

Supplementary Information

of "A theoretical Study of an Electronically Mismatched Diels -Alder Cycloadditions"

Qian Liu^a, Long-Jiu Cheng^a, Kun Wang^{*a,b}

^aDepartment of Chemistry, Anhui University, Hefei, Anhui 230601, P. R. China

^bState Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081 P. R. China

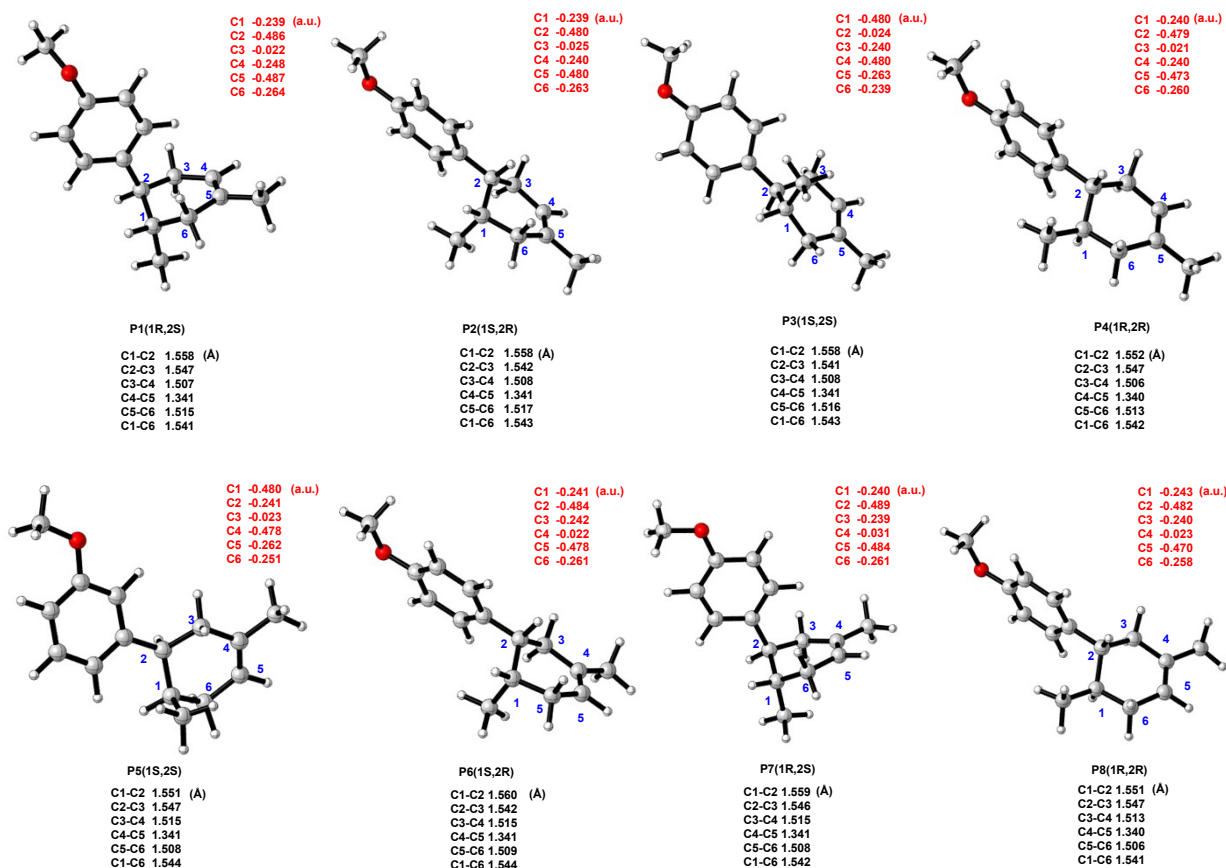


Figure S1. Proposed conformations of the products from the different reagents based on the optic activities of diene and the different substitution sites of -CH₃ on dienophile.

*^a Corresponding authors: Kun Wang, Tel & Fax: +86 551 63861279.

E-mail: wangkun@ahu.edu.cn

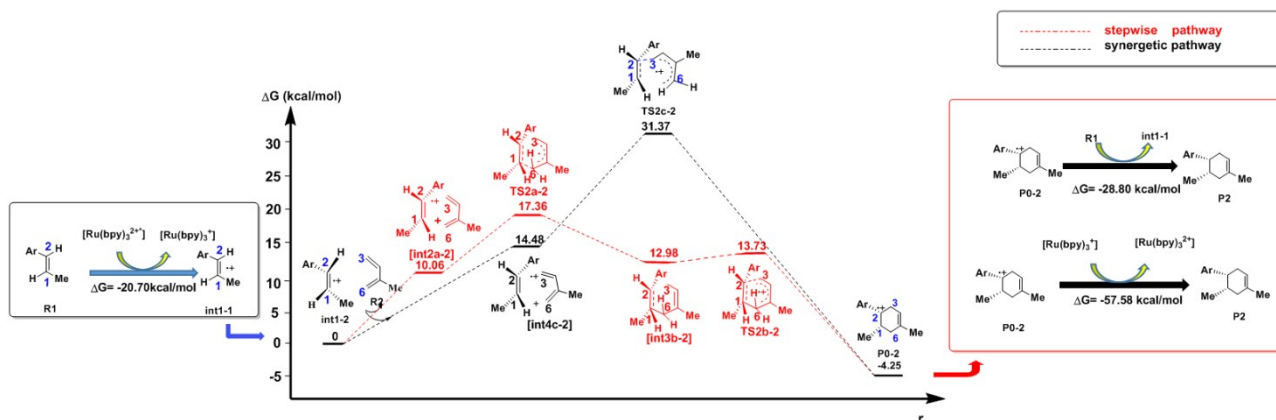


Figure S2. Schematic energy profiles of the C-C cycloaddition reaction between (1S,2R)-R1⁺ and R2 (5-Me). The red line is designed as stepwise pathway and the black line is regarded as synergetic pathway. [int2a-2] and [int4c-2] are the pre-reaction compounds after the molecular orientations in the corresponding pathways which are stationary points on the potential energy surface.

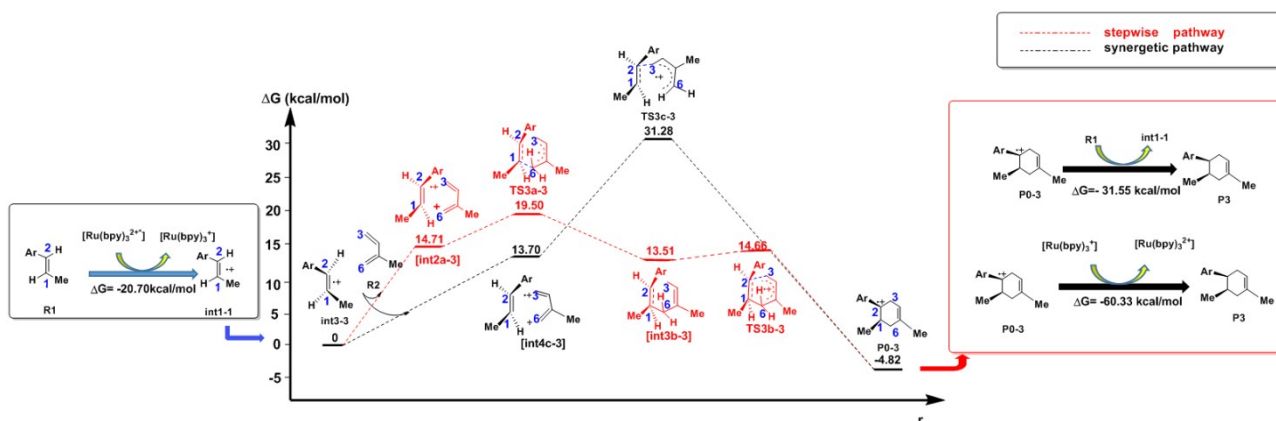


Figure S3. Schematic energy profiles of the C-C cycloaddition reaction between (1S,2S)-R1⁺ and R2 (5-Me). The red line is designed as stepwise pathway and the black line is regarded as synergetic pathway. [int2a-3] and [int4c-3] are the pre-reaction compounds after the molecular orientations in the corresponding pathways which are stationary points on the potential energy surface.

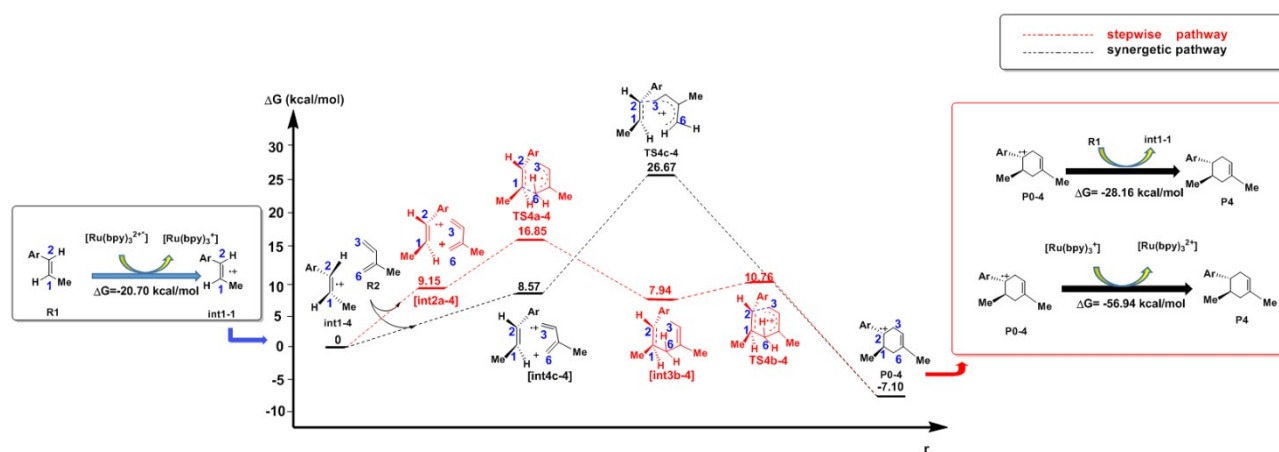


Figure S4. Schematic energy profiles of the C-C cycloaddition reaction between (1R,2R)-R1⁺ and R2 (5-Me). The red line is designed as stepwise pathway and the black line is regarded as synergetic pathway. [int2a-4] and [int4c-4] are the pre-reaction compounds after the molecular orientations in the corresponding pathways which are stationary points on the potential energy surface.

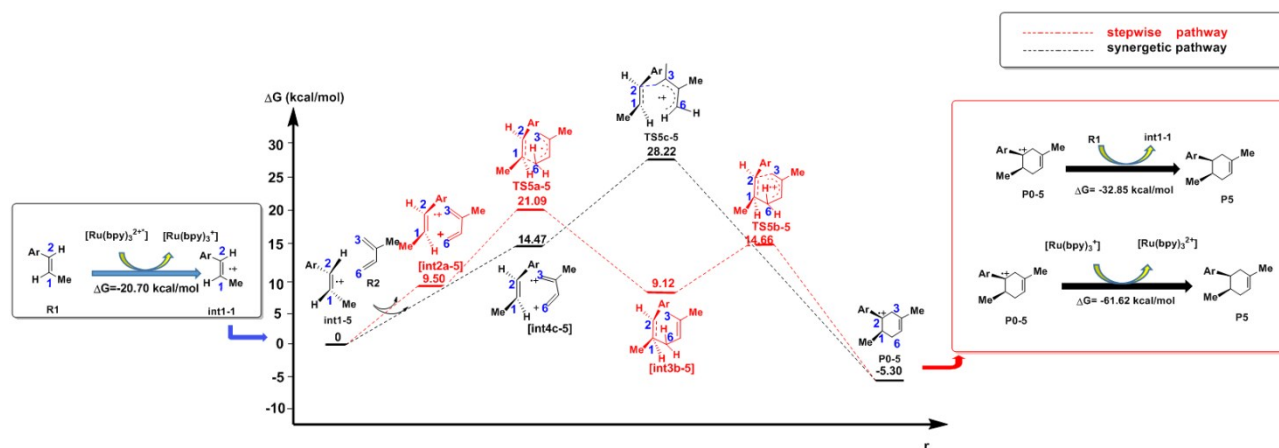


Figure S5. Schematic energy profiles of the C-C cycloaddition reaction between (1S,2S)-R1⁺ and R2 (4-Me). The red line is designed as stepwise pathway and the black line is regarded as synergetic pathway. [int2a-5] and [int4c-5] are the pre-reaction compounds after the molecular orientations in the corresponding pathways which are stationary points on the potential energy surface.

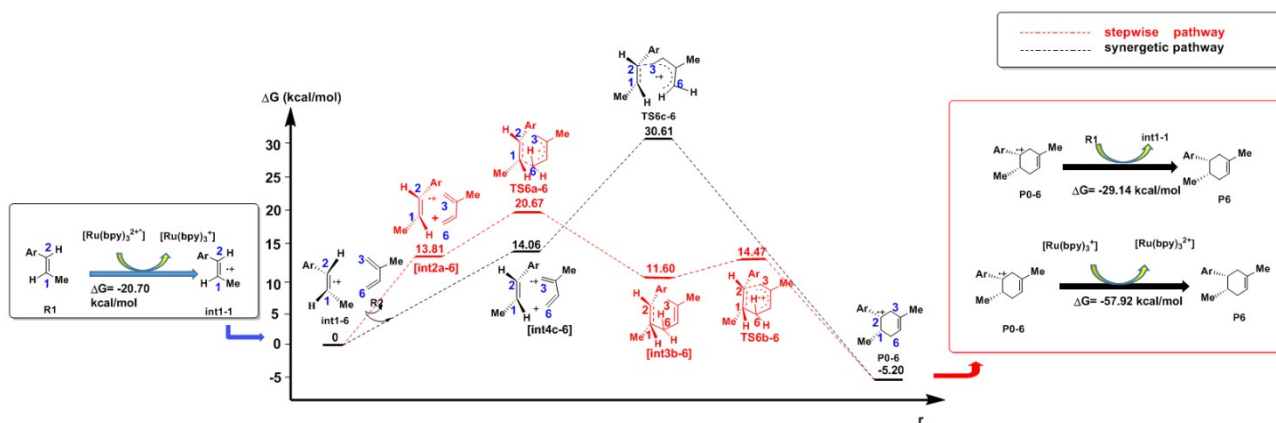


Figure S6. Schematic energy profiles of the C-C cycloaddition reaction between (1S,2R)- R1⁺ and R2 (4-Me). The red line is designed as stepwise pathway and the black line is regarded as synergetic pathway. [int2a-6] and [int4c-6] are the pre-reaction compounds after the molecular orientations in the corresponding pathways which are stationary points on the potential energy surface.

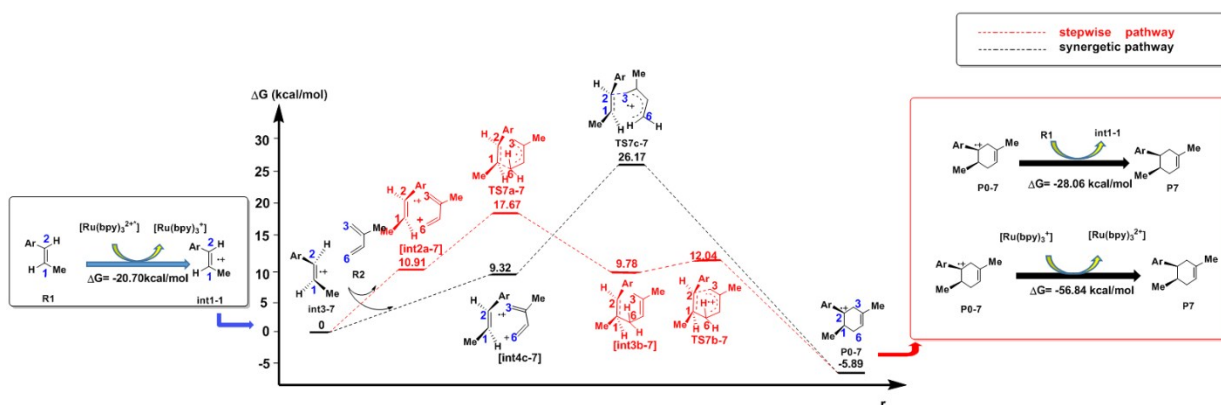


Figure S7. Schematic energy profiles of the C-C cycloaddition reaction between (1R,2S)- R1⁺ and R2 (4-Me). The red line is designed as stepwise pathway and the black line is regarded as synergetic pathway. [int2a-7] and [int4c-7] are the pre-reaction compounds after the molecular orientations in the corresponding pathways which are stationary points on the potential energy surface.

