	1.155439	2.724774	0.062067
1	-1.718183	-4.527507	-3.091291	6	1.948611	3.640669	-0.632458
6	0.309030	-0.896464	1.923001	6	0.986933	2.894001	-2.720244
6	-0.569970	-1.182941	4.573409	1	-0.459191	1.316028	-2.591126
6	1.217101	-1.227275	2.937475	1	1.233944	2.665148	1.141778
6	-1.045119	-0.703281	2.249861	1	2.636417	4.278183	-0.084484
6	-1.481364	-0.855350	3.564224	1	0.923903	2.947250	-3.803142
6	0.776658	-1.364992	4.257317	1	2.495016	4.429763	-2.562370
1	2.266195	-1.376741	2.704331	6	-0.353430	0.749868	1.986467
1	-1.754196	-0.427942	1.476657	6	0.326953	0.753513	4.710058
1	-2.532621	-0.711496	3.798641	6	-1.306291	1.097543	2.953173
1	1.490700	-1.617882	5.036393	6	0.944645	0.397024	2.397513
1	-0.909200	-1.293685	5.599666	6	1.282797	0.408519	3.749097
6	2.588478	-1.113408	0.106418	6	-0.965072	1.094806	4.309088
6	5.261492	-1.942192	0.008249	1	-2.313766	1.368720	2.654931
6	3.602951	-0.185800	-0.163412	1	1.688414	0.110267	1.661816
6	2.920213	-2.464657	0.310424	1	2.292585	0.141666	4.048743
6	4.250958	-2.874171	0.267723	1	-1.713498	1.362760	5.049945
6	4.935634	-0.604042	-0.212154	1	0.588930	0.754550	5.764539
1	3.351088	0.845311	-0.380063	6	-2.447889	1.314481	0.025331
1	2.135956	-3.193076	0.497893	6	-5.020044	2.396768	-0.200120
1	4.499730	-3.919630	0.428376	6	-3.517550	0.506383	-0.380621
1	5.715025	0.118558	-0.436951	6	-2.670951	2.675132	0.300629
1	6.298524	-2.264326	-0.033046	6	-3.952647	3.210503	0.194482
1	1.065584	4.500350	-0.865364	6	-4.799806	1.050799	-0.492499
1	1.711273	1.776705	2.476574	1	-3.340603	-0.527906	-0.650045
1	-0.913527	2.353893	2.393562	1	-1.840643	3.312207	0.593139
9	-6.012185	-0.762961	0.697799				

1	-4.118354	4.262280	0.411201
1	-5.621548	0.421294	-0.822088
1	-6.017955	2.817427	-0.290296
1	-1.556854	-4.281628	-1.253480
1	-1.867239	-1.814318	2.327242
1	0.653452	-2.727781	2.189484
1	4.535519	-2.114581	1.781897
1	5.700863	0.061286	1.316777

Cycloadduct **1a-2d**

Energy = -1847.37554308

77	-0.090890	-1.470365	-0.229264
15	-0.721800	0.694778	0.189446
6	0.825846	-3.395976	0.726116
6	0.524588	-2.517571	1.809992
6	-0.400349	-3.746916	0.072414
6	-0.894777	-2.317391	1.807077
6	-1.473438	-3.093276	0.759046
1	-2.522884	-3.163175	0.510619
1	1.806857	-3.749870	0.437984
6	-0.785957	-1.477802	-2.122096
8	-1.884033	-1.806383	-2.515410
8	0.159912	-1.132602	-3.090896
7	1.425616	-0.741257	-2.591713
6	1.505964	-0.803437	-1.307468
6	2.750076	-0.247285	-0.711282
6	5.004478	0.936243	0.494851
6	3.256736	0.976921	-1.181750
6	3.397068	-0.868319	0.368867
6	4.517996	-0.288087	0.961983
6	4.370036	1.563118	-0.580011
1	2.752400	1.471140	-2.004209
1	3.010677	-1.806420	0.747956
1	4.735120	2.518529	-0.947812
6	0.040611	2.053394	-0.787349
6	1.155971	4.066895	-2.387158
6	-0.093726	2.004548	-2.184240
6	0.725519	3.125256	-0.199611
6	1.280854	4.126880	-0.998944
6	0.463602	3.005460	-2.977325
1	-0.611741	1.178859	-2.659063
1	0.836801	3.181977	0.877398
1	1.814935	4.950102	-0.532237
1	0.366300	2.946753	-4.057403
1	1.595563	4.842664	-3.008272
6	-0.321733	1.077816	1.947476
6	0.389131	1.449316	4.637784
6	-1.308009	1.314779	2.913767
6	1.027494	1.023302	2.342140
6	1.378489	1.217693	3.676455
6	-0.951186	1.495174	4.253908
1	-2.353861	1.356419	2.627967
1	1.801348	0.822615	1.608554
1	2.425885	1.180660	3.963512
1	-1.725735	1.673212	4.994991
1	0.663336	1.591909	5.679489
6	-2.514082	1.057717	0.011495

