

Supplementary data

[3+2] vs [4+1] Annulation: Revisiting mechanism studies on phosphine-catalyzed domino sequence of alkynoates and activated methylenes

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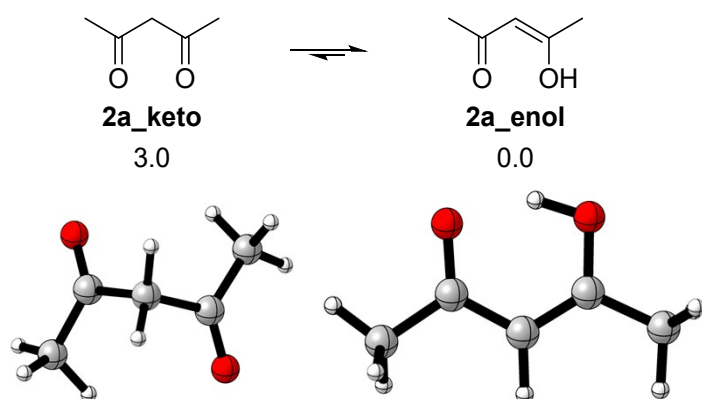
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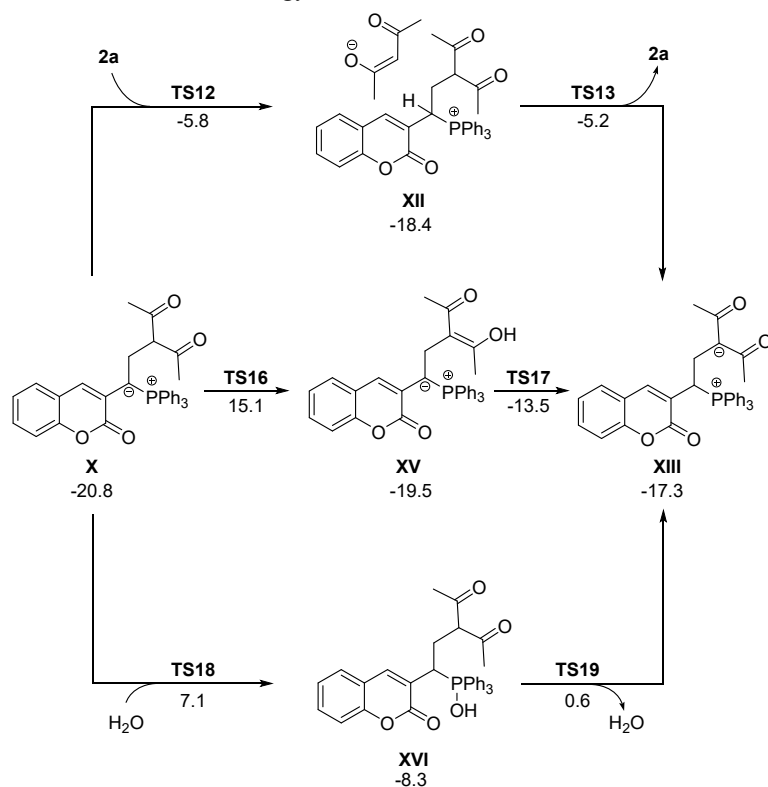
1. Stability of diketone structures



Obviously, the enol configuration **2a_enol** is more stable than the diketone configuration by 3.0 kcal/mol, which is also consistent with previous theoretical results.

2. Studies on [1,3]-proton shift of intermediate X

Several stepwise [1,3]-proton shift pathway was considered, and the **2a**-mediated pathway is most favorable with a free energy barrier about 15.6 kcal/mol.



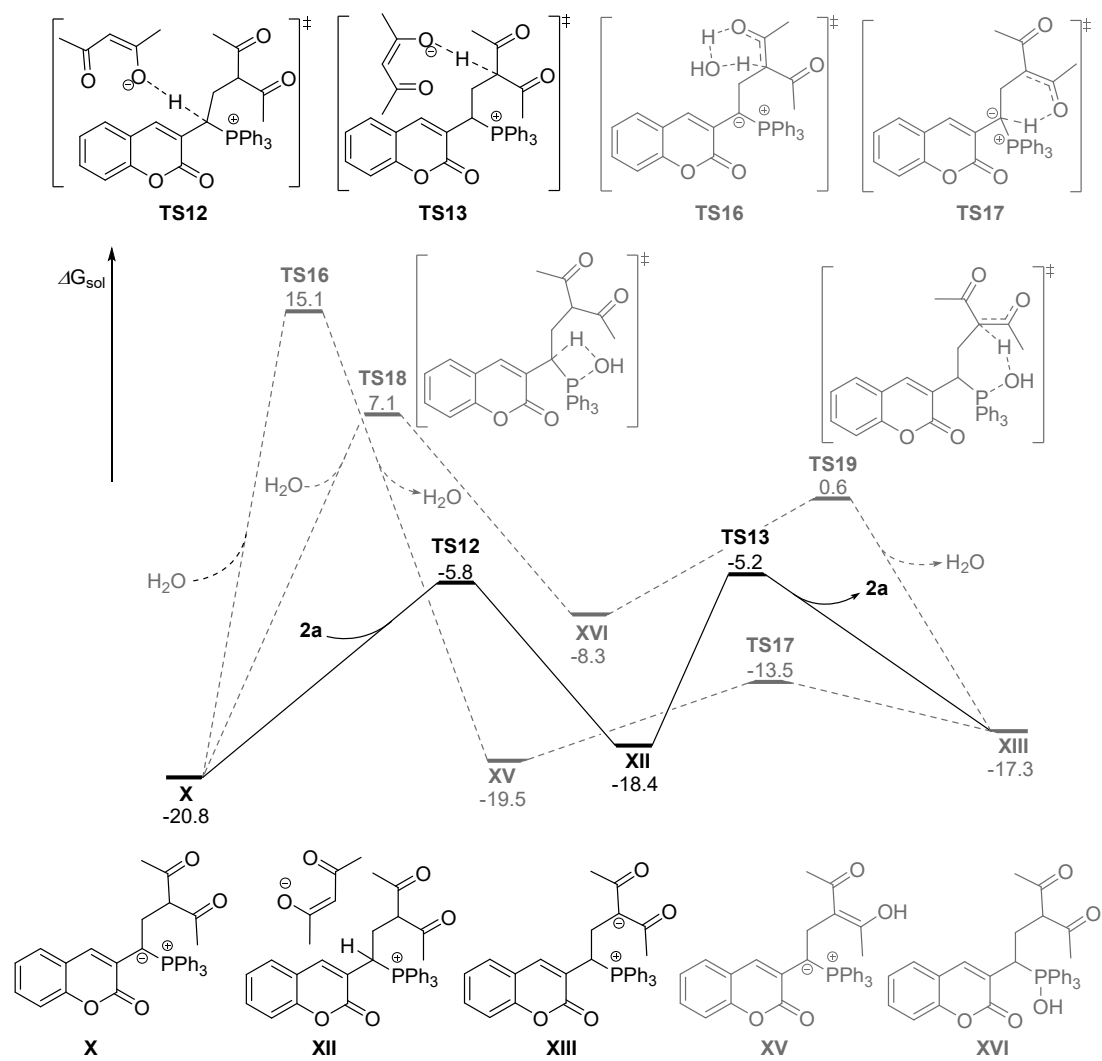


Figure S1. Free energy profiles of [1,3]-proton shift of intermediate X.

3. Studies on phosphine-catalyzed Knoevenagel condensation

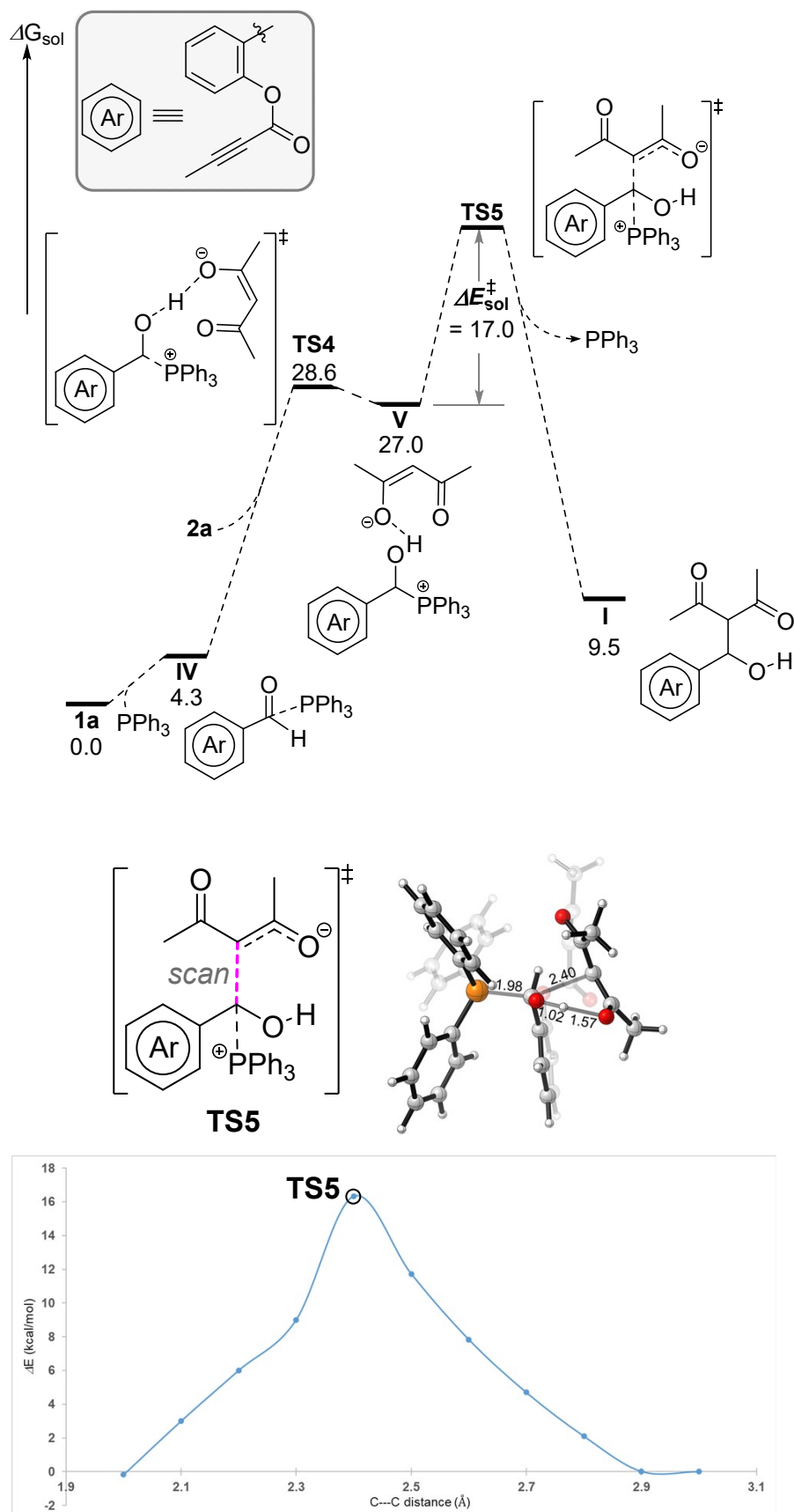


Figure S2. Energy profile during the scanning of forming C-C bond via **TS5**.

4. Isomerization of vinyl anion VI.

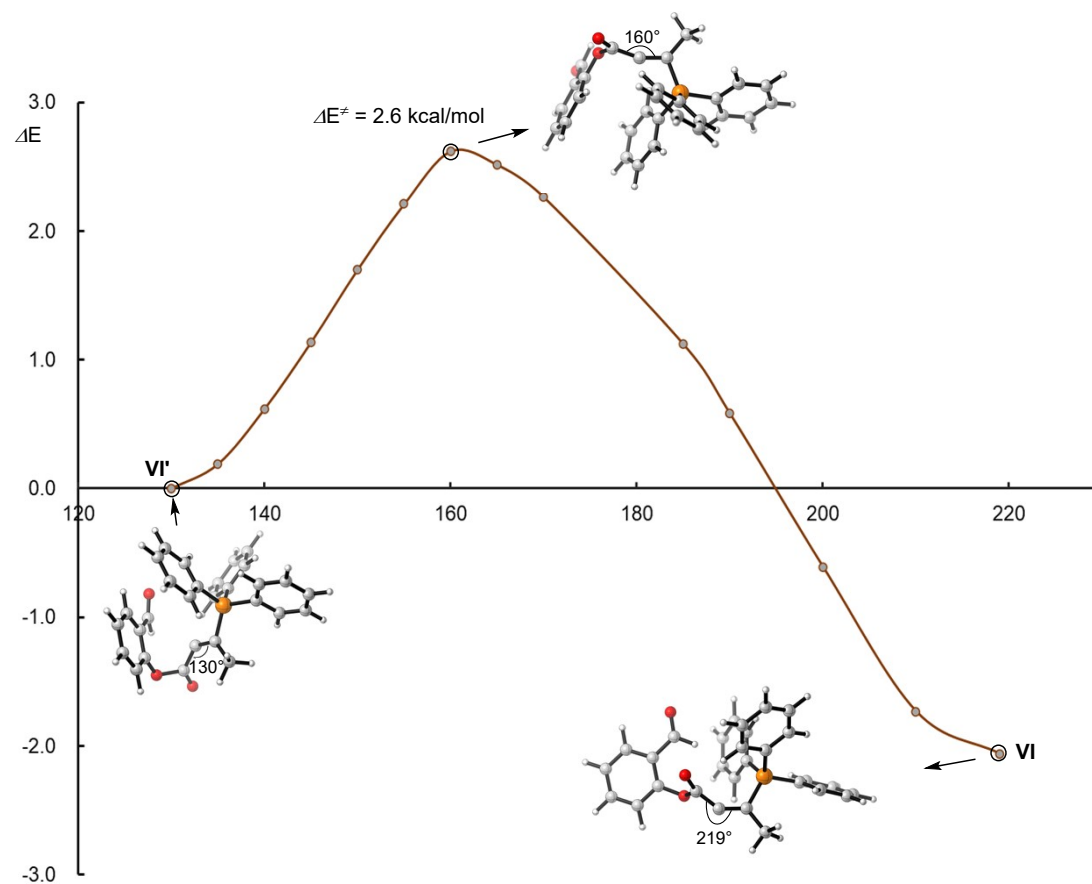


Figure S3. Energy profile for isomerization of adduct intermediate VI.

After extensive efforts, the transition state responding to the isomerization of VI to VI' could not be located. The energy barrier was estimated by scanning the reaction coordinates (angle $\text{C}(\text{Me})-\text{C}-\text{C}(\text{O}_2)$, to be about 2.6 kcal/mol.

5. Substrate-mediated [1,5]-H shift.

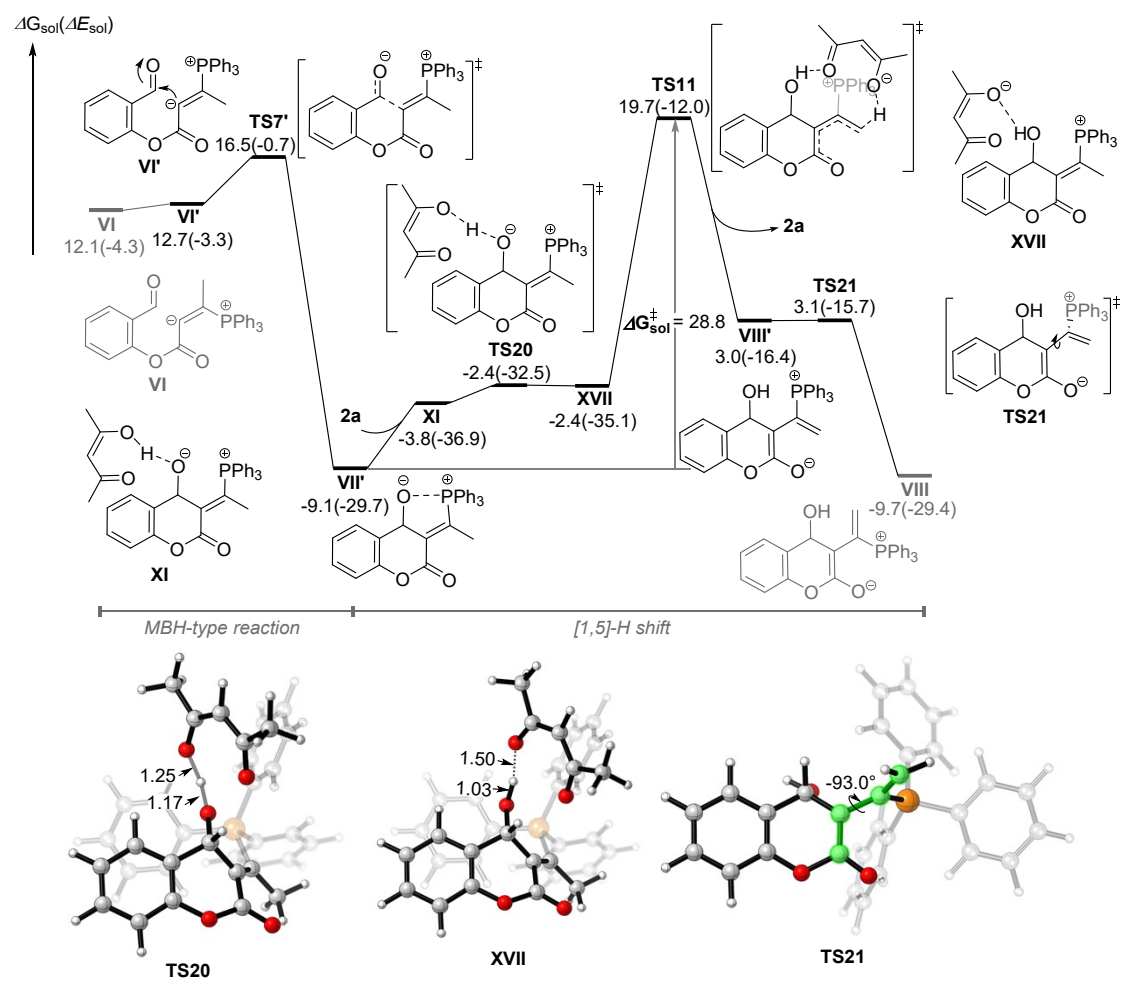


Figure S4. Free energy profile of the alternative [4+1] annulation pathway.

