

Electronic Supplementary Information

Understanding the Insertion Reactions of CO₂, Aldehyde and Alkene into Cu-X (X = B, C, O) Bonds

Xueying Guo and Zhenyang Lin*

Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay,
Kowloon, Hong Kong, P.R. China.

*Corresponding author e-mail: chzlin@ust.hk (Z. Y. Lin)

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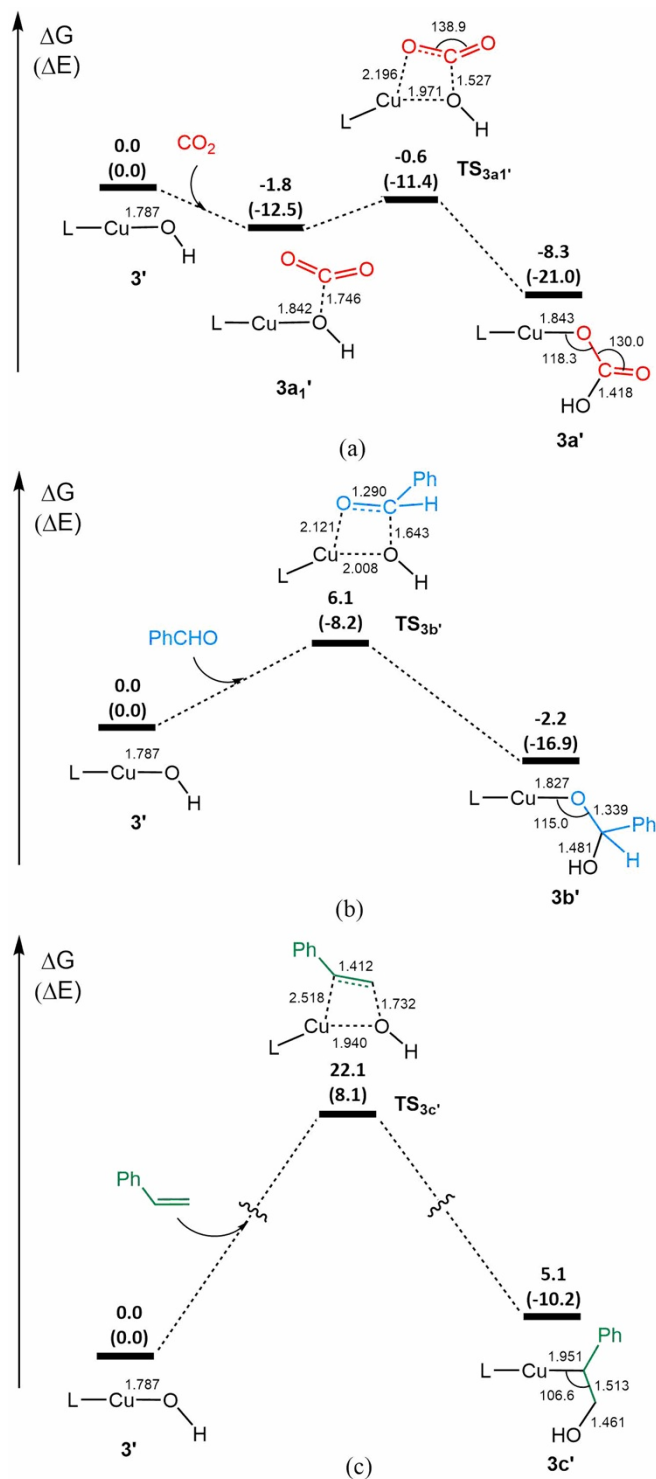


Figure S1. Energy profiles calculated for the insertion of (a) CO₂, (b) PhCHO, and (c) styrene into the Cu-OH bond in (NHC)CuOH (**3'**). Relative free energies and electronic energies (in parenthesis) are given in kcal/mol.