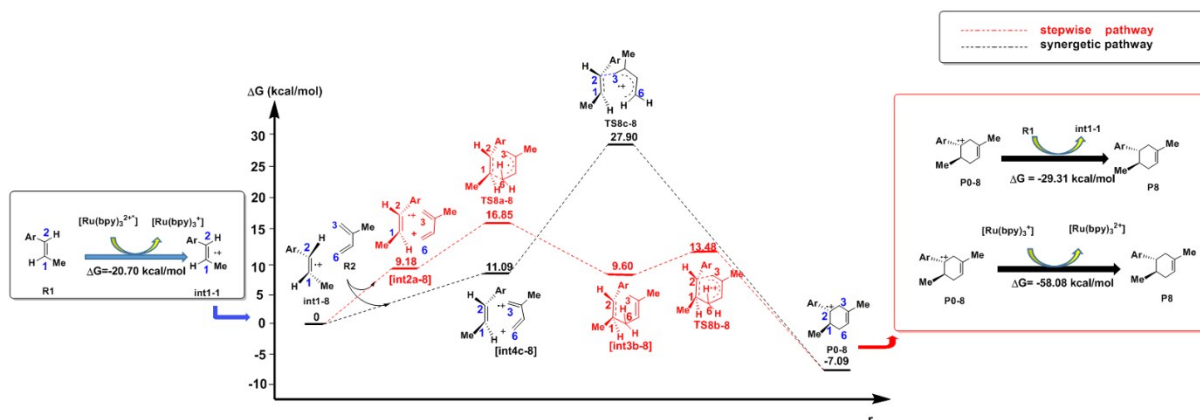


Figure S8. Schematic energy profiles of the C-C cycloaddition reaction between (1R,2R)-R1⁺ and R2 (4-Me). The red line is designed as stepwise pathway and the black line is regard as synergetic pathway. **[int2a-8]** and **[int4c-8]** are the pre-reaction compounds after the molecular orientation in the corresponding pathways which are stationary points on the potential energy surface.

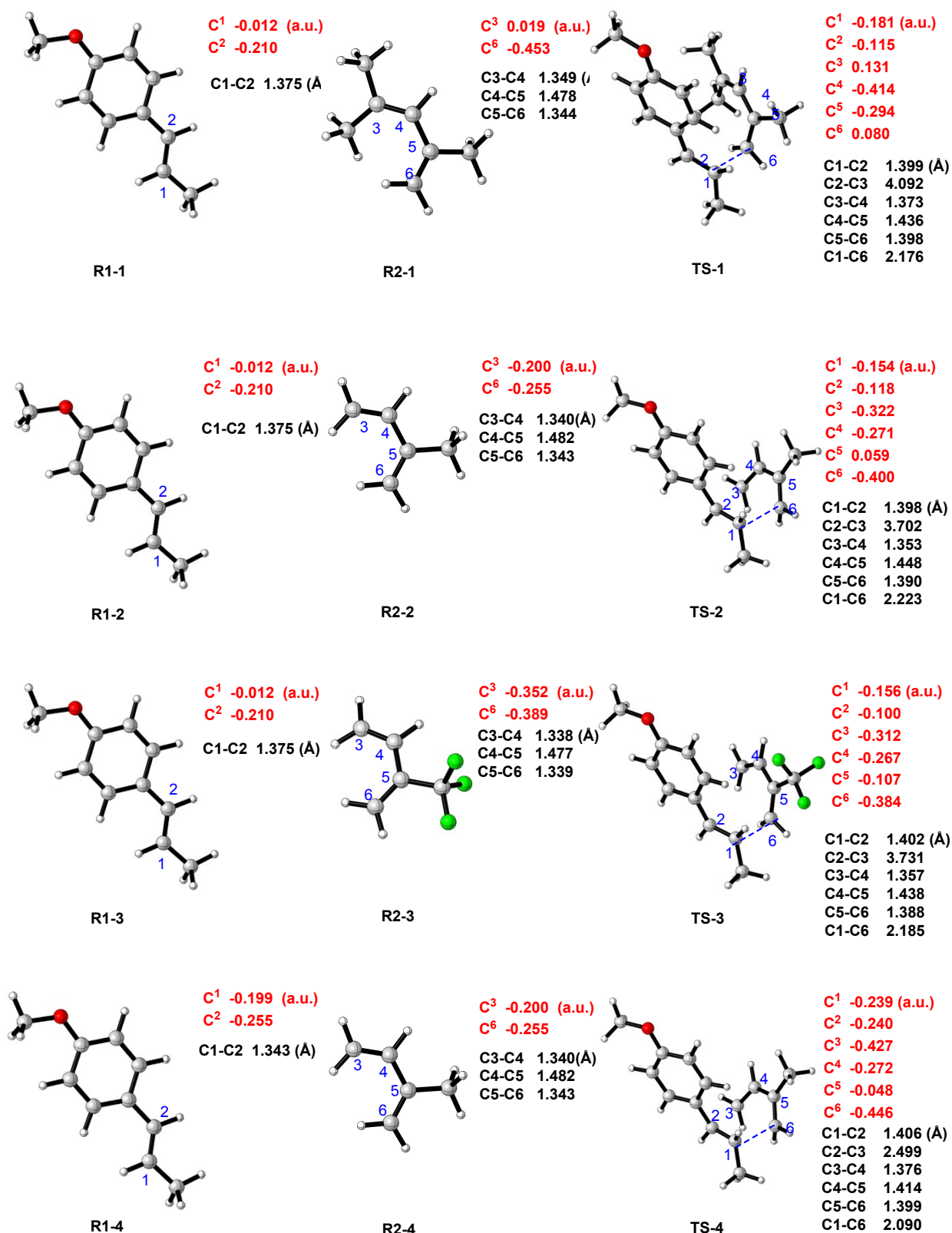
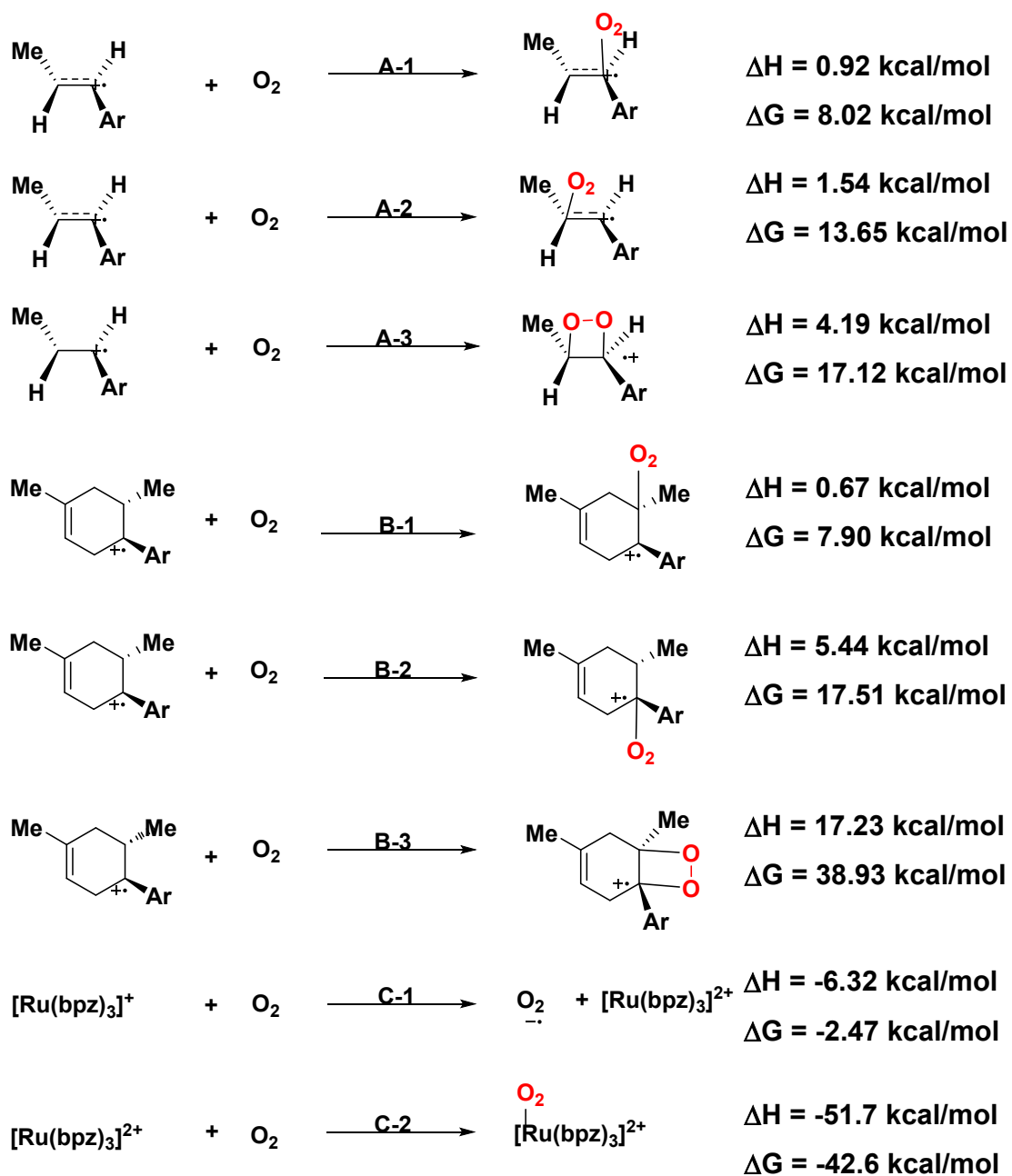


Figure S9. The optimized structures of the reagents and transition states including the typical bond lengths (black) and NBO atomic charges (red) with different substituents of different electronic properties.



Scheme S1 The proposed oxygen-participated reactions and the corresponding thermodynamic properties

Cartesian coordinates of all the complexes under the theoretical level of M062X/cc-pVTZ

Atom	x	y	z	Atom	x	y	z
Int 1-1				Int2a-5			
C	-1.231007	1.487973	-0.000062	C	-1.987000	-2.356367	0.358632
C	0.135861	1.529640	-0.000049	C	-3.897729	0.299811	0.511897
C	0.916284	0.329059	-0.000095	C	-3.265460	1.095615	-0.368796
C	0.220205	-0.924187	-0.000240	C	-2.216574	2.095397	-0.086104
C	-1.150329	-0.981762	-0.000286	C	-1.645154	2.249366	1.124025
C	-1.899548	0.228615	-0.000106	C	-0.943768	-1.725136	1.008655
H	-1.832573	2.390693	0.000013	H	-4.665682	-0.393751	0.180895
H	0.652011	2.484646	0.000025	H	-3.706857	0.336496	1.581480
H	0.781020	-1.851862	3.001193	H	-0.878474	3.001515	1.290382
H	-1.652215	-1.941514	-0.000450	H	-1.927681	1.648868	1.984837
O	-3.218618	0.292809	0.000053	C	-2.154140	-2.685103	-1.085990
C	-4.023571	-0.909373	0.000311	H	-1.897265	-1.847166	-1.741613
H	-5.054700	-0.558856	0.000798	H	-1.504288	-3.528767	-1.365092
H	-3.824907	-1.497001	-0.899589	H	-3.184539	-2.985321	-1.291461
H	-3.824110	-1.497178	0.899919	H	-2.794612	-2.679271	1.011975
C	2.336084	0.448614	0.000022	C	0.292740	-1.217196	0.514087
C	3.243999	-0.584098	0.000051	C	0.783095	-1.373057	-0.822658
C	4.713595	-0.392128	0.000197	C	1.122672	-0.507033	1.443503
H	5.156586	-0.889392	0.875815	C	1.992564	-0.847625	-1.192049
H	5.156687	-0.889196	-0.875495	H	0.210183	-1.923928	-1.555466
H	5.002297	0.662268	0.000315	C	2.335351	0.029397	1.084670
H	2.893153	-1.614062	-0.000042	H	0.771212	-0.392465	2.464608
H	2.726266	1.464860	0.000133	C	2.787063	-0.132481	-0.249757
Int2a-1				H	2.375348	-0.964116	-2.200535
C	1.940959	2.203332	-0.481572	H	2.933338	0.563676	1.812699
C	3.675045	-1.115915	-0.072383	H	-1.090056	-1.579792	2.076779
C	2.599109	-1.916683	-0.163735	O	3.933276	0.336037	-0.719022
C	1.800895	-2.318611	1.015257	C	4.823913	1.085972	0.136706
C	1.638825	-1.613850	2.143101	H	5.670705	1.348582	-0.496610
C	0.865467	2.066158	0.364545	H	4.327360	1.990417	0.498001
H	4.242687	-0.828349	-0.954209	H	5.157906	0.467153	0.974154
H	4.039314	-0.750829	0.884677	H	-3.547410	1.013360	-1.418738
H	1.904524	1.764698	-1.476461	C	-1.798592	2.946022	-1.262957
H	1.282043	-3.273841	0.921100	H	-1.012360	3.656039	-0.989930
H	0.940611	2.512248	1.354780	H	-1.426595	2.321298	-2.086246
C	-0.348667	1.379746	0.074626	H	-2.650329	3.513390	-1.661129
C	-1.343373	1.294943	1.100161	Int 3b-5			
C	-0.629617	0.760696	-1.187557	C	-2.083571	-1.801614	0.329852
C	-2.532316	0.636209	0.905246	C	-3.270464	-0.734993	0.515675
H	-1.141067	1.767147	2.056945	C	-3.193647	0.450349	-0.377820
C	-1.810553	0.105089	-1.396923	C	-2.709706	1.725284	-0.029144
H	0.096841	0.813765	-1.990334	C	-2.284869	2.046324	1.245418

C	-2.780396	0.024261	-0.353063	C	-0.858887	-1.273097	0.968258
H	-3.266193	0.584912	1.700494	H	-4.177301	-1.307122	0.288610
H	-2.038934	-0.368302	-2.345884	H	-3.315038	-0.456104	1.571950
O	-3.879480	-0.642997	-0.658015	H	-1.902219	3.037080	1.472677
C	-4.929377	-0.823053	0.320288	H	-2.333451	1.343623	2.070701
H	-5.694341	-1.406186	-0.190684	C	-2.039699	-2.359541	-1.094733
H	-4.548163	-1.373142	1.184563	H	-1.926552	-1.580786	-1.853684
H	-5.334251	0.145818	0.624170	H	-1.229752	-3.086506	-1.213635
C	3.182369	2.932793	-0.129008	H	-2.983350	-2.877278	-1.298896
H	3.344970	3.757393	-0.839162	H	-2.397136	-2.612314	1.004823
H	3.161139	3.334049	0.887639	C	0.377221	-0.868623	0.478738
H	4.052828	2.270464	-0.240054	C	0.771122	-0.862487	-0.905442
C	2.141552	-2.487362	-1.486008	C	1.343495	-0.411102	1.441183
H	2.158686	-3.585588	-1.463101	C	2.015634	-0.434789	-1.277394
H	1.105288	-2.197956	-1.706699	H	0.081175	-1.193361	-1.667923
H	2.776670	-2.154585	-2.312728	C	2.595488	0.014352	1.075935
H	1.041934	-1.999222	2.965895	H	1.065161	-0.406561	2.491035
H	2.091727	-0.635028	2.285313	C	2.947900	0.007198	-0.298225
Int3a-1				H	2.321911	-0.423220	-2.318022
C	2.047017	1.245803	-0.301240	H	3.297558	0.352764	1.827959
C	3.290620	0.370913	0.154437	H	-0.966300	-1.175723	2.048461
C	3.126030	-1.082237	-0.143644	O	4.122355	0.392646	-0.771505
C	2.392730	-1.921697	0.707650	C	5.151361	0.867474	0.123947
C	1.858584	-1.557048	1.924959	H	5.997056	1.109551	-0.519003
C	0.866445	1.070265	0.572228	H	4.812216	1.762780	0.652348
H	4.146266	0.770572	-0.399201	H	5.431333	0.083333	0.832407
H	3.471030	0.562002	1.217471	H	-3.506265	0.301497	-1.409561
H	1.817482	0.982597	-1.336955	C	-2.650845	2.776510	-1.123688
H	2.205044	-2.936489	0.357917	H	-2.330962	3.746581	-0.731770
H	0.997588	1.403408	1.601770	H	-1.949125	2.483823	-1.914604
C	-0.417247	0.659759	0.215252	H	-3.630986	2.909322	-1.597191
C	-1.454083	0.706396	1.203987				
C	-0.772486	0.202986	-1.098145	Int 4c-5			
C	-2.746596	0.334583	0.920899	C	1.298071	1.656242	0.760497
H	-1.201690	1.047948	2.203912	C	3.215911	-0.060732	-1.224068
C	-2.056897	-0.175734	-1.385936	C	3.758541	-1.055820	-0.495256
H	-0.018881	0.150150	-1.875522	C	4.970074	-0.870597	0.330383
C	-3.062938	-0.115067	-0.385158	C	5.946709	0.022123	0.116451
H	-3.509112	0.383412	1.689003	C	0.367378	0.676227	1.058599
H	-2.336789	-0.524583	-2.374295	H	2.343229	-0.231140	-1.849132
O	-4.273504	-0.503258	-0.772100	H	3.642598	0.938547	-1.239838
C	-5.369638	-0.491035	0.164438	H	5.071046	-1.559327	1.170306
H	-6.231553	-0.846715	-0.399765	H	0.710712	-0.082828	1.758087
H	-5.166789	-1.165701	1.001517	C	-0.968522	0.491090	0.602250
H	-5.553905	0.524431	0.527095	C	-1.661635	-0.672919	1.072442