6	-5.240815	1.639441	-0.248582
6	-3.417436	0.047798	-0.343249
6	-2.982765	2.367449	0.216770
6	-4.340395	2.653846	0.094348
6	-4.777571	0.343263	-0.473191
1	-3.054788	-0.948912	-0.564187
1	-2.283392	3.160524	0.467729
1	-4.695559	3.667794	0.257124
1	-5.469504	-0.442031	-0.764305
1	-6.298681	1.865694	-0.352028
1	-0.498091	-4.398329	-0.785662
1	-1.434699	-1.681355	2.496914
1	1.227371	-2.069947	2.497732
1	5.009100	-0.789791	1.792077
1	5.869068	1.396604	0.965808

Cycloadduct **1b-2d**

Energy = -2306.97116484

77	0.773673	-1.437302	0.140160
15	0.806584	0.838477	-0.168172
6	0.192914	-3.422154	-0.972506
6	0.244354	-2.404599	-1.966952
6	1.499091	-3.565976	-0.398519
6	1.596450	-1.917258	-2.000974
6	2.378458	-2.648141	-1.062896
1	3.431879	-2.517108	-0.859160
1	-0.676433	-3.998196	-0.684242
6	1.666629	-1.429030	1.948168
8	2.848951	-1.506354	2.202124
8	0.783709	-1.420245	3.033963
7	-0.585145	-1.290621	2.699924
6	-0.793308	-1.257011	1.429207
6	-2.182101	-0.937364	1.007545
6	-4.699584	-0.126368	0.086944
6	-2.863162	0.128980	1.620035
6	-2.803410	-1.595762	-0.064256
6	-4.059989	-1.206740	-0.522841
6	-4.112900	0.542439	1.160834
1	-2.388994	0.656314	2.439889
1	-2.287427	-2.408083	-0.560877
1	-4.619790	1.383204	1.622292
6	-0.036527	1.936305	1.041330
6	-1.245568	3.568549	2.975130
6	0.253021	1.756290	2.403053
6	-0.918356	2.956531	0.656514
6	-1.522098	3.765093	1.621294
6	-0.350936	2.567545	3.362495
1	0.928826	0.973028	2.724379
1	-1.147787	3.119220	-0.390693
1	-2.210823	4.546155	1.310985
1	-0.129386	2.405349	4.413236
1	-1.722240	4.193658	3.725290
6	0.001184	1.186139	-1.788577
6	-1.275420	1.416539	-4.279548
6	0.743190	1.478979	-2.941253
6	-1.389281	1.006699	-1.897429
6	-2.022099	1.127980	-3.132978

6	0.105607	1.591153	-4.180131
1	1.817376	1.620628	-2.877013
1	-1.977652	0.768925	-1.019089
1	-3.098195	0.991468	-3.195527
1	0.692481	1.817352	-5.066253
1	-1.768472	1.505516	-5.243658
6	2.478617	1.591323	-0.288109
6	5.014288	2.767216	-0.448181
6	3.622177	0.836910	0.005516
6	2.610981	2.945506	-0.641682
6	3.873510	3.527220	-0.728380
6	4.885935	1.429484	-0.075028
1	3.525454	-0.190579	0.337496
1	1.726244	3.541474	-0.849466
1	3.968619	4.572931	-1.007887
1	5.767349	0.841798	0.165840
1	5.998522	3.223527	-0.511233
1	1.777444	-4.264600	0.378997
1	1.957208	-1.129634	-2.649493
1	-0.573272	-2.052729	-2.580588
1	-4.533747	-1.722485	-1.351417
17	-6.261411	0.409780	-0.523332

Cycloadduct **1c-2d**

Energy = -1946.60922391

77	-0.434338	-1.471680	-0.173252
15	-0.774370	0.769220	0.185716
6	0.300583	-3.447120	0.850183
6	0.088938	-2.508487	1.901343
6	-0.953588	-3.694852	0.201990
6	-1.306709	-2.170425	1.890593
6	-1.958006	-2.920195	0.869375
1	-3.009143	-2.894366	0.618881
1	1.241734	-3.904709	0.575470
6	-1.215754	-1.448402	-2.033140
8	-2.363678	-1.646036	-2.365151
8	-0.281714	-1.260221	-3.055162
7	1.045066	-1.021423	-2.628025
6	1.180239	-1.047200	-1.346574
6	2.515979	-0.634763	-0.838768
6	4.959729	0.270113	0.161780
6	3.183901	0.448970	-1.438172
6	3.109918	-1.247680	0.275840
6	4.333861	-0.807848	0.778818
6	4.402305	0.906698	-0.941372
1	2.723992	0.945206	-2.284552
1	2.602964	-2.072528	0.760206
1	4.914586	1.752695	-1.387544
6	0.152939	1.977307	-0.844472
6	1.506133	3.766488	-2.525581
6	-0.025674	1.915367	-2.236180
6	1.006512	2.947811	-0.303300
6	1.680548	3.837427	-1.143306
6	0.649031	2.805121	-3.069548
1	-0.671226	1.162574	-2.675068
1	1.156229	3.012233	0.768808
1	2.344249	4.582192	-0.712642