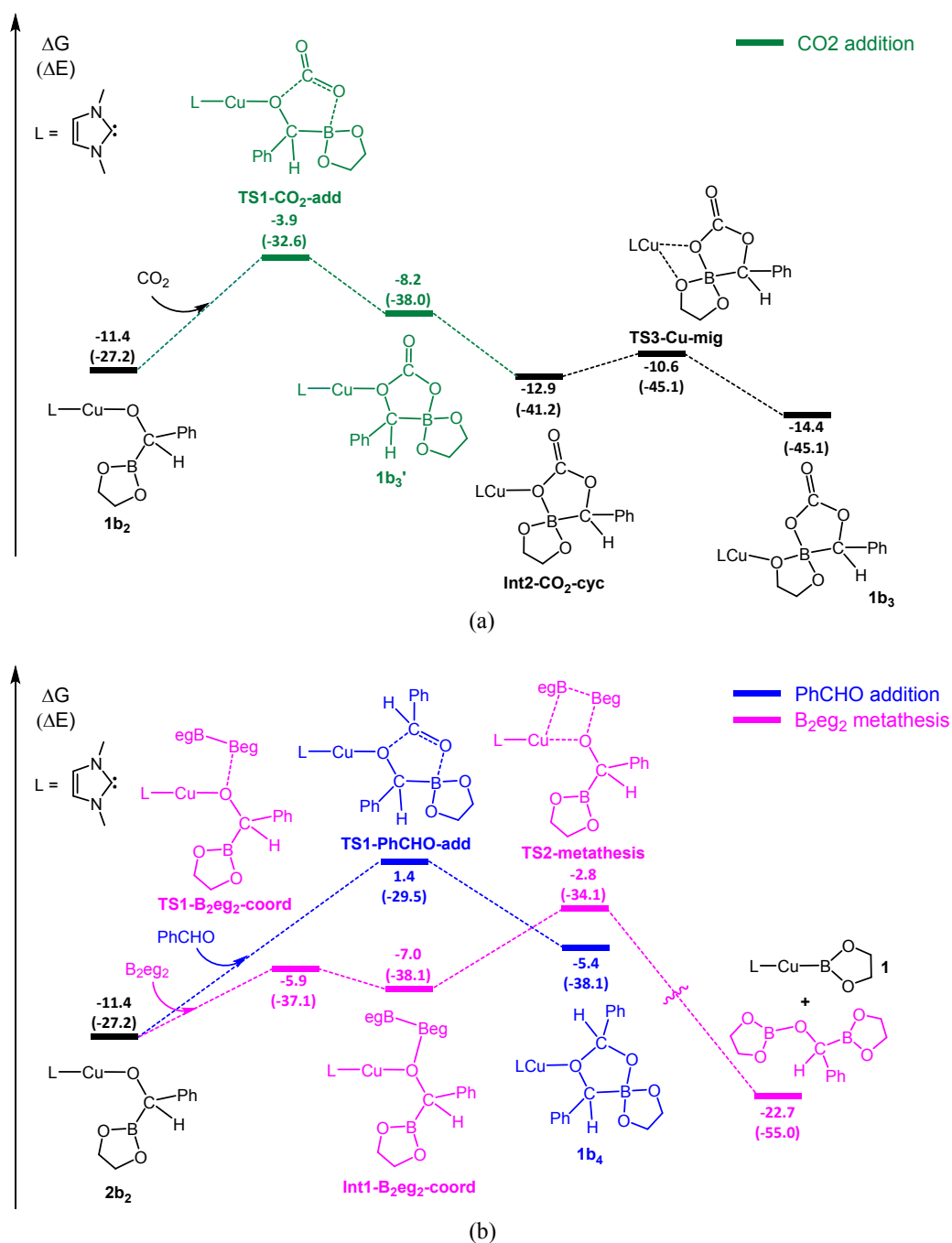


Figure S2. Energy profiles calculated for other possible pathways and processes that are relevant to the reaction mechanism for the reactions shown equation (2). (a) [2+3] cycloaddition of one CO_2 C=O double bond with the O-C-B unit of $\mathbf{1b}_2$ and (b) [2+3] cycloaddition of one PhCHO C=O double bond with the O-C-B unit of $\mathbf{1b}_2$ and the possible metathesis reaction of $\mathbf{1b}_2$ with B_2eg_2 . Relative free energies and electronic energies (in parenthesis) are given in kcal/mol.

Table S1. NPA charges of LCu, Beg and the CO₂, PhCHO and styrene fragments in reactants, rate-determining transition states and products in the reactions of **1** with small molecules.

	LCu	Beg	CO ₂
1	0.513	-0.513	0.000
TS_{1a2}	0.946	-0.260	-0.685
1a₂	0.823	0.103	-0.926
	LCu	Beg	PhCHO
1	0.513	-0.513	0.000
TS_{1b2}	1.046	-0.180	-0.866
1b₂	0.805	0.255	-1.061
	LCu	Beg	styrene
1	0.513	-0.513	0.000
TS_{1c2}	1.067	-0.176	-0.892
1c₂	0.747	0.279	-1.026

Table S2. NPA charges of LCu, CH₃ and the CO₂, PhCHO and styrene fragments in reactants, rate-determining transition states and products in the reactions of **2** with small molecules.

	LCu	CH ₃	CO ₂
2	0.655	-0.655	0.000
TS_{2a}	0.918	-0.378	-0.540
2a	0.821	-0.117	-0.704
	LCu	CH ₃	PhCHO
2	0.655	-0.655	0.000
TS_{2b2}	0.947	-0.354	-0.593
2b₂	0.797	-0.041	-0.756
	LCu	CH ₃	styrene
2	0.655	-0.655	0.000
TS_{2c2}	0.954	-0.254	-0.700
2c₂	0.742	-0.023	-0.720

Table S3. NPA charges of LCu, OR (R = CHPhBeg) and the CO₂, PhCHO and styrene fragments in reactants, rate-determining transition states and products in the reactions of **3** with small molecules.