C	2.459336	2.739132	-0.251195	C	-1.678114	1.372058	-0.277784
H	1.643142	3.385638	-0.588584	C	-2.950058	-0.961309	0.695887
H	2.739850	3.036903	0.765135	H	-1.140034	-1.346492	1.745933
H	3.320334	2.898462	-0.909194	C	-2.964041	1.097812	-0.659078
C	3.679121	-1.593421	-1.438044	H	-1.205721	2.270431	-0.648625
H	4.778562	-1.544179	-1.437717	C	-3.621765	-0.073950	-0.184613
H	3.385945	-2.629508	-1.633039	H	-3.442432	-1.852289	1.065981
H	3.350382	-0.973113	-2.284835	H	-3.509601	1.758820	-1.324265
H	1.236250	-2.250996	2.482616	O	-4.858864	-0.244729	-0.621442
H	2.074889	-0.609761	2.406549	C	-5.630326	-1.395771	-0.209359
Int4a-1				H	-6.590428	-1.287049	-0.712323
C	-0.823862	2.028757	-0.072322	H	-5.138006	-2.317196	-0.531513
C	-2.539674	-1.443736	0.573160	H	-5.770048	-1.389441	0.874957
C	-3.687419	-1.518304	-0.114544	C	3.145337	-2.435131	-0.457705
C	-4.965470	-0.863701	0.243649	H	3.856552	-3.191382	-0.815895
C	-5.321523	-0.626972	1.517024	H	2.882388	-2.718583	0.570688
C	-0.050977	1.080291	-0.701159	H	2.241979	-2.495213	-1.072305
H	-1.651622	-1.978578	0.245790	H	6.801564	0.089670	0.784373
H	-2.449403	-0.859074	1.486164	H	5.936411	0.702886	-0.732071
H	-0.426085	2.570906	0.782855	C	1.186950	2.825244	-0.158697
H	-0.482756	0.568209	-1.558815	H	0.879253	2.527904	-1.168569
C	1.275049	0.701515	-0.343912	H	0.434559	3.539308	0.207264
C	1.935326	-0.284326	-1.145253	H	2.141011	3.352185	-0.228209
C	1.989519	1.248102	0.772895	H	2.238821	1.561610	1.296992
C	3.212969	-0.705344	-0.871903				
H	1.402025	-0.704260	-1.993057	TS5a-5			
C	3.262280	0.838454	1.056363	C	1.526571	-0.188562	0.298336
H	1.521510	1.992158	1.407331	C	2.709994	-0.806327	-1.414456
C	3.898166	-0.144334	0.239579	C	2.325139	-0.079453	-2.537411
H	3.688647	-1.453225	-1.494551	C	1.356780	-0.466724	-3.530644
H	3.815751	1.241514	1.897899	C	0.699874	-1.659728	-3.481942
O	5.126939	-0.467594	0.601171	C	0.300623	-0.812821	0.015843
C	5.877607	-1.460116	-0.137115	H	3.603083	-0.482848	-0.888093
H	6.832604	-1.534071	0.381542	H	2.488202	-1.865322	-1.333877
H	5.358061	-2.421374	-0.111382	H	-0.040088	-1.918370	-4.233766
H	6.030755	-1.127839	-1.167221	H	0.886256	-2.401596	-2.712314
C	-2.201507	2.379643	-0.489540	C	1.793992	1.288238	0.437232
H	-2.264068	3.455574	-0.709573	H	1.549423	1.862017	-0.459455
H	-2.534187	1.811257	-1.361802	H	1.204778	1.695855	1.269748
H	-2.900491	2.207169	0.342120	H	2.849888	1.457250	0.667246
H	-6.257962	-0.130545	1.760233	H	2.187061	-0.817683	0.891236
H	-4.699869	-0.934355	2.354408	C	-0.941738	-0.300482	-0.451424
H	-3.700397	-2.088804	-1.044694	C	-1.242829	1.076875	-0.679440
C	-5.863599	-0.502141	-0.916808	C	-1.988208	-1.241206	-0.685971
H	-5.363656	0.190579	-1.607105	C	-2.486857	1.467338	-1.117076

H	-6.121871	-1.394806	-1.502835	H	-0.495844	1.837527	-0.500519
H	-6.793817	-0.036402	-0.577351	C	-3.240098	-0.860011	-1.124707
P0-1				H	-1.788671	-2.295128	-0.512622
C	1.780650	1.253295	-0.676365	C	-3.503368	0.508913	-1.345833
C	2.138578	-0.110485	-1.292271	H	-2.717974	2.513913	-1.287932
C	2.751377	-1.092081	-0.316103	H	-4.005670	-1.608215	-1.290456
C	2.652444	-0.915351	1.012527	H	0.307596	-1.891586	0.162200
C	1.951459	0.241287	1.672214	O	-4.674809	1.001431	-1.762581
C	1.065978	1.065408	0.716899	C	-5.772509	0.109286	-2.020024
H	1.251476	-0.572455	-1.751362	H	-6.598868	0.750376	-2.328294
H	2.837351	0.055267	-2.124429	H	-5.525213	-0.588212	-2.826562
H	1.076658	1.760602	-1.346732	H	-6.049482	-0.439941	-1.114432
H	3.109937	-1.643966	1.681501	H	2.763230	0.909832	-2.659205
H	1.355893	-0.115981	2.523036	C	1.085585	0.525068	-4.639171
H	2.696980	0.919283	2.113224	H	0.354326	0.138191	-5.354401
C	3.013734	2.156438	-0.524555	H	0.703130	1.469950	-4.233382
H	2.752754	3.111882	-0.054220	H	2.007220	0.760992	-5.185658
H	3.797028	1.683355	0.077336				
H	3.438980	2.373625	-1.511478	TS5b-5			
C	3.451902	-2.279754	-0.919635	C	1.558447	-0.302527	-0.246830
H	4.308538	-1.962884	-1.530998	C	2.806207	-0.797031	-1.098814
H	3.816203	-2.972433	-0.153795	C	2.826847	-0.147343	-2.437147
H	2.781696	-2.834412	-1.591920	C	1.832980	-0.365961	-3.383083
H	0.944646	2.077895	1.124736	C	0.913020	-1.398897	-3.180587
C	-0.321607	0.528336	0.529451	C	0.279456	-0.909530	-0.727997
C	-1.340735	1.430079	0.082932	H	3.705195	-0.543392	-0.531362
C	-0.676722	-0.833661	0.748774	H	2.756754	-1.890716	-1.166849
C	-2.624985	1.016534	-0.158702	H	0.022673	-1.477575	-3.799517
H	-1.079723	2.473200	-0.068202	H	1.163847	-2.276969	-2.598617
C	-1.953907	-1.273353	0.513480	C	1.629638	1.204886	0.014124
H	0.072997	-1.534713	1.095891	H	1.556824	1.795195	-0.904082
C	-2.950339	-0.357123	0.047436	H	0.844716	1.530379	0.703502
H	-3.376867	1.717885	-0.498682	H	2.594553	1.437598	0.477555
H	-2.243265	-2.307220	0.670996	H	1.703063	-0.814499	0.719411
O	-4.139008	-0.880959	-0.156762	C	-1.011664	-0.372874	-0.928308
C	-5.248870	-0.074818	-0.631521	C	-1.331965	1.015070	-1.075539
H	-5.009108	0.343749	-1.611839	C	-2.099284	-1.300889	-0.982966
H	-6.084526	-0.768587	-0.706348	C	-2.631696	1.426398	-1.238505
H	-5.469323	0.715071	0.090014	H	-0.548267	1.759135	-1.076727
PI				C	-3.407357	-0.895464	-1.132728
C	1.912979	1.226949	-0.627929	H	-1.882899	-2.361465	-0.888275
C	2.273240	-0.154516	-1.207488	C	-3.689867	0.483225	-1.259156
C	2.792353	-1.130865	-0.171633	H	-2.877873	2.477072	-1.353290
C	2.556781	-0.944889	1.135623	H	-4.202806	-1.630615	-1.153736
C	1.795519	0.223511	1.711189	H	0.291318	-1.994210	-0.644804

C	1.047374	1.074831	0.658746	O	-4.912820	0.994118	-1.408629
H	1.392732	-0.594623	-1.700384	C	-6.056008	0.119032	-1.421234
H	3.021973	-0.033157	-2.003595	H	-6.916537	0.772666	-1.563752
H	1.306901	1.759323	-1.372783	H	-5.990931	-0.594145	-2.248763
H	2.947503	-1.666578	1.854521	H	-6.146201	-0.411928	-0.468384
H	1.087486	-0.133033	2.472021	H	3.541092	0.655144	-2.605914
H	2.498439	0.870294	2.258194	C	1.669507	0.564500	-4.566952
C	3.168287	2.074110	-0.366608	H	1.701568	0.013532	-5.513765
H	2.906092	3.045610	0.071165	H	0.701233	1.078664	-4.523602
H	3.865241	1.574689	0.315748	H	2.455286	1.325729	-4.585823
H	3.706187	2.264853	-1.303501				
C	3.558018	-2.319204	-0.693197	TS5c-5			
H	4.467901	-2.004389	-1.223980	C	0.554033	0.517659	0.790858
H	3.853028	-3.001193	0.112115	C	1.103171	0.234277	-1.747664
H	2.960417	-2.890024	-1.418800	C	2.355133	-0.444646	-1.697692
H	0.926893	2.083367	1.075433	C	3.534779	0.134478	-1.122591
C	-0.359920	0.580305	0.333723	C	3.636972	1.384148	-0.601032
C	-1.323044	1.507931	-0.099874	C	-0.010197	-0.267586	-0.247990
C	-0.750825	-0.763642	0.427022	H	0.404336	-0.147902	-2.486113
C	-2.621828	1.119272	-0.425722	H	1.103943	1.318121	-1.684180
H	-1.050368	2.558383	-0.180851	H	4.414682	-0.505981	-1.096765
C	-2.050355	-1.166609	0.107548	H	0.309059	-1.308904	-0.208555
H	-0.035781	-1.512735	0.753178	C	-1.420614	-0.122110	-0.704083
C	-2.988438	-0.226332	-0.320758	C	-2.224762	-1.269343	-0.766999
H	-3.351530	1.849957	-0.764507	C	-1.987063	1.105350	-1.100298
H	-2.342229	-2.210717	0.182378	C	-3.558316	-1.208337	-1.170693
O	-4.256522	-0.642742	-0.677898	H	-1.807425	-2.232371	-0.482368
C	-5.261071	-0.398690	0.310518	C	-3.308478	1.180089	-1.514935
H	-5.351392	0.671075	0.540765	H	-1.386661	2.010197	-1.102815
H	-6.205166	-0.755833	-0.109315	C	-4.109820	0.024550	-1.547464
H	-5.046571	-0.946296	1.238416	H	-4.150832	-2.115500	-1.192703
R2				H	-3.743545	2.125700	-1.823955
C	-0.835763	-0.618763	0.000005	O	-5.387735	0.204155	-1.962860
C	0.454382	0.111108	-0.000021	C	-6.253456	-0.931340	-2.020756
C	-2.071251	-0.100278	-0.000003	H	-7.213832	-0.552201	-2.374718
C	0.555613	1.450439	0.000003	H	-5.878560	-1.683865	-2.724402
C	1.685163	-0.766413	-0.000004	H	-6.385066	-1.383738	-1.030736
H	1.702214	-1.423680	0.880342	C	2.440279	-1.862704	-2.174631
H	1.701973	-1.424127	-0.880010	H	3.264807	-1.973794	-2.891250
H	2.605415	-0.174120	-0.000255	H	2.670662	-2.538841	-1.338517
H	-2.946603	-0.744582	0.000007	H	1.515927	-2.197669	-2.651226
H	-2.260803	0.971078	-0.000025	H	4.570739	1.721238	-0.160420
H	1.525169	1.942062	-0.000024	H	2.820658	2.100956	-0.608171
H	-0.314894	2.102143	0.000065	C	0.013763	1.754575	1.395752
H	-0.741334	-1.705334	0.000023	H	0.499445	2.640147	0.952060

TS1a-1				H	-1.065140	1.864452	1.268763
C	-2.255984	-1.472286	-0.465085	H	0.269437	1.781414	2.462063
C	-3.212705	0.388009	0.288040	H	1.527583	0.192217	1.151638
C	-2.437230	1.494185	-0.039461				
C	-1.455543	2.063050	0.859858	P0-5			
C	-1.206372	1.670362	2.130887	C	1.556944	-1.426029	0.295131
C	-1.110518	-1.562797	0.330628	C	1.949356	1.076175	-0.102958
H	-4.064342	0.156327	-0.342791	C	3.414186	0.750556	-0.306892
H	-3.278145	0.037382	1.312336	C	3.846996	-0.517727	-0.369494
H	-2.154747	-1.083418	-1.474835	C	2.966026	-1.734346	-0.245549
H	-0.873199	2.890218	0.456679	C	1.046033	-0.123092	-0.438384
H	-1.213710	-2.091511	1.277989	H	1.671825	1.929872	-0.736182
C	0.180367	-1.033002	0.053762	H	1.798766	1.412336	0.932157
C	1.212498	-1.212990	1.015835	H	4.908272	-0.704944	-0.532769
C	0.513257	-0.341631	-1.148870	H	1.169882	-0.347432	-1.507669
C	2.494366	-0.739721	0.812067	C	0.420173	0.083479	-0.224345
H	0.979633	-1.740101	1.937150	C	1.331672	-0.699540	-1.005900
C	1.784752	0.138547	-1.359756	C	0.960924	0.993651	0.728110
H	-0.237134	-0.201371	-1.919597	C	2.690495	-0.595661	-0.865002
C	2.793265	-0.052995	-0.383618	H	0.920760	-1.389388	-1.737018
H	3.254223	-0.896451	1.568093	C	2.316707	1.117195	0.890043
H	2.045384	0.662071	-2.274128	H	0.299379	1.601300	1.333800
O	3.995940	0.449157	-0.690497	C	3.207225	0.323452	0.095321
C	5.087825	0.280694	0.228446	H	3.357479	-1.192984	-1.474561
H	5.945701	0.752276	-0.251859	H	2.749338	1.805765	1.608296
H	4.877702	0.778687	1.181031	O	4.485557	0.520241	0.326891
H	5.295293	-0.781260	0.395623	C	5.505638	-0.212867	-0.402187
C	-3.404664	-2.419511	-0.239476	H	6.450433	0.153525	-0.004672
H	-3.171809	-3.375854	-0.729059	H	5.426429	0.007084	-1.469612
H	-3.564251	-2.621787	0.824515	H	5.397707	-1.283388	-0.211576
H	-4.336530	-2.052141	-0.677749	C	4.342074	1.930474	-0.425643
C	-2.566806	2.131768	-1.394770	H	5.385986	1.615931	-0.528177
H	-2.896602	3.175031	-1.292718	H	4.085268	2.553860	-1.293966
H	-1.597530	2.166256	-1.909015	H	4.268604	2.583322	0.455953
H	-3.285296	1.607634	-2.030356	H	2.892597	-2.232950	-1.224279
H	-0.437179	2.162930	2.718741	H	3.444856	-2.467574	0.419458
H	-1.754038	0.871739	2.623009	C	1.537620	-1.310821	1.825109
TS1b-1				H	2.241536	-0.555310	2.190146
C	2.036087	1.152211	-0.398124	H	0.540922	-1.061670	2.206665
C	3.361681	0.449147	0.101254	H	1.828242	-2.270762	2.267486
C	3.254348	-1.035459	-0.003521	H	0.890813	-2.247907	0.007223
C	2.375088	-1.718645	0.836073	P5			
C	1.728735	-1.121128	1.904702	C	1.556944	-1.426029	0.295131
C	0.876655	0.993277	0.521939	C	1.949356	1.076175	-0.102958
H	4.176035	0.819682	-0.527933	C	3.414186	0.750556	-0.306892