6. Studies on the transformation from intermediate IX to X

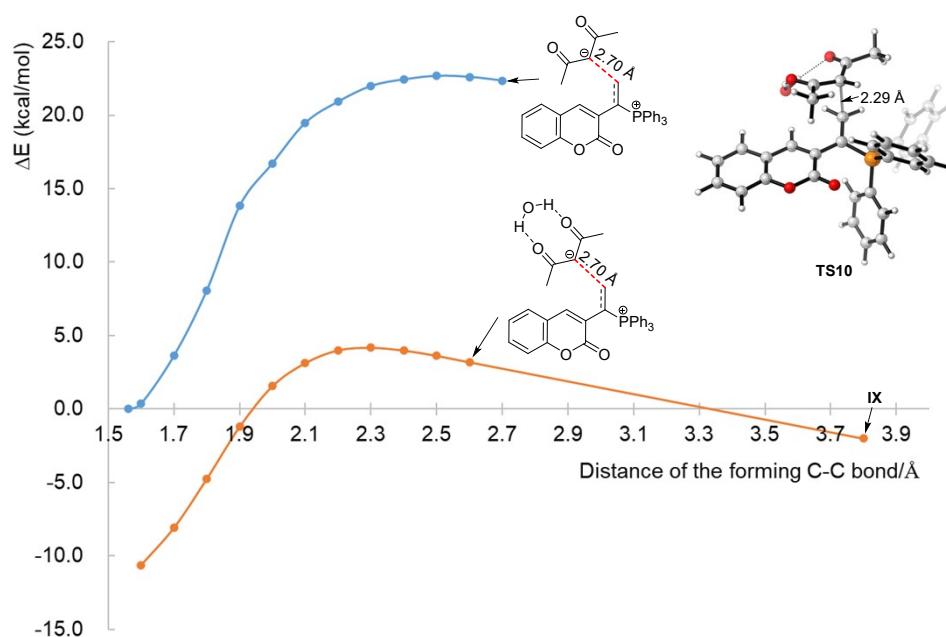


Fig. S5. Energy profile when scanning the forming C-C bond from **IX** to **X**

The conversion of **IX** to **X** was driven by the favorable electrostatic interaction between dicarbonyl anion and vinyl phosphonium. It is nearly a barrier-less process when the coordinated water is released (blue line in Fig. S5), while there is a low barrier when approaching the dicarbonyl anion—water complex to the vinyl phosphonium (orange line in Fig. S5). After extensive efforts, the corresponding transition state **TS10** was successfully optimized, with a free energy barrier about 6.1 kcal/mol. And the forming C—C bond is 2.29 Å in length.

7. Tables of energies and other thermodynamic parameters.

Table S1

	E_{ele}	$E_{\text{ele}}(\text{SP})$	ZPE	H	G(T)	$q_{\text{h}}G(\text{T})$
2a_enol	-345.83634	-345.93782	0.12325	-345.70422	-345.74418	-345.74269
2a_keto	-345.83226	-345.93229	0.12243	-345.70057	-345.74037	-345.73931
1a	-649.65560	-649.82307	0.16123	-649.48096	-649.53241	-649.53013
PPh₃	-1036.41021	-1036.59399	0.27426	-1036.11915	-1036.17905	-1036.17515
3a	-919.12020	-919.35560	0.26579	-918.83616	-918.89634	-918.89428
H₂O	-76.42315	-76.46360	0.02109	-76.39828	-76.41735	-76.41735
TS1	-995.46323	-995.73211	0.28203	-995.15832	-995.23354	-995.22751
I	-995.50205	-995.76892	0.28862	-995.19051	-995.26625	-995.25968
TS2	-1071.89893	-1072.20157	0.31145	-1071.56395	-1071.63797	-1071.63335
II	-995.49608	-995.76364	0.29054	-995.18372	-995.25341	-995.24939
TS3	-995.46294	-995.73028	0.28639	-995.15492	-995.22333	-995.22013
III	-919.05595	-919.29383	0.25997	-918.77425	-918.84708	-918.84116
IV	-1686.08151	-1686.43057	0.43669	-1685.61263	-1685.71181	-1685.70065
TS4	-2031.90184	-2032.34959	0.55802	-2031.30344	-2031.41971	-2031.40736
V	-2031.90886	-2032.35755	0.56344	-2031.30505	-2031.42094	-2031.40894
TS6	-1686.06443	-1686.41551	0.43718	-1685.59683	-1685.68749	-1685.68005
VI	-1686.07392	-1686.42395	0.43905	-1685.60468	-1685.69377	-1685.68720
TS7	-1686.05515	-1686.40543	0.43833	-1685.58764	-1685.67483	-1685.66823
VII	-1686.08438	-1686.43183	0.44178	-1685.61379	-1685.69903	-1685.69328
TS8	-1686.06155	-1686.41248	0.43623	-1685.59730	-1685.68129	-1685.67524
VIII	-1686.11365	-1686.46385	0.44219	-1685.64279	-1685.72787	-1685.72188
TS9	-2031.95570	-2032.40462	0.56523	-2031.35321	-2031.45698	-2031.44903
IX	-2031.97021	-2032.42363	0.56521	-2031.36563	-2031.47540	-2031.46597
TS10	-2031.96035	-2032.41379	0.56490	-2031.35669	-2031.46589	-2031.45619
X	-1955.54385	-1955.95982	0.54170	-1954.96621	-1955.06900	-1955.06011
TS12	-2301.38239	-2301.89163	0.66190	-2300.67537	-2300.79862	-2300.78714
XII	-2301.40663	-2301.91713	0.66758	-2300.69375	-2300.81643	-2300.80582
TS13	-2301.38029	-2301.89293	0.66284	-2300.67303	-2300.79219	-2300.78276
XIII	-1955.53653	-1955.95548	0.54255	-1954.95847	-1955.06009	-1955.05153
TS14	-1955.52559	-1955.94586	0.54236	-1954.94869	-1955.04714	-1955.03956
XIV	-1955.53259	-1955.95356	0.54332	-1954.95434	-1955.05325	-1955.04570
TS15	-1955.52852	-1955.94613	0.54236	-1954.95144	-1955.05027	-1955.04251
TS16	-2031.930729	-2032.380541	0.562057	-2031.3317	-2031.4347	-2031.42695
XV	-1955.543778	-1955.960929	0.543421	-1954.96548	-1955.0643	-1955.05679
TS17	-1955.529303	-1955.945777	0.538031	-1954.95624	-1955.05654	-1955.04805
TS18	-2031.948252	-2032.396627	0.565005	-2031.34652	-2031.4485	-2031.44105
XVI	-2031.978745	-2032.424127	0.569054	-2031.37219	-2031.47757	-2031.46865
TS19	-2031.956292	-2032.405616	0.563975	-2031.35531	-2031.45826	-2031.45046
VI'	-1686.07064	-1686.42224	0.43846	-1685.60182	-1685.69207	-1685.68476
TS7'	-1686.06803	-1686.41818	0.43890	-1685.60003	-1685.68615	-1685.68008
VII'	-1686.12207	-1686.46439	0.44293	-1685.65095	-1685.73427	-1685.72875

XI	-2031.97421	-2032.41366	0.56700	-2031.36892	-2031.47711	-2031.46726
TS20	-2031.96309	-2032.40666	0.56212	-2031.36299	-2031.47050	-2031.46089
XVII	-2031.96515	-2032.41073	0.56655	-2031.36036	-2031.46836	-2031.45889
TS11	-2031.92793	-2032.37401	0.56257	-2031.32834	-2031.43072	-2031.42328
VIII'	-1686.08806	-1686.44319	0.44145	-1685.61794	-1685.70219	-1685.69668
TS21	-1686.08892	-1686.44211	0.44072	-1685.61990	-1685.70417	-1685.69845

Notes: E_{elec} , ZPE, H, G(T), and ${}_{\text{qh}}G(T)$ were the electronic energies, zero-point energies, sum of electronic and thermal enthalpies, sum of electronic and thermal free energies, and sum of electronic and thermal free energies using Grimme's quasiharmonic approximation, respectively, which were given at the B3LYP-D3(BJ)/6-31+G(d) level. $E_{\text{elec}}(\text{SP})$ were electronic energies with solvent correction at the SMD(1,4-dioxane)-B3LYP-D3(BJ)/6-311++G(d,p) level.

8. Coordinates of all stationary points.

1a				H	1.974630	-0.333984	-0.586247
C	-1.254579	-1.642064	-0.455518	H	1.812152	0.603229	-2.113923
C	-0.803312	-0.337582	-0.275290	H	1.159924	-1.056113	-1.972156
C	-1.691303	0.717909	-0.023375	C	0.005904	0.438973	-0.960764
C	-3.065907	0.434834	0.044758	C	-0.688534	-0.351891	0.155829
C	-3.531342	-0.863354	-0.127695	H	-0.435887	-1.413711	0.095867
C	-2.622657	-1.900270	-0.376993	H	-1.767224	-0.201937	0.061919
H	-0.544521	-2.438609	-0.645647	C	-0.176440	0.189363	1.497233
H	-3.744738	1.259766	0.237217	C	-0.940780	1.352334	2.082347
H	-4.595076	-1.073983	-0.070480	H	-1.938180	1.015137	2.394108
H	-2.980641	-2.916846	-0.512819	H	-0.408780	1.762452	2.943140
O	-1.952494	3.050927	0.388104	H	-1.091286	2.124324	1.317776
O	0.550242	-0.026929	-0.422489	O	-0.483281	1.469794	-1.385937
C	1.463588	-0.628031	0.409708	O	0.817743	-0.283941	2.017095
C	2.792307	-0.185620	0.088647				
C	3.934097	0.156626	-0.127778	3a			
O	1.174689	-1.408258	1.287427	C	-3.364228	-1.000235	0.004590
C	5.306829	0.566653	-0.389822	C	-2.284030	-0.140470	-0.183953
H	5.339727	1.444237	-1.045139	C	-0.982930	-0.621374	-0.365972
H	5.822864	0.812606	0.545540	C	-0.790116	-2.006870	-0.368522
H	5.861985	-0.244447	-0.875989	C	-1.859593	-2.881469	-0.178364
C	-1.211410	2.106239	0.171140	C	-3.149468	-2.377017	0.009116
H	-0.118809	2.254209	0.109814	H	-4.352389	-0.575041	0.146951
				H	0.210514	-2.403669	-0.503175
2a_enol				H	-1.683961	-3.953200	-0.174175
C	-0.368443	0.108939	-2.620557	H	-3.987517	-3.051500	0.159094
H	0.516027	-0.474146	-2.903546	C	0.108377	0.387521	-0.630262
H	-0.468643	0.973076	-3.280491	H	0.232677	0.442968	-1.725144
H	-1.241968	-0.543794	-2.745568	C	-0.273601	1.767359	-0.146901
C	-0.270788	0.568958	-1.183398	C	-1.676927	2.212477	-0.116290
C	0.002068	-0.413289	-0.159915	O	-2.611456	1.216603	-0.204879
H	0.140615	-1.452343	-0.435955	O	-2.047399	3.359975	-0.016575
C	0.087711	-0.052818	1.162232	C	1.540436	0.192773	-0.010375
C	0.364168	-1.009313	2.278236	C	0.781722	2.478122	0.259673
H	0.489447	-2.029514	1.908327	H	0.739904	3.500430	0.619581
H	1.272039	-0.704955	2.812302	C	2.050737	1.672419	0.171493
H	-0.460507	-0.985964	3.000393	H	2.679329	1.781132	1.063827
O	-0.435088	1.778612	-0.905380	H	2.665296	2.002900	-0.675568
O	-0.070984	1.205054	1.563967	C	1.487604	-0.379298	1.425708
H	-0.249824	1.747500	0.733844	C	2.387142	-0.673979	-0.948623
				C	3.013695	-0.036818	-2.172739
2a_keto				H	3.959305	0.443666	-1.888716
C	1.327540	-0.108791	-1.442830	H	3.231263	-0.815299	-2.906848

H	2.378785	0.734741	-2.619845	C	-0.133054	4.082427	-1.924480
C	2.778424	-0.898804	2.027231	H	-1.540968	4.471869	-0.334077
H	2.762168	-0.731405	3.106880	H	1.298602	3.393688	-3.384428
H	2.839562	-1.975128	1.834669	H	-0.186249	5.089183	-2.330312
H	3.669037	-0.440686	1.585113				
O	0.464113	-0.329064	2.077589	I			
O	2.519019	-1.868124	-0.736419	C	-1.973697	-1.343342	3.863429
				C	-1.672935	-1.581923	2.525217
H₂O				C	-1.078462	-0.610584	1.708681
O	-0.796527	1.717580	0.000000	C	-0.775410	0.628014	2.282730
H	0.171805	1.751364	0.000000	C	-1.080215	0.892190	3.619395
H	-1.087917	2.641648	0.000000	C	-1.680629	-0.091150	4.406743
				H	-2.433165	-2.117517	4.463801
PPh₃				H	-0.277746	1.371701	1.671288
P	0.019981	-0.207029	-0.110269	H	-0.839605	1.861968	4.045482
C	1.457417	-0.988969	-0.969545	H	-1.917563	0.106649	5.448102
C	2.728068	-0.788033	-0.405601	C	-0.748045	-0.912471	0.259450
C	1.350741	-1.764315	-2.133155	H	-0.210329	-1.872045	0.225598
C	3.867851	-1.329053	-1.002003	O	-1.858091	-2.837174	1.929770
H	2.823185	-0.201056	0.505337	C	-3.015208	-3.547506	2.099777
C	2.490215	-2.317892	-2.723470	C	-2.981679	-4.731733	1.279350
H	0.376798	-1.935772	-2.580787	H	-3.937120	-6.911916	-0.892281
C	3.751035	-2.098571	-2.163493	C	-3.027253	-5.737098	0.604626
H	4.844179	-1.158550	-0.555764	C	-3.081982	-6.946252	-0.206866
H	2.391137	-2.918121	-3.624433	H	-3.200380	-7.831169	0.429446
H	4.636068	-2.528637	-2.624841	H	-2.168769	-7.070186	-0.799822
C	-1.403332	-1.009689	-0.973951	C	-2.032060	-1.124420	-0.594585
C	-2.056611	-0.462471	-2.087661	H	-2.590109	-1.960980	-0.171328
C	-1.848983	-2.241455	-0.466952	C	-3.051169	0.039769	-0.626124
C	-3.124999	-1.136729	-2.685285	C	-1.695975	-1.498603	-2.040394
H	-1.730564	0.491310	-2.490546	C	-2.559035	1.449031	-0.834743
C	-2.906914	-2.921933	-1.071400	H	-1.933922	1.759300	0.006976
H	-1.360748	-2.669918	0.405652	H	-1.924297	1.506226	-1.725966
C	-3.550036	-2.368935	-2.182868	H	-3.417810	2.116165	-0.934538
H	-3.622521	-0.698809	-3.546979	O	-3.932781	-3.226171	2.818504
H	-3.235050	-3.877157	-0.669792	O	0.085004	0.116608	-0.244969
H	-4.380114	-2.892377	-2.649841	O	-4.236215	-0.225294	-0.531173
C	0.009286	1.476010	-0.874000	O	-0.682564	-1.087076	-2.592044
C	-0.814325	2.445341	-0.278251	H	0.227624	-0.093787	-1.187783
C	0.770169	1.834567	-1.996102	C	-2.682651	-2.396676	-2.740595
C	-0.893888	3.735689	-0.803910	H	-3.707078	-2.046368	-2.569419
H	-1.398422	2.184628	0.601658	H	-2.461651	-2.448992	-3.808593
C	0.701366	3.130379	-2.515061	H	-2.617992	-3.401741	-2.302163
H	1.417011	1.100967	-2.467033				

II				C	-1.906737	1.584180	-0.530727
C	-2.597436	0.811483	2.552012	C	-2.390967	1.941001	0.729970
C	-2.132802	-0.444398	2.169978	H	-2.702034	1.271925	2.773837
C	-1.550222	-0.672128	0.916521	H	-0.963303	0.052881	-1.717500
C	-1.475934	0.424171	0.045715	H	-1.951679	2.292629	-1.352509
C	-1.939339	1.688047	0.404855	H	-2.820748	2.924709	0.894742
C	-2.501750	1.884653	1.668069	C	-0.672877	-1.944734	0.159711
H	-3.022110	0.928924	3.543815	H	-0.053219	-2.258596	0.997109
H	-1.037367	0.271061	-0.937081	O	-1.673771	-1.109678	2.640754
H	-1.857953	2.514387	-0.295075	C	-2.531767	-2.178969	2.652034
H	-2.862465	2.864567	1.966360	C	-2.256372	-3.037666	3.771398
C	-1.067739	-2.021533	0.395740	C	-2.068463	-3.805121	4.689804
H	-0.367216	-1.808794	-0.420647	C	-1.849014	-4.725805	5.796935
O	-2.175652	-1.429166	3.166552	H	-1.876728	-5.765110	5.449451
C	-2.945339	-2.530894	2.983602	C	-0.864787	-2.817289	-0.849888
C	-2.765735	-3.463176	4.053545	C	-0.254300	-4.175850	-0.851949
C	-2.579132	-4.290213	4.917953	C	-1.805534	-2.537702	-2.006559
C	-2.331281	-5.275980	5.958907	C	0.745010	-4.553664	0.226160
H	-1.263589	-5.309689	6.205231	H	1.116576	-5.558027	0.014514
C	-0.389260	-2.950039	1.412984	H	1.585993	-3.851878	0.256091
H	-2.952716	-2.600941	0.329941	H	0.271610	-4.549103	1.215631
C	-0.528977	-4.318020	1.354340	O	-3.393655	-2.366561	1.822677
C	0.580168	-2.373722	2.365071	O	-0.577747	-4.979782	-1.719084
C	0.137200	-5.316464	2.255074	O	-1.418836	-1.931264	-2.989704
H	0.065967	-6.301741	1.786722	C	-3.215398	-3.036969	-1.833163
H	1.177845	-5.058472	2.458123	H	-3.822340	-2.760095	-2.698264
H	-0.368031	-5.341532	3.225896	H	-3.198631	-4.127519	-1.719526
O	-3.691510	-2.692113	2.031762	H	-3.642247	-2.621394	-0.911507
O	-2.187108	-2.648673	-0.282194	H	-0.880473	-4.545741	6.276762
O	-1.285500	-4.942386	0.434996	H	-2.632894	-4.604755	6.554114
O	0.926130	-2.948416	3.398325	IV			
H	-1.757348	-4.250862	-0.097419	C	-3.491457	-0.941606	-2.688237
C	1.225020	-1.028091	2.044130	C	-3.130007	-0.615944	-1.383310
H	0.681627	-0.220178	2.546297	C	-3.450311	0.630208	-0.823159
H	2.241690	-1.046555	2.445629	C	-4.158839	1.553382	-1.605301
H	1.255802	-0.797368	0.975060	C	-4.543031	1.237833	-2.904357
H	-2.880663	-5.016324	6.871759	C	-4.207158	-0.009234	-3.442187
H	-2.649754	-6.275251	5.641418	H	-3.225618	-1.905558	-3.103407
III				H	-4.385728	2.519527	-1.165981
C	-2.325056	1.028424	1.785745	H	-5.091018	1.960325	-3.501669
C	-1.770778	-0.222498	1.559182	H	-4.497024	-0.261369	-4.458397
C	-1.274492	-0.612921	0.304618	O	-3.263377	2.087477	1.054473
C	-1.355232	0.320651	-0.743367	O	-2.332978	-1.458260	-0.610720