	LCu	OR	CO ₂
3(1b₂)	0.805	-0.805	0.000
TS_{3a}	0.882	-0.464	-0.418
3a	0.840	-0.376	-0.464
	LCu	OR	PhCHO
3(1b₂)	0.805	-0.805	0.000
TS_{3b}	0.876	-0.522	-0.354
3b	0.825	-0.418	-0.407
	LCu	OR	styrene
3(1b₂)	0.805	-0.805	0.000
TS_{3c}	0.879	-0.573	-0.306
3c	0.761	-0.363	-0.398

Cartesian coordinates for all optimized structures

I				TS_{1a2}			
Cu	-0.223904	-0.000001	0.000005	Cu	-0.031710	-0.498503	-0.146806
B	-2.206704	0.000000	0.000005	B	1.874592	0.097491	0.116694
O	-3.006104	1.139401	0.075905	O	2.498392	0.159689	1.342394
O	-3.006105	-1.139399	-0.075895	O	2.302795	1.081589	-0.756506
C	1.693696	-0.000002	0.000005	C	-1.802308	0.166803	-0.022606
N	2.536095	-1.071902	0.014905	N	-2.261104	1.426305	-0.254806
N	2.536096	1.071898	-0.014895	N	-2.911910	-0.534993	0.335194
C	3.866195	-0.679203	0.009505	C	-3.628103	1.509410	-0.044306
C	3.866196	0.679197	-0.009495	C	-4.039408	0.269311	0.330094
C	-4.392904	0.770702	0.049505	C	3.472996	1.216685	1.292794
C	-4.392905	-0.770698	-0.049595	C	3.486797	1.670085	-0.184306
C	2.067097	2.451598	-0.034795	C	-2.894015	-1.954993	0.678594
C	2.067094	-2.451602	0.034805	C	-1.415400	2.538502	-0.677106
H	2.415194	-2.963702	0.937405	C	1.578585	-1.755108	-0.485506
H	4.682195	-1.385703	0.019505	O	2.733185	-1.822512	-0.855606
H	4.682197	1.385697	-0.019495	O	0.620183	-2.538205	-0.371706
H	-4.881305	-1.135698	-0.961595	H	-4.180700	2.426512	-0.179606
H	-4.877805	-1.249498	0.810205	H	-5.019309	-0.103086	0.586694
H	-4.877804	1.249502	-0.810195	H	4.439794	0.827582	1.625894
H	-4.881304	1.135702	0.961605	H	3.162098	2.016986	1.975794
H	2.415197	2.963698	-0.937395	H	4.361496	1.289882	-0.724106
H	0.976097	2.423799	-0.030295	H	3.442301	2.757485	-0.302406
H	2.421797	2.991498	0.848905	H	-3.592217	-2.504390	0.040594
H	0.976094	-2.423701	0.030305	H	-1.882617	-2.329996	0.513794
H	2.421694	-2.991502	-0.848895	H	-3.171016	-2.095992	1.727694
CO₂				H			
C	0.000000	0.000000	0.000000	H	-0.387901	2.177298	-0.742906
O	0.000000	0.000000	1.160443	H	-1.734799	2.906503	-1.656806
O	0.000000	0.000000	-1.160443	H	-1.470697	3.352502	0.052094
TS_{1a1}				1a₂			
Cu	-0.057103	0.256896	-0.048906	Cu	-0.388015	-0.958125	-0.181529
B	-1.910903	-0.338105	0.211094	B	2.611499	-0.034111	0.070606
O	-2.679503	-0.097505	1.333594	O	3.378852	0.255950	1.166816
O	-2.549902	-1.190505	-0.673706	O	2.123561	1.101602	-0.555097
C	1.841397	-0.212002	0.024294	C	-1.961659	0.003676	-0.039124
N	2.359198	-1.433902	-0.285706	N	-2.203212	1.269963	-0.479708
N	2.924297	0.509198	0.424394	N	-3.148805	-0.392660	0.500727
C	3.729698	-1.472801	-0.086606	C	-3.509903	1.653287	-0.221418
C	4.087297	-0.242501	0.364494	C	-4.107576	0.603303	0.399115
C	-3.917602	-0.820306	1.220994	C	3.393293	1.678329	1.352765
C	-3.877502	-1.458606	-0.185506	C	2.718086	2.246923	0.083812