H	3.559685	0.781756	1.127193	C	3.846996	-0.517727	-0.369494
H	1.803049	0.746765	-1.386504	C	2.966026	-1.734346	-0.245549
H	2.122770	-2.748120	0.585882	C	1.046033	-0.123092	-0.438384
H	0.981228	1.486894	1.486695	H	1.671825	1.929872	-0.736182
C	-0.425102	0.578300	0.184664	H	1.798766	1.412336	0.932157
C	-1.474224	0.772460	1.134293	H	4.908272	-0.704944	-0.532769
C	-0.770495	-0.023245	-1.066771	H	1.169882	-0.347432	-1.507669
C	-2.776216	0.408414	0.868328	C	0.420173	0.083479	-0.224345
H	-1.231088	1.224378	2.092029	C	1.331672	-0.699540	-1.005900
C	-2.064267	-0.394756	-1.337380	C	0.960924	0.993651	0.728110
H	-0.004426	-0.197165	-1.814329	C	2.690495	-0.595661	-0.865002
C	-3.086037	-0.184429	-0.377219	H	0.920760	-1.389388	-1.737018
H	-3.548143	0.576569	1.609226	C	2.316707	1.117195	0.890043
H	-2.333871	-0.852359	-2.283785	H	0.299379	1.601300	1.333800
O	-4.307581	-0.580930	-0.742460	C	3.207225	0.323452	0.095321
C	-5.410952	-0.424265	0.168122	H	3.357479	-1.192984	-1.474561
H	-6.277201	-0.825756	-0.358063	H	2.749338	1.805765	1.608296
H	-5.239174	-0.992712	1.087803	O	4.485557	0.520241	0.326891
H	-5.575571	0.632949	0.399501	C	5.505638	-0.212867	-0.402187
C	2.311657	2.669875	-0.547449	H	6.450433	0.153525	-0.004672
H	1.432381	3.196362	-0.931744	H	5.426429	0.007084	-1.469612
H	2.588501	3.115777	0.414379	H	5.397707	-1.283388	-0.211576
H	3.137824	2.822878	-1.250266	C	4.342074	1.930474	-0.425643
C	3.957307	-1.723422	-1.127510	H	5.385986	1.615931	-0.528177
H	5.047175	-1.632696	-1.009355	H	4.085268	2.553860	-1.293966
H	3.703801	-2.785926	-1.186926	H	4.268604	2.583322	0.455953
H	3.718681	-1.248414	-2.090380	H	2.892597	-2.232950	-1.224279
H	0.932018	-1.642114	2.428321	H	3.444856	-2.467574	0.419458
H	2.101374	-0.221315	2.379532	C	1.537620	-1.310821	1.825109
TS1c-1				H	2.241536	-0.555310	2.190146
C	-1.421875	1.510642	0.395181	H	0.540922	-1.061670	2.206665
C	-1.526496	-0.974790	-0.355203	H	1.828242	-2.270762	2.267486
C	-2.901341	-0.984845	-0.762080	H	0.890813	-2.247907	0.007223
C	-4.028396	-0.828543	0.091735				
C	-3.876407	-0.640864	1.440951	Int2a-6			
C	-0.697575	0.639953	-0.472173	C	-1.177501	2.085785	0.846115
H	-0.871741	-1.490480	-1.056061	C	-3.237064	0.618439	-1.484477
H	-1.324547	-1.261517	0.673933	C	-4.188901	0.026300	-0.747456
H	-1.106301	1.609463	1.431596	C	-4.162577	-1.360756	-0.235723
H	-0.871380	0.861245	-1.526965	C	-3.514489	-2.351725	-0.870861
C	0.746396	0.361516	-0.173288	C	-0.399698	0.966867	1.085046
C	1.664391	0.342433	-1.229344	H	-3.354435	1.639223	-1.838936
C	1.219992	0.103230	1.125672	H	-2.323994	0.101555	-1.771314
C	3.020443	0.091486	-1.013891	H	-2.140675	2.077865	1.350448
H	1.319941	0.533435	-2.242919	C	-0.882142	3.294897	0.026011

C	2.564126	-0.150747	1.355692	H	0.020611	3.808527	0.384602
H	0.534004	0.096054	1.968948	H	-0.703933	3.037065	-1.026368
C	3.478562	-0.159273	0.286701	H	-1.714720	4.000581	0.067221
H	3.701843	0.092820	-1.856333	H	-3.496997	-3.363418	-0.472795
H	2.931205	-0.349728	2.358013	H	-2.997943	-2.189398	-1.813701
O	4.768875	-0.420407	0.615356	C	0.900333	0.621153	0.618886
C	5.743593	-0.464794	-0.428754	C	1.707503	1.408425	-0.267391
H	6.691253	-0.695406	0.061134	C	1.444306	-0.624888	1.077820
H	5.510981	-1.249991	-1.158154	C	2.946688	0.977667	-0.656744
H	5.824773	0.501197	-0.941172	H	1.344372	2.355016	-0.642027
C	-2.571939	2.306221	-0.064381	C	2.685820	-1.067563	0.697423
H	-2.180850	3.277136	-0.421317	H	0.846785	-1.231715	1.750981
H	-3.077923	1.848719	-0.922993	C	3.459013	-0.266440	-0.183391
H	-3.282717	2.524574	0.737191	H	3.564646	1.563451	-1.329062
H	-4.739054	-0.469746	2.078526	H	3.067008	-2.012375	1.064268
H	-2.909630	-0.666430	1.933570	O	4.663220	-0.585602	-0.623158
H	-3.097616	-1.066759	-1.829923	C	5.291810	-1.826174	-0.223533
C	-5.402339	-0.846304	-0.541892	H	4.676691	-2.677731	-0.526233
H	-5.498846	-0.058938	-1.298950	H	6.243351	-1.842523	-0.753510
H	-5.583762	-1.803331	-1.045605	H	5.460485	-1.831770	0.856612
H	-6.187436	-0.700988	0.205078	H	-0.853555	0.225000	1.738851
[Ru(bpz)₃]²⁺				H	-5.064970	0.611653	-0.463555
Ru	0.229870	0.016553	-0.013491	C	-4.942598	-1.604209	1.035559
N	-1.327801	-0.855382	1.063734	H	-6.000812	-1.342916	0.898969
N	-0.070898	-1.753961	-1.073225	H	-4.889259	-2.651316	1.348620
N	-1.158123	1.179988	-1.045971	H	-4.571432	-0.978631	1.858494
C	-1.949406	-0.330886	2.129299				
H	-1.626776	0.644968	2.469124	Int3-6			
C	-2.973029	-1.031581	2.765688	C	1.741589	1.679641	-0.494546
H	-3.473404	-0.602298	3.628115	C	2.887010	1.152478	0.495117
C	-2.759982	-2.749438	1.283191	C	3.723572	0.037114	-0.025194
H	-3.099081	-3.721074	0.940390	C	3.597574	-1.325859	0.300084
C	-1.723675	-2.079179	0.621913	C	2.629236	-1.807140	1.161368
C	-1.010065	-2.588209	-0.553098	C	0.766173	0.586071	-0.688171
C	-1.234281	-3.833235	-1.152411	H	3.521509	2.032637	0.652510
H	-1.966698	-4.523617	-0.746694	H	2.418301	0.913011	1.453730
C	0.341942	-3.392581	-2.739127	H	2.247526	1.778654	-1.467144
H	0.887315	-3.708748	-3.623155	C	1.262370	3.062186	-0.048901
C	0.599824	-2.149726	-2.163671	H	0.460407	3.440068	-0.691366
H	1.339415	-1.472020	-2.569965	H	0.914515	3.064053	0.989634
C	-1.840817	0.819823	-2.142088	H	2.099125	3.765426	-0.113518
H	-1.657395	-0.168959	-2.543020	H	2.548344	-2.869835	1.370867
C	-2.751329	1.698570	-2.727140	H	1.925020	-1.156637	1.670528
H	-3.299743	1.403898	-3.616667	C	0.583037	0.433964	-0.390681
C	-2.307730	3.267341	-1.134011	C	1.430393	1.409293	0.245138

H	-2.507797	4.253738	-0.727166	C	1.184657	-0.821054	-0.755906
C	-1.371901	2.419406	-0.530005	C	2.749396	1.140453	0.484648
N	1.911625	0.661598	-1.068894	H	1.030562	2.367136	0.543894
C	1.926514	1.483801	-2.127789	C	2.509529	-1.093674	-0.528235
H	0.975529	1.852618	-2.490394	H	0.559272	-1.572608	-1.228470
C	3.131266	1.840401	-2.730574	C	3.312440	-0.108885	0.100700
H	3.136207	2.508456	-3.586466	H	3.395975	1.866931	0.965525
C	4.288357	0.568740	-1.236249	H	2.929255	-2.047926	-0.821218
H	5.244848	0.199495	-0.883407	O	4.597631	-0.257981	0.375805
C	3.099634	0.194625	-0.599708	C	5.283039	-1.482240	0.030563
C	3.017971	-0.697506	0.560494	H	4.841451	-2.329263	0.562802
N	1.763459	-0.949511	1.019105	H	6.311717	-1.331639	0.356183
C	-0.562966	2.762065	0.642082	H	5.251586	-1.646133	-1.050196
N	0.285995	1.792055	1.074841	H	1.217910	-0.290206	-1.150439
C	1.064404	2.053183	2.134078	H	4.490978	0.312114	-0.747684
H	1.738925	1.272850	2.462371	C	4.572108	-2.295680	-0.345187
C	0.990081	3.286975	2.778304	H	5.603886	-2.070671	-0.048819
H	1.617627	3.491286	3.640377	H	4.358134	-3.329655	-0.058667
C	-0.603204	3.990885	1.309369	H	4.532364	-2.231632	-1.439371
H	-1.267524	4.780123	0.974470				
C	1.621219	-1.775610	2.065171	Int 4-6			
C	2.738937	-2.342114	2.674834	C	-1.215398	1.890653	0.166426
C	4.117301	-1.277733	1.204469	C	-3.148694	-0.889834	1.148787
H	5.129805	-1.080401	0.866340	C	-3.841375	-1.132708	0.020900
H	2.618829	-3.008433	3.523523	C	-5.133170	-0.478255	-0.278407
H	0.615860	-1.975543	2.412431	C	-6.032754	-0.054763	0.619650
N	-3.379189	-2.234807	2.346690	C	-0.144844	1.369246	0.870851
N	-0.565258	-4.235250	-2.234460	H	-2.216774	-1.407251	1.362248
N	4.309038	1.384103	-2.291716	H	-3.499838	-0.184026	1.897320
N	0.160871	4.253919	2.370769	H	-2.041980	2.224414	0.789314
N	-2.991217	2.914312	-2.223933	H	-5.367360	-0.371307	-1.338758
N	3.982921	-2.091708	2.252842	C	-1.388841	2.084918	-1.301370
O	-4.503803	0.274626	0.251772	H	-0.572710	2.683236	-1.727649
O	-4.254269	-0.544659	-0.609671	H	-1.391325	1.123919	-1.834193
				H	-2.333566	2.590504	-1.512166
Int2a-2				C	-3.327946	-2.081145	-1.036734
C	1.426785	2.076228	0.670113	H	-4.038685	-2.899296	-1.213802
C	3.300285	0.072905	-1.171588	H	-3.203780	-1.564825	-1.998638
C	3.902731	-0.776329	-0.316232	H	-2.365265	-2.518426	-0.755011
C	3.297346	-2.060750	0.092388	H	-6.957116	0.423844	0.306299
C	2.425725	-2.790147	-0.618558	H	-5.886834	-0.180934	1.690350
C	0.566135	1.063332	1.054080	C	1.097263	0.838398	0.420905
H	3.783092	0.996227	-1.481569	C	2.028409	0.422511	1.430045
H	2.328380	-0.142174	-1.607236	C	1.490606	0.678418	-0.948279
H	2.360686	2.107793	1.226149	C	3.257358	-0.103997	1.121468

H	3.633341	-2.447354	1.055643	H	1.744378	0.537043	2.471906
C	1.257312	3.129217	-0.371223	C	2.713543	0.155632	-1.270515
H	0.527722	3.884328	-0.040423	H	0.819016	0.962783	-1.745800
H	0.891561	2.724850	-1.321529	C	3.619033	-0.245389	-0.244310
H	2.203832	3.644642	-0.550450	H	3.937382	-0.404286	1.909000
C	5.240445	-0.456695	0.306601	H	3.020637	0.028102	-2.303254
H	5.985219	-1.223201	0.054135	O	4.769004	-0.739917	-0.668129
H	5.168711	-0.442838	1.402833	C	5.763920	-1.206739	0.273035
H	5.621261	0.513955	-0.025168	H	5.359314	-2.025073	0.874691
H	2.031188	-3.726502	-0.232276	H	6.588372	-1.564206	-0.342583
H	2.091846	-2.492203	-1.610115	H	6.097725	-0.382877	0.909324
C	0.748666	0.742995	0.610913	H	-0.266283	1.366307	1.951720
C	1.332215	-0.463382	1.120508				
C	1.539585	1.532017	-0.286626	P0-6			
C	2.585514	-0.884337	0.750687	C	1.878378	1.642920	0.112295
H	0.752192	-1.064597	1.813815	C	2.187587	-0.476045	-1.263308
C	2.793598	1.127415	-0.658365	C	2.919330	-1.054198	-0.073021
H	1.157525	2.467691	-0.670389	C	2.934935	-0.432498	1.118230
C	3.335829	-0.090724	-0.154781	C	2.266201	0.887377	1.389223
H	2.992915	-1.805812	1.147510	C	1.210592	0.684295	-0.948057
H	3.401774	1.717967	-1.335489	H	1.659658	-1.279347	-1.795509
H	0.961365	0.388126	1.810223	H	2.927195	-0.092894	-1.982251
O	4.549289	-0.391527	-0.587002	H	2.809734	1.953987	-0.379495
C	5.205645	-1.604637	-0.153206	H	3.461874	-0.896470	1.951723
H	4.611843	-2.478923	-0.433039	C	1.059601	2.900801	0.410699
H	6.158188	-1.614156	-0.681681	H	0.814003	3.449194	-0.506406
H	5.373733	-1.578248	0.926803	H	0.122694	2.668709	0.931478
				H	1.634973	3.576166	1.055027
Int3b-2				C	3.629611	-2.360764	-0.311760
C	1.889153	1.270578	-0.322264	H	4.361805	-2.269040	-1.126611
C	3.004165	0.611134	0.621381	H	4.159778	-2.703564	0.582703
C	3.715842	-0.570376	0.046965	H	2.925129	-3.147383	-0.616697
C	3.360006	-1.892836	0.359385	H	1.387108	0.739435	2.036776
C	2.359090	-2.298930	1.216574	H	2.945848	1.525195	1.972683
C	0.804858	0.289577	-0.542557	C	-0.165308	0.227154	-0.563433
H	3.724204	1.420774	0.785411	C	-1.295830	1.003397	-0.973824
H	2.535565	0.389003	1.583802	C	-0.404607	-0.950984	0.203237
H	2.383615	1.357879	-1.303420	C	-2.579973	0.661195	-0.632571
H	3.930776	-2.674236	-0.142545	H	-1.123607	1.892425	-1.572044
C	1.558159	2.677094	0.179285	C	-1.676720	-1.314650	0.559458
H	0.815214	3.169312	-0.456178	H	0.432460	-1.564683	0.514402
H	1.194979	2.670914	1.212544	C	-2.789798	-0.514000	0.147216
H	2.467505	3.286426	0.155489	H	-3.417085	1.269807	-0.952395
C	4.821794	-0.288664	-0.926104	H	-1.876451	-2.206992	1.143574
H	5.218212	-1.204155	-1.375959	O	-3.966909	-0.957054	0.531128

H	4.480427	0.372640	-1.737178	C	-5.192127	-0.267944	0.169614
H	5.653754	0.239586	-0.436810	H	-5.307783	-0.267821	-0.916907
H	2.154010	-3.355472	1.361472	H	-5.986288	-0.846774	0.638180
H	1.755954	-1.603418	1.792406	H	-5.177366	0.750741	0.563490
C	-0.566778	0.294095	-0.303682	H	1.090363	1.289393	-1.854729
C	-1.295007	-0.879434	-0.706201				
C	-1.323782	1.359358	0.299550	P6			
C	-2.652997	-0.993792	-0.542982	C	1.878378	1.642920	0.112295
H	-0.744497	-1.699517	-1.158091	C	2.187587	-0.476045	-1.263308
C	-2.676460	1.249292	0.471803	C	2.919330	-1.054198	-0.073021
H	-0.829037	2.261443	0.628251	C	2.934935	-0.432498	1.118230
C	-3.364266	0.078320	0.051000	C	2.266201	0.887377	1.389223
H	-3.168328	-1.891697	-0.861297	C	1.210592	0.684295	-0.948057
H	-3.253872	2.046741	0.927354	H	1.659658	-1.279347	-1.795509
H	1.169274	-0.629978	-0.996768	H	2.927195	-0.092894	-1.982251
O	-4.672604	0.083367	0.258775	H	2.809734	1.953987	-0.379495
C	-5.474302	-1.051470	-0.133376	H	3.461874	-0.896470	1.951723
H	-5.171134	-1.943337	0.422047	C	1.059601	2.900801	0.410699
H	-6.497189	-0.780895	0.127274	H	0.814003	3.449194	-0.506406
H	-5.395452	-1.222612	-1.210675	H	0.122694	2.668709	0.931478
				H	1.634973	3.576166	1.055027
Int4c-2				C	3.629611	-2.360764	-0.311760
C	-1.046181	2.208798	-0.005168	H	4.361805	-2.269040	-1.126611
C	-2.842900	-0.585481	1.735345	H	4.159778	-2.703564	0.582703
C	-3.330160	-1.212770	0.655455	H	2.925129	-3.147383	-0.616697
C	-4.608266	-0.912531	-0.026687	H	1.387108	0.739435	2.036776
C	-5.126756	0.325613	-0.075432	H	2.945848	1.525195	1.972683
C	0.043551	1.748343	0.710632	C	-0.165308	0.227154	-0.563433
H	-1.890734	-0.875606	2.172165	C	-1.295830	1.003397	-0.973824
H	-3.386242	0.215130	2.232536	C	-0.404607	-0.950984	0.203237
H	-1.789693	2.729089	0.595048	C	-2.579973	0.661195	-0.632571
C	-1.340464	2.119124	-1.461993	H	-1.123607	1.892425	-1.572044
H	-0.464801	2.340089	-2.081775	C	-1.676720	-1.314650	0.559458
H	-1.678145	1.104311	-1.723588	H	0.432460	-1.564683	0.514402
H	-2.145549	2.807500	-1.730258	C	-2.789798	-0.514000	0.147216
H	-6.077628	0.522740	-0.564751	H	-3.417085	1.269807	-0.952395
H	-4.618092	1.180052	0.364258	H	-1.876451	-2.206992	1.143574
C	1.177283	0.993773	0.295858	O	-3.966909	-0.957054	0.531128
C	2.212432	0.788618	1.268385	C	-5.192127	-0.267944	0.169614
C	1.357125	0.404671	-0.998984	H	-5.307783	-0.267821	-0.916907
C	3.355822	0.085999	0.983806	H	-5.986288	-0.846774	0.638180
H	2.083423	1.218328	2.257334	H	-5.177366	0.750741	0.563490
C	2.489941	-0.303023	-1.294828	H	1.090363	1.289393	-1.854729
H	0.588116	0.499688	-1.753197				
C	3.512938	-0.469539	-0.314203	TS 6a-6			