C	-2.599651	-2.796776	-0.511165				
C	-1.587807	-3.427690	0.294846	V			
C	-0.744207	-3.986155	0.960795	C	-3.413088	-1.539428	-2.628803
O	-3.543788	-3.357649	-1.018578	C	-2.723741	-0.929670	-1.582812
C	0.279183	-4.644883	1.760703	C	-2.743427	0.460027	-1.384297
H	1.195828	-4.044744	1.796756	C	-3.528146	1.237373	-2.246097
H	-0.072536	-4.788371	2.789352	C	-4.236989	0.639771	-3.289121
H	0.524174	-5.630491	1.348376	C	-4.169995	-0.740552	-3.487707
C	-3.044859	0.992273	0.558617	H	-3.376401	-2.613104	-2.754119
H	-2.546757	0.200325	1.139426	H	-3.580647	2.311936	-2.089671
P	-0.033309	1.231495	-0.613624	H	-4.843423	1.258042	-3.945143
C	1.127952	0.029288	-1.391534	H	-4.716780	-1.206892	-4.302525
C	1.143356	-1.274083	-0.870933	O	-2.545097	2.131762	0.432603
C	1.966881	0.337062	-2.473298	O	-1.914630	-1.650019	-0.697532
C	1.990269	-2.245400	-1.407474	C	-2.246003	-2.880895	-0.213178
H	0.474548	-1.531174	-0.055087	C	-1.230490	-3.312895	0.715787
C	2.811322	-0.635650	-3.013487	C	-0.412110	-3.707109	1.517414
H	1.954188	1.337001	-2.896906	O	-3.233114	-3.515113	-0.506934
C	2.827244	-1.928176	-2.480866	C	0.565956	-4.185637	2.485755
H	1.982890	-3.253284	-0.999931	H	1.415865	-3.498445	2.567543
H	3.455973	-0.384256	-3.851945	H	0.107639	-4.279996	3.477333
H	3.481004	-2.685051	-2.906291	H	0.945863	-5.173029	2.198032
C	-0.233681	2.475862	-1.958747	C	-1.953812	1.088193	-0.248080
C	0.305209	3.769042	-1.916234	H	-1.716746	0.312005	0.486590
C	-1.023454	2.107207	-3.061238	P	-0.217200	1.620192	-0.851005
C	0.066386	4.670889	-2.957710	C	0.646068	0.226172	-1.637581
H	0.913531	4.074091	-1.070643	C	0.879872	-0.921614	-0.863080
C	-1.252040	3.002921	-4.104405	C	1.116472	0.277619	-2.956581
H	-1.459640	1.113058	-3.104634	C	1.547649	-2.012793	-1.411984
C	-0.708858	4.290847	-4.055259	H	0.537770	-0.967801	0.164869
H	0.490994	5.670505	-2.910047	C	1.789728	-0.818169	-3.501253
H	-1.863608	2.698505	-4.949890	H	0.973082	1.169936	-3.554540
H	-0.893131	4.993029	-4.864042	C	2.000636	-1.965056	-2.733853
C	1.031876	2.123338	0.594773	H	1.705388	-2.901710	-0.808636
C	0.372029	2.882626	1.576551	H	2.151019	-0.770161	-4.524521
C	2.433291	2.081262	0.593231	H	2.520839	-2.817751	-3.161401
C	1.103035	3.603960	2.522324	C	-0.328615	3.000320	-1.999444
H	-0.715229	2.908783	1.597667	C	0.085097	4.270958	-1.577783
C	3.162753	2.793187	1.548826	C	-0.908626	2.826748	-3.267939
H	2.955614	1.491624	-0.154025	C	-0.080189	5.363951	-2.427084
C	2.500348	3.559541	2.511582	H	0.475748	4.415151	-0.578538
H	0.580627	4.192454	3.272001	C	-1.061538	3.924967	-4.109946
H	4.249070	2.751269	1.538437	H	-1.262811	1.853233	-3.587129
H	3.069479	4.114624	3.252724	C	-0.648730	5.192544	-3.689934

H	0.210768	6.352055	-2.086381	O	-1.508855	2.626690	-2.080935
H	-1.518518	3.792586	-5.086539	O	-0.700899	-1.119946	-0.496198
H	-0.787358	6.050433	-4.342183	C	0.472256	-0.599235	0.104844
C	0.785899	2.056873	0.589574	C	1.525549	-1.512340	0.069404
C	0.190349	2.531145	1.766793	C	2.647357	-1.763522	-0.586144
C	2.184204	1.929649	0.499996	O	0.448355	0.494922	0.677961
C	1.001774	2.861096	2.854798	C	3.675782	-2.811486	-0.208397
H	-0.880770	2.679581	1.810680	H	3.888150	-3.507068	-1.029783
C	2.981138	2.270290	1.589703	H	4.631696	-2.361863	0.094378
H	2.645044	1.562635	-0.412082	H	3.284066	-3.376780	0.640987
C	2.388133	2.732960	2.770508	P	3.101114	-0.707835	-2.021828
H	0.539503	3.241488	3.760591	C	4.315924	-1.492276	-3.129179
H	4.061029	2.174638	1.518682	C	5.638215	-1.677493	-2.690536
H	3.011700	3.000283	3.619609	C	3.930884	-1.986371	-4.383914
C	-1.368249	7.143285	1.618422	C	6.558841	-2.342394	-3.497500
H	-1.792658	8.103316	1.306366	H	5.949622	-1.296521	-1.722418
H	-0.273439	7.213760	1.609403	C	4.856657	-2.655479	-5.187644
H	-1.668958	6.943862	2.654309	H	2.914423	-1.843922	-4.735690
C	-1.807258	5.969476	0.739446	C	6.169389	-2.834904	-4.747625
C	-2.714918	6.256683	-0.321294	H	7.579501	-2.477133	-3.150766
H	-2.995923	7.295920	-0.461425	H	4.549928	-3.031656	-6.159539
C	-3.283131	5.326386	-1.206561	H	6.888131	-3.354452	-5.375039
C	-4.168236	5.859431	-2.326962	C	1.640724	-0.337502	-3.024358
H	-4.269036	6.949193	-2.314760	C	1.545985	0.888627	-3.701286
H	-3.745199	5.551773	-3.291541	C	0.637478	-1.304668	-3.177605
H	-5.164543	5.406923	-2.250948	C	0.451080	1.144098	-4.525301
O	-1.321703	4.846229	1.002467	H	2.308324	1.648674	-3.563814
O	-3.139564	4.063218	-1.191615	C	-0.457222	-1.039450	-4.000423
H	-2.698165	2.971641	-0.121981	H	0.693946	-2.238618	-2.629893
				C	-0.550216	0.180830	-4.674103
				H	0.362312	2.105566	-5.020785
				H	-1.246989	-1.778716	-4.095028
				H	-1.415342	0.392559	-5.295779
				C	3.820110	0.874942	-1.495206
				C	3.291615	1.515183	-0.362714
				C	4.836644	1.492046	-2.243106
				C	3.791880	2.762089	0.016258
				H	2.480176	1.070225	0.207359
				C	5.331703	2.735776	-1.850817
				H	5.239846	1.007698	-3.126511
				C	4.810993	3.371106	-0.719651
				H	3.374096	3.255983	0.888628
				H	6.119869	3.207941	-2.430760
				H	5.196473	4.340796	-0.416591
VI							
C	-2.847210	-1.215980	0.495155				
C	-1.907143	-0.498365	-0.246045				
C	-2.227773	0.765977	-0.771459				
C	-3.506770	1.294300	-0.529137				
C	-4.446070	0.584478	0.209817				
C	-4.113029	-0.677310	0.720327				
H	-2.565590	-2.188094	0.887476				
H	-3.734307	2.273804	-0.938953				
H	-5.431202	1.004849	0.390986				
H	-4.840280	-1.240324	1.299478				
C	-1.264329	1.534749	-1.586424				
H	-0.287995	1.062410	-1.751874				

				H	0.543050	-4.296417	2.014249
VII				H	2.478520	-1.348265	4.483123
C	-5.273612	-0.376338	1.096800	H	1.627618	-3.662568	4.162669
C	-4.092278	0.013706	0.477268	C	2.630305	-0.295650	-1.161889
C	-3.987248	0.161905	-0.905767	C	3.028202	0.645582	-2.125303
C	-5.115887	-0.102670	-1.681549	C	3.321397	-1.509588	-1.059642
C	-6.318748	-0.496748	-1.086774	C	4.092857	0.368829	-2.980421
C	-6.395669	-0.630042	0.302412	H	2.507669	1.595613	-2.201876
H	-5.303718	-0.475709	2.177431	C	4.390737	-1.782758	-1.917035
H	-5.050023	0.016640	-2.760844	H	3.035442	-2.239447	-0.310103
H	-7.191957	-0.693353	-1.702698	C	4.776001	-0.847482	-2.878657
H	-7.327350	-0.932356	0.772509	H	4.391961	1.103444	-3.722689
C	-2.678446	0.679009	-1.450599	H	4.923132	-2.725527	-1.827238
H	-2.597418	0.445401	-2.525167	H	5.608404	-1.060965	-3.543475
C	-1.516409	0.173780	-0.630058				
O	-3.004229	0.259155	1.311570	VIII			
O	-2.423655	1.989261	-1.117294	C	-4.695950	-1.610037	-1.657197
C	-1.747076	0.381610	0.824613	C	-3.729348	-1.512424	-0.650324
O	-0.839918	0.562229	1.621153	C	-3.454310	-0.294474	-0.022047
C	-0.271881	-0.151219	-1.105257	C	-4.170622	0.838509	-0.433332
C	-0.056751	-0.493312	-2.567502	C	-5.132426	0.761534	-1.437246
H	0.216589	0.385977	-3.167148	C	-5.396074	-0.472503	-2.047648
H	0.734339	-1.236015	-2.703801	H	-4.875194	-2.577289	-2.116374
H	-0.974668	-0.909534	-2.987774	H	-3.971008	1.783637	0.065191
P	1.191981	0.095128	-0.098272	H	-5.676982	1.650914	-1.741491
C	1.488249	1.829108	0.351571	H	-6.145935	-0.546227	-2.830756
C	2.738059	2.203595	0.870021	C	-2.448127	-0.212888	1.096118
C	0.509549	2.797119	0.084224	H	-1.791358	0.654839	0.943198
C	2.996574	3.542702	1.159890	C	-1.638478	-1.463112	1.193383
H	3.515340	1.460291	1.024625	O	-3.073488	-2.675023	-0.327555
C	0.787293	4.136746	0.366291	O	-3.108380	0.144529	2.350683
H	-0.455585	2.528142	-0.343756	C	-1.985802	-2.648690	0.530890
C	2.017925	4.510195	0.910706	O	-1.367559	-3.729424	0.632523
H	3.961904	3.829897	1.567520	C	-0.424848	-1.440139	1.973793
H	0.028522	4.885734	0.159089	C	-0.044999	-0.441187	2.817894
H	2.220539	5.554629	1.132485	H	0.929098	-0.403589	3.285446
C	1.322621	-1.060744	1.299842	H	-0.744606	0.353771	3.052747
C	0.823373	-2.357947	1.123996	H	-3.648682	-0.620597	2.610626
C	1.916888	-0.697567	2.512488	P	0.770183	-2.804602	1.728752
C	0.937585	-3.293701	2.152760	C	0.435160	-4.314612	2.677033
H	0.327983	-2.626388	0.194820	C	1.447906	-5.271147	2.830655
C	2.027900	-1.637249	3.537846	C	-0.801299	-4.493650	3.308067
H	2.258884	0.318740	2.672528	C	1.212803	-6.418401	3.590351
C	1.544547	-2.936025	3.359226	H	2.422134	-5.117465	2.375638

C	-1.021169	-5.629049	4.086618	O	-0.853755	2.211880	4.240481
H	-1.583291	-3.754353	3.180940	C	-1.917280	-2.509037	0.077903
C	-0.020711	-6.596224	4.221146	O	-1.334254	-3.575087	0.209447
H	1.996204	-7.163394	3.697338	C	-0.178815	-1.198773	1.376397
H	-1.980145	-5.763888	4.578562	C	0.149631	-0.130414	2.138581
H	-0.201168	-7.484943	4.819670	H	1.089316	-0.049867	2.661155
C	1.137716	-3.049244	-0.026922	H	-0.516998	0.713458	2.253583
C	1.099168	-1.926578	-0.864542	H	-1.660187	1.846802	3.822016
C	1.467279	-4.305916	-0.545411	P	0.961141	-2.603061	1.416135
C	1.399000	-2.065925	-2.221296	C	0.434973	-3.975090	2.476527
H	0.820874	-0.956342	-0.464113	C	1.370952	-4.972251	2.793397
C	1.772252	-4.435144	-1.899463	C	-0.848775	-4.014644	3.028103
H	1.452130	-5.182470	0.093196	C	1.005080	-6.026619	3.629160
C	1.739890	-3.317066	-2.738799	H	2.384772	-4.917674	2.406578
H	1.357061	-1.196901	-2.871864	C	-1.201559	-5.063004	3.876652
H	2.018468	-5.413189	-2.303122	H	-1.560108	-3.221342	2.835092
H	1.968987	-3.424200	-3.795417	C	-0.284061	-6.073849	4.168777
C	2.362895	-2.256325	2.459261	H	1.729030	-6.800193	3.868777
C	2.548084	-2.345644	3.849325	H	-2.194264	-5.078055	4.316262
C	3.392549	-1.733790	1.664982	H	-0.565800	-6.889851	4.828498
C	3.736671	-1.908251	4.432333	C	1.379402	-3.120326	-0.268973
H	1.762961	-2.758052	4.475273	C	1.565970	-2.116918	-1.229800
C	4.584367	-1.302003	2.251159	C	1.528393	-4.466578	-0.618664
H	3.271225	-1.668216	0.589480	C	1.913551	-2.463312	-2.536362
C	4.758105	-1.385369	3.634021	H	1.431952	-1.072794	-0.960105
H	3.865586	-1.979304	5.508722	C	1.879421	-4.805414	-1.925105
H	5.376644	-0.903107	1.623835	H	1.341063	-5.244742	0.113043
H	5.686102	-1.049061	4.088204	C	2.074520	-3.806860	-2.883655
				H	2.052711	-1.684376	-3.280560
				H	1.986307	-5.851355	-2.197869
				H	2.341450	-4.076167	-3.901700
				C	2.521017	-2.067143	2.190754
				C	2.527350	-1.794501	3.570835
				C	3.707873	-1.969623	1.452279
				C	3.714213	-1.413446	4.193342
				H	1.606179	-1.832578	4.146696
				C	4.894682	-1.597367	2.088327
				H	3.713715	-2.188336	0.390109
				C	4.898904	-1.318131	3.456133
				H	3.708008	-1.184525	5.254908
				H	5.812742	-1.526323	1.511925
				H	5.822253	-1.024144	3.947586
				C	-1.006997	-2.304577	6.078649
				H	-1.844962	-2.963264	6.326577
IX							
C	-5.084965	-1.556217	-1.462184				
C	-3.867491	-1.407440	-0.801028				
C	-3.422002	-0.160574	-0.333882				
C	-4.245950	0.964165	-0.539008				
C	-5.462540	0.831544	-1.192785				
C	-5.879550	-0.428772	-1.655103				
H	-5.389587	-2.539742	-1.804531				
H	-3.920035	1.925396	-0.152825				
H	-6.097607	1.699659	-1.340302				
H	-6.833640	-0.529765	-2.164204				
C	-2.166872	-0.105775	0.351455				
H	-1.818975	0.861873	0.687295				
C	-1.431184	-1.234742	0.589363				
O	-3.105131	-2.528812	-0.610118				

H	-0.723347	-1.742426	6.976659	H	1.531654	-7.544263	3.678314
H	-0.146190	-2.919868	5.792525	H	-2.518236	-6.162727	4.159509
C	-1.324194	-1.309193	4.962393	H	-0.779385	-7.904140	4.529966
C	-2.646970	-1.316771	4.452686	C	1.106049	-3.412101	0.068581
H	-3.302637	-2.071283	4.877625	C	1.243294	-2.313576	-0.790716
C	-3.256991	-0.445693	3.509182	C	1.391841	-4.698641	-0.401006
C	-4.697458	-0.766667	3.110974	C	1.688428	-2.498171	-2.100697
H	-5.132479	-1.595832	3.677519	H	0.980263	-1.320794	-0.435200
H	-5.315689	0.128045	3.245724	C	1.835722	-4.879782	-1.711539
H	-4.728722	-1.016085	2.043314	H	1.241532	-5.561161	0.238240
O	-0.361814	-0.580494	4.589579	C	1.990335	-3.781703	-2.562039
O	-2.740640	0.560958	2.955629	H	1.788374	-1.641210	-2.761266
H	-0.465400	1.387795	4.591678	H	2.048132	-5.882534	-2.072314
				H	2.330903	-3.927689	-3.583478
X				C	2.072356	-2.621580	2.686408
C	-5.230835	-1.548025	-1.230388	C	2.118569	-2.786807	4.079675
C	-4.095330	-1.510808	-0.428303	C	3.172571	-2.055714	2.030272
C	-3.737842	-0.387525	0.336846	C	3.234406	-2.371922	4.804547
C	-4.595164	0.734442	0.273152	H	1.282663	-3.245985	4.598421
C	-5.734774	0.714728	-0.520920	C	4.292684	-1.646229	2.757421
C	-6.056352	-0.424868	-1.277154	H	3.158618	-1.931004	0.952959
H	-5.450636	-2.446291	-1.798948	C	4.323539	-1.796702	4.144624
H	-4.344685	1.614533	0.859791	H	3.253112	-2.496078	5.883785
H	-6.381257	1.587146	-0.556942	H	5.138314	-1.205380	2.237012
H	-6.947408	-0.436439	-1.897743	H	5.191106	-1.468129	4.709844
C	-2.545828	-0.440808	1.123429	C	-0.241745	0.539311	6.587886
H	-2.299951	0.439245	1.704801	H	-1.061828	1.266555	6.614867
C	-1.736471	-1.565077	1.161067	H	0.578873	0.906681	7.208398
O	-3.304574	-2.638436	-0.390327	H	-0.626906	-0.405705	6.989418
C	-2.183898	-2.728258	0.373822	C	0.223695	0.387636	5.153893
O	-1.597789	-3.803793	0.379640	C	-0.605828	-0.543053	4.255590
C	-0.527409	-1.697474	1.924483	H	-0.475630	-1.557756	4.657207
C	-0.081892	-0.537212	2.788280	C	-2.088503	-0.186119	4.323841
H	1.002772	-0.484925	2.869097	C	-3.067812	-1.333036	4.394303
H	-0.371374	0.415527	2.330189	H	-2.812874	-2.084973	3.640933
P	0.541824	-3.064376	1.774691	H	-2.985006	-1.818169	5.377176
C	0.099362	-4.644700	2.598572	H	-4.088998	-0.975785	4.247909
C	1.081673	-5.620114	2.824757	O	1.220757	0.952837	4.746130
C	-1.193524	-4.846584	3.090450	O	-2.447112	0.982164	4.313432
C	0.764262	-6.793304	3.511195				
H	2.100657	-5.456966	2.485689	XII			
C	-1.509014	-6.014916	3.785047	C	-5.982000	-0.955000	0.099882
H	-1.950679	-4.089726	2.924924	C	-4.615880	-0.905553	0.376047
C	-0.532747	-6.993057	3.991615	C	-4.062601	0.095609	1.189989