C	2.866096	1.894298	0.881694	C	-3.362452	-1.702268	1.104238
C	1.559299	-2.552103	-0.774806	C	-1.209312	2.094244	-1.160803
H	4.320599	-2.354601	-0.282006	C	2.341868	-1.511691	-0.448626
H	5.050697	0.156500	0.643294	O	3.291267	-2.151503	-0.880725
H	-4.751503	-0.121907	1.346294	O	1.117098	-1.968868	-0.373469
H	-3.967802	-1.568006	2.022094	H	-3.895322	2.622530	-0.496346
H	-4.603002	-1.006507	-0.871406	H	-5.112778	0.482311	0.771196
H	-4.042601	-2.541606	-0.168406	H	4.426404	2.017920	1.471394
H	3.567295	2.506799	0.307394	H	2.839233	1.924472	2.266514
H	1.855196	2.266198	0.722394	H	3.438923	2.700860	-0.605529
H	3.120796	1.953399	1.944694	H	1.940203	-2.984200	0.308053
H	0.510099	-2.256003	-0.728806	H	-4.164810	-2.236090	0.587789
H	1.825499	-2.791302	-1.809106	H	-2.433597	-2.264624	1.005356
H	1.718399	-3.432802	-0.145406	H	-3.615036	-1.602073	2.163552
C	-1.188404	2.038196	-0.723506	H	-0.249579	1.576589	-1.122942
O	-2.315004	2.155895	-1.058306	H	-1.495680	2.254208	-2.204299
O	-0.078005	2.489396	-0.591006	H	-1.119197	3.062485	-0.660506
1a₁				PhCHO			
Cu	0.074088	-0.557905	-0.138444	C	0.043051	-1.099601	0.000048
B	1.790039	0.327545	0.180632	C	0.532824	0.212712	0.000067
O	2.534584	0.253774	1.335503	C	-0.359539	1.288918	0.000055
O	2.332018	1.217924	-0.731544	C	-1.732363	1.059436	-0.000053
C	-1.719366	0.235773	-0.015961	C	-2.213856	-0.248491	-0.000061
N	-2.086161	1.511203	-0.319415	C	-1.325928	-1.327731	0.000033
N	-2.868854	-0.339115	0.433206	H	0.754472	-1.916984	0.000048
C	-3.431513	1.726399	-0.065280	H	0.026108	2.303928	0.000135
C	-3.926557	0.555931	0.413805	H	-2.424521	1.893525	-0.000115
C	3.668532	1.132606	1.221677	H	-3.282993	-0.429409	-0.000137
C	3.587316	1.702775	-0.213010	H	-1.707737	-2.342289	0.000100
C	-2.966608	-1.720250	0.897053	C	1.992540	0.465463	0.000035
C	-1.186008	2.520869	-0.869827	H	2.272474	1.541738	0.000047
C	1.147475	-2.196813	-0.543847	O	2.842727	-0.394344	-0.000102
O	2.286373	-2.522150	-0.650637	TS_{1b1}			
O	-0.021146	-2.585319	-0.630566	C	2.195653	0.293623	0.123127
H	-3.911614	2.675378	-0.249126	N	2.709420	0.311065	1.387612
H	-4.920842	0.286738	0.736121	C	4.082602	0.126723	1.386252
H	4.582763	0.557173	1.398113	H	4.667027	0.100752	2.293288
H	3.592890	1.911164	1.990010	C	4.449091	-0.002599	0.085073
H	4.396143	1.339214	-0.856192	H	5.418222	-0.154445	-0.365213
H	3.586873	2.797805	-0.238586	N	3.288995	0.100892	-0.666375
H	-3.798601	-2.222395	0.395134	C	1.898104	0.493406	2.585482
H	-2.038193	-2.234202	0.649043	H	2.356815	1.243293	3.236588
H	-3.127219	-1.748536	1.979559	H	0.912868	0.841270	2.269984
H	-0.170658	2.122978	-0.865810	H	1.794086	-0.449185	3.132779
H	-1.475358	2.767712	-1.896180	C	3.257391	0.064383	-2.125715
H	-1.224054	3.426300	-0.256606	H	3.876094	-0.763672	-2.483613