H	4.122008	-0.039086	1.739019	C	1.640319	-0.600847	0.505891
H	2.636153	-0.758504	-2.268631	C	2.497489	-0.606668	-1.512751
O	4.564918	-1.162053	-0.711984	C	1.638262	0.058710	-2.382177
C	5.666654	-1.420996	0.189641	C	0.635402	-0.527539	-3.235870
H	5.320250	-2.000566	1.049304	C	0.441125	-1.873209	-3.311577
H	6.378374	-2.001949	-0.395224	C	0.695338	-1.623058	0.326169
H	6.120240	-0.480220	0.512488	H	3.338169	-0.047895	-1.113929
H	0.043917	2.011448	1.766073	H	2.644720	-1.679601	-1.581146
H	-2.766053	-2.050319	0.241745	H	1.233575	0.396114	0.360300
C	-5.290138	-2.089091	-0.686148	C	2.884157	-0.652583	1.353161
H	-4.631392	-2.557099	-1.430399	H	2.612125	-0.802299	2.406972
H	-5.534129	-2.868176	0.048475	H	3.565628	-1.458621	1.066182
H	-6.214657	-1.789485	-1.188826	H	3.426701	0.294079	1.284177
TS2a-2				H	-0.331352	-2.290393	-3.951479
C	1.605702	-0.685104	0.557167	H	1.048892	-2.583391	-2.759788
C	2.715213	-0.632063	-1.669673	C	0.689171	-2.994922	0.708465
C	1.819726	0.086471	-2.473247	C	1.673015	-3.644436	1.514154
C	0.833753	-0.670473	-3.382363	C	-0.413690	-3.783836	0.269478
C	0.805453	-2.025334	-3.371416	C	1.557501	-4.976515	1.837012
C	0.570577	-1.526800	0.128229	H	2.521202	-3.093444	1.896132
H	3.424839	-0.111008	-1.061534	C	-0.538938	-5.121972	0.586879
H	2.689313	-1.701736	-1.664265	H	-1.180276	-3.312837	-0.339849
H	1.634602	0.334627	0.234345	C	0.454120	-5.735925	1.378777
H	0.171037	-0.126671	-4.022665	H	2.303076	-5.470009	2.452230
C	2.701605	-1.227813	1.493148	H	-1.393790	-5.683649	0.230236
H	2.404547	-1.084287	2.511017	O	0.442129	-7.020291	1.753022
H	2.844660	-2.271770	1.307169	C	-0.641711	-7.868525	1.338374
H	3.617048	-0.704459	1.311584	H	-0.685036	-7.938570	0.246848
C	1.887151	1.624304	-2.519344	H	-0.420176	-8.848597	1.761780
H	2.116394	1.941572	-3.515180	H	-1.594960	-7.502766	1.733031
H	0.942973	2.031734	-2.223662	H	-0.185001	-1.318892	-0.236515
H	2.648934	1.968101	-1.851220	H	1.690910	1.146545	-2.386163
H	0.120394	-2.551263	-4.003074	C	-0.208274	0.430378	-4.046596
H	1.468169	-2.569136	-2.731114	H	0.422675	1.058644	-4.687563
C	0.532727	-2.862362	0.551031	H	-0.920243	-0.101170	-4.683970
C	-0.502398	-3.704057	0.122096	H	-0.771557	1.107013	-3.391549
C	1.530002	-3.356229	1.402771				
C	-0.538999	-4.995591	0.530958	TS6b-6			
H	-1.263840	-3.326979	-0.528226	C	1.644330	-0.560298	0.061244
C	1.493401	-4.647762	1.811634	C	2.633649	-0.554024	-1.182816
H	2.320342	-2.713575	1.730275	C	1.947420	0.037261	-2.362753
C	0.458276	-5.489458	1.382696	C	0.833027	-0.545413	-2.955245
H	-1.329341	-5.638244	0.203457	C	0.485294	-1.851842	-2.604472
H	2.254843	-5.024841	2.461955	C	0.563820	-1.603579	-0.012137
H	-0.190863	-1.149722	-0.522095	H	3.503415	0.048759	-0.909015

O	0.423131	-6.729624	1.775298	H	2.982273	-1.578438	-1.359304
C	-0.633120	-7.588497	1.337608	H	1.128527	0.404546	0.040383
H	-0.966456	-7.278860	0.369149	C	2.450245	-0.605071	1.380273
H	-0.275808	-8.595785	1.286634	H	1.783615	-0.652553	2.247393
H	-1.447435	-7.533498	2.029536	H	3.134639	-1.455867	1.426438
TS2b-2				H	3.044701	0.311121	1.460906
C	1.632250	-0.222504	-0.203041	H	-0.471965	-2.273779	-2.901763
C	3.068394	-0.256687	-0.757949	H	1.226629	-2.556549	-2.254250
C	3.069408	0.252552	-2.211316	C	0.636938	-2.976709	0.303890
C	2.889523	-0.648363	-3.269576	C	1.852990	-3.716040	0.461830
C	2.714681	-1.967708	-3.013986	C	-0.589262	-3.695030	0.457297
C	0.727837	-1.124248	-1.063562	C	1.832914	-5.055444	0.761198
H	3.696784	0.369850	-0.160054	H	2.808373	-3.224593	0.326921
H	3.437139	-1.260794	-0.731589	C	-0.619743	-5.036716	0.770819
H	2.890227	-0.294542	-4.279383	H	-1.526024	-3.159326	0.330273
C	3.268096	1.751807	-2.501759	C	0.599092	-5.735270	0.926651
H	4.311718	1.957346	-2.617977	H	2.751778	-5.621076	0.877112
H	2.750897	2.012411	-3.401476	H	-1.569238	-5.543493	0.892767
H	2.879724	2.327353	-1.687626	O	0.695603	-7.032200	1.221259
H	2.577339	-2.655578	-3.821992	C	-0.498449	-7.815953	1.401132
H	2.713976	-2.321530	-2.004180	H	-1.093631	-7.829555	0.482872
C	0.556549	-2.611598	-0.702938	H	-0.149507	-8.822941	1.630505
C	1.427072	-3.568167	-1.242462	H	-1.092061	-7.429340	2.235221
C	-0.469847	-3.008518	0.164753	H	-0.448346	-1.216159	-0.098290
C	1.271202	-4.921656	-0.914292	H	2.209332	1.056761	-2.638385
H	2.210749	-3.265111	-1.904962	C	-0.059481	0.252911	-3.882100
C	-0.625719	-4.362006	0.492922	H	0.337259	1.258880	-4.047879
H	-1.134512	-2.278156	0.576691	H	-0.164062	-0.240339	-4.855078
C	0.244807	-5.318575	-0.046599	H	-1.067069	0.352513	-3.459701
H	1.935868	-5.652017	-1.326228				
H	-1.409393	-4.665062	1.155425	TS6c-6			
O	0.085757	-6.699685	0.288270	C	0.515990	0.172365	0.596106
C	0.531360	-7.509159	-0.803100	C	1.424129	-0.121925	-1.891923
H	1.563446	-7.306336	-0.999471	C	2.828570	-0.025727	-1.676057
H	0.412350	-8.542577	-0.552534	C	3.441875	1.130886	-1.085274
H	-0.048293	-7.284255	-1.673916	C	2.805137	2.279535	-0.740905
H	0.218459	-0.717365	-1.912020	C	0.449008	-0.851452	-0.390782
C	1.631236	-0.731742	1.250326	H	1.118657	-0.895901	-2.591546
H	0.622371	-0.867204	1.580085	H	0.871433	0.805251	-2.011144
H	2.151597	-1.665286	1.301515	H	-0.020954	1.087004	0.354765
H	2.119037	-0.016558	1.879183	H	4.512018	1.060574	-0.898943
H	1.263505	0.781603	-0.229401	C	1.248009	0.135163	1.882377
TS2c-2				H	1.131813	-0.831307	2.387973
C	0.602076	0.609251	0.482190	H	2.329114	0.268963	1.717737
C	1.172148	0.517130	-1.992915	H	0.916282	0.940806	2.542557

C	2.379892	-0.193696	-1.994784	C	3.713361	-1.169942	-2.060839
C	3.475767	0.284915	-1.264092	H	4.202970	-0.933510	-3.019019
C	3.367586	1.435141	-0.555682	H	4.516797	-1.329104	-1.333174
C	0.085800	-0.376463	-0.369720	H	3.153536	-2.097482	-2.200021
H	0.335423	0.151700	-2.550815	H	3.353548	3.091743	-0.272465
H	1.086733	1.425290	-1.433585	H	1.749505	2.455014	-0.925348
H	4.204311	1.800571	0.002219	C	0.832211	-2.267795	-0.150134
H	2.445447	1.977872	-0.554253	C	-0.020334	-3.272917	-0.633774
C	4.802957	-0.496213	-1.266145	C	1.996908	-2.669925	0.535242
H	4.802797	-1.201771	-0.461728	C	0.243813	-4.626198	-0.427501
H	4.909936	-1.015177	-2.195732	H	-0.920463	-2.992699	-1.176305
H	5.618279	0.185578	-1.142402	C	2.276085	-4.012143	0.744486
H	2.465306	-1.101857	-2.554111	H	2.703861	-1.931335	0.897060
C	1.447017	0.204967	1.704577	C	1.399059	-5.004687	0.271455
H	2.155732	0.977267	1.919462	H	-0.446975	-5.368498	-0.809551
H	0.806450	0.063445	2.549885	H	3.174384	-4.317949	1.272282
H	1.965939	-0.706709	1.493704	O	1.759870	-6.284388	0.533502
H	0.409194	1.642763	0.283322	C	0.915343	-7.342428	0.074682
C	0.363401	-1.863948	-0.083495	H	0.837182	-7.343790	-1.018955
C	-0.152876	-2.849661	-0.935404	H	1.394976	-8.265770	0.404344
C	1.132291	-2.231846	1.028881	H	-0.085700	-7.274580	0.516431
C	0.099737	-4.203273	-0.674937	H	-0.472191	-0.773741	-0.970365
H	-0.739941	-2.568763	-1.784728				
C	1.384906	-3.585458	1.289348	Int 2a-7			
H	1.526479	-1.479232	1.679333	C	-2.244909	-2.340025	-0.290620
C	0.868627	-4.571172	0.437440	C	-3.496208	1.265247	-0.450762
H	-0.294450	-4.955888	-1.325389	C	-2.358286	1.904303	-0.756622
H	1.971970	-3.866357	2.138671	C	-1.455579	2.594004	0.190870
O	1.126393	-5.952409	0.703224	C	-1.333724	2.225190	1.477385
C	2.329933	-6.348829	0.040470	C	-1.258172	-1.942823	0.581078
H	3.146340	-5.758015	0.400081	H	-4.096016	0.788415	-1.221927
H	2.522808	-7.382342	0.239344	H	-3.880021	1.217129	0.566059
H	2.221204	-6.202753	-1.013920	H	-2.063397	-2.313679	-1.362954
H	-0.501268	-0.095564	-1.219041	H	-1.479618	-1.987847	1.646052
P0-2				C	0.037799	-1.466134	0.229554
C	-1.600695	-0.892435	0.666511	C	0.924249	-1.076172	1.284339
C	-1.735382	1.335208	-0.589299	C	0.506995	-1.346799	-1.119821
C	-3.219983	1.092750	-0.676344	C	2.186294	-0.597091	1.033396
C	-3.825233	-0.046411	-0.309271	H	0.580144	-1.167971	2.310124
C	-3.044337	-1.221993	0.240845	C	1.761233	-0.872398	-1.384152
C	-0.962405	0.009914	-0.463999	H	-0.133523	-1.632761	-1.946178
H	-1.520744	2.000268	0.258565	C	2.621053	-0.481910	-0.313962
H	-1.393147	1.872646	-1.483555	H	2.835931	-0.311565	1.851687
H	-1.033711	-1.830454	0.698561	H	2.130623	-0.774446	-2.399491
C	-1.537966	-0.254632	2.061024	O	3.803956	-0.022480	-0.682715

H	-0.510861	-0.009159	2.353594	C	4.753865	0.445802	0.302688
H	-2.137741	0.659650	2.124362	H	5.619435	0.772213	-0.272379
H	-1.931966	-0.958099	2.803666	H	4.332658	1.285396	0.862151
H	-3.577747	-1.638146	1.108022	H	5.033759	-0.368772	0.975476
H	-3.040478	-2.026063	-0.510832	C	-3.578770	-2.825640	0.136395
C	0.518408	0.134794	-0.293147	H	-3.740073	-3.848791	-0.234577
C	1.347685	-0.934308	-0.766239	H	-3.704805	-2.813704	1.222289
C	1.149017	1.244961	0.339019	H	-4.367916	-2.216395	-0.327333
C	2.710711	-0.918101	-0.626588	H	-0.678965	2.761571	2.159968
H	0.871338	-1.778851	-1.254850	H	-1.882250	1.381860	1.888968
C	2.510500	1.286779	0.491892	H	-2.063234	1.963425	-1.805508
H	0.551160	2.071628	0.703781	C	-0.654353	3.737500	-0.386754
C	3.317527	0.204125	0.011187	H	-1.312619	4.520112	-0.787037
H	3.315335	-1.736870	-0.997218	H	0.000768	4.191325	0.363222
H	3.009257	2.123607	0.969115	H	-0.031449	3.396015	-1.224962
O	4.609462	0.343632	0.205000				
C	5.553360	-0.668467	-0.235988	Int3b-7			
H	5.494859	-0.781199	-1.321041	C	-2.256351	-1.512112	-0.398776
H	6.528955	-0.284836	0.057439	C	-3.200787	-0.258624	-0.100755
H	5.344301	-1.613619	0.270736	C	-2.672231	1.043441	-0.580902
H	-1.119592	-0.559895	-1.390672	C	-2.127567	2.070897	0.211077
H	-3.819631	1.912223	-1.071560	C	-2.041014	1.994823	1.588041
C	-5.312415	-0.245834	-0.440489	C	-1.081292	-1.453723	0.489662
H	-5.776393	-0.424890	0.539612	H	-4.125698	-0.495685	-0.641544
H	-5.801049	0.622188	-0.895720	H	-3.439810	-0.251695	0.966356
H	-5.540604	-1.127280	-1.056686	H	-1.964969	-1.449375	-1.450463
P2				H	-1.258569	-1.761277	1.521033
C	-1.600695	-0.892435	0.666511	C	0.200209	-1.021097	0.184830
C	-1.735382	1.335208	-0.589299	C	1.190159	-1.001902	1.225302
C	-3.219983	1.092750	-0.676344	C	0.592727	-0.566457	-1.122076
C	-3.825233	-0.046411	-0.309271	C	2.470502	-0.565541	0.997990
C	-3.044337	-1.221993	0.240845	H	0.905409	-1.342404	2.216823
C	-0.962405	0.009914	-0.463999	C	1.865662	-0.124136	-1.354729
H	-1.520744	2.000268	0.258565	H	-0.123102	-0.578831	-1.935604
H	-1.393147	1.872646	-1.483555	C	2.823370	-0.119006	-0.302676
H	-1.033711	-1.830454	0.698561	H	3.198349	-0.559739	1.800353
C	-1.537966	-0.254632	2.061024	H	2.178922	0.219950	-2.334608
H	-0.510861	-0.009159	2.353594	O	4.026486	0.318097	-0.638308
H	-2.137741	0.659650	2.124362	C	5.091469	0.347145	0.337006
H	-1.931966	-0.958099	2.803666	H	5.958016	0.730402	-0.200845
H	-3.577747	-1.638146	1.108022	H	4.835228	1.017863	1.161702
H	-3.040478	-2.026063	-0.510832	H	5.295791	-0.660919	0.708258
C	0.518408	0.134794	-0.293147	C	-3.052493	-2.809622	-0.162958
C	1.347685	-0.934308	-0.766239	H	-2.438955	-3.692310	-0.371215
C	1.149017	1.244961	0.339019	H	-3.407760	-2.874092	0.871859