C	-4.923891	1.066457	1.734539	H	3.218775	-5.999882	-0.674411
C	-6.286177	1.026414	1.473847	H	3.069765	-5.081481	-2.984502
C	-6.812620	0.015196	0.652419	C	-1.857139	-0.862627	0.837308
H	-6.364727	-1.741361	-0.542319	C	0.303905	0.280910	1.654836
H	-4.497524	1.859030	2.343364	H	-0.312265	0.562530	2.513910
H	-6.943127	1.783425	1.891214	H	1.272023	-0.007703	2.060282
H	-7.877463	-0.009542	0.439588	C	0.532435	1.472674	0.703720
C	-2.641857	0.091290	1.398493	C	0.769201	2.748442	1.508796
H	-2.221862	0.893748	1.991143	C	1.688373	1.179943	-0.250752
O	-3.828014	-1.884585	-0.161686	C	-0.469176	3.447572	2.029131
C	-2.465229	-1.878208	-0.018109	H	-0.196184	4.408221	2.471948
O	-1.830522	-2.763068	-0.570513	H	-1.199297	3.567839	1.220741
P	0.350699	-2.559680	1.323292	H	-0.950577	2.829890	2.799860
C	-0.938118	-3.625903	2.021578	C	1.893152	2.158168	-1.374006
C	-1.164335	-4.916526	1.530356	H	2.832256	1.947716	-1.890639
C	-1.746700	-3.114654	3.048340	H	1.050849	2.025114	-2.063966
C	-2.182230	-5.697197	2.077645	H	1.882756	3.190628	-1.011237
H	-0.573041	-5.295378	0.704354	O	1.893329	3.172944	1.728309
C	-2.767578	-3.898113	3.587462	O	2.364394	0.165081	-0.139838
H	-1.590869	-2.106463	3.420112	C	-0.346972	-0.881906	0.881882
C	-2.984020	-5.190797	3.104064	H	-0.051420	-0.773975	-0.170696
H	-2.360478	-6.695141	1.687938	C	-1.629387	-1.167928	-3.548762
H	-3.395266	-3.494831	4.376844	H	-1.600006	-2.142929	-3.045993
H	-3.783051	-5.798365	3.519457	H	-0.748912	-1.099265	-4.198169
C	1.650222	-2.435692	2.597907	H	-2.534954	-1.122531	-4.161793
C	2.892827	-1.890920	2.227559	C	-1.560272	-0.067679	-2.491151
C	1.452899	-2.894238	3.907736	C	-2.744055	0.680848	-2.269822
C	3.915036	-1.794685	3.169501	H	-3.579021	0.441588	-2.921710
H	3.045861	-1.518439	1.220237	C	-2.949030	1.770857	-1.382996
C	2.485398	-2.797440	4.843646	C	-4.271141	2.526532	-1.525430
H	0.508929	-3.339508	4.199940	H	-5.024002	1.972454	-2.095386
C	3.714393	-2.245989	4.477691	H	-4.668623	2.763070	-0.534105
H	4.867374	-1.361022	2.879030	H	-4.080911	3.477717	-2.039942
H	2.326263	-3.158364	5.855871	O	-0.453342	0.071465	-1.898334
H	4.515182	-2.169827	5.208036	O	-2.155833	2.184862	-0.497032
C	1.179890	-3.334461	-0.085260	H	-0.366728	1.624804	0.083982
C	1.099724	-2.808503	-1.380767				
C	1.954910	-4.479274	0.170132				
C	1.787723	-3.444347	-2.415724	XIII			
H	0.528811	-1.912234	-1.602679	C	-5.655031	-0.628797	-0.431418
C	2.624740	-5.112641	-0.874246	C	-4.310601	-0.644399	-0.064360
H	2.044582	-4.866989	1.181264	C	-3.702403	0.446534	0.576103
C	2.540387	-4.593730	-2.170450	C	-4.482854	1.589838	0.840332
H	1.730650	-3.028314	-3.417170	C	-5.823254	1.620324	0.480654
				C	-6.407113	0.509684	-0.152632

H	-6.083532	-1.493917	-0.926670	C	0.404512	0.179574	1.966217
H	-4.014944	2.443946	1.322242	H	-0.333554	0.278913	2.766937
H	-6.420265	2.503911	0.684113	H	1.312683	-0.193921	2.442369
H	-7.455636	0.537746	-0.434493	C	0.681410	1.504219	1.281166
C	-2.314814	0.336257	0.924666	C	0.164766	2.733426	1.817324
H	-1.837482	1.191537	1.382432	C	1.591472	1.445973	0.185435
O	-3.581251	-1.765518	-0.355994	C	-0.506841	2.706045	3.206685
C	-2.242276	-1.875051	-0.069219	H	-0.661863	3.741781	3.517088
O	-1.676897	-2.896100	-0.426561	H	-1.485984	2.205941	3.200160
P	0.477828	-2.600936	1.368999	H	0.110516	2.194034	3.955661
C	-0.801417	-3.505067	2.275105	C	1.988189	2.687638	-0.588139
C	-1.223839	-4.785691	1.901655	H	2.756144	2.405198	-1.314360
C	-1.400640	-2.855542	3.365317	H	1.124224	3.122487	-1.102256
C	-2.228641	-5.421535	2.631028	H	2.355093	3.475177	0.077546
H	-0.794614	-5.267282	1.030290	O	0.239776	3.848541	1.261847
C	-2.409625	-3.494686	4.086559	O	2.114750	0.341840	-0.177821
H	-1.083438	-1.856281	3.650596	C	-0.111190	-0.888152	0.948110
C	-2.820866	-4.779468	3.722180	H	0.474463	-0.686365	0.038407
H	-2.559475	-6.413169	2.336304				
H	-2.873790	-2.987733	4.927536	XIV			
H	-3.608073	-5.276022	4.282481	C	-5.227928	-0.593609	-0.416025
C	1.933460	-2.516026	2.460792	C	-3.869788	-0.558570	-0.076540
C	3.073335	-1.840639	1.986406	C	-3.204809	0.665883	0.078284
C	1.968668	-3.184773	3.689995	C	-3.932235	1.848336	-0.102499
C	4.233257	-1.833781	2.756988	C	-5.281601	1.827096	-0.450176
H	3.030172	-1.285728	1.050586	C	-5.927931	0.594815	-0.607111
C	3.140757	-3.174029	4.452179	H	-5.707058	-1.560822	-0.532478
H	1.094526	-3.713312	4.055169	H	-3.423746	2.801574	0.025578
C	4.270856	-2.500541	3.987270	H	-5.823710	2.756836	-0.596577
H	5.107210	-1.298530	2.397407	H	-6.979864	0.560127	-0.877866
H	3.165250	-3.692802	5.406418	C	-1.760331	0.673229	0.473780
H	5.179923	-2.490881	4.582417	H	-1.649862	1.394622	1.296823
C	1.132882	-3.522711	-0.049174	O	-3.251526	-1.769946	0.057598
C	1.115342	-3.001885	-1.347025	C	-1.892583	-1.867841	0.463043
C	1.758395	-4.753056	0.205672	O	-1.433281	-3.017305	0.426304
C	1.707541	-3.718885	-2.386458	P	0.784437	-0.523979	2.711841
H	0.655320	-2.044256	-1.553966	C	-0.188858	0.766968	3.515581
C	2.328959	-5.474935	-0.841657	C	-1.494610	0.436112	3.916222
H	1.814573	-5.140231	1.219252	C	0.249635	2.098072	3.583113
C	2.304710	-4.956817	-2.139431	C	-2.354964	1.438786	4.363753
H	1.700971	-3.304970	-3.390281	H	-1.838135	-0.590078	3.851803
H	2.803929	-6.430948	-0.640775	C	-0.610402	3.091244	4.051625
H	2.760060	-5.512621	-2.954340	H	1.251812	2.362863	3.261908
C	-1.591764	-0.783756	0.650376	C	-1.915436	2.763397	4.431414

H	-3.370700	1.184474	4.651241				
H	-0.266958	4.120379	4.103658	XV			
H	-2.589527	3.540815	4.779967	C	-5.178954	-1.503715	-1.625598
C	2.548870	-0.101647	2.841809	C	-4.153125	-1.463645	-0.687939
C	3.396853	-0.444881	1.777400	C	-3.943868	-0.371691	0.171787
C	3.089279	0.493959	3.992454	C	-4.841107	0.714748	0.055676
C	4.766074	-0.188512	1.862084	C	-5.873530	0.692158	-0.873496
H	2.995499	-0.910431	0.882918	C	-6.046583	-0.415733	-1.719705
C	4.458061	0.748602	4.071981	H	-5.284147	-2.378365	-2.259959
H	2.445052	0.765573	4.822856	H	-4.706640	1.574263	0.707887
C	5.297632	0.408765	3.007099	H	-6.550998	1.538473	-0.946060
H	5.413977	-0.454708	1.032144	H	-6.854079	-0.430294	-2.445481
H	4.868360	1.212011	4.964762	C	-2.851469	-0.419780	1.091813
H	6.363348	0.609307	3.070634	H	-2.721207	0.434907	1.746778
C	0.517761	-2.060529	3.625901	C	-1.976620	-1.498073	1.152580
C	0.076781	-3.226441	2.987849	O	-3.321162	-2.559125	-0.606788
C	0.796373	-2.065205	5.004913	C	-2.289702	-2.640216	0.272626
C	-0.077226	-4.396076	3.739575	O	-1.661420	-3.691342	0.297322
H	-0.203942	-3.227312	1.935481	C	-0.832616	-1.609169	2.004644
C	0.641382	-3.236653	5.740094	C	-0.395384	-0.391180	2.814080
H	1.122250	-1.157948	5.505378	H	0.665656	-0.221379	2.623630
C	0.206945	-4.406673	5.104898	H	-0.881428	0.491000	2.379757
H	-0.433896	-5.294424	3.244439	P	0.273469	-2.957898	1.939238
H	0.854143	-3.237554	6.805428	C	-0.216647	-4.560002	2.687666
H	0.083477	-5.320139	5.680418	C	0.773656	-5.472633	3.082204
C	-1.262295	-0.687772	0.863628	C	-1.560451	-4.857053	2.938546
C	0.625060	0.723682	0.220672	C	0.420539	-6.672926	3.700673
H	0.861884	1.512717	0.939779	H	1.823031	-5.241442	2.925325
H	1.485916	0.587196	-0.433470	C	-1.911831	-6.051573	3.567923
C	-0.636105	1.112883	-0.582402	H	-2.329256	-4.159157	2.634585
C	-0.685218	2.587455	-0.949372	C	-0.923678	-6.963901	3.946069
C	-0.678469	0.257684	-1.876281	H	1.196085	-7.373067	3.998972
C	-0.458576	3.620131	0.143832	H	-2.958836	-6.269891	3.758856
H	-0.931448	4.558780	-0.155514	H	-1.199051	-7.894458	4.434788
H	-0.832816	3.303296	1.120682	C	1.030856	-3.272074	0.300483
H	0.619550	3.801279	0.245577	C	1.193289	-2.170882	-0.550006
C	-1.945661	0.169917	-2.691857	C	1.451959	-4.538711	-0.116998
H	-2.479051	-0.744552	-2.405444	C	1.792326	-2.331832	-1.800270
H	-2.609391	1.020698	-2.546134	H	0.831336	-1.195134	-0.236192
H	-1.667206	0.082097	-3.745265	C	2.049263	-4.697042	-1.368650
O	-0.903495	2.953370	-2.095644	H	1.293658	-5.404447	0.516575
O	0.322454	-0.347925	-2.222875	C	2.225179	-3.595492	-2.210326
C	0.229458	-0.615749	0.939347	H	1.910781	-1.473400	-2.455928
H	0.710491	-1.492574	0.491060	H	2.366792	-5.685068	-1.690829

H	2.685857	-3.723636	-3.186006	C	-1.106902	-1.700876	2.793946
C	1.711437	-2.512160	2.994825	C	-0.597921	-0.295300	3.208807
C	1.602566	-2.622653	4.390365	H	0.410833	-0.089914	2.843442
C	2.920330	-2.073789	2.437924	H	-1.244047	0.461728	2.757424
C	2.677183	-2.287407	5.212889	P	0.376498	-2.965087	2.712012
H	0.678603	-2.973244	4.836619	C	0.116750	-4.797204	2.794978
C	3.999585	-1.744985	3.263288	C	0.994829	-5.673525	2.142826
H	3.027669	-1.996810	1.361495	C	-0.947807	-5.329662	3.535275
C	3.878942	-1.848122	4.650518	C	0.824917	-7.055600	2.242038
H	2.569707	-2.358746	6.290883	H	1.812331	-5.287370	1.546435
H	4.932569	-1.409965	2.818425	C	-1.137376	-6.710591	3.605457
H	4.715851	-1.586843	5.292186	H	-1.638416	-4.664885	4.035766
C	1.539413	1.112604	4.435365	C	-0.247497	-7.578394	2.968059
H	2.246967	0.444442	3.931490	H	1.524877	-7.719775	1.742029
H	2.077602	1.683265	5.194796	H	-1.983452	-7.105565	4.161126
H	1.133030	1.794181	3.679884	H	-0.390400	-8.653784	3.033227
C	0.449108	0.316578	5.121089	C	0.427053	-2.887148	0.783194
C	-0.561271	-0.377462	4.336974	C	1.016644	-1.787559	0.139344
C	-1.610579	-0.968844	5.019391	C	-0.341593	-3.758589	-0.002955
C	-2.802750	-1.648401	4.422176	C	0.858173	-1.571652	-1.231735
H	-2.630942	-2.730501	4.392374	H	1.605995	-1.076112	0.711693
H	-3.661926	-1.468502	5.075951	C	-0.509234	-3.548198	-1.375315
H	-3.032353	-1.311400	3.413991	H	-0.836152	-4.608883	0.455951
O	0.459379	0.298881	6.378685	C	0.091453	-2.453102	-1.997092
O	-1.658469	-0.994177	6.352094	H	1.328225	-0.709562	-1.699249
H	-0.827841	-0.513356	6.679439	H	-1.118727	-4.238249	-1.953299
				H	-0.045927	-2.281654	-3.061129
XVI				C	2.158448	-2.440657	2.897185
C	-4.429477	-2.086370	-1.812231	C	2.564758	-1.572764	3.922527
C	-3.629402	-1.899322	-0.684987	C	3.140363	-2.922864	2.015652
C	-2.733909	-0.822336	-0.585873	C	3.899328	-1.184557	4.052183
C	-2.657300	0.085221	-1.659132	H	1.834919	-1.202338	4.627112
C	-3.446925	-0.088397	-2.787445	C	4.481727	-2.570640	2.168797
C	-4.331969	-1.177460	-2.862182	H	2.862477	-3.560363	1.185984
H	-5.107700	-2.932760	-1.846585	C	4.866341	-1.690611	3.182429
H	-1.960489	0.916555	-1.592084	H	4.179407	-0.489494	4.839006
H	-3.380895	0.614835	-3.612188	H	5.221822	-2.973129	1.482346
H	-4.949726	-1.313425	-3.745249	H	5.907838	-1.399970	3.290292
C	-1.913407	-0.740699	0.588515	C	-0.127925	1.720941	6.541603
H	-1.196867	0.071813	0.648759	H	-1.161642	2.048747	6.709481
C	-1.979711	-1.673053	1.573289	H	0.547758	2.554264	6.745444
O	-3.748621	-2.802746	0.332345	H	0.071183	0.897673	7.238250
C	-2.966460	-2.753238	1.471537	C	0.028879	1.266738	5.104874
O	-3.157521	-3.607603	2.314731	C	-0.640299	-0.057070	4.722949