H	2.228096	-0.095505	-2.445596	C	-2.808073	-1.515678	0.970226
H	3.641335	1.004216	-2.536705	C	-4.742736	0.103409	-0.209257
O	-1.440793	2.722665	0.897275	H	-3.274847	0.468967	-1.739293
O	-2.499343	1.699396	-0.847178	C	-4.057219	-1.372511	1.566865
C	-2.741960	3.331014	0.840705	H	-2.051729	-2.172238	1.382679
C	-3.395900	2.741881	-0.426329	C	-5.029000	-0.559559	0.983825
B	-1.330390	1.743194	-0.083988	H	-5.499639	0.720697	-0.682362
C	-0.780294	-0.859889	-1.677685	H	-4.280330	-1.907005	2.484694
O	0.326915	-1.076701	-2.183848	H	-6.004397	-0.454685	1.446553
H	-1.484761	-0.143742	-2.122983	Cu	0.745103	-0.714180	-0.161077
C	-1.347311	-1.742878	-0.620979	H	-0.702093	3.675794	0.710160
C	-2.669186	-1.577673	-0.189851	H	-2.293826	2.976407	0.320688
C	-0.589725	-2.811284	-0.127806	H	-1.694401	3.327082	-1.984853
C	-3.217990	-2.458434	0.734916	H	0.028576	3.518810	-1.581324
H	-3.239156	-0.735994	-0.566274				
C	-1.137706	-3.686779	0.802927	1b₂/3			
H	0.421511	-2.936448	-0.495663	C	2.529085	0.095311	0.043900
C	-2.452857	-3.513141	1.235728	N	2.743310	0.460561	1.341013
H	-4.241492	-2.326126	1.068300	C	4.069882	0.287429	1.704673
H	-0.547059	-4.512847	1.184261	H	4.434232	0.518345	2.694023
H	-2.882031	-4.199807	1.957324	C	4.712846	-0.197141	0.611097
Cu	0.315436	0.658062	-0.293841	H	5.747247	-0.465633	0.460181
H	-2.630440	4.419885	0.796472	N	3.759535	-0.309832	-0.389092
H	-3.294653	3.078369	1.754227	C	1.690127	0.934659	2.231460
H	-4.386448	2.314296	-0.236402	H	1.976434	1.893762	2.674402
H	-3.488304	3.479201	-1.233167	H	0.780716	1.062757	1.642276
				H	1.507896	0.207412	3.029245
1b₁				C	4.015017	-0.794524	-1.738790
C	2.342403	-0.343830	0.158674	H	4.490421	-1.779547	-1.705858
N	2.992181	0.248400	1.197911	H	3.051254	-0.873081	-2.244677
C	4.333168	-0.101869	1.222077	H	4.657856	-0.098328	-2.287100
H	5.011316	0.259138	1.980057	O	-1.148698	1.916413	0.309210
C	4.537119	-0.928892	0.164693	O	-3.247423	2.050245	-0.596198
H	5.430692	-1.420056	-0.189035	C	-1.698351	3.142585	0.815992
N	3.312112	-1.067186	-0.467764	C	-3.161237	3.160636	0.307182
C	2.353368	1.091665	2.205530	B	-2.074593	1.335950	-0.537615
H	3.050655	1.878919	2.505628	C	-1.817998	-0.001293	-1.338573
H	1.456306	1.546478	1.783098	O	-0.550334	-0.021649	-1.926636
H	2.084835	0.497852	3.085598	H	-2.579681	-0.046548	-2.138541
C	3.093005	-1.864918	-1.672030	C	-2.126273	-1.196818	-0.422252
H	3.582089	-2.836702	-1.559512	C	-3.384653	-1.348851	0.176435
H	2.019138	-2.014166	-1.795172	C	-1.148716	-2.158260	-0.166262
H	3.506104	-1.354031	-2.548371	C	-3.653807	-2.432011	1.007550
O	-0.310640	2.477555	0.716276	H	-4.158741	-0.612099	-0.019774
O	-0.984383	2.261487	-1.455993	C	-1.416963	-3.247812	0.661598
C	-1.060630	3.674775	0.433463	H	-0.194135	-2.049086	-0.667537
C	-1.337712	3.605250	-1.081722	C	-2.667568	-3.388120	1.257366