C	2.710711	-0.918101	-0.626588	H	-3.923235	-2.834133	-0.826695
H	0.871338	-1.778851	-1.254850	H	-1.602976	2.804673	2.164155
C	2.510500	1.286779	0.491892	H	-2.413589	1.145505	2.151267
H	0.551160	2.071628	0.703781	H	-2.688902	1.198246	-1.658932
C	3.317527	0.204125	0.011187	C	-1.602641	3.304204	-0.502806
H	3.315335	-1.736870	-0.997218	H	-2.350416	3.710448	-1.193970
H	3.009257	2.123607	0.969115	H	-1.333022	4.093254	0.205390
O	4.609462	0.343632	0.205000	H	-0.710939	3.065610	-1.096231
C	5.553360	-0.668467	-0.235988				
H	5.494859	-0.781199	-1.321041	Int4c-7			
H	6.528955	-0.284836	0.057439	C	-1.011397	2.079102	-0.381470
H	5.344301	-1.613619	0.270736	C	-2.685915	-1.119250	1.025768
H	-1.119592	-0.559895	-1.390672	C	-3.733588	-1.328468	0.210420
H	-3.819631	1.912223	-1.071560	C	-4.927642	-0.454345	0.210640
C	-5.312415	-0.245834	-0.440489	C	-5.428535	0.199869	1.267510
H	-5.776393	-0.424890	0.539612	C	-0.212879	1.089429	-0.907193
H	-5.801049	0.622188	-0.895720	H	-1.827788	-1.787316	1.028478
H	-5.540604	-1.127280	-1.056686	H	-2.655780	-0.282312	1.719002
Int 2a-3				H	-0.658815	2.667080	0.463198
C	-1.901869	1.963055	-0.782319	H	-5.451299	-0.378509	-0.743747
C	-3.680964	-0.530282	-0.735824	H	-0.602958	0.524956	-1.752202
C	-3.176776	-1.172951	0.343144	C	1.091138	0.730720	-0.459140
C	-2.120784	-2.195922	0.255794	C	1.777655	-0.319396	-1.147876
C	-1.386539	-2.510177	-0.824896	C	1.761194	1.360707	0.641123
C	-0.801662	1.291620	-1.282903	C	3.039047	-0.722676	-0.785459
H	-4.475249	0.202849	-0.627957	H	1.280165	-0.805787	-1.981400
H	-3.373831	-0.767980	-1.750087	C	3.016864	0.968979	1.013249
H	-1.919652	-2.729617	1.184443	H	1.273285	2.158092	1.190122
C	-3.684068	-0.876674	1.732303	C	3.680535	-0.077823	0.306150
H	-4.108240	-1.781063	2.189426	H	3.533697	-1.521187	-1.324599
H	-2.866883	-0.552636	2.391140	H	3.536256	1.436544	1.843124
H	-4.455276	-0.101255	1.727867	O	4.891698	-0.374702	0.743743
H	-0.629916	-3.288597	-0.776682	C	5.674331	-1.410069	0.104139
H	-1.517673	-2.020686	-1.786623	H	6.611944	-1.436780	0.657867
C	-2.137845	2.530504	0.578034	H	5.162195	-2.372699	0.181920
H	-1.943321	1.807686	1.377839	H	5.859312	-1.151660	-0.941851
H	-1.475002	3.390736	0.754354	C	-2.355372	2.419931	-0.902627
H	-3.167970	2.882285	0.671663	H	-2.377879	3.475877	-1.210999
H	-2.684661	2.149643	-1.513309	H	-2.651429	1.792051	-1.746871
C	0.431322	0.922913	-0.666710	H	-3.106421	2.329668	-0.104247
C	0.832597	1.264107	0.664169	C	-3.757588	-2.467659	-0.782069
C	1.352541	0.161293	-1.455580	H	-4.604174	-3.140024	-0.589685
C	2.045919	0.861217	1.158800	H	-3.883382	-2.092729	-1.807097
H	0.185841	1.858698	1.294044	H	-2.836130	-3.056845	-0.743630
C	2.572437	-0.249263	-0.971103	H	-6.311876	0.826545	1.174035

H	1.071091	-0.098312	-2.471895	H	-4.989589	0.118355	2.259651
C	2.934728	0.095582	0.353893				
H	2.358348	1.118646	2.165561	P0-7			
H	3.241690	-0.825836	-1.597627	C	-1.717835	1.453894	0.100967
H	-0.888678	0.987097	-2.323863	C	-1.785753	-1.119287	0.461117
O	4.079653	-0.241540	0.934662	C	-3.249464	-1.102567	0.104809
C	5.064586	-1.008164	0.209531	C	-3.885321	0.079598	0.221281
H	5.886357	-1.151717	0.910406	C	-3.137908	1.278719	0.731680
H	4.652668	-1.976653	-0.087729	C	-1.082122	0.074062	-0.293713
H	5.411409	-0.452129	-0.666271	H	-1.313619	-2.065466	0.178685
Int 3b-3				H	-1.636566	-0.986006	1.540679
C	-2.030086	-0.986735	1.081642	H	-1.085862	1.924058	0.862539
C	-3.290806	-0.019481	0.853748	H	-4.940143	0.172704	-0.029804
C	-3.374499	0.580152	-0.510258	H	-1.273008	-0.090409	-1.359216
C	-2.582015	1.681921	-0.871645	C	0.394759	0.025007	-0.082499
C	-1.789789	2.417174	-0.018591	C	1.269249	-0.240270	-1.177040
C	-0.781657	-0.213587	1.280244	C	0.967125	0.211050	1.211011
H	-4.168600	-0.643890	1.043618	C	2.633781	-0.294274	-1.020424
H	-3.255695	0.747258	1.634560	H	0.837195	-0.394860	-2.160909
H	-2.588173	1.965747	-1.923567	C	2.323240	0.159740	1.394910
C	-4.291769	-0.053511	-1.511265	H	0.317394	0.397815	2.059860
H	-5.340714	0.067112	-1.199763	C	3.182029	-0.093885	0.278580
H	-4.182097	0.389986	-2.505931	H	3.278994	-0.486810	-1.868867
H	-4.124047	-1.135835	-1.590525	H	2.778465	0.302456	2.369402
H	-1.154955	3.210354	-0.402972	O	4.469187	-0.127536	0.559720
H	-1.811881	2.296613	1.058685	C	5.455263	-0.382838	-0.471992
C	-2.042474	-2.188475	0.134828	H	6.415807	-0.312737	0.035885
H	-1.941495	-1.903954	-0.916120	H	5.313116	-1.386146	-0.880912
H	-1.243750	-2.894233	0.384168	H	5.382841	0.374302	-1.256696
H	-2.994876	-2.717680	0.243855	C	-1.755322	2.382242	-1.119930
H	-2.236271	-1.360645	2.098691	H	-0.763822	2.490829	-1.575635
C	0.484700	-0.259884	0.689536	H	-2.437977	1.995592	-1.886978
C	0.862853	-1.058703	-0.442537	H	-2.101513	3.382311	-0.833565
C	1.502472	0.567169	1.273435	C	-3.887719	-2.359765	-0.410625
C	2.143644	-1.027531	-0.929681	H	-3.811083	-3.172168	0.325491
H	0.136900	-1.691095	-0.932378	H	-4.946246	-2.206976	-0.645319
C	2.790222	0.598548	0.794337	H	-3.382833	-2.716119	-1.319819
H	1.238809	1.188222	2.125068	H	-3.716950	2.195151	0.578318
C	3.127679	-0.205712	-0.321020	H	-3.011705	1.174223	1.820309
H	2.433875	-1.625761	-1.787277				
H	3.530033	1.233896	1.265977	P7			
H	-0.851832	0.469671	2.125251	C	-1.717835	1.453894	0.100967
O	4.335818	-0.258710	-0.872774	C	-1.785753	-1.119287	0.461117
C	5.407691	0.546897	-0.343815	C	-3.249464	-1.102567	0.104809
H	6.268846	0.326338	-0.974424	C	-3.885321	0.079598	0.221281

H	5.159095	1.609988	-0.410455	C	-3.137908	1.278719	0.731680
H	5.623295	0.268134	0.691981	C	-1.082122	0.074062	-0.293713
Int4c-3				H	-1.313619	-2.065466	0.178685
C	1.031905	1.614642	0.819739	H	-1.636566	-0.986006	1.540679
C	2.874424	-0.857731	-1.321400	H	-1.085862	1.924058	0.862539
C	3.773411	-1.249662	-0.407354	H	-4.940143	0.172704	-0.029804
C	5.097812	-0.636905	-0.163397	H	-1.273008	-0.090409	-1.359216
C	5.338697	0.669213	-0.364102	C	0.394759	0.025007	-0.082499
C	0.140795	0.577120	1.026329	C	1.269249	-0.240270	-1.177040
H	1.922919	-1.371791	-1.431033	C	0.967125	0.211050	1.211011
H	3.065837	-0.032025	-2.003311	C	2.633781	-0.294274	-1.020424
H	0.518399	-0.232692	1.646561	H	0.837195	-0.394860	-2.160909
C	-1.194623	0.390879	0.569230	C	2.323240	0.159740	1.394910
C	-1.882269	-0.780116	1.034446	H	0.317394	0.397815	2.059860
C	-1.901202	1.262936	-0.323477	C	3.182029	-0.093885	0.278580
C	-3.172581	-1.066500	0.667454	H	3.278994	-0.486810	-1.868867
H	-1.356909	-1.453523	1.705003	H	2.778465	0.302456	2.369402
C	-3.186594	0.986527	-0.702087	O	4.469187	-0.127536	0.559720
H	-1.421257	2.147222	-0.718001	C	5.455263	-0.382838	-0.471992
C	-3.847319	-0.179307	-0.212853	H	6.415807	-0.312737	0.035885
H	-3.664870	-1.955656	1.041918	H	5.313116	-1.386146	-0.880912
H	-3.729265	1.637077	-1.379764	H	5.382841	0.374302	-1.256696
O	-5.085166	-0.348485	-0.641336	C	-1.755322	2.382242	-1.119930
C	-5.861424	-1.494500	-0.219498	H	-0.763822	2.490829	-1.575635
H	-6.824288	-1.380414	-0.715635	H	-2.437977	1.995592	-1.886978
H	-5.376082	-2.418835	-0.543265	H	-2.101513	3.382311	-0.833565
H	-5.991676	-1.483152	0.865784	C	-3.887719	-2.359765	-0.410625
H	6.325402	1.095016	-0.198350	H	-3.811083	-3.172168	0.325491
H	4.561906	1.353816	-0.695908	H	-4.946246	-2.206976	-0.645319
C	0.851528	2.895226	0.080103	H	-3.382833	-2.716119	-1.319819
H	0.752639	2.715760	-1.000751	H	-3.716950	2.195151	0.578318
H	-0.053024	3.427465	0.399126	H	-3.011705	1.174223	1.820309
H	1.712104	3.550097	0.232599				
H	2.005085	1.467972	1.283035	TS7a-7			
C	6.166280	-1.575523	0.348129	C	1.445309	-0.539969	0.931513
H	5.855030	-2.047189	1.290200	C	2.222875	-0.755456	-1.100915
H	6.350135	-2.391646	-0.363373	C	1.435713	-0.075164	-2.021625
H	7.112166	-1.054009	0.523240	C	0.381609	-0.623765	-2.836086
H	3.544036	-2.123397	0.205036	C	0.031176	-1.940450	-2.785322
				C	0.253322	-1.267740	0.853285
TS3a-3				H	3.123570	-0.261036	-0.752660
C	1.547969	-0.243765	0.271149	H	2.250358	-1.840121	-1.083085
C	2.777603	-0.925762	-1.405968	H	1.393064	0.544000	0.875526
C	2.442687	-0.222581	-2.563121	H	0.318289	-2.333666	1.070922
C	1.428250	-0.674584	-3.490698	C	-1.035997	-0.784410	0.503617

C	0.713124	-1.819735	-3.402931	C	-2.120643	-1.704919	0.456219
C	0.304645	-0.833905	-0.011448	C	-1.317110	0.583557	0.212773
H	3.675763	-0.630213	-0.872074	C	-3.404920	-1.307097	0.140673
H	2.498022	-1.967924	-1.297372	H	-1.926027	-2.750859	0.677626
H	1.230180	-0.010611	-4.330751	C	-2.590815	0.989445	-0.110070
C	3.111032	1.086409	-2.874464	H	-0.524710	1.322996	0.259470
H	3.625865	1.023057	-3.843268	C	-3.652434	0.051609	-0.150731
H	2.373733	1.894700	-2.971431	H	-4.205440	-2.036588	0.117268
H	3.844196	1.367159	-2.114863	H	-2.813816	2.029074	-0.327713
H	-0.040657	-2.057521	-4.147903	O	-4.850788	0.554254	-0.468578
H	0.859616	-2.550670	-2.613446	C	-5.997542	-0.312026	-0.503406
C	1.848545	1.224946	0.413731	H	-6.838348	0.332175	-0.762178
H	1.623653	1.805396	-0.483685	H	-5.877259	-1.088077	-1.266535
H	1.257306	1.644522	1.239282	H	-6.169094	-0.768765	0.476649
H	2.904249	1.372725	0.657086	C	2.614272	-1.098107	1.701461
H	2.189247	-0.888719	0.867557	H	2.452502	-0.911171	2.772308
C	-0.931530	-0.287112	-0.459504	H	2.715330	-2.179535	1.563895
C	-1.203233	1.096879	-0.683724	H	3.556093	-0.614079	1.428346
C	-2.005339	-1.200739	-0.675157	H	-0.777288	-2.324987	-3.400392
C	-2.445908	1.517735	-1.098278	H	0.537082	-2.658330	-2.147439
H	-0.434702	1.840282	-0.522405	H	1.610102	0.994973	-2.124168
C	-3.255401	-0.788902	-1.091916	C	-0.329733	0.333130	-3.765521
H	-1.829452	-2.259509	-0.505292	H	0.378281	0.795418	-4.464627
C	-3.489856	0.585464	-1.307948	H	-1.102758	-0.174351	-4.349141
H	-2.653340	2.569807	-1.266258	H	-0.802670	1.147674	-3.203490
H	-4.041532	-1.518407	-1.244500				
H	0.283990	-1.912944	0.130628	TS7b-7			
O	-4.658174	1.106009	-1.702980	C	1.408399	-0.535643	0.192706
C	-5.776744	0.237009	-1.945986	C	2.499429	-0.773852	-0.923819
H	-6.595676	0.894946	-2.238301	C	2.085613	-0.154715	-2.211555
H	-5.556059	-0.461892	-2.759212	C	1.001362	-0.616008	-2.948307
H	-6.050563	-0.311206	-1.038628	C	0.397239	-1.824202	-2.595108
TS3b-3				C	0.151701	-1.305435	-0.022220
C	1.556971	-0.294921	-0.261174	H	3.430118	-0.325658	-0.565593
C	2.790884	-0.816929	-1.126010	H	2.667467	-1.854738	-1.011378
C	2.852967	-0.158944	-2.464318	H	1.202501	0.537436	0.225889
C	1.834798	-0.394125	-3.391354	H	0.253947	-2.386807	0.050809
C	0.890684	-1.394797	-3.253084	C	-1.164795	-0.812735	0.027675
C	0.264136	-0.897574	-0.697244	C	-2.243174	-1.747089	0.105716
H	3.694665	-0.603778	-0.548889	C	-1.494631	0.580185	0.019313
H	2.700600	-1.906251	-1.210367	C	-3.556398	-1.340094	0.181049
H	1.746988	0.287388	-4.236741	H	-2.011550	-2.808586	0.109456
C	3.923365	0.851336	-2.724088	C	-2.800973	0.994492	0.086732
H	4.910647	0.365991	-2.714064	H	-0.707474	1.323081	-0.046633
H	3.796049	1.349448	-3.689913	C	-3.850653	0.043562	0.169817