H	-0.093529	-0.858642	5.233111	O	-1.066027	-0.721930	-2.399368
C	-2.096381	-0.105081	5.220163	H	-0.362515	-0.282413	-1.394643
C	-2.426796	-1.140613	6.266780	C	-2.554298	-2.567249	-2.602289
H	-2.103164	-2.129780	5.920571	H	-3.121734	-2.268495	-3.493348
H	-1.855569	-0.933903	7.182120	H	-1.700107	-3.161801	-2.942688
H	-3.495716	-1.136531	6.489487	H	-3.208592	-3.172290	-1.968400
O	0.679832	1.908112	4.299935				
O	-2.929427	0.657371	4.761577	TS2			
O	0.179306	-2.898299	4.534896	C	-4.662976	-2.103705	2.422332
H	-1.703365	-2.136240	3.594250	C	-3.560937	-1.855551	1.610083
H	0.778976	-3.530520	4.962618	C	-2.943417	-2.837611	0.832186
				C	-3.491344	-4.126542	0.893959
TS1				C	-4.590183	-4.406369	1.705505
C	-1.895000	-1.467557	3.919688	C	-5.178376	-3.397765	2.474745
C	-1.542219	-1.730807	2.604438	H	-5.106457	-1.295269	2.994798
C	-0.976436	-0.747641	1.779421	H	-3.036010	-4.912694	0.304162
C	-0.770988	0.537171	2.309155	H	-4.989549	-5.416057	1.736980
C	-1.122658	0.815449	3.626684	H	-6.036504	-3.611955	3.104874
C	-1.682769	-0.184075	4.430236	C	-1.701083	-2.512144	-0.001492
H	-2.337330	-2.250457	4.526002	H	-1.782122	-1.462395	-0.285569
H	-0.347720	1.296848	1.661280	O	-3.094071	-0.520199	1.491083
H	-0.965014	1.811455	4.029184	C	-2.532341	0.085189	2.551529
H	-1.959724	0.033572	5.457622	C	-2.233413	1.459254	2.279461
C	-0.635223	-1.046406	0.389571	C	-1.940715	2.619435	2.088898
H	-0.605894	-2.094997	0.092876	C	-1.584566	4.011643	1.859826
O	-1.703043	-3.011575	2.063931	H	-1.811732	4.620026	2.742742
C	-2.977478	-3.429349	1.778969	C	-0.462559	-2.684129	0.894896
C	-2.951059	-4.702507	1.114300	H	-1.316166	-4.113611	-0.995937
H	-4.044774	-7.452541	-0.177612	C	0.093214	-4.034067	0.973532
C	-2.989042	-5.761891	0.527648	C	0.378464	-1.521506	1.125794
C	-3.030758	-7.037353	-0.173968	C	1.386395	-4.324426	1.715619
H	-2.359840	-7.763126	0.299953	H	1.828805	-5.222021	1.277153
H	-2.708620	-6.912599	-1.214732	H	2.095055	-3.494327	1.692351
C	-2.700782	-0.906279	-0.690990	H	1.166535	-4.539487	2.769197
H	-3.421133	-1.600475	-0.268592	O	-2.286164	-0.462689	3.620748
C	-2.875662	0.495573	-0.284521	O	-1.655987	-3.223591	-1.225720
C	-2.073196	-1.321241	-1.897682	O	-0.496267	-4.987571	0.426926
C	-3.925710	0.727179	0.791724	O	1.059023	-1.387401	2.180548
H	-4.927333	0.637338	0.350496	H	-0.861582	-2.815761	2.482576
H	-3.857893	-0.019506	1.589834	C	0.415086	-0.381298	0.128200
H	-3.810271	1.732704	1.202069	H	-0.374889	0.346128	0.355703
O	-3.975020	-2.794858	2.039940	H	1.374196	0.132667	0.232957
O	-0.004646	-0.172888	-0.310228	H	0.277172	-0.724733	-0.900453
O	-2.236030	1.428594	-0.762493	O	-0.686569	-2.595979	3.555289

H	-1.367426	-1.900033	3.774188	TS4			
H	0.186193	-2.086948	3.339282	C	-3.413856	-1.545524	-2.567881
H	-0.509976	4.099165	1.659039	C	-2.749923	-0.880039	-1.540642
H	-2.128143	4.423107	1.002190	C	-2.800122	0.513790	-1.391109
				C	-3.588408	1.237646	-2.294475
TS3				C	-4.270052	0.587947	-3.324719
C	-2.676571	0.920202	2.294432	C	-4.175810	-0.798059	-3.467794
C	-2.195182	-0.363328	2.069060	H	-3.351393	-2.622864	-2.649916
C	-1.514816	-0.701386	0.884642	H	-3.660722	2.313383	-2.180956
C	-1.361058	0.312894	-0.074478	H	-4.877705	1.167593	-4.014333
C	-1.827438	1.607678	0.140943	H	-4.703019	-1.306377	-4.270261
C	-2.492381	1.911929	1.329908	O	-2.492981	2.367886	0.205197
H	-3.182808	1.129012	3.231230	O	-1.927691	-1.554355	-0.629310
H	-0.862457	0.067221	-1.007997	C	-2.286517	-2.734914	-0.051089
H	-1.680754	2.370251	-0.617768	C	-1.254587	-3.146514	0.869462
H	-2.868235	2.914671	1.510287	C	-0.417596	-3.514777	1.664020
C	-1.045218	-2.064220	0.530730	O	-3.308242	-3.345878	-0.267004
H	-0.630725	-2.092147	-0.476671	C	0.585371	-3.958130	2.623588
O	-2.304458	-1.256408	3.138597	H	0.938083	-4.966917	2.378490
C	-3.141503	-2.329650	3.074740	H	1.449219	-3.283631	2.636710
C	-2.902887	-3.203224	4.175040	H	0.161483	-3.988698	3.634306
C	-2.470936	-3.994489	4.985144	C	-2.038740	1.206245	-0.270629
C	-1.898021	-4.924194	5.941450	H	-1.844434	0.480665	0.533985
H	-0.825925	-5.020558	5.729592	P	-0.187882	1.535542	-0.911662
C	-0.471878	-3.022980	1.462974	C	0.682670	0.143760	-1.700263
H	-3.226028	-2.802088	0.575570	C	0.914010	-1.005160	-0.925733
C	-0.408085	-4.372040	0.973068	C	1.125780	0.177430	-3.029675
C	0.154144	-2.675150	2.743554	C	1.558054	-2.108057	-1.479508
C	0.391564	-5.464409	1.637472	H	0.585172	-1.041359	0.106753
H	0.557074	-6.253282	0.898845	C	1.774083	-0.930658	-3.580472
H	1.337167	-5.106597	2.049727	H	0.982116	1.067091	-3.631873
H	-0.176912	-5.877961	2.477570	C	1.986535	-2.075465	-2.810358
O	-3.947663	-2.506580	2.175928	H	1.716199	-2.995185	-0.873009
O	-2.570602	-2.773391	-0.159897	H	2.115512	-0.893741	-4.611193
O	-1.050155	-4.703629	-0.075258	H	2.487138	-2.937568	-3.242555
O	0.352804	-3.523747	3.621391	C	-0.249374	2.928905	-2.056823
H	-2.104517	-3.715016	-0.255125	C	0.205670	4.188161	-1.644624
C	0.715591	-1.277954	2.993531	C	-0.866192	2.779459	-3.310874
H	0.181340	-0.808718	3.825346	C	0.053255	5.288210	-2.487903
H	1.756909	-1.408025	3.306811	H	0.630270	4.318490	-0.657154
H	0.688375	-0.612781	2.129077	C	-1.006561	3.882708	-4.149395
H	-2.012886	-4.550298	6.965738	H	-1.257687	1.817201	-3.622207
H	-2.366622	-5.912248	5.876495	C	-0.548109	5.137433	-3.738226
				H	0.384387	6.266524	-2.153470

H	-1.489308	3.764728	-5.115528	O	-1.460608	-5.600998	-0.662069
H	-0.672606	5.999693	-4.387893	C	-1.084425	-1.310812	-1.680646
C	0.809503	1.964173	0.539507	O	-1.572431	-0.538649	-2.489479
C	0.190485	2.479942	1.687598	C	-1.862611	-1.529626	0.822454
C	2.202629	1.777324	0.508379	C	-2.768163	-2.145705	1.830667
C	0.971105	2.792447	2.802539	H	-2.211524	-2.546307	2.685831
H	-0.876273	2.673315	1.681114	H	-3.488251	-1.410207	2.209474
C	2.970700	2.098529	1.625519	H	-3.321507	-2.965470	1.360934
H	2.681942	1.378210	-0.380332	P	-0.658618	-0.059664	2.048239
C	2.353431	2.603243	2.775842	C	0.572660	0.648037	0.921140
H	0.490917	3.203980	3.685404	C	1.943505	0.651674	1.220675
H	4.047569	1.955791	1.598625	C	0.128660	1.160641	-0.307862
H	2.954301	2.855114	3.645915	C	2.856605	1.171883	0.303622
C	-1.540637	7.140812	1.783714	H	2.294229	0.243678	2.163237
H	-1.553654	8.128635	1.308721	C	1.048125	1.664336	-1.229537
H	-0.578917	6.978377	2.278089	H	-0.926580	1.153913	-0.559417
H	-2.328036	7.134547	2.549575	C	2.411121	1.672602	-0.924413
C	-1.800531	6.012772	0.785742	H	3.916579	1.178200	0.543496
C	-2.745464	6.299342	-0.264408	H	0.694331	2.030173	-2.188441
H	-3.091445	7.326245	-0.334234	H	3.126379	2.061263	-1.644190
C	-3.245964	5.428992	-1.215286	C	-1.413572	1.337653	2.944868
C	-4.124896	5.974327	-2.320780	C	-2.368375	1.055546	3.938669
H	-4.267844	7.056019	-2.250444	C	-1.135238	2.674694	2.623139
H	-3.667969	5.736541	-3.289318	C	-3.016148	2.091600	4.608872
H	-5.103098	5.478970	-2.294286	H	-2.596291	0.024110	4.195032
O	-1.195788	4.939295	0.925645	C	-1.795426	3.709262	3.290000
O	-3.065601	4.146904	-1.324167	H	-0.401197	2.906880	1.858502
H	-2.696528	3.387956	-0.519979	C	-2.733839	3.422570	4.283620
				H	-3.745769	1.860804	5.380213
TS6				H	-1.570348	4.740939	3.033675
C	1.995195	-2.256449	-0.765674	H	-3.244712	4.229719	4.800992
C	0.771249	-2.777489	-1.184864	C	0.282582	-1.003999	3.289290
C	0.330251	-4.031885	-0.730454	C	0.703148	-2.295212	2.930351
C	1.156335	-4.764373	0.138532	C	0.589725	-0.505843	4.564542
C	2.389482	-4.261345	0.540125	C	1.428567	-3.071729	3.832972
C	2.803697	-3.000032	0.092371	H	0.467402	-2.689815	1.947276
H	2.293030	-1.275899	-1.119599	C	1.309483	-1.290922	5.467141
H	0.803491	-5.734264	0.476306	H	0.270167	0.491529	4.849717
H	3.027787	-4.841608	1.200416	C	1.729779	-2.573775	5.103804
H	3.757747	-2.592799	0.415803	H	1.750510	-4.066985	3.541652
C	-0.974139	-4.595101	-1.155462	H	1.544811	-0.898184	6.452678
H	-1.493795	-4.061405	-1.968409	H	2.287982	-3.183212	5.809225
C	-1.570226	-1.598939	-0.398901				
O	0.041173	-2.046463	-2.101287	TS7			

C	-4.641455	-1.470814	-1.590129	H	1.913809	-3.654586	-3.704482
C	-3.478256	-1.226729	-0.860526	C	2.387899	-2.351094	2.595869
C	-3.329183	-0.061864	-0.097617	C	2.523260	-2.393441	3.993840
C	-4.400734	0.838367	-0.038307	C	3.408405	-1.782453	1.821148
C	-5.575173	0.600587	-0.750692	C	3.661867	-1.871880	4.604257
C	-5.689232	-0.550204	-1.539095	H	1.741619	-2.836858	4.603240
H	-4.715699	-2.388474	-2.165191	C	4.547725	-1.261257	2.438049
H	-4.273452	1.731995	0.565231	H	3.321820	-1.753037	0.740423
H	-6.394727	1.312480	-0.702394	C	4.676342	-1.303174	3.827570
H	-6.598756	-0.741107	-2.102430	H	3.756721	-1.908768	5.685741
C	-2.026722	0.277057	0.547191	H	5.334974	-0.825960	1.829143
H	-1.160471	0.016650	-0.101493	H	5.563436	-0.896641	4.304965
C	-1.547787	-1.708997	1.231663				
O	-2.506554	-2.217891	-0.925173	TS8			
O	-1.901031	1.175529	1.395031	C	-5.226145	-1.654151	-0.848101
C	-1.855991	-2.677336	0.212402	C	-3.884004	-1.447887	-0.547816
O	-1.677591	-3.888285	0.293742	C	-3.422168	-0.244598	-0.009465
C	-0.509925	-1.754124	2.077160	C	-4.339768	0.769887	0.252731
C	-0.367362	-0.828366	3.263015	C	-5.696206	0.582174	-0.032209
H	-0.532362	-1.366167	4.207730	C	-6.135536	-0.623778	-0.588428
H	0.621591	-0.360918	3.319878	H	-5.542645	-2.604618	-1.266658
H	-1.117638	-0.039067	3.170246	H	-3.964745	1.698654	0.672432
P	0.850853	-2.966605	1.837124	H	-6.408948	1.376772	0.171911
C	0.521417	-4.542263	2.671966	H	-7.188026	-0.769712	-0.816030
C	1.579435	-5.421277	2.954955	C	-1.926597	-0.120367	0.188575
C	-0.787698	-4.875836	3.040625	H	-1.497636	-0.126381	-0.845613
C	1.323176	-6.634362	3.592803	C	-1.415402	-1.488584	0.693229
H	2.598020	-5.155186	2.687483	O	-3.001087	-2.500991	-0.810670
C	-1.034826	-6.086994	3.688561	O	-1.446447	0.978607	0.832036
H	-1.602057	-4.201561	2.804419	C	-1.859052	-2.647264	-0.059150
C	0.015507	-6.966483	3.961128	O	-1.332189	-3.754732	-0.029943
H	2.142395	-7.314867	3.807061	C	-0.458092	-1.551931	1.678373
H	-2.050906	-6.344260	3.972895	C	-0.396138	-0.475124	2.650800
H	-0.182612	-7.909963	4.462324	H	-1.247787	-0.460268	3.336351
C	1.191134	-3.220999	0.080004	H	0.546068	-0.316047	3.171641
C	1.189404	-2.101635	-0.765903	H	-0.803858	0.492893	1.852122
C	1.444092	-4.495507	-0.439753	P	0.842712	-2.838249	1.605875
C	1.455323	-2.260350	-2.126095	C	0.378631	-4.386925	2.425473
H	0.961578	-1.116591	-0.369315	C	1.372121	-5.326913	2.739072
C	1.710437	-4.645957	-1.800085	C	-0.952195	-4.623374	2.788057
H	1.402857	-5.366580	0.205293	C	1.027428	-6.510367	3.391658
C	1.717723	-3.531008	-2.643142	H	2.411083	-5.129221	2.490598
H	1.441547	-1.393645	-2.780411	C	-1.288234	-5.802746	3.452953
H	1.894510	-5.636937	-2.204835	H	-1.716411	-3.893695	2.547149

C	-0.303138	-6.748317	3.748535	O	-1.230497	-2.858974	1.706097
H	1.797211	-7.239128	3.629013	C	0.632018	-0.724113	1.433213
H	-2.321637	-5.984019	3.733410	C	1.454494	0.335697	1.629530
H	-0.570195	-7.667937	4.261769	H	2.517846	0.229173	1.796784
C	1.426278	-3.083466	-0.088904	H	1.051969	1.342929	1.647995
C	1.529702	-1.950438	-0.910045	H	-2.318383	2.030530	2.411296
C	1.765989	-4.347279	-0.584012	P	1.378901	-2.380849	1.617345
C	1.987643	-2.087319	-2.221383	C	1.134785	-3.105256	3.256693
H	1.239347	-0.972809	-0.535297	C	1.892808	-4.227948	3.623666
C	2.224517	-4.474533	-1.894554	C	0.263523	-2.503638	4.173316
H	1.643185	-5.229123	0.035490	C	1.757851	-4.767119	4.902719
C	2.337893	-3.346880	-2.713145	H	2.599668	-4.668423	2.925984
H	2.059798	-1.210345	-2.858184	C	0.155357	-3.038823	5.457572
H	2.478168	-5.457256	-2.281637	H	-0.338648	-1.638246	3.910428
H	2.687349	-3.452065	-3.736400	C	0.889944	-4.169596	5.821708
C	2.263378	-2.234892	2.568527	H	2.337811	-5.641984	5.182832
C	2.193358	-2.268487	3.971394	H	-0.517176	-2.566984	6.167247
C	3.399060	-1.701182	1.944465	H	0.791575	-4.583438	6.821667
C	3.246302	-1.769577	4.736502	C	0.955784	-3.440539	0.212466
H	1.320148	-2.686809	4.462150	C	0.810833	-2.838637	-1.044788
C	4.451901	-1.205510	2.715849	C	0.788958	-4.821965	0.356800
H	3.467086	-1.676300	0.862429	C	0.509645	-3.625369	-2.157987
C	4.376801	-1.236978	4.110011	H	0.910935	-1.762375	-1.150222
H	3.183190	-1.796270	5.820544	C	0.494090	-5.601362	-0.760821
H	5.330329	-0.796877	2.224644	H	0.851987	-5.281342	1.337141
H	5.197180	-0.849633	4.707712	C	0.356418	-5.006350	-2.018472
				H	0.386786	-3.155800	-3.129832
				H	0.354776	-6.672493	-0.646118
TS9				H	0.117883	-5.616754	-2.884912
C	-4.805160	-0.602592	-0.015498	C	3.195920	-2.170228	1.529926
C	-3.476209	-0.542642	0.405808	C	3.898124	-1.779593	2.682619
C	-2.714975	0.622176	0.252157	C	3.897044	-2.367955	0.332278
C	-3.314305	1.740157	-0.349778	C	5.277066	-1.579043	2.631318
C	-4.634618	1.694437	-0.779219	H	3.367457	-1.635482	3.618386
C	-5.380058	0.518912	-0.604657	C	5.278569	-2.171279	0.286708
H	-5.362309	-1.521631	0.133325	H	3.371841	-2.683589	-0.562363
H	-2.735047	2.654354	-0.448131	C	5.969957	-1.774332	1.433233
H	-5.090922	2.569110	-1.232543	H	5.809184	-1.274243	3.527924
H	-6.416413	0.479919	-0.928665	H	5.812759	-2.332598	-0.645364
C	-1.338842	0.637196	0.751016	H	7.045109	-1.622594	1.395637
H	-0.679200	1.356041	0.272590	C	-6.042966	1.892767	2.987673
C	-0.777637	-0.628580	1.090895	H	-6.768004	1.133292	3.293754
O	-2.950978	-1.677550	0.960043	H	-6.209269	2.144708	1.934033
O	-1.374830	1.630181	2.283702	H	-6.210538	2.805718	3.570967
C	-1.613099	-1.761697	1.284322				