B	-0.338786	1.641956	-0.397237	H	-4.635695	-2.535257	1.458399
C	-1.069265	-1.170065	-1.151516	H	-0.646720	-3.992389	0.838144
O	-0.077240	-1.982458	-0.971688	H	-2.877451	-4.235216	1.901620
H	-1.247169	-0.762328	-2.156320	Cu	0.940080	0.081030	-0.897773
C	-2.285494	-1.247835	-0.297397	H	-1.109212	3.982134	0.429023
C	-3.369338	-0.390558	-0.527377	H	-1.630075	3.143219	1.908997
C	-2.384559	-2.213200	0.710382	H	-3.887019	3.018334	1.116024
C	-4.523276	-0.490107	0.240755	H	-3.413303	4.081668	-0.228049
H	-3.286659	0.366276	-1.300800				
C	-3.540755	-2.311348	1.479189	Styrene			
H	-1.548292	-2.884841	0.863648	C	-1.952494	-0.527619	-0.000363
C	-4.613703	-1.451543	1.249100	C	-2.972223	0.334342	0.000456
H	-5.355834	0.180224	0.055151	C	-0.513831	-0.220093	-0.000220
H	-3.609592	-3.066630	2.255060	C	0.406032	-1.279005	0.000002
H	-5.514963	-1.531143	1.847006	C	1.777815	-1.043969	0.000224
Cu	0.471544	-0.166973	-0.407900	C	2.260945	0.261034	0.000179
H	-0.468578	4.549385	0.722512	C	1.359787	1.326617	-0.000079
H	-1.981068	3.663932	1.029355	C	-0.008409	1.090261	-0.000289
H	-2.388111	3.785013	-1.332175	H	-2.185251	-1.590530	-0.001169
H	-0.719640	4.308800	-1.653157	H	-3.996715	-0.017193	0.000256
				H	-2.832815	1.409726	0.001404
TS_{1b2}				H	0.035285	-2.298888	0.000027
C	2.510149	-0.281370	0.242664	H	2.468081	-1.880083	0.000418
N	3.037282	0.491869	1.234161	H	3.328483	0.449219	0.000324
C	4.419918	0.555873	1.139688	H	1.728175	2.346468	-0.000153
H	5.021075	1.112409	1.842159	H	-0.690982	1.931867	-0.000572
C	4.773141	-0.183588	0.057040				
H	5.740574	-0.386350	-0.376001	TS_{1c1}			
N	3.597643	-0.690830	-0.474740	C	1.139415	1.620003	-0.261498
C	2.246496	1.114517	2.290014	N	1.635669	2.765211	0.293327
H	2.681453	2.085315	2.543488	C	2.879123	3.093191	-0.228013
H	1.226576	1.258673	1.928140	H	3.428374	3.968487	0.083837
H	2.231025	0.484127	3.185509	C	3.177386	2.132643	-1.139514
C	3.501358	-1.542848	-1.653649	H	4.039674	2.005631	-1.776235
H	4.261888	-2.327452	-1.610009	N	2.107908	1.249394	-1.147682
H	2.509014	-1.999809	-1.655201	C	0.932575	3.538084	1.307204
H	3.632645	-0.958896	-2.570467	H	0.858183	4.586444	1.002066
O	-0.765746	1.603464	0.569280	H	-0.071132	3.121619	1.406259
O	-0.637884	1.561585	-1.720065	H	1.448476	3.477874	2.271397
C	-1.216386	2.900502	0.133712	C	2.025210	0.060420	-1.988524
C	-0.877196	2.936962	-1.370803	H	0.996179	-0.299304	-1.961402
B	-0.527467	0.827010	-0.556486	H	2.297069	0.314124	-3.017598
C	-1.153774	-1.042149	-0.863728	H	2.684151	-0.728933	-1.615080
O	-0.487171	-2.162512	-0.494706	O	-3.550497	1.274695	-0.558300
H	-1.231787	-0.891783	-1.953220	O	-3.053023	-0.903485	-0.090359
C	-2.506628	-0.839222	-0.214582	C	-4.809832	0.584983	-0.594208
C	-3.491465	-0.037912	-0.803635	C	-4.449229	-0.905754	-0.430321
				B	-2.530123	0.391870	-0.224094