1	0.512904	2.736983	-4.144905
1	2.035693	4.455448	-3.178064
6	-0.306742	1.159029	1.924719
6	0.493952	1.574833	4.582139
6	-1.223720	1.628177	2.873784
6	1.016310	0.892238	2.320373
6	1.414989	1.109601	3.637476
6	-0.822748	1.829432	4.198460
1	-2.249286	1.835828	2.587067
1	1.728347	0.509369	1.596453
1	2.443471	0.909787	3.925936
1	-1.543960	2.188636	4.927545
1	0.802982	1.735845	5.611299
6	-2.506093	1.354432	0.007550
6	-5.142256	2.265955	-0.236078
6	-3.544956	0.445592	-0.230939
6	-2.793699	2.727300	0.106119
6	-4.106672	3.178505	-0.008705
6	-4.859120	0.905099	-0.352732
1	-3.322017	-0.605425	-0.369747
1	-1.989336	3.439846	0.267716
1	-4.321601	4.240722	0.069997
1	-5.657032	0.196007	-0.554320
1	-6.164930	2.620089	-0.334358
1	-1.116235	-4.364640	-0.631646
1	-1.781847	-1.464654	2.560123
1	0.831230	-2.112977	2.579624
9	6.134576	0.716397	0.656932
1	4.803505	-1.281824	1.634641

Cycloadduct **1d-2d**

Energy = -1946.60963861

77	-0.581292	-1.429398	-0.287988
15	-0.652833	0.811441	0.205284
6	-0.229543	-3.539247	0.663303
6	-0.390791	-2.627299	1.747474
6	-1.447418	-3.568852	-0.091805
6	-1.717462	-2.087412	1.649358
6	-2.381694	-2.683893	0.538093
1	-3.393143	-2.490377	0.210089
1	0.655342	-4.118516	0.435222
6	-1.156776	-1.197470	-2.208724
8	-2.279919	-1.218042	-2.662308
8	-0.104586	-1.080747	-3.122777
7	1.189526	-1.042823	-2.554986
6	1.184168	-1.167055	-1.273206
6	2.493350	-0.955389	-0.598329
6	4.875231	-0.355119	0.794583
6	3.285658	0.137048	-0.985045
6	2.914964	-1.748898	0.481666
6	4.098109	-1.457782	1.160308
6	4.445673	0.419230	-0.277387
1	2.982823	0.779268	-1.802111
1	2.302347	-2.583874	0.796755
9	5.171979	1.502683	-0.632193
6	0.483671	1.953851	-0.678336
6	2.185002	3.627275	-2.148303

6	0.400840	1.993402	-2.079467
6	1.413476	2.770900	-0.020817
6	2.262924	3.600810	-0.755660
6	1.248150	2.826373	-2.807798
1	-0.303703	1.360269	-2.607741
1	1.490043	2.756366	1.060514
1	2.991607	4.216948	-0.236732
1	1.185170	2.835260	-3.891953
1	2.854226	4.265061	-2.719023
6	-0.254305	1.010520	1.993304
6	0.405119	1.093980	4.720984
6	-1.192853	1.452485	2.934808
6	1.017920	0.602011	2.432225
6	1.346826	0.653696	3.785052
6	-0.862637	1.488914	4.293237
1	-2.181249	1.766276	2.615640
1	1.746540	0.236890	1.716611
1	2.337496	0.343186	4.105821
1	-1.600527	1.829361	5.014626
1	0.659174	1.126436	5.776915
6	-2.280680	1.630597	-0.023209
6	-4.750441	2.908046	-0.350875
6	-3.391777	0.906378	-0.474092
6	-2.408950	3.005236	0.243134
6	-3.640032	3.637854	0.087016
6	-4.622487	1.549009	-0.637153
1	-3.285145	-0.137699	-0.743715
1	-1.544214	3.577160	0.569057
1	-3.732550	4.699713	0.298099
1	-5.475861	0.984311	-1.001939
1	-5.708664	3.404154	-0.479805
1	-1.632558	-4.166248	-0.974368
1	-2.141230	-1.351119	2.320139
1	0.344522	-2.372397	2.496739
1	4.415551	-2.086052	1.988153
1	5.788104	-0.091578	1.318099