C	-4.594472	1.453140	3.162505	H	2.135391	-7.238744	3.258285
C	-4.382795	0.142331	3.665430	H	-1.914759	-6.000577	4.042619
H	-5.295449	-0.421393	3.825983	H	-0.094885	-7.682826	4.268335
C	-3.208088	-0.545490	4.044096	C	1.273937	-3.045889	-0.269724
C	-3.386831	-1.955091	4.592045	C	1.324012	-1.910439	-1.091218
H	-4.434114	-2.262916	4.654531	C	1.528027	-4.312151	-0.808339
H	-2.846855	-2.659570	3.948900	C	1.645930	-2.043515	-2.442769
H	-2.940222	-2.012452	5.591978	H	1.095599	-0.932085	-0.678216
O	-3.734826	2.321427	2.831563	C	1.851721	-4.437862	-2.159083
O	-2.000287	-0.143614	3.991325	H	1.442793	-5.197549	-0.188247
H	-1.482956	0.916947	3.015109	C	1.914527	-3.305975	-2.976761
TS10				H	1.677335	-1.162047	-3.076858
C	-4.916631	-1.372876	-1.643973	H	2.040010	-5.422958	-2.576355
C	-3.782693	-1.334879	-0.836770	H	2.159741	-3.409551	-4.030041
C	-3.373048	-0.164542	-0.176774	C	2.414939	-2.268998	2.300018
C	-4.152543	1.001020	-0.336357	C	2.533341	-2.407300	3.692332
C	-5.286869	0.977431	-1.135882	C	3.461274	-1.685617	1.573846
C	-5.666443	-0.207361	-1.790742	C	3.677394	-1.955973	4.348219
H	-5.193838	-2.300445	-2.134326	H	1.729370	-2.860041	4.264024
H	-3.848375	1.903119	0.187342	C	4.609621	-1.242747	2.233546
H	-5.886416	1.875225	-1.252429	H	3.387127	-1.580833	0.496956
H	-6.555575	-0.220470	-2.414520	C	4.718292	-1.373623	3.619673
C	-2.191612	-0.212132	0.626777	H	3.752704	-2.055955	5.426985
H	-1.893957	0.705102	1.129118	H	5.417712	-0.795222	1.661975
C	-1.486733	-1.376172	0.793041	H	5.610462	-1.023688	4.131257
O	-3.059458	-2.493287	-0.693558	C	0.827643	-0.066906	6.113701
O	-1.916321	2.328436	2.592950	H	0.771576	0.492248	7.053564
C	-1.955765	-2.579344	0.109283	H	1.750258	0.243037	5.606587
O	-1.420554	-3.676177	0.212046	H	0.888087	-1.137494	6.334260
C	-0.305965	-1.480239	1.667059	C	-0.373920	0.309893	5.244500
C	-0.052226	-0.511471	2.632026	C	-1.112174	-0.783089	4.645587
H	0.910205	-0.477629	3.123107	H	-0.767888	-1.778913	4.912739
H	-0.574264	0.438036	2.601614	C	-2.492599	-0.720408	4.211663
H	-2.465384	1.734845	3.158392	C	-3.191752	-2.058483	3.987036
P	0.867869	-2.802583	1.482616	H	-3.060842	-2.348730	2.935996
C	0.530058	-4.384720	2.318743	H	-2.797077	-2.862136	4.616711
C	1.564017	-5.322621	2.464013	H	-4.263874	-1.937916	4.163160
C	-0.720241	-4.632909	2.891931	O	-0.592794	1.513390	5.044616
C	1.334161	-6.512467	3.154728	O	-3.142434	0.313041	3.977838
H	2.550314	-5.119401	2.056448	H	-1.244732	2.607174	3.238467
C	-0.941457	-5.816255	3.596993	TS11			
H	-1.513977	-3.906558	2.784808	C	-6.231189	-0.370895	-1.672882
C	0.080963	-6.759652	3.723159	C	-4.852114	-0.304267	-1.495809

C	-4.265228	0.714082	-0.739276	C	-1.162177	3.591067	-5.170599
C	-5.074087	1.681531	-0.151224	C	1.618542	3.732995	-5.400093
C	-6.460526	1.631819	-0.321812	H	1.675059	3.077859	-3.355061
C	-7.035395	0.607026	-1.079048	C	-0.578240	4.000910	-6.371027
H	-6.654090	-1.177207	-2.263915	H	-2.242261	3.554657	-5.091322
H	-4.604916	2.472650	0.423807	C	0.810912	4.069016	-6.490218
H	-7.089729	2.391166	0.134243	H	2.700283	3.787999	-5.482389
H	-8.113279	0.564199	-1.210454	H	-1.213209	4.269346	-7.210627
C	-2.768520	0.634222	-0.626105	H	1.262948	4.387816	-7.425292
O	-2.175023	1.822702	-0.142015	H	-2.537453	-0.175105	0.088341
C	-2.185668	0.182342	-1.953593	C	-0.812557	-1.160781	2.928596
O	-4.075265	-1.300155	-2.067989	H	-1.777051	-0.690004	3.150519
C	-2.750679	-1.057050	-2.460129	H	-0.100514	-0.806011	3.683871
O	-2.248548	-1.884729	-3.199231	H	-0.909311	-2.246730	3.016936
C	-0.162045	0.209407	-3.437063	C	-0.333033	-0.707003	1.555542
H	-0.409089	-0.788123	-3.796849	C	0.015806	-1.728296	0.614668
H	0.383700	0.819761	-4.149899	H	-0.178078	-2.750948	0.920542
H	0.630646	-0.177378	-2.283142	C	0.537537	-1.563267	-0.664115
C	-1.162699	0.825610	-2.628578	C	0.655756	-2.755485	-1.581804
P	-1.068887	2.664378	-2.487692	H	0.493463	-3.697564	-1.051729
C	-2.754760	3.338060	-2.440590	H	-0.101138	-2.677673	-2.372515
C	-3.086181	4.423366	-1.622075	H	1.642622	-2.768350	-2.057766
C	-3.735662	2.755325	-3.257610	O	-0.292705	0.529087	1.342984
C	-4.382186	4.938583	-1.643689	O	0.946613	-0.418557	-1.133747
H	-2.351271	4.842111	-0.944665	H	-1.447114	1.528865	0.458618
C	-5.029964	3.273127	-3.271661				
H	-3.501049	1.881283	-3.855878	TS12			
C	-5.353320	4.368781	-2.470126	C	-10.682333	-0.204960	-0.930476
H	-4.636370	5.774152	-0.997595	C	-9.434712	-0.400326	-0.342664
H	-5.788711	2.800173	-3.887537	C	-8.909761	0.481335	0.613087
H	-6.365818	4.762169	-2.471335	C	-9.686009	1.600102	0.978213
C	0.049674	3.433427	-1.286939	C	-10.933229	1.809270	0.403778
C	0.226056	4.828096	-1.340451	C	-11.431808	0.906498	-0.550687
C	0.803741	2.656625	-0.404088	H	-11.042344	-0.916924	-1.666320
C	1.125396	5.443576	-0.473589	H	-9.280954	2.299771	1.704416
H	-0.319170	5.426595	-2.064499	H	-11.522381	2.676227	0.688292
C	1.709620	3.285462	0.455016	H	-12.406629	1.073746	-0.999745
H	0.695357	1.578298	-0.367937	C	-7.605114	0.214710	1.144450
C	1.866649	4.670956	0.428902	H	-7.222489	0.935522	1.854368
H	1.254412	6.521768	-0.508397	O	-8.717267	-1.506502	-0.717615
H	2.281566	2.676205	1.148104	C	-7.469051	-1.771476	-0.230937
H	2.569008	5.153171	1.103529	O	-6.938417	-2.810281	-0.600383
C	-0.357802	3.247189	-4.076475	P	-4.976386	-2.810894	1.354782
C	1.039738	3.328722	-4.198326	C	-6.329473	-3.812545	2.041718

C	-6.584583	-5.122540	1.621119	H	-1.893277	2.613183	0.017859
C	-7.151373	-3.216338	3.009467	H	-3.466986	2.143923	-0.711606
C	-7.643399	-5.837784	2.181315	H	-3.405662	3.477713	0.436624
H	-5.975363	-5.571656	0.844268	O	-6.156460	2.927912	2.673404
C	-8.209939	-3.935358	3.566112	O	-2.313292	1.040223	1.982505
H	-6.972576	-2.190803	3.318280	C	-5.440592	-1.083037	1.099272
C	-8.455200	-5.247761	3.154262	H	-4.488536	-0.724216	0.019294
H	-7.842445	-6.852294	1.847516	C	-1.767231	-0.879764	-2.104453
H	-8.845832	-3.466998	4.312097	H	-1.556640	-0.762501	-3.171070
H	-9.283364	-5.805587	3.582606	H	-1.623251	-1.929476	-1.822450
C	-3.642209	-2.848821	2.603833	H	-1.046657	-0.285785	-1.529213
C	-2.400101	-2.286889	2.261808	C	-3.168005	-0.448589	-1.742556
C	-3.826277	-3.413852	3.871223	C	-4.037101	-0.012533	-2.720056
C	-1.361138	-2.283882	3.189130	H	-3.676491	-0.054755	-3.743445
H	-2.263374	-1.825356	1.288457	C	-5.356058	0.549008	-2.516693
C	-2.775241	-3.416900	4.792830	C	-6.157455	0.864542	-3.773531
H	-4.779325	-3.856497	4.140406	H	-5.550334	1.394258	-4.517392
C	-1.544530	-2.851345	4.454254	H	-6.498252	-0.070732	-4.237713
H	-0.413275	-1.824216	2.925700	H	-7.030482	1.466066	-3.509821
H	-2.922382	-3.861629	5.773265	O	-3.406853	-0.548319	-0.460586
H	-0.730774	-2.848867	5.174417	O	-5.852209	0.784615	-1.405355
C	-4.192111	-3.726385	-0.022985	H	-5.299115	1.518273	0.806034
C	-4.327616	-3.362986	-1.366516				
C	-3.395336	-4.833364	0.314436	TS13			
C	-3.670144	-4.091498	-2.357027	C	-5.537907	0.084043	-0.058372
H	-4.941285	-2.519850	-1.643809	C	-4.202505	-0.070816	0.312659
C	-2.756119	-5.572597	-0.681416	C	-3.635463	0.673572	1.359581
H	-3.261519	-5.114773	1.354285	C	-4.452844	1.590623	2.048094
C	-2.888710	-5.199223	-2.020996	C	-5.784579	1.752867	1.692299
H	-3.773346	-3.786227	-3.394475	C	-6.323838	0.999680	0.635509
H	-2.147563	-6.429753	-0.406956	H	-5.932704	-0.506693	-0.878439
H	-2.382221	-5.766244	-2.797516	H	-4.017162	2.179207	2.851306
C	-6.851255	-0.844155	0.716577	H	-6.407207	2.466431	2.223199
C	-4.952128	-0.135352	2.211217	H	-7.364218	1.131925	0.353040
H	-5.687258	-0.100447	3.030896	C	-2.240916	0.484624	1.644711
H	-4.019768	-0.474475	2.656777	H	-1.802800	1.098042	2.422355
C	-4.689705	1.310073	1.685977	O	-3.456743	-0.986153	-0.373668
C	-5.118797	2.293643	2.783515	C	-2.115691	-1.169616	-0.133137
C	-3.214410	1.538871	1.328532	O	-1.532462	-2.004180	-0.801621
C	-4.251161	2.405359	4.018205	P	0.551090	-2.305063	1.312691
H	-4.815398	2.883624	4.821654	C	-0.888159	-3.300218	1.795950
H	-3.871699	1.428445	4.333094	C	-1.253729	-4.453391	1.092576
H	-3.369101	3.015813	3.786694	C	-1.678450	-2.855840	2.867911
C	-2.965422	2.500472	0.193342	C	-2.391078	-5.166826	1.472259

H	-0.671706	-4.773727	0.235911	O	2.090446	3.893922	1.524539
C	-2.816584	-3.570424	3.241199	O	2.656918	0.118859	0.168773
H	-1.412129	-1.951090	3.406356	C	0.014158	-0.533625	1.044215
C	-3.172401	-4.728245	2.544183	H	0.392297	-0.347210	0.034806
H	-2.674811	-6.056916	0.918319	C	-1.032264	-0.058199	-3.550638
H	-3.425801	-3.218991	4.068979	H	-1.827007	0.330710	-4.194794
H	-4.062229	-5.281800	2.830606	H	-1.322541	-1.059020	-3.205626
C	1.769668	-2.477290	2.658707	H	-0.106337	-0.156486	-4.125976
C	3.068346	-1.983254	2.437906	C	-0.775281	0.810796	-2.327263
C	1.466116	-3.136661	3.857385	C	-1.814858	1.722940	-1.940858
C	4.040951	-2.138232	3.423442	H	-2.680390	1.770027	-2.593308
H	3.294804	-1.457006	1.515309	C	-1.816406	2.612297	-0.877298
C	2.450034	-3.287805	4.837947	C	-2.969871	3.584773	-0.745396
H	0.477244	-3.546324	4.027920	H	-3.747443	3.414726	-1.494815
C	3.735347	-2.787730	4.623943	H	-3.411279	3.506454	0.253272
H	5.039335	-1.746447	3.251694	H	-2.588280	4.607372	-0.852992
H	2.208817	-3.801980	5.764090	O	0.301800	0.666530	-1.718679
H	4.498791	-2.906347	5.387999	O	-0.943959	2.756867	0.073107
C	1.372436	-3.026278	-0.128994	H	0.052990	2.138916	0.324144
C	1.448692	-2.368634	-1.361885				
C	1.980180	-4.281974	0.045420	TS14			
C	2.120359	-2.984430	-2.419328	C	-5.138895	-1.036599	-0.717824
H	1.018796	-1.385512	-1.512943	C	-3.840202	-0.884943	-0.222186
C	2.636689	-4.891594	-1.021369	C	-3.339730	0.385556	0.109178
H	1.950681	-4.776415	1.012634	C	-4.175154	1.501614	-0.057689
C	2.706054	-4.240792	-2.257468	C	-5.467610	1.361252	-0.553804
H	2.188819	-2.466052	-3.371151	C	-5.945189	0.086136	-0.886808
H	3.101720	-5.863691	-0.884009	H	-5.489233	-2.033762	-0.964831
H	3.226477	-4.709819	-3.088209	H	-3.786680	2.486841	0.182182
C	-1.485281	-0.386846	0.931757	H	-6.097012	2.235740	-0.689526
C	0.718312	0.484043	1.975235	H	-6.951554	-0.032697	-1.279355
H	0.045871	0.776058	2.781870	C	-1.961744	0.485245	0.599411
H	1.568723	0.009559	2.468443	H	-1.814263	1.302289	1.305299
C	1.209607	1.692552	1.170302	O	-3.106493	-2.025558	-0.068979
C	1.339536	2.980545	1.877329	C	-1.783960	-1.997866	0.408286
C	2.275811	1.303802	0.231393	O	-1.200669	-3.081276	0.396211
C	0.443306	3.221650	3.096006	P	0.762943	-0.446641	2.701436
H	0.539823	4.269860	3.387035	C	-0.081020	0.929327	3.517350
H	-0.606637	3.007914	2.866096	C	-1.405670	0.731159	3.943273
H	0.745513	2.591560	3.942795	C	0.510959	2.194580	3.638810
C	2.890081	2.321514	-0.698405	C	-2.128585	1.797064	4.476568
H	3.330230	1.792820	-1.548009	H	-1.868985	-0.243587	3.833936
H	2.151893	3.051344	-1.038238	C	-0.214351	3.252700	4.188244
H	3.664336	2.882561	-0.163489	H	1.528707	2.358423	3.300327

C	-1.534215	3.056398	4.601821	H	0.682526	-1.452646	0.524617
H	-3.156977	1.643727	4.789844				
H	0.247856	4.231317	4.278700	TS15			
H	-2.100272	3.884189	5.019476	C	-5.367129	0.209143	0.074603
C	2.556414	-0.149700	2.778385	C	-4.008576	-0.014584	0.324415
C	3.348824	-0.433638	1.656492	C	-3.062661	0.996387	0.109820
C	3.168053	0.279600	3.967333	C	-3.516786	2.245086	-0.331789
C	4.734788	-0.276310	1.721147	C	-4.866009	2.481496	-0.586662
H	2.894920	-0.778639	0.734119	C	-5.793278	1.452669	-0.384526
C	4.551566	0.436858	4.026304	H	-6.065438	-0.604195	0.245731
H	2.567103	0.494584	4.845434	H	-2.795289	3.042342	-0.491203
C	5.336671	0.160412	2.902442	H	-5.191396	3.455347	-0.940661
H	5.340094	-0.496674	0.846826	H	-6.848639	1.619666	-0.581903
H	5.016732	0.772503	4.948770	C	-1.621837	0.732671	0.432627
H	6.414954	0.283009	2.950223	H	-1.343637	1.434259	1.233093
C	0.416208	-1.929022	3.677737	O	-3.691894	-1.268648	0.788834
C	0.161988	-3.159349	3.058143	C	-2.366356	-1.655597	1.055853
C	0.478156	-1.839541	5.079836	O	-2.230211	-2.823366	1.426170
C	-0.028072	-4.295546	3.849634	P	0.812053	-0.661937	2.924241
H	0.043499	-3.232737	1.980119	C	-0.435334	0.439023	3.632223
C	0.292220	-2.980080	5.856816	C	-1.716950	-0.094212	3.852763
H	0.650886	-0.883100	5.564425	C	-0.248699	1.831965	3.693498
C	0.041995	-4.211556	5.240620	C	-2.789218	0.754268	4.138679
H	-0.245784	-5.243157	3.366026	H	-1.882298	-1.165442	3.803134
H	0.334250	-2.907388	6.939937	C	-1.320119	2.670602	3.994480
H	-0.108885	-5.099661	5.848268	H	0.725566	2.264002	3.490345
C	-1.294508	-0.756366	0.888884	C	-2.595270	2.133941	4.206244
C	0.560021	0.745415	0.164593	H	-3.778029	0.331360	4.289185
H	0.869189	1.534817	0.852658	H	-1.164018	3.744702	4.046044
H	1.408561	0.529349	-0.488281	H	-3.433804	2.791499	4.416944
C	-0.640996	1.204344	-0.660709	C	2.450337	0.101958	3.163227
C	-0.952625	2.647847	-0.735484	C	3.425311	-0.118051	2.177479
C	-0.831074	0.347915	-1.866327	C	2.785467	0.849461	4.304927
C	-0.376204	3.579233	0.327464	C	4.710818	0.404827	2.326072
H	-0.814187	4.569605	0.186131	H	3.180904	-0.698616	1.292434
H	-0.600487	3.227027	1.340830	C	4.070115	1.374749	4.448368
H	0.714883	3.657260	0.244584	H	2.046877	1.012405	5.083720
C	-1.833772	0.688622	-2.942401	C	5.033488	1.155414	3.459140
H	-1.906883	-0.165133	-3.620667	H	5.456307	0.228347	1.556046
H	-2.811545	0.927153	-2.515747	H	4.319902	1.950112	5.335615
H	-1.519184	1.583919	-3.488351	H	6.032673	1.566311	3.572967
O	-1.723049	3.126015	-1.570716	C	0.853336	-2.224304	3.856428
O	-0.190839	-0.704638	-1.932325	C	-0.050549	-3.247544	3.527254
C	0.189365	-0.575259	0.956058	C	1.795503	-2.427517	4.881147