C	0.589160	-0.858013	1.942793	H	-1.788802	-1.491211	1.070279
H	1.409223	-0.303976	2.391807	C	-4.816200	0.036451	0.861158
C	0.979910	-1.942124	1.039777	H	-5.568943	1.022772	-0.901239
C	2.302858	-2.416662	1.048960	H	-3.778979	-1.035587	2.410947
C	0.074473	-2.513051	0.124427	H	-5.696834	0.235737	1.461010
C	2.708084	-3.438120	0.196525	Cu	0.345468	-0.027574	-0.634715
H	3.014302	-1.980321	1.743483	C	-0.340496	-1.796658	-1.179857
C	0.484974	-3.535313	-0.725854	H	-0.752542	-2.583237	-0.544587
H	-0.946500	-2.152957	0.073533	H	0.152350	-2.220386	-2.052685
C	1.798285	-4.004432	-0.696561	H	2.695143	-2.348043	2.436651
H	3.731670	-3.795982	0.230876	H	4.028876	-2.923712	0.519008
H	-0.227146	-3.965443	-1.422104	H	2.867414	-4.168466	0.002569
H	2.109317	-4.802796	-1.361256	H	1.843907	-3.885805	2.160697
Cu	-0.609343	0.821093	0.029277	1c₂			
C	-0.675538	-0.487897	2.220806	C	-2.321657	-0.464796	-0.043696
H	-1.533390	-1.057092	1.893172	N	-3.307486	0.475750	-0.008402
H	-0.868156	0.322461	2.914220	C	-4.468311	-0.024416	0.560905
H	-4.592102	-1.475709	-1.357072	H	-5.360762	0.571236	0.678163
H	-5.313721	0.799595	-1.543216	C	-4.208369	-1.313980	0.899307
H	-5.444106	0.954166	0.221808	H	-4.828715	-2.059763	1.372543
H	-5.016822	-1.398608	0.366721	N	-2.897208	-1.563011	0.523840
1c₁				C	-3.148298	1.827007	-0.534580
C	0.368637	1.491248	-0.004955	H	-3.546448	2.552700	0.180950
N	1.183256	2.467739	-0.500830	H	-2.082461	2.010236	-0.679981
C	0.990468	3.673948	0.155668	H	-3.676316	1.935034	-1.487896
H	1.535959	4.567745	-0.105112	C	-2.203099	-2.831255	0.713386
C	0.035149	3.455032	1.093747	H	-1.173797	-2.701596	0.376063
H	-0.409660	4.116820	1.820786	H	-2.203122	-3.111197	1.771178
N	-0.336689	2.122768	0.975849	H	-2.682064	-3.622435	0.127871
C	2.147396	2.246130	-1.574459	O	0.232393	2.667707	-0.080236
H	2.806306	3.115066	-1.640450	O	2.476758	2.810678	0.338341
H	2.740619	1.354353	-1.354712	C	0.344237	3.505967	1.078806
H	1.633616	2.118479	-2.532527	C	1.867175	3.707728	1.273974
C	-1.293847	1.464598	1.857328	B	1.499498	2.238512	-0.444928
H	-1.707285	0.593823	1.350345	C	1.236977	-0.193798	-1.458829
H	-0.807451	1.148660	2.786564	H	1.191125	-0.653457	-2.454313
H	-2.108073	2.155207	2.091424	C	2.029346	-1.105092	-0.586324
O	3.431264	-0.753954	-0.409791	C	1.915041	-2.504527	-0.755676
O	2.384546	-1.943552	1.237612	C	2.902564	-0.671357	0.430210
C	4.489497	-1.447114	0.279160	C	2.597624	-3.405357	0.049068
C	3.789959	-2.156075	1.458742	H	1.271583	-2.876030	-1.549465
B	2.203066	-1.098809	0.155279	C	3.583932	-1.577206	1.243617
C	-1.231894	-0.969403	-1.571702	H	3.057910	0.388861	0.590525
H	-1.277619	-0.378267	-2.481426	C	3.438234	-2.950049	1.068987
C	-2.451590	-0.929655	-0.756064	H	2.484392	-4.471656	-0.124107
C	-3.474121	-0.013508	-1.071227	H	4.246683	-1.199083	2.016546
C	-2.662565	-1.769235	0.356460	H	3.974277	-3.650685	1.699464
C	-4.639246	0.065524	-0.318263	Cu	-0.575085	-0.296385	-0.746889
H	-3.342287	0.643126	-1.925727	C	1.777912	1.252577	-1.624192
C	-3.828244	-1.686548	1.111268	H	2.854650	1.254301	-1.854090
H	-1.904204	-2.490270	0.638141	H	1.275126	1.679669	-2.502394
C	-4.826312	-0.768937	0.784362	H	2.202000	3.457033	2.285491
H	-5.408327	0.779530	-0.594628	H	-0.122235	2.998324	1.931688
H	-3.960011	-2.348771	1.960800	H	-0.189111	4.445272	0.898103
H	-5.735230	-0.710596	1.372231	H	2.187055	4.730931	1.045381
Cu	0.450804	-0.382769	-0.516036	2			
C	-0.230551	-1.959517	-1.479660	Cu	-1.439043	0.000091	0.000970
H	-0.353009	-2.816138	-0.827418	C	0.448280	0.000004	0.000690
H	0.391771	-2.151398	-2.346818	N	1.292641	1.072554	0.000107
H	4.067859	-1.728487	2.429902	N	1.292547	-1.072621	-0.000271
H	5.244468	-0.722513	0.604061	C	2.622579	0.678900	-0.001228
H	4.964359	-2.151892	-0.413981	C	2.622519	-0.679085	-0.001454
H	3.990696	-3.232565	1.487072	C	0.827665	-2.453111	0.000822
TS_{1c2}				C	0.827879	2.453084	0.000667
C	1.141495	1.571823	-0.071216	H	1.177364	2.977976	-0.894149
N	2.410989	2.029565	-0.281679	H	3.438475	1.385618	-0.001831
C	2.602434	3.269539	0.309559	H	3.438354	-1.385874	-0.002163
H	3.536958	3.804592	0.240411	H	1.180379	-2.977953	0.894395
C	1.433805	3.593871	0.920127	H	-0.263298	-2.426624	0.001215
H	1.155720	4.460065	1.500446	H	1.179986	-2.979243	-0.892137
N	0.553101	2.553047	0.672860	H	-0.263080	2.426694	0.004480
C	3.410715	1.320119	-1.068642	H	1.183516	2.979105	0.892372
H	4.404322	1.519987	-0.658356	C	-3.360044	-0.000062	-0.001609
H	3.205963	0.248506	-1.014713	H	-3.785922	-0.877593	-0.514678
H	3.385482	1.641059	-2.115776	H	-3.797059	-0.001860	1.009781
C	-0.821099	2.479355	1.158795	H	-3.786051	0.879196	-0.511604
H	-1.411702	1.893656	0.452066	TS_{2a}			
H	-0.863315	1.997210	2.140467	Cu	0.720559	-0.498552	-0.188750
H	-1.234074	3.488472	1.230515	C	-1.093603	-0.032772	-0.038234
O	2.383912	-2.229855	-0.544043	N	-2.171923	-0.852815	0.111263
O	0.983550	-2.220375	1.275871	N	-1.622802	1.220547	-0.025604
C	2.964791	-3.150071	0.398431	C	-3.347711	-0.127314	0.214268
C	2.150330	-2.944377	1.694039	C	-2.998744	1.182727	0.128016
B	1.189596	-1.757775	-0.014564	C	-0.841803	2.452487	-0.149237
C	-1.324024	-0.723856	-1.538040	C	-2.080490	-2.305662	0.157381
H	-1.428731	-0.519589	-2.597307	C	2.687726	0.463467	0.214815
C	-2.504929	-0.499075	-0.723671	O	2.248653	1.244483	-0.629994
C	-3.616259	0.215504	-1.235967	O	3.289897	0.473706	1.253403
C	-2.607438	-0.938415	0.620889	H	-4.311391	-0.597050	0.337850
C	-4.738122	0.476699	-0.464203	H	-3.600007	2.078293	0.162332
H	-3.581362	0.562658	-2.264592	H	-0.977620	3.067776	0.745091
C	-3.739291	-0.675341	1.387075	H	0.213116	2.194324	-0.258986