H	3.953769	1.613285	-1.933204	H	-4.349477	-2.074693	0.246825
H	0.033044	-1.440885	-3.918371	H	-3.060950	2.048017	0.080398
H	1.054812	-2.263798	-2.627792	O	-5.080741	0.552969	0.231749
C	1.639726	1.212790	-0.008019	C	-6.218480	-0.327320	0.305431
H	1.547063	1.802023	-0.924832	H	-7.087514	0.329757	0.339354
H	0.867471	1.539500	0.695087	H	-6.270569	-0.967303	-0.580994
H	2.611613	1.446949	0.439200	H	-6.177756	-0.936074	1.214063
H	1.726762	-0.801316	0.704089	C	1.991127	-0.964644	1.562825
C	-1.025489	-0.359735	-0.890473	H	1.280551	-0.777369	2.374041
C	-1.345550	1.027614	-1.045529	H	2.246911	-2.030099	1.565982
C	-2.115519	-1.285769	-0.934240	H	2.901568	-0.389982	1.764821
C	-2.645371	1.439049	-1.211069	H	-0.549805	-2.121192	-3.038903
H	-0.561361	1.771210	-1.054306	H	0.932192	-2.595634	-2.054664
C	-3.423411	-0.879542	-1.086996	H	2.542184	0.792438	-2.490506
H	-1.901005	-2.345917	-0.830352	C	0.402707	0.225893	-4.055431
C	-3.704385	0.497732	-1.226070	H	0.981044	1.140386	-4.216402
H	-2.889811	2.489213	-1.334478	H	0.365457	-0.327695	-5.000561
H	-4.219543	-1.614200	-1.101986	H	-0.626656	0.514990	-3.808976
H	0.279919	-1.983337	-0.623556	TS7c-7			
O	-4.927844	1.009002	-1.383396	C	0.573418	0.286945	0.886422
C	-6.069423	0.133173	-1.395212	C	1.029327	-0.097579	-1.705431
H	-6.930212	0.784346	-1.547911	C	2.383044	-0.531245	-1.605456
H	-5.999816	-0.586994	-2.216507	C	3.449945	0.344275	-1.215104
H	-6.165402	-0.390632	-0.438854	C	3.331834	1.673549	-0.963572
				C	-0.001244	-0.490808	-0.152680
TS3c-3				H	0.411227	-0.707427	-2.360217
C	0.510412	0.386536	0.716822	H	0.842290	0.966430	-1.814214
C	1.005494	0.354150	-1.783608	H	0.168373	1.274477	1.095961
C	2.318649	-0.218337	-1.798626	H	4.431714	-0.114342	-1.112575
C	3.500103	0.337770	-1.234779	H	0.240064	-1.552874	-0.087622
C	3.498278	1.565983	-0.626525	C	-1.406529	-0.234076	-0.585715
C	-0.030457	-0.313564	-0.398262	C	-2.218661	-1.323316	-0.927416
H	0.358763	-0.023902	-2.572459	C	-1.954035	1.059136	-0.682943
H	0.928076	1.433194	-1.677172	C	-3.541538	-1.150289	-1.334705
H	0.318424	-1.345944	-0.442811	H	-1.816041	-2.331494	-0.865697
C	-1.465298	-0.180067	-0.796389	C	-3.265904	1.247815	-1.090315
C	-2.253567	-1.334804	-0.880534	H	-1.350375	1.930676	-0.444499
C	-2.061160	1.055270	-1.111708	C	-4.073890	0.143925	-1.419935
C	-3.602648	-1.274415	-1.232611	H	-4.141191	-2.018950	-1.579409
H	-1.812120	-2.303377	-0.657516	H	-3.689072	2.244843	-1.166561
C	-3.399211	1.130847	-1.470907	O	-5.340357	0.434324	-1.807758
H	-1.470731	1.967212	-1.088168	C	-6.200666	-0.640505	-2.191265
C	-4.185389	-0.033732	-1.526840	H	-7.146333	-0.175087	-2.474570
H	-4.182933	-2.188652	-1.276909	H	-5.794077	-1.188955	-3.049289
H	-3.859200	2.083743	-1.714522	H	-6.371599	-1.332466	-1.358025

O	-5.482675	0.145909	-1.880333	C	1.693622	-0.191713	1.722303
C	-6.336838	-0.997631	-1.941600	H	1.274519	-0.586372	2.664905
H	-7.316884	-0.618950	-2.237378	H	2.246521	-1.011460	1.251571
H	-5.986219	-1.719145	-2.689153	H	2.376475	0.616926	2.002065
H	-6.416614	-1.489283	-0.964651	C	2.710640	-1.967541	-1.877311
H	4.398979	1.959528	-0.164245	H	3.184095	-2.054458	-2.867341
H	2.620348	2.203389	-0.591700	H	3.432799	-2.362423	-1.153256
C	-0.088836	1.500193	1.473242	H	1.818192	-2.599719	-1.882704
H	0.423980	2.443728	1.220822	H	4.196278	2.252514	-0.651584
H	-1.158463	1.626968	1.302303	H	2.398125	2.217871	-1.069764
H	0.109247	1.347708	2.543260				
H	1.511341	0.086881	1.021632	Int2a-8			
C	4.764920	-0.490686	-1.304799	C	1.308689	2.353754	0.339594
H	4.637910	-1.446233	-0.781927	C	2.810621	-0.638255	2.035128
H	5.019563	-0.724203	-2.345513	C	3.614093	-1.024444	1.034411
H	5.612266	0.035126	-0.856578	C	3.200713	-1.756487	-0.183528
H	2.403232	-1.216295	-2.226094	C	2.195742	-2.647324	-0.181056
P0-3				C	0.540456	1.788778	-0.651076
C	1.600089	-0.891693	0.667097	H	3.204236	-0.119684	2.905857
C	1.735575	1.334825	-0.591341	H	1.739955	-0.831142	2.022242
C	3.220212	1.091907	-0.677562	H	1.895287	-3.165451	-1.088749
C	3.825054	-0.046975	-0.308737	H	1.656275	-2.902180	0.727901
C	3.043898	-1.221932	0.242404	C	2.590407	3.056790	0.094104
C	0.962680	0.009452	-0.464625	H	2.860477	3.084085	-0.964913
H	1.393770	1.870760	-1.486609	H	2.534618	4.084926	0.481032
H	1.520524	2.001236	0.255293	H	3.396282	2.568122	0.660526
H	1.119874	-0.561294	-1.390662	H	0.978031	2.302380	1.374566
C	-0.518145	0.134657	-0.293878	C	-0.699877	1.110930	-0.473309
C	-1.347625	-0.934404	-0.766815	C	-1.327052	0.925071	0.801978
C	-1.148526	1.244697	0.338679	C	-1.361341	0.585379	-1.629533
C	-2.710610	-0.918115	-0.626997	C	-2.525612	0.268729	0.921400
H	-0.871398	-1.779067	-1.255338	H	-0.851093	1.308804	1.697362
C	-2.509974	1.286653	0.491675	C	-2.558394	-0.068073	-1.526150
H	-0.550570	2.071273	0.703539	H	-0.894554	0.716831	-2.600903
C	-3.317228	0.204026	0.011138	C	-3.163166	-0.236528	-0.246417
H	-3.315361	-1.736810	-0.997552	H	-2.979643	0.140183	1.896470
H	-3.008646	2.123438	0.969079	H	-3.070396	-0.468755	-2.394546
O	-4.609044	0.343551	0.205501	H	0.903295	1.861561	-1.674920
C	-5.553247	-0.668417	-0.235093	O	-4.319323	-0.875527	-0.249475
H	-6.528668	-0.284455	0.058432	C	-5.033952	-1.120738	0.984307
H	-5.494859	-0.781625	-1.320098	H	-5.285519	-0.174383	1.470055
H	-5.344368	-1.613478	0.271874	H	-5.941475	-1.643635	0.684734
H	3.040601	-2.026892	-0.508285	H	-4.435924	-1.752260	1.646649
H	3.577018	-1.636829	1.110347	H	4.672333	-0.762783	1.086430
H	3.820280	1.910773	-1.073391	C	3.996919	-1.453949	-1.431968

C	5.312240	-0.246641	-0.439003	H	3.930226	-0.390265	-1.697926
H	5.540898	-1.128289	-1.054737	H	5.062859	-1.669990	-1.277647
H	5.801259	0.621252	-0.894068	H	3.649836	-2.043954	-2.285728
H	5.775591	-0.425368	0.541485				
H	1.032776	-1.829456	0.699979	Int3b-8			
C	1.536791	-0.252161	2.060785	C	-1.463064	1.647847	-0.017852
H	0.509544	-0.006115	2.352341	C	-2.558309	1.111381	-1.042878
H	1.930218	-0.954755	2.804554	C	-3.664718	0.304951	-0.457359
H	2.136767	0.662025	2.123444	C	-3.714320	-1.098735	-0.376363
P3				C	-2.702758	-1.911648	-0.851961
C	1.600269	-0.892294	0.666337	C	-0.688371	0.521858	0.539983
C	3.043698	-1.222520	0.240295	H	-2.974599	2.022809	-1.488596
C	3.825059	-0.046698	-0.308940	H	-2.033703	0.571575	-1.836935
C	3.220225	1.092735	-0.676092	H	-2.759029	-2.991316	-0.746913
C	1.735575	1.335550	-0.589709	H	-1.830724	-1.519212	-1.365183
C	0.962566	0.010068	-0.464278	C	-2.118345	2.460732	1.119856
H	3.576962	-1.639345	1.107216	H	-2.757881	1.832236	1.747913
H	3.039624	-2.025988	-0.512005	H	-1.357044	2.919774	1.758863
H	1.520579	2.001100	0.257642	H	-2.732196	3.259760	0.689415
H	1.393895	1.872540	-1.484404	H	-0.818059	2.312057	-0.599055
C	1.537936	-0.254186	2.060729	C	0.656352	0.225184	0.367822
H	2.138167	0.659775	2.124080	C	1.546706	1.011848	-0.437238
H	0.510884	-0.008259	2.353083	C	1.201983	-0.923567	1.042030
H	1.931586	-0.957765	2.803453	C	2.874505	0.688573	-0.556829
H	1.032792	-1.829990	0.698651	H	1.168648	1.881204	-0.963564
C	-0.518277	0.135084	-0.293421	C	2.525245	-1.248375	0.933509
C	-1.148930	1.245165	0.338791	H	0.538720	-1.532457	1.649488
C	-1.347540	-0.934173	-0.766289	C	3.383847	-0.442262	0.137044
C	-2.510417	1.286984	0.491501	H	3.527872	1.296947	-1.169624
H	-0.551220	2.071933	0.703627	H	2.949073	-2.107808	1.442004
C	-2.710529	-0.918113	-0.626569	H	-1.248148	-0.159047	1.180845
H	-0.871126	-1.778762	-1.254757	O	4.650059	-0.823937	0.102594
C	-3.317450	0.204145	0.011089	C	5.621694	-0.070277	-0.656383
H	-3.009245	2.123832	0.968631	H	5.695488	0.950967	-0.272444
H	-3.315114	-1.736995	-0.996996	H	6.565028	-0.595013	-0.508395
H	1.119589	-0.559712	-1.390933	H	5.357394	-0.066054	-1.717308
O	-4.609366	0.343736	0.204709	H	-4.496655	0.858936	-0.027197
C	-5.553226	-0.668953	-0.235048	C	-4.936280	-1.725993	0.271548
H	-6.528658	-0.285755	0.059457	H	-5.105953	-1.323179	1.277164
H	-5.495820	-0.781951	-1.320141	H	-5.840149	-1.517663	-0.314172
H	-5.343076	-1.613892	0.271602	H	-4.833552	-2.812125	0.353346
H	3.820396	1.912120	-1.070689				
C	5.312211	-0.246340	-0.439450	Int4c-8			
H	5.540771	-1.127145	-1.056399	C	1.347839	2.361042	0.350982
H	5.801391	0.622112	-0.893283	C	3.573696	-0.522231	-1.281577

H	5.775534	-0.426462	0.540800	C	3.062690	-1.516113	-0.535561
int2a-4				C	3.735311	-2.024212	0.680554
C	-1.281188	2.323935	-0.174531	C	4.491250	-1.308673	1.523096
C	-2.837233	-0.785745	-1.557602	C	0.425174	1.843053	-0.527802
C	-3.549803	-1.159531	-0.480692	H	3.060896	-0.158981	-2.169039
C	-2.929635	-1.795428	0.702639	H	4.530322	-0.062318	-1.046739
C	-1.845239	-2.581972	0.701132	H	3.559031	-3.077439	0.905336
C	-0.534132	1.619126	0.740086	C	1.774238	-2.211749	-0.907830
H	-3.316385	-0.341658	-2.427011	H	1.947276	-3.282699	-1.081222
H	-1.759592	-0.919149	-1.606927	H	1.035703	-2.143293	-0.097650
H	-3.442929	-1.618297	1.649229	H	1.331980	-1.788124	-1.815011
C	-5.040851	-0.932151	-0.393360	H	4.959414	-1.769137	2.389519
H	-5.578271	-1.880638	-0.260298	H	4.665556	-0.243848	1.382419
H	-5.291281	-0.307401	0.474952	H	1.193630	2.248680	1.422116
H	-5.428979	-0.441765	-1.291338	C	2.570562	3.087178	-0.065283
H	-1.454876	-3.004170	1.623824	H	2.677242	3.146078	-1.151687
H	-1.321755	-2.844493	-0.215828	H	2.557245	4.105587	0.351546
C	-2.578691	2.968641	0.138455	H	3.460759	2.604739	0.363008
H	-2.886397	2.814337	1.176174	C	-0.773520	1.156620	-0.179238
H	-2.518628	4.048192	-0.064823	C	-1.613486	0.678239	-1.235155
H	-3.359450	2.582563	-0.532565	C	-1.193453	0.923764	1.172019
H	-0.917664	2.439875	-1.193388	C	-2.789603	0.016477	-0.983054
C	0.724009	0.994775	0.500809	H	-1.302668	0.849013	-2.261760
C	1.390698	1.013996	-0.767337	C	-2.362588	0.267731	1.437669
C	1.365232	0.315168	1.585660	H	-0.584309	1.276206	1.996666
C	2.610480	0.411385	-0.943738	C	-3.183221	-0.195726	0.365938
H	0.927935	1.513662	-1.611089	H	-3.406089	-0.337825	-1.800242
C	2.580105	-0.292501	1.423735	H	-2.695979	0.087465	2.454260
H	0.869508	0.292430	2.551268	H	0.616091	1.966033	-1.592326
C	3.227778	-0.250130	0.154735	O	-4.293355	-0.810934	0.731816
H	3.095745	0.441766	-1.911467	C	-5.216394	-1.319804	-0.259144
H	3.075831	-0.807996	2.239299	H	-6.027812	-1.765647	0.314493
H	-0.929439	1.523726	1.749611	H	-5.594736	-0.501280	-0.876773
O	4.401348	-0.855155	0.099673	H	-4.727684	-2.079321	-0.875134
C	5.178891	-0.856843	-1.120398	P0			
H	5.417195	0.168190	-1.416117	C	1.735895	1.364476	0.349898
H	6.090485	-1.399408	-0.873167	C	1.847471	-1.164088	0.044501
H	4.635628	-1.374875	-1.915284	C	3.352350	-1.031278	-0.046707
				C	3.947495	0.168323	-0.094722
Int3b-4				C	3.211755	1.480962	-0.063620
C	1.686646	-1.254287	0.060233	C	1.105975	0.137706	-0.383440
C	2.691028	-0.626885	-1.014669	H	1.561665	-1.434846	1.070501
C	3.650928	0.396339	-0.505517	H	1.510556	-1.995087	-0.589235
C	3.242328	1.718686	-0.270162	H	5.033486	0.219997	-0.170971
C	1.999779	2.233137	-0.569499	C	4.122863	-2.325875	-0.074220