C	-0.022212	-4.449485	4.240070	O	-1.881913	-4.164253	1.332425
H	-0.775251	-3.123493	2.724225	C	-0.194758	-1.936756	1.937509
C	1.817665	-3.633346	5.579408	C	0.460868	-0.711536	2.558814
H	2.511986	-1.652922	5.132292	H	1.516378	-0.902161	2.758545
C	0.906116	-4.646211	5.263000	H	0.434794	0.117850	1.838996
H	-0.729097	-5.232294	3.980110	P	0.747046	-3.394669	1.744594
H	2.548210	-3.781895	6.370047	C	0.579415	-4.733174	2.977565
H	0.927280	-5.585829	5.808506	C	1.530375	-5.761140	3.044302
C	-1.366379	-0.683501	0.875435	C	-0.471007	-4.700019	3.897853
C	0.694481	0.239235	0.112729	C	1.411082	-6.764164	4.007620
H	1.150916	0.979779	0.775283	H	2.374366	-5.771612	2.360375
H	1.461301	-0.122081	-0.573915	C	-0.586227	-5.698990	4.862956
C	-0.484507	0.891395	-0.660825	H	-1.184320	-3.885629	3.862394
C	-0.212207	2.341925	-1.051249	C	0.349804	-6.735080	4.916109
C	-0.746945	0.062131	-1.951215	H	2.150515	-7.559157	4.053216
C	0.292450	3.303525	0.013145	H	-1.403211	-5.664191	5.578201
H	0.031962	4.323220	-0.280775	H	0.259219	-7.512167	5.670442
H	-0.099923	3.086312	1.010102	C	0.552044	-4.099767	0.066820
H	1.386866	3.234401	0.064091	C	0.353215	-3.211294	-0.999362
C	-2.067843	0.173546	-2.670839	C	0.604289	-5.475400	-0.182235
H	-2.813087	-0.446977	-2.159533	C	0.226595	-3.694317	-2.302700
H	-2.442726	1.197673	-2.683390	H	0.277818	-2.145759	-0.802627
H	-1.938501	-0.200280	-3.689090	C	0.478100	-5.954973	-1.486597
O	-0.386129	2.734977	-2.194739	H	0.710800	-6.175374	0.638531
O	0.129071	-0.673958	-2.371562	C	0.293226	-5.067554	-2.549826
C	0.037087	-0.918300	0.906265	H	0.066890	-2.997798	-3.121403
H	0.395547	-1.929037	0.720803	H	0.510492	-7.025609	-1.669402
TS16				H	0.189004	-5.445087	-3.563393
C	-5.636714	-1.740786	0.395722	C	2.528351	-2.963306	1.840568
C	-4.290267	-1.713791	0.740277	C	3.183979	-2.949370	3.081868
C	-3.593990	-0.517940	1.003422	C	3.242901	-2.627435	0.681648
C	-4.331684	0.686929	0.911017	C	4.532677	-2.599354	3.156164
C	-5.678864	0.675761	0.569118	H	2.633148	-3.181889	3.984714
C	-6.337519	-0.536673	0.308850	C	4.592215	-2.277794	0.761748
H	-6.113730	-2.696632	0.202513	H	2.755637	-2.648560	-0.286742
H	-3.821546	1.627334	1.106786	C	5.240126	-2.262898	1.999078
H	-6.224430	1.612961	0.502657	H	5.028062	-2.587107	4.123190
H	-7.389916	-0.542723	0.042039	H	5.135811	-2.024254	-0.144381
C	-2.209808	-0.594084	1.350790	H	6.291234	-1.993487	2.060713
H	-1.687146	0.338452	1.524956	C	-0.309779	-0.699597	6.436834
C	-1.535827	-1.808419	1.480907	H	-0.405563	0.378523	6.582507
O	-3.628625	-2.918473	0.824726	H	0.403638	-1.121206	7.148819
C	-2.322321	-3.034188	1.210799	H	-1.291478	-1.145568	6.639953
				C	0.148320	-1.083610	5.037454

C	-0.245217	-0.295210	3.855823	H	-2.878170	-6.395695	3.895972
H	-1.726811	-0.867950	3.999809	H	-1.276465	-8.298749	3.930022
C	-0.701044	1.064453	4.006061	C	1.181350	-3.271207	0.375516
C	-0.100365	2.195348	3.201720	C	1.678287	-2.065964	-0.143472
H	0.970424	2.060235	3.027970	C	1.242367	-4.438936	-0.392617
H	-0.592939	2.266530	2.222266	C	2.253023	-2.036743	-1.414470
H	-0.284671	3.134235	3.730210	H	1.613848	-1.152103	0.441088
O	0.857410	-2.087895	4.903583	C	1.821626	-4.405277	-1.661543
O	-1.678968	1.371956	4.764962	H	0.812410	-5.360252	-0.016394
O	-2.797811	-0.767825	4.386965	C	2.330257	-3.208187	-2.172681
H	-2.541425	0.230242	4.732753	H	2.635010	-1.100547	-1.811674
H	-3.339757	-0.670515	3.577183	H	1.861672	-5.312964	-2.257047
				H	2.775542	-3.185551	-3.163431
TS17				C	1.802388	-2.915436	3.192816
C	-5.168501	-1.386936	-1.242699	C	1.496220	-2.781800	4.558458
C	-4.094415	-1.451040	-0.358319	C	3.138184	-2.891723	2.774241
C	-3.807631	-0.419834	0.550614	C	2.520933	-2.604338	5.485084
C	-4.652786	0.709108	0.554636	H	0.463144	-2.801568	4.893678
C	-5.728984	0.788374	-0.319479	C	4.161237	-2.719750	3.711093
C	-5.986457	-0.259412	-1.219414	H	3.385402	-3.002690	1.723982
H	-5.346087	-2.211556	-1.925487	C	3.854779	-2.572108	5.064494
H	-4.447035	1.513975	1.255361	H	2.275968	-2.487630	6.536838
H	-6.373766	1.662079	-0.306898	H	5.195376	-2.699597	3.378427
H	-6.828653	-0.194677	-1.902026	H	4.650671	-2.432210	5.790780
C	-2.676041	-0.575643	1.417635	C	0.546069	2.197110	3.347970
H	-2.468481	0.210882	2.136851	H	1.477509	1.638476	3.192587
C	-1.885623	-1.694799	1.383244	H	0.775147	3.173620	3.779605
O	-3.304858	-2.572748	-0.396058	H	0.091747	2.348322	2.359397
C	-2.234369	-2.754383	0.436372	C	-0.414557	1.468599	4.292156
O	-1.617863	-3.804901	0.330879	C	-0.716264	0.073490	4.003243
C	-0.740952	-1.879111	2.301744	C	-1.492254	-0.695685	4.871653
C	-0.095248	-0.537209	2.747064	C	-2.102737	-0.177192	6.148647
H	0.981477	-0.665802	2.902645	H	-2.826497	0.618256	5.944973
H	-0.183990	0.162818	1.905345	H	-2.595920	-1.011764	6.654907
P	0.423631	-3.206158	2.027494	H	-1.347107	0.274993	6.797460
C	-0.164367	-4.837693	2.570537	O	-0.879575	2.109237	5.247076
C	0.748920	-5.900740	2.618328	O	-1.747090	-1.962850	4.638055
C	-1.470609	-5.018692	3.037091	H	-1.283460	-2.164518	3.485278
C	0.345174	-7.147733	3.095013				
H	1.777144	-5.753930	2.299475	TS18			
C	-1.864765	-6.263208	3.528566	C	-5.140181	-1.654869	1.087512
H	-2.175447	-4.195968	3.033291	C	-3.915033	-1.114901	0.700976
C	-0.963588	-7.330180	3.549938	C	-3.789678	-0.284467	-0.423669
H	1.055094	-7.969586	3.122969	C	-4.948526	0.007876	-1.170251

C	-6.176442	-0.524144	-0.798449	C	3.757778	-0.709509	-3.424088
C	-6.270339	-1.356090	0.329838	H	2.196423	-1.934850	-2.599764
H	-5.188583	-2.290118	1.965928	C	4.523026	0.448709	-3.277039
H	-4.863306	0.667402	-2.029661	H	4.891736	2.200514	-2.065795
H	-7.066105	-0.291349	-1.375777	H	3.924097	-1.372997	-4.268200
H	-7.232131	-1.768789	0.620248	H	5.285714	0.693402	-4.011339
C	-2.491954	0.245479	-0.733932	C	-2.579469	3.253203	0.680515
H	-2.422702	0.895808	-1.596742	H	-1.935822	2.852449	1.466048
C	-1.404515	-0.007769	0.047241	H	-3.520107	2.700872	0.594544
O	-2.815279	-1.422388	1.456153	H	-2.841901	4.288230	0.938029
C	-1.566804	-0.916914	1.188026	C	-1.903733	3.265406	-0.671439
O	-0.650249	-1.285891	1.899686	C	-0.385841	3.116277	-0.852379
C	-0.063004	0.640805	-0.108242	H	-0.192519	3.706408	-1.761434
C	0.028166	1.672135	-1.250979	C	0.607958	3.709757	0.171242
H	1.057699	1.769485	-1.584320	C	0.218856	4.995307	0.872040
H	-0.547262	1.365897	-2.132304	H	0.137644	5.791817	0.116426
P	1.322969	-0.569356	-0.096937	H	-0.727817	4.917665	1.403633
C	2.322235	-0.595460	1.422088	H	1.009276	5.268012	1.575369
C	3.608148	-1.158508	1.342171	O	-2.577780	3.365049	-1.692659
C	1.857521	-0.085830	2.641012	O	1.802024	3.408685	0.050768
C	4.416251	-1.221523	2.475974	O	0.004983	2.384394	1.875572
H	3.982003	-1.539468	0.396678	H	0.092176	1.322744	0.900975
C	2.681747	-0.136649	3.766698	H	0.881020	2.541209	2.261689
H	0.870636	0.352102	2.710264				
C	3.954243	-0.705711	3.690418	TS19			
H	5.407137	-1.661449	2.406803	C	5.550271	-0.826890	0.745241
H	2.319598	0.270334	4.706439	C	4.157434	-0.899336	0.710641
H	4.587712	-0.744348	4.572587	C	3.480201	-1.571925	-0.320442
C	0.734137	-2.245776	-0.472447	C	4.240289	-2.179465	-1.338004
C	-0.126385	-2.419918	-1.567067	C	5.626570	-2.111932	-1.317626
C	1.092234	-3.344759	0.316044	C	6.279105	-1.434603	-0.273374
C	-0.614423	-3.689947	-1.876088	H	6.033719	-0.300734	1.561894
H	-0.420301	-1.567454	-2.172082	H	3.721512	-2.695916	-2.141378
C	0.603803	-4.613026	0.001046	H	6.206814	-2.582434	-2.105564
H	1.724893	-3.205322	1.185675	H	7.364025	-1.384186	-0.256189
C	-0.248251	-4.787683	-1.092776	C	2.045943	-1.566532	-0.289613
H	-1.283733	-3.818380	-2.721970	H	1.516758	-2.068563	-1.093875
H	0.877574	-5.462353	0.620344	C	1.354133	-0.917959	0.681651
H	-0.633631	-5.775557	-1.329285	O	3.466944	-0.290845	1.718652
C	2.556720	-0.179695	-1.386928	C	2.081630	-0.234347	1.754896
C	3.333464	0.982427	-1.235778	O	1.573803	0.388877	2.663322
C	2.775424	-1.025934	-2.482224	C	-0.148991	-0.823039	0.711482
C	4.306828	1.292995	-2.183438	C	-0.813925	-2.098725	0.127885
H	3.152666	1.661887	-0.408903	H	-0.774404	-2.117870	-0.961009

H	-0.188922	-2.926888	0.475901	H	-4.307683	-2.382090	2.627249
P	-0.723908	0.826812	-0.073537	H	-4.049938	-4.090049	2.244715
C	-0.721013	2.267350	1.045818	H	-3.364085	-3.410105	3.738848
C	-0.475487	3.540127	0.504830	O	-2.750817	-3.061790	-1.599953
C	-0.941207	2.130651	2.421528	O	-1.238067	-2.910193	2.648936
C	-0.468409	4.665364	1.329192	O	-2.574662	0.180697	1.184357
H	-0.282497	3.655632	-0.557024	H	-0.459200	-0.711713	1.750227
C	-0.906324	3.256176	3.244634	H	-3.375064	0.621424	0.858587
H	-1.143836	1.156629	2.842110				
C	-0.678224	4.523218	2.703138	TS20			
H	-0.288901	5.646360	0.898089	C	-5.106031	-1.536966	-2.438744
H	-1.059606	3.137809	4.313271	C	-3.783479	-1.108480	-2.452874
H	-0.659830	5.396830	3.349246	C	-3.298261	-0.177292	-1.535816
C	0.757868	1.219722	-1.138035	C	-4.171842	0.358626	-0.591895
C	0.839648	0.758739	-2.458432	C	-5.506003	-0.054355	-0.560643
C	1.898803	1.812825	-0.568324	C	-5.969601	-1.002457	-1.478178
C	2.030669	0.867173	-3.183786	H	-5.441707	-2.267510	-3.167850
H	-0.023404	0.311337	-2.937368	H	-3.795514	1.104581	0.101015
C	3.086429	1.920894	-1.289780	H	-6.183866	0.366506	0.176464
H	1.867537	2.181070	0.451418	H	-7.006368	-1.326078	-1.453118
C	3.159792	1.440544	-2.600165	C	-1.834934	0.210378	-1.642626
H	2.069825	0.500087	-4.205956	O	-1.530813	1.449332	-1.114049
H	3.957382	2.371568	-0.822099	C	-1.515077	0.253657	-3.112170
H	4.088982	1.513562	-3.158253	O	-2.940142	-1.666601	-3.421752
C	-2.067743	0.942897	-1.317295	C	-1.811362	-1.014977	-3.843091
C	-2.344029	-0.088435	-2.222397	O	-1.154008	-1.498303	-4.734278
C	-2.839497	2.115905	-1.359807	C	-0.791400	1.520625	-5.171888
C	-3.378520	0.047255	-3.150602	H	-0.944365	0.566506	-5.675918
H	-1.802987	-1.023461	-2.196903	H	-1.397647	2.293832	-5.653640
C	-3.862554	2.250404	-2.298696	H	0.255091	1.809348	-5.316670
H	-2.659975	2.917553	-0.652605	C	-1.112052	1.392121	-3.704701
C	-4.136811	1.217088	-3.198643	P	-1.121401	2.938346	-2.671577
H	-3.589927	-0.779483	-3.822221	C	-2.796270	3.424244	-2.144838
H	-4.450797	3.163933	-2.317508	C	-2.995998	4.113621	-0.943998
H	-4.940281	1.320781	-3.922557	C	-3.891916	3.046312	-2.929615
C	-4.644925	-3.012765	-0.190785	C	-4.292525	4.436757	-0.543382
H	-4.857034	-4.031147	0.155558	H	-2.155303	4.349918	-0.300891
H	-5.168283	-2.870825	-1.139913	C	-5.186424	3.366912	-2.518889
H	-5.033481	-2.313867	0.553772	H	-3.743354	2.481028	-3.845287
C	-3.154824	-2.838796	-0.452450	C	-5.388757	4.066843	-1.327918
C	-2.248848	-2.320095	0.599388	H	-4.445306	4.960593	0.396052
H	-2.637356	-1.086858	0.857680	H	-6.033633	3.055157	-3.122936
C	-2.282501	-2.843521	1.996947	H	-6.396980	4.310201	-1.004515
C	-3.586295	-3.203725	2.689721	C	0.252130	3.365774	-1.551331

C	0.437277	4.714434	-1.212039	C	-6.315531	-1.537316	0.085356
C	1.120448	2.388545	-1.055481	H	-6.593670	-1.441927	-2.062597
C	1.469348	5.075200	-0.346493	H	-3.706196	-0.128815	1.747897
H	-0.216200	5.479577	-1.619964	H	-5.742852	-1.486036	2.172410
C	2.169650	2.762540	-0.215240	H	-7.208406	-2.132944	0.256629
H	0.953123	1.340095	-1.267257	C	-2.823633	0.882499	-0.629227
C	2.339875	4.099535	0.148373	O	-3.096878	2.284572	-0.226450
H	1.596257	6.117229	-0.066354	C	-2.449425	0.876150	-2.061424
H	2.831339	1.997366	0.177649	O	-4.559083	-0.073359	-2.737133
H	3.145477	4.382012	0.820699	C	-3.324842	0.523100	-3.093011
C	-0.765192	4.214364	-3.986504	O	-3.162343	0.678065	-4.314242
C	0.556905	4.358438	-4.442250	C	-0.030885	0.920130	-2.703334
C	-1.756576	5.031848	-4.544037	H	0.043569	-0.158942	-2.595015
C	0.874891	5.278177	-5.439065	H	0.863318	1.449707	-3.025780
H	1.348256	3.754855	-4.006030	C	-1.202342	1.522856	-2.463816
C	-1.438687	5.959912	-5.541403	P	-1.165392	3.376977	-2.687659
H	-2.781673	4.959377	-4.199262	C	-2.816442	4.113762	-2.745285
C	-0.125477	6.082646	-5.994666	C	-3.123575	5.211051	-1.927503
H	1.903186	5.372447	-5.777292	C	-3.795293	3.574680	-3.594042
H	-2.221634	6.588237	-5.957414	C	-4.395236	5.779946	-1.976327
H	0.121234	6.804020	-6.768835	H	-2.388919	5.608712	-1.237352
H	-1.213526	-0.560453	-1.160529	C	-5.065734	4.149965	-3.631040
C	1.905753	-1.314128	1.737502	H	-3.590141	2.688441	-4.188944
H	2.417851	-1.068890	2.673258	C	-5.367787	5.252163	-2.829281
H	2.643949	-1.440112	0.937749	H	-4.628530	6.626333	-1.336298
H	1.396268	-2.278141	1.860326	H	-5.822559	3.716037	-4.278025
C	0.879886	-0.264550	1.316708	H	-6.361738	5.690659	-2.857384
C	0.560622	0.755563	2.270436	C	-0.242714	4.159185	-1.331587
H	1.102864	0.725384	3.209752	C	0.208165	5.483762	-1.457280
C	-0.387425	1.768151	2.150604	C	-0.006015	3.453108	-0.145775
C	-0.555882	2.737840	3.304476	C	0.894314	6.091006	-0.406518
H	0.080798	2.494223	4.159292	H	0.028058	6.035772	-2.375041
H	-0.316367	3.751447	2.959174	C	0.682909	4.065753	0.902720
H	-1.604045	2.744970	3.626256	H	-0.364572	2.436409	-0.042939
O	0.384838	-0.362368	0.175584	C	1.133162	5.381428	0.774709
O	-1.180712	2.019948	1.165143	H	1.242887	7.114597	-0.510709
H	-1.238302	1.538181	0.014591	H	0.865451	3.513063	1.819872
				H	1.670124	5.854439	1.592301
				C	-0.264233	3.792060	-4.214992
TS21				C	1.126362	3.988662	-4.189271
C	-5.984198	-1.154293	-1.211410	C	-0.940462	3.799037	-5.444272
C	-4.833893	-0.388643	-1.441359	C	1.825582	4.204058	-5.377071
C	-4.014764	0.006091	-0.374662	H	1.663735	3.980429	-3.246480
C	-4.355583	-0.409746	0.919365	C	-0.235253	4.015781	-6.627450
C	-5.496290	-1.173008	1.161811				