C	0.772079	-0.257174	0.662331	H	3.859921	-2.929111	-0.954680
H	3.237756	-1.486223	-1.415763	H	5.203516	-2.149782	-0.091858
H	2.071895	-0.223872	-1.822475	H	3.892210	-2.943252	0.805643
H	3.960731	2.378873	0.214806	H	3.715914	2.168408	0.630674
C	5.058803	-0.026586	-0.217230	H	3.280364	1.966035	-1.051069
H	5.575906	-0.298443	-1.150410	H	1.696740	1.157713	1.428319
H	5.635690	0.766317	0.268531	C	0.988006	2.672698	0.069409
H	5.090480	-0.922851	0.416150	H	0.942420	2.879169	-1.007641
H	1.737190	3.246551	-0.279701	H	-0.038058	2.650310	0.453945
H	1.267142	1.693570	-1.159220	H	1.502513	3.514789	0.547328
C	2.451969	-1.998279	1.174403	C	-0.365177	-0.003544	-0.150072
H	3.050421	-1.311722	1.782110	C	-1.274298	0.016187	-1.251079
H	1.755129	-2.519861	1.839099	C	-0.894098	-0.171216	1.165938
H	3.119549	-2.745057	0.731461	C	-2.629601	-0.105818	-1.073518
H	1.114449	-1.986956	-0.514471	H	-0.873747	0.133077	-2.253233
C	-0.602309	-0.125338	0.454296	C	-2.241227	-0.294069	1.371722
C	-1.343399	-0.920570	-0.477224	H	-0.217026	-0.192084	2.013348
C	-1.328474	0.853876	1.214427	C	-3.136189	-0.257757	0.251571
C	-2.699450	-0.757146	-0.641504	H	-3.302976	-0.088058	-1.921423
H	-0.835188	-1.672595	-1.070724	H	-2.665375	-0.412417	2.363328
C	-2.679420	1.016443	1.063049	H	1.265884	0.279333	-1.459108
H	-0.784630	1.472806	1.922545	O	-4.409881	-0.369546	0.551750
C	-3.386853	0.211615	0.131654	C	-5.439185	-0.313406	-0.472074
H	-3.233977	-1.373291	-1.354145	H	-6.377508	-0.409115	0.071534
H	-3.233370	1.751011	1.638232	H	-5.390910	0.646467	-0.991776
H	1.209006	0.396098	1.414661	H	-5.312760	-1.144987	-1.169139
O	-4.694312	0.438934	0.056951	TS8a-8			
C	-5.512206	-0.326133	-0.851204	C	1.429909	-0.599682	0.414363
H	-5.481423	-1.389163	-0.594162	C	2.598989	-0.957643	-1.402782
H	-6.523011	0.059062	-0.717984	C	2.046685	-0.224671	-2.443825
H	-5.187957	-0.171914	-1.884447	C	1.059538	-0.672796	-3.397924
				C	0.581630	-1.945695	-3.404505
Int4c-4				C	0.332549	-1.439802	0.189951
C	-1.175615	1.895629	-0.795530	H	3.471528	-0.547993	-0.902214
C	-3.119269	-0.642910	1.510157	H	2.503872	-2.037648	-1.365738
C	-3.345766	-1.431276	0.445354	H	-0.179376	-2.252560	-4.116475
C	-4.600041	-1.386839	-0.339432	H	0.941956	-2.709423	-2.722975
C	-5.453168	-0.357396	-0.432111	C	1.261657	0.894868	0.459686
C	-0.272558	1.776115	0.234811	H	0.506098	1.244612	-0.250140
H	-2.183663	-0.694612	2.061428	H	0.934326	1.182782	1.468708
H	-3.865221	0.056167	1.880098	H	2.204021	1.415251	0.265420
H	-4.817518	-2.289605	-0.911961	H	2.256446	-0.992741	1.001521
C	-2.328100	-2.447496	-0.018491	C	0.229884	-2.830858	0.470176
H	-2.740212	-3.464396	0.035197	C	1.265415	-3.596475	1.076253
H	-2.048549	-2.280603	-1.067539	C	-0.983302	-3.505405	0.139528

H	-1.418529	-2.417042	0.589239	C	1.108383	-4.943398	1.336271
H	-6.356493	-0.431010	-1.032292	H	2.200843	-3.121100	1.351783
H	-5.288572	0.585471	0.085088	C	-1.152718	-4.844703	0.399147
C	-2.462456	2.622323	-0.692419	H	-1.786407	-2.940268	-0.324948
H	-2.636933	3.034185	0.304961	C	-0.108154	-5.583352	1.003605
H	-2.486973	3.438457	-1.430304	H	1.915299	-5.498434	1.799681
H	-3.294098	1.955931	-0.963755	H	-2.076345	-5.358403	0.152707
H	-0.956282	1.444597	-1.760735	H	-0.543652	-0.985871	-0.271532
C	0.983521	1.104761	0.181274	O	-0.367258	-6.877163	1.222144
C	1.793895	1.076210	1.361824	C	0.627844	-7.709452	1.841358
C	1.488827	0.458567	-0.994241	H	0.877840	-7.338762	2.840505
C	3.010647	0.450685	1.374343	H	0.171711	-8.696749	1.918170
H	1.424591	1.562791	2.259363	H	1.528710	-7.765207	1.221874
C	2.707200	-0.171707	-0.995895	H	2.340812	0.820791	-2.521603
H	0.904934	0.464837	-1.907849	C	0.562227	0.353397	-4.391028
C	3.489512	-0.184888	0.192224	H	0.072389	1.191082	-3.878414
H	3.631675	0.422518	2.263371	H	1.395031	0.775377	-4.967129
H	3.069780	-0.652933	-1.895774	H	-0.152641	-0.082592	-5.094211
O	4.674278	-0.760596	0.298004				
C	5.268521	-1.439743	-0.832980	TS8b-8			
H	5.434230	-0.735038	-1.652189	C	1.763026	-0.698044	-0.058760
H	6.220993	-1.819076	-0.465196	C	2.729296	-0.391302	-1.282362
H	4.630956	-2.267674	-1.154456	C	2.030365	0.183614	-2.461053
H	-0.529253	2.239603	1.185950	C	1.103454	-0.546878	-3.194351
				C	0.937280	-1.905580	-2.906845
TS4a-4				C	0.594632	-1.575680	-0.383041
C	1.308110	-0.482513	0.426096	H	3.493868	0.296206	-0.910963
C	2.677711	-0.825060	-1.282175	H	3.231409	-1.332091	-1.538549
C	2.193146	-0.150574	-2.397441	H	0.103475	-2.464627	-3.324322
C	1.254442	-0.744619	-3.330542	H	1.728330	-2.494280	-2.459494
C	0.745833	-1.994324	-3.264833	C	1.243693	0.615237	0.562279
C	0.247146	-1.351033	0.141208	H	0.625370	1.175172	-0.148171
H	3.500529	-0.380470	-0.730337	H	0.640665	0.417752	1.455059
H	2.592487	-1.903626	-1.210617	H	2.088559	1.247464	0.857308
H	0.929605	-0.098756	-4.144925	H	2.400350	-1.199946	0.673967
C	2.590924	1.274015	-2.658216	C	0.389320	-2.898825	0.056100
H	3.044289	1.360879	-3.655380	C	1.399558	-3.691511	0.678633
H	1.712900	1.934468	-2.663183	C	-0.900645	-3.494812	-0.127292
H	3.306344	1.646086	-1.921182	C	1.149366	-4.982970	1.090933
H	0.027353	-2.337584	-4.003870	H	2.389861	-3.277849	0.835758
H	1.030931	-2.709317	-2.499046	C	-1.161626	-4.775181	0.287474
C	1.090080	1.004363	0.460261	H	-1.682899	-2.910653	-0.604161
H	0.368130	1.332086	-0.293815	C	-0.138049	-5.540220	0.902191
H	0.687969	1.277834	1.446441	H	1.935456	-5.559005	1.563678
H	2.023482	1.558284	0.329189	H	-2.139161	-5.227723	0.157035

H	2.109177	-0.851064	1.061973	H	-0.287019	-1.070053	-0.767522
C	0.175016	-2.748230	0.404635	O	-0.486822	-6.773238	1.269116
C	1.203522	-3.486299	1.054722	C	0.482251	-7.641736	1.885690
C	-0.992622	-3.461783	-0.000006	H	0.838296	-7.215574	2.828386
C	1.085932	-4.844088	1.280242	H	-0.049595	-8.573723	2.077681
H	2.102561	-2.981738	1.392493	H	1.321395	-7.825192	1.207799
C	-1.121811	-4.812575	0.222611	H	2.147249	1.244475	-2.669749
H	-1.791913	-2.918563	-0.496557	C	0.204293	0.124972	-4.209380
C	-0.081111	-5.524472	0.864162	H	0.397225	1.200425	-4.263760
H	1.886681	-5.376877	1.779247	H	0.350984	-0.300462	-5.209025
H	-2.009456	-5.355971	-0.084976	H	-0.851930	-0.018689	-3.950228
H	-0.619157	-0.918447	-0.357408	TS8c-8			
O	-0.294285	-6.835201	1.033297	C	0.363539	0.090141	0.631754
C	0.708118	-7.640202	1.675365	C	1.316133	0.191324	-1.862346
H	0.882065	-7.300325	2.701435	C	2.707974	-0.058110	-1.721293
H	0.302841	-8.652361	1.686929	C	3.546528	0.707500	-0.842620
H	1.643699	-7.624197	1.107044	C	3.151129	1.784228	-0.118860
				C	0.294989	-0.767376	-0.496528
TS4b-4				H	0.842029	-0.291037	-2.713515
C	1.709145	-0.681206	-0.045393	H	0.956320	1.201016	-1.685416
C	2.707016	-0.415586	-1.258677	H	4.575255	0.366499	-0.743727
C	2.062289	0.189473	-2.459388	C	3.327873	-1.202342	-2.459930
C	1.128747	-0.561059	-3.174517	H	3.861439	-0.810921	-3.340745
C	0.892420	-1.902314	-2.921595	H	4.072868	-1.724854	-1.850350
C	0.545195	-1.567460	-0.355062	H	2.581249	-1.914557	-2.819456
H	3.494830	0.236255	-0.870638	H	3.843680	2.279044	0.556055
H	3.169272	-1.377772	-1.507726	H	2.158843	2.217381	-0.195549
H	0.502911	-0.048010	-3.903306	H	1.061098	-0.141656	1.433344
C	2.338635	1.618137	-2.795725	C	-0.482602	1.292703	0.801694
H	3.402333	1.750941	-3.042818	H	-1.067020	1.531871	-0.091362
H	1.741226	1.966084	-3.643467	H	-1.184189	1.112517	1.632866
H	2.146620	2.271565	-1.933388	H	0.112637	2.164231	1.104020
H	0.049052	-2.411993	-3.379201	C	0.743422	-2.181801	-0.403255
H	1.623467	-2.534601	-2.432893	C	0.054125	-3.162096	-1.130027
C	1.192493	0.647633	0.541678	C	1.822347	-2.592907	0.403984
H	0.564672	1.187633	-0.175454	C	0.405034	-4.510775	-1.058818
H	0.595855	0.468284	1.442538	H	-0.783345	-2.870512	-1.759599
H	2.035095	1.290584	0.818877	C	2.184495	-3.928460	0.483894
H	2.338769	-1.166254	0.705289	H	2.390237	-1.862388	0.973303
C	0.360329	-2.895428	0.080258	C	1.478059	-4.902483	-0.246413
C	1.379458	-3.673073	0.705938	H	-0.158957	-5.238995	-1.629657
C	-0.915166	-3.516324	-0.117669	H	3.015106	-4.245404	1.107276
C	1.151987	-4.974444	1.104049	H	-0.624268	-0.644921	-1.070568
H	2.359355	-3.241195	0.878470	O	1.911456	-6.178495	-0.098683
C	-1.152890	-4.806728	0.282057	C	1.232727	-7.218059	-0.806986

H	-1.705149	-2.945095	-0.597320	H	1.745724	-8.142656	-0.536428
C	-0.119570	-5.557604	0.896332	H	0.180545	-7.284053	-0.506122
H	1.946385	-5.537339	1.578881	H	1.297610	-7.069407	-1.891467
H	-2.119678	-5.277859	0.137251	P8			
H	-0.339899	-1.073826	-0.747653	C	1.735895	1.364476	0.349898
O	-0.445214	-6.804955	1.243792	C	1.847471	-1.164088	0.044501
C	0.540335	-7.659909	1.850362	C	3.352350	-1.031278	-0.046707
H	0.877432	-7.245812	2.805558	C	3.947495	0.168323	-0.094722
H	0.032680	-8.610116	2.017608	C	3.211755	1.480962	-0.063620
H	1.390939	-7.807157	1.177696	C	1.105975	0.137706	-0.383440
TS4c-4				H	1.561665	-1.434846	1.070501
C	0.521922	0.267524	0.804787	H	1.510556	-1.995087	-0.589235
C	1.115329	0.194164	-1.785245	H	5.033486	0.219997	-0.170971
C	2.486374	-0.180450	-1.829088	C	4.122863	-2.325875	-0.074220
C	3.506742	0.531805	-1.113518	H	3.859921	-2.929111	-0.954680
C	3.318216	1.667354	-0.396011	H	5.203516	-2.149782	-0.091858
C	0.219769	-0.615549	-0.264824	H	3.892210	-2.943252	0.805643
H	0.488180	-0.262380	-2.546951	H	3.715914	2.168408	0.630674
H	0.877347	1.238642	-1.605263	H	3.280364	1.966035	-1.051069
H	4.504406	0.097844	-1.142439	H	1.696740	1.157713	1.428319
C	2.893781	-1.404620	-2.585849	C	0.988006	2.672698	0.069409
H	3.455317	-1.102179	-3.483475	H	0.942420	2.879169	-1.007641
H	3.570521	-2.035105	-1.996997	H	-0.038058	2.650310	0.453945
H	2.035556	-1.996374	-2.911389	H	1.502513	3.514789	0.547328
H	4.142734	2.117621	0.149331	C	-0.365177	-0.003544	-0.150072
H	2.368915	2.192206	-0.355172	C	-1.274298	0.016187	-1.251079
C	-0.187640	1.545794	1.035917	C	-0.894098	-0.171216	1.165938
H	-0.864779	1.810353	0.218811	C	-2.629601	-0.105818	-1.073518
H	-0.783447	1.452618	1.959104	H	-0.873747	0.133077	-2.253233
H	0.515406	2.368168	1.221987	C	-2.241227	-0.294069	1.371722
H	1.307338	0.004696	1.509245	H	-0.217026	-0.192084	2.013348
C	0.532366	-2.067989	-0.171132	C	-3.136189	-0.257757	0.251571
C	-0.338666	-2.986446	-0.786878	H	-3.302976	-0.088058	-1.921423
C	1.639407	-2.576717	0.523956	H	-2.665375	-0.412417	2.363328
C	-0.119097	-4.353665	-0.704609	H	1.265884	0.279333	-1.459108
H	-1.205654	-2.619951	-1.331205	O	-4.409881	-0.369546	0.551750
C	1.874687	-3.948237	0.615471	C	-5.439185	-0.313406	-0.472074
H	2.341524	-1.903231	1.007328	H	-6.377508	-0.409115	0.071534
C	0.991621	-4.848934	-0.000610	H	-5.390910	0.646467	-0.991776
H	-0.797362	-5.058873	-1.175148	H	-5.312760	-1.144987	-1.169139
H	2.739644	-4.301513	1.164917				
O	1.121320	-6.198357	0.024854				
C	2.242600	-6.767785	0.703263				
H	2.226485	-6.528367	1.773154				
H	2.149567	-7.847378	0.572906				

H	3.188250	-6.429047	0.263626
H	-0.757701	-0.420493	-0.708417

P0-4

C	-1.702361	1.027694	-0.367339
C	-3.217451	0.987363	-0.104684
C	-3.834583	-0.392909	-0.137863
C	-3.074361	-1.495996	-0.117255
C	-1.570205	-1.494218	-0.054146
C	-1.018564	-0.120018	0.437349
H	-3.435757	1.453473	0.869819
H	-3.716772	1.626274	-0.847526
H	-3.549097	-2.477103	-0.131514
C	-5.339009	-0.448635	-0.174900
H	-5.730580	0.036239	-1.080078
H	-5.709153	-1.478958	-0.151836
H	-5.775527	0.090176	0.678112
H	-1.222714	-2.285775	0.621825
H	-1.144727	-1.731361	-1.039934
C	-1.131172	2.409036	-0.027271
H	-1.208863	2.615476	1.047868
H	-0.076505	2.497440	-0.312489
H	-1.683845	3.193974	-0.557040
H	-1.535335	0.829787	-1.435204
C	0.474604	-0.116060	0.359644
C	1.147102	-0.173180	-0.903559
C	1.260244	-0.084040	1.546112
C	2.515333	-0.178081	-0.993094
H	0.555073	-0.206991	-1.812307
C	2.628599	-0.090820	1.486274
H	0.758548	-0.049406	2.507868
C	3.281856	-0.130224	0.210731
H	3.004355	-0.218978	-1.958789
H	3.246449	-0.060611	2.377440
H	-1.301992	-0.002508	1.490135
O	4.594375	-0.114924	0.260971
C	5.403550	-0.122996	-0.944772
H	5.169966	0.753619	-1.553297
H	6.431947	-0.080591	-0.590637
H	5.228031	-1.046287	-1.501540

P4

H	-3.549097	-2.477103	-0.131514
C	-5.339009	-0.448635	-0.174900
H	-5.730580	0.036239	-1.080078
H	-5.709153	-1.478958	-0.151836

H	-5.775527	0.090176	0.678112
H	-1.222714	-2.285775	0.621825
H	-1.144727	-1.731361	-1.039934
C	-1.131172	2.409036	-0.027271
H	-1.208863	2.615476	1.047868
H	-0.076505	2.497440	-0.312489
H	-1.683845	3.193974	-0.557040
H	-1.535335	0.829787	-1.435204
C	0.474604	-0.116060	0.359644
C	1.147102	-0.173180	-0.903559
C	1.260244	-0.084040	1.546112
C	2.515333	-0.178081	-0.993094
H	0.555073	-0.206991	-1.812307
C	2.628599	-0.090820	1.486274
H	0.758548	-0.049406	2.507868
C	3.281856	-0.130224	0.210731
H	3.004355	-0.218978	-1.958789
H	3.246449	-0.060611	2.377440
H	-1.301992	-0.002508	1.490135
O	4.594375	-0.114924	0.260971
C	5.403550	-0.122996	-0.944772