H	-2.009754	3.627786	-5.483215	C	-2.446117	0.125744	3.427179
C	1.146667	4.219955	-6.597947	C	-1.631319	2.374456	3.008579
H	2.900396	4.359696	-5.346140	C	-3.538024	0.648885	4.118311
H	-0.768536	4.018672	-7.573615	H	-2.360208	-0.947685	3.287240
H	1.692446	4.387323	-7.522255	C	-2.728396	2.891476	3.696939
H	-1.985440	0.557214	0.009708	H	-0.920043	3.042238	2.536452
H	-3.423682	2.281968	0.689455	C	-3.675668	2.031395	4.259957
				H	-4.290611	-0.022303	4.520733
TS7'				H	-2.851932	3.967605	3.777808
C	-4.969345	-1.852488	0.107067	H	-4.531955	2.439657	4.789835
C	-3.834946	-1.202632	-0.368150	C	1.073567	-0.296612	3.421822
C	-3.561618	0.131985	-0.028287	C	2.360156	-0.738598	3.072079
C	-4.453265	0.797281	0.816462	C	0.676116	-0.311635	4.763963
C	-5.599985	0.161073	1.296078	C	3.233345	-1.197881	4.055414
C	-5.860486	-1.163108	0.936825	H	2.678361	-0.715910	2.033192
H	-5.141897	-2.885366	-0.179500	C	1.556529	-0.771028	5.747438
H	-4.220562	1.822753	1.085296	H	-0.311823	0.038073	5.044043
H	-6.285873	0.696860	1.946841	C	2.831788	-1.215748	5.395670
H	-6.752638	-1.666134	1.300521	H	4.226470	-1.539114	3.777654
C	-2.357551	0.864572	-0.562750	H	1.243373	-0.776896	6.787647
H	-2.146385	0.664137	-1.628975	H	3.514233	-1.572609	6.161960
C	-1.175748	-0.906321	-0.035363				
O	-2.999852	-1.921985	-1.215826	VI'			
O	-1.967023	1.926534	-0.041488	C	-4.594030	-1.940028	0.283186
C	-1.620612	-1.860893	-1.019912	C	-3.694825	-1.114746	-0.389558
O	-0.914565	-2.491726	-1.784070	C	-3.661311	0.268556	-0.129181
C	-0.525806	-1.185963	1.097448	C	-4.546958	0.799690	0.816029
C	-0.198427	-2.556330	1.667415	C	-5.457785	-0.017696	1.481114
H	0.881764	-2.735932	1.714128	C	-5.480850	-1.389516	1.212200
H	-0.587514	-2.688278	2.685687	H	-4.591546	-3.002605	0.060898
H	-0.638568	-3.322802	1.024326	H	-4.500690	1.865781	1.011924
P	-0.036260	0.253099	2.084206	H	-6.144774	0.409942	2.205737
C	0.922615	1.493459	1.180287	H	-6.189719	-2.035256	1.724164
C	1.674238	2.423416	1.918872	C	-2.725420	1.170862	-0.847094
C	0.928848	1.535006	-0.218131	H	-2.311972	0.786148	-1.792748
C	2.417739	3.398058	1.256359	C	-1.001776	-0.894041	-0.075591
H	1.686934	2.380134	3.004288	O	-2.881063	-1.691208	-1.343574
C	1.687333	2.505917	-0.873397	O	-2.480776	2.313875	-0.480101
H	0.348876	0.814330	-0.780732	C	-1.475039	-1.687400	-1.156923
C	2.424425	3.438479	-0.141870	O	-0.811490	-2.226330	-2.025338
H	2.994812	4.118362	1.829279	C	-0.494223	-1.273697	1.097519
H	1.691103	2.535747	-1.958892	C	-0.377804	-2.663012	1.701268
H	3.007530	4.195927	-0.658634	H	0.663248	-2.958281	1.877257
C	-1.482084	0.988757	2.888283	H	-0.901081	-2.747378	2.663510

H	-0.820866	-3.381576	1.005540	H	-4.314508	2.323994	0.306982
P	-0.012004	0.148157	2.098569	H	-6.763021	1.820170	0.233977
C	0.949338	1.422553	1.228565	H	-7.558057	-0.274516	-0.852806
C	1.804563	2.236650	1.992455	C	-2.259729	0.761096	-0.694861
C	0.822277	1.640830	-0.149168	O	-1.861813	2.076172	-0.562160
C	2.526701	3.257973	1.377505	C	-1.744432	0.242799	-2.015386
H	1.911344	2.071961	3.060143	O	-3.344952	-1.546591	-1.912864
C	1.555613	2.661096	-0.756734	C	-2.105739	-1.153177	-2.361109
H	0.150725	1.011228	-0.721407	O	-1.427369	-1.945910	-2.971310
C	2.403541	3.470768	0.000903	C	-0.640855	0.847758	-4.199161
H	3.186623	3.883157	1.972419	H	-0.817713	-0.198230	-4.456919
H	1.452255	2.824918	-1.825313	H	-1.103446	1.497629	-4.948234
H	2.967063	4.267352	-0.477410	H	0.436528	1.033987	-4.257551
C	-1.473423	0.937882	2.827096	C	-1.158086	1.139025	-2.821297
C	-2.375761	0.143948	3.553583	P	-1.298152	2.895418	-2.126192
C	-1.704680	2.310461	2.687869	C	-2.997371	3.559817	-2.318853
C	-3.476920	0.730146	4.171044	C	-3.431700	4.649722	-1.555886
H	-2.223645	-0.928802	3.628667	C	-3.898416	2.917703	-3.177065
C	-2.816959	2.890730	3.302176	C	-4.751573	5.093461	-1.656629
H	-1.038186	2.918961	2.087659	H	-2.749594	5.139172	-0.867884
C	-3.693311	2.107072	4.053415	C	-5.219228	3.358549	-3.270557
H	-4.173808	0.111716	4.728909	H	-3.579281	2.060823	-3.763038
H	-3.000395	3.954170	3.179800	C	-5.649495	4.448799	-2.511862
H	-4.556672	2.562635	4.530759	H	-5.080109	5.938802	-1.057603
C	1.052506	-0.374571	3.483263	H	-5.911902	2.841899	-3.929104
C	2.254074	-1.027320	3.161095	H	-6.678732	4.789958	-2.581194
C	0.723351	-0.152263	4.825646	C	-0.175979	3.862239	-1.010568
C	3.110885	-1.456630	4.172050	C	-0.009511	5.237738	-1.229126
H	2.519990	-1.191053	2.119780	C	0.539635	3.243841	0.021955
C	1.585726	-0.584848	5.837073	C	0.834893	5.986876	-0.408931
H	-0.196924	0.360970	5.083648	H	-0.531008	5.726515	-2.045649
C	2.776214	-1.237429	5.512943	C	1.420085	3.986100	0.812198
H	4.038049	-1.961014	3.915383	H	0.396195	2.187190	0.211772
H	1.325593	-0.407499	6.876853	C	1.561468	5.360358	0.607002
H	3.444456	-1.573354	6.300931	H	0.936789	7.055712	-0.576286
				H	1.984003	3.490247	1.597738
				H	2.234428	5.939851	1.233342
VII'				C	-0.540984	3.712959	-3.689088
C	-5.582800	-0.937523	-1.385777	C	0.851869	3.634103	-3.862707
C	-4.227007	-0.631184	-1.327024	C	-1.282790	4.377972	-4.672741
C	-3.760333	0.526110	-0.701980	C	1.479882	4.181289	-4.979841
C	-4.682905	1.407908	-0.142391	H	1.461588	3.145413	-3.105008
C	-6.048785	1.123787	-0.195674	C	-0.659443	4.937198	-5.795643
C	-6.495959	-0.049914	-0.810694	H	-2.358391	4.474534	-4.572083
H	-5.904124	-1.849060	-1.879605				

C	0.722039	4.837690	-5.955911	C	1.546347	3.665698	0.562329
H	2.558866	4.102772	-5.087276	H	0.739836	2.000007	-0.551646
H	-1.259803	5.452751	-6.541253	C	1.532357	5.051859	0.741331
H	1.206939	5.270834	-6.826730	H	0.705326	6.928902	0.068556
H	-1.818403	0.165134	0.126372	H	2.205747	3.043756	1.161148
				H	2.174896	5.510410	1.487658
VIII'				C	-0.449060	3.854535	-3.990277
C	-5.897027	-0.604415	-1.437360	C	0.924982	4.138504	-4.065189
C	-4.522331	-0.375384	-1.351522	C	-1.267812	4.118947	-5.098415
C	-4.018498	0.668334	-0.566784	C	1.470228	4.665775	-5.236149
C	-4.903875	1.500957	0.115190	H	1.568398	3.948691	-3.212177
C	-6.282594	1.288228	0.029291	C	-0.718674	4.653581	-6.263404
C	-6.774701	0.230264	-0.741519	H	-2.331553	3.913643	-5.052810
H	-6.255510	-1.423521	-2.053138	C	0.650568	4.924258	-6.337184
H	-4.503930	2.323432	0.699245	H	2.534877	4.876245	-5.285098
H	-6.967621	1.943172	0.561097	H	-1.362570	4.857788	-7.114115
H	-7.845700	0.056142	-0.808822	H	1.075610	5.338037	-7.247337
C	-2.517383	0.796982	-0.532111	H	-2.128579	0.097546	0.231362
O	-2.146788	2.125106	-0.101810	H	-1.450988	2.050444	0.565478
C	-1.942951	0.469858	-1.894721				
O	-3.679454	-1.199732	-2.047486	XI			
C	-2.456011	-0.662331	-2.575657	C	-5.249402	-1.630365	-3.073915
O	-2.031878	-1.241087	-3.570769	C	-3.919818	-1.225901	-3.133861
C	-0.018153	0.837716	-3.460748	C	-3.339837	-0.448097	-2.131108
H	0.130511	-0.225736	-3.602295	C	-4.125036	-0.046717	-1.051942
H	0.529431	1.513067	-4.106870	C	-5.463771	-0.435739	-0.974378
C	-0.945672	1.267700	-2.557418	C	-6.021904	-1.231225	-1.980042
P	-1.129782	3.090816	-2.478039	H	-5.660893	-2.236763	-3.874549
C	-2.888173	3.515425	-2.433064	H	-3.679967	0.587742	-0.292923
C	-3.411077	4.536362	-1.632771	H	-6.072061	-0.112943	-0.134316
C	-3.745061	2.731694	-3.222383	H	-7.062931	-1.536478	-1.921253
C	-4.782993	4.786145	-1.637256	C	-1.879108	-0.070132	-2.296477
H	-2.764636	5.108536	-0.977357	O	-1.489857	1.074535	-1.627307
C	-5.116674	2.984545	-3.216960	C	-1.666709	0.160330	-3.771012
H	-3.350284	1.907388	-3.807325	O	-3.179051	-1.646399	-4.245509
C	-5.635949	4.010415	-2.426558	C	-2.078415	-0.943680	-4.672822
H	-5.187520	5.571582	-1.005047	O	-1.542368	-1.269194	-5.706507
H	-5.777827	2.355655	-3.804976	C	-1.090711	1.841885	-5.561369
H	-6.706868	4.190791	-2.407570	H	-1.332198	1.032395	-6.252791
C	-0.131661	3.870708	-1.173078	H	-1.701909	2.720178	-5.790902
C	-0.116021	5.263473	-1.018394	H	-0.051518	2.138284	-5.737899
C	0.717649	3.074660	-0.392925	C	-1.284599	1.390853	-4.143170
C	0.704701	5.849466	-0.053321	P	-1.257551	2.588019	-2.684440
H	-0.723301	5.892993	-1.661755	C	-2.943420	3.093206	-2.169787

C	-3.182056	3.590930	-0.883737	H	-1.532219	2.701864	3.409768
C	-4.019147	2.888122	-3.042290	O	-0.245315	-0.751767	0.260449
C	-4.484921	3.891641	-0.483263	O	-1.234034	1.612523	1.067881
H	-2.362166	3.705067	-0.183202	H	-1.106894	0.923805	0.358888
C	-5.321600	3.181143	-2.635000				
H	-3.848252	2.483437	-4.035764	XVII			
C	-5.557880	3.687317	-1.355330	C	-5.152986	-1.470141	-2.380073
H	-4.662176	4.272037	0.519411	C	-3.854331	-1.001107	-2.218155
H	-6.149734	3.003724	-3.315627	C	-3.544391	0.024577	-1.325931
H	-6.571976	3.911927	-1.036182	C	-4.570404	0.607525	-0.586176
C	0.122175	2.972588	-1.512722	C	-5.883800	0.154210	-0.733256
C	0.239591	4.266224	-0.988579	C	-6.173094	-0.883027	-1.625389
C	1.053687	1.994336	-1.146232	H	-5.349275	-2.276111	-3.079958
C	1.251666	4.566212	-0.075335	H	-4.322522	1.420704	0.088104
H	-0.455486	5.042420	-1.292783	H	-6.680807	0.611420	-0.153713
C	2.090983	2.308187	-0.266926	H	-7.193327	-1.238960	-1.738030
H	0.945690	0.982702	-1.518146	C	-2.091325	0.438533	-1.230192
C	2.184996	3.589395	0.281743	O	-1.905363	1.700802	-0.675992
H	1.318917	5.567081	0.343003	C	-1.528458	0.376313	-2.629274
H	2.811541	1.542367	0.006191	O	-2.849628	-1.620382	-2.966666
H	2.981690	3.826244	0.982103	C	-1.662784	-0.988702	-3.238527
C	-0.855961	4.128046	-3.755197	O	-0.847552	-1.556214	-3.923309
C	0.461149	4.278054	-4.223911	C	-0.410647	1.331871	-4.687399
C	-1.785571	5.116395	-4.101089	H	-0.403609	0.298503	-5.029706
C	0.833617	5.358873	-5.020711	H	-0.933864	1.959127	-5.415789
H	1.215756	3.542184	-3.952910	H	0.629037	1.677387	-4.660017
C	-1.418701	6.210032	-4.895745	C	-1.030884	1.425189	-3.312333
H	-2.808823	5.049331	-3.748163	P	-1.193298	3.130546	-2.629731
C	-0.110578	6.333397	-5.362217	C	-2.921810	3.544759	-2.257613
H	1.859438	5.445929	-5.370088	C	-3.242148	4.399992	-1.198004
H	-2.160657	6.964837	-5.144693	C	-3.936069	2.989706	-3.046777
H	0.175317	7.181056	-5.979390	C	-4.577578	4.710270	-0.943829
H	-1.256163	-0.912471	-1.951191	H	-2.462407	4.784714	-0.549578
C	1.362339	-1.920338	1.599109	C	-5.270379	3.301673	-2.784180
H	2.395883	-1.566700	1.705236	H	-3.693996	2.292320	-3.843274
H	1.308616	-2.653325	0.791342	C	-5.592494	4.165564	-1.736371
H	1.086689	-2.399995	2.546655	H	-4.825555	5.363750	-0.112296
C	0.432523	-0.759212	1.303196	H	-6.054309	2.850911	-3.385379
C	0.374897	0.318005	2.266162	H	-6.631983	4.400984	-1.526165
H	0.994688	0.262758	3.154633	C	0.041030	3.669822	-1.422958
C	-0.432486	1.412606	2.107096	C	0.180791	5.047263	-1.178303
C	-0.495112	2.536307	3.095241	C	0.896858	2.747332	-0.815491
H	0.120171	2.333939	3.974849	C	1.163079	5.491798	-0.297105
H	-0.144826	3.458253	2.615584	H	-0.459375	5.766616	-1.680966

C	1.896724	3.208471	0.044690	H	-1.527753	-0.302406	-0.642253
H	0.769321	1.678756	-0.958529	C	2.126395	-1.558584	0.883364
C	2.024823	4.571010	0.311180	H	2.695235	-1.633616	1.815579
H	1.262030	6.554241	-0.093000	H	2.820630	-1.429866	0.044407
H	2.542972	2.485159	0.530881	H	1.594427	-2.503047	0.715138
H	2.792838	4.921063	0.995688	C	1.115480	-0.413736	0.880901
C	-0.786536	4.213972	-4.063508	C	0.984513	0.343223	2.077846
C	0.563692	4.446056	-4.375917	H	1.636824	0.060672	2.898057
C	-1.779831	4.797311	-4.861198	C	0.074373	1.386610	2.345755
C	0.910539	5.231078	-5.473537	C	0.135979	2.031193	3.725762
H	1.345664	4.020688	-3.754298	H	0.891389	1.583036	4.378298
C	-1.429593	5.587301	-5.959451	H	0.351315	3.100867	3.610331
H	-2.827586	4.649645	-4.625898	H	-0.846680	1.951807	4.205980
C	-0.086420	5.802474	-6.270309	O	0.475808	-0.226339	-0.185827
H	1.958626	5.401203	-5.702913	O	-0.804797	1.876069	1.572291
H	-2.210408	6.037422	-6.566056	H	-1.353773	1.644017	0.192466
H	0.184363	6.417969	-7.123628				