H	-1.171763	3.013249	-1.028780	H	-1.890266	-0.848154	1.999451
H	-1.025252	-2.565523	0.061310	C	-4.783068	0.663857	1.029288
H	-2.462829	-2.685514	1.109639	H	-5.402150	0.915552	-1.017525
H	-2.643627	-2.754122	-0.666819	H	-3.909152	0.255753	2.953341
C	2.556520	-1.371587	-0.365117	H	-5.665547	1.141462	1.440403
H	3.357601	-1.245199	-1.096341	Cu	0.297678	-0.085995	-0.664679
H	2.901200	-1.973451	0.476020	C	-0.207801	1.275030	-1.976470
H	1.787659	-1.962461	-0.925793	H	-0.724952	0.849718	-2.848323
2a				H	-0.897948	2.013266	-1.540354
Cu	-0.526693	-0.349653	0.015848	H	0.662042	1.825202	-2.365369
C	1.292211	-0.003339	0.003732	TS_{2b2}			
N	1.949737	1.190590	0.006296	C	2.379958	0.092879	0.055811
N	2.292145	-0.930681	-0.011130	N	3.091776	1.234950	0.285600
C	3.324603	1.011340	-0.006859	C	4.422630	0.959934	0.562561
C	3.540621	-0.329113	-0.017784	H	5.143044	1.735241	0.774340
C	2.059635	-2.370609	-0.018578	C	4.558860	-0.390016	0.505733
C	1.282814	2.486492	0.021143	H	5.422325	-1.019801	0.656450
C	-3.333341	-0.097326	-0.005109	N	3.308053	-0.900142	0.200117
O	-2.273526	-0.857943	0.028604	C	2.520416	2.573532	0.245710
O	-4.479942	-0.504015	-0.000538	H	2.991295	3.169165	-0.542931
H	4.016754	1.839341	-0.007081	H	1.455032	2.477843	0.037919
H	4.458030	-0.897379	-0.029405	H	2.658066	3.076165	1.208286
H	2.502933	-2.834494	0.867607	C	2.990154	-2.316847	0.058009
H	0.980584	-2.530814	-0.009253	H	3.281198	-2.862405	0.960752
H	2.485789	-2.822592	-0.919219	H	1.910717	-2.395442	-0.085376
H	0.207381	2.306281	0.032886	H	3.508208	-2.743081	-0.807018
H	1.565220	3.052263	0.914139	C	-1.497075	-0.738633	-0.894753
H	1.543961	3.062138	-0.872035	O	-0.765202	-1.600328	-0.233653
C	-3.044554	1.415560	-0.050727	H	-1.632049	-0.934227	-1.969786
H	-2.434978	1.657053	-0.932335	C	-2.780226	-0.303819	-0.231508
H	-3.973406	1.990016	-0.090361	C	-3.886268	0.122453	-0.971759
H	-2.475537	1.716386	0.839853	C	-2.894805	-0.388735	1.158496
TS_{2b1}				C	-5.074017	0.479062	-0.338011
C	1.947803	0.141494	-0.108567	H	-3.820428	0.167419	-2.054940
N	2.414290	1.368753	-0.482106	C	-4.077191	-0.026901	1.796233
C	3.628872	1.661123	0.119050	H	-2.046192	-0.768379	1.714809
H	4.149839	2.592220	-0.043855	C	-5.171532	0.411741	1.050832
C	3.942609	0.586655	0.887530	H	-5.925605	0.802305	-0.927380
H	4.796829	0.393931	1.518536	H	-4.151613	-0.096958	2.876529
N	2.908919	-0.324097	0.737280	H	-6.095800	0.687643	1.546834
C	1.703386	2.264177	-1.385168	Cu	0.589967	-0.192084	-0.355647
H	2.378267	2.622558	-2.168311	C	-0.813563	1.198565	-1.349579
H	0.887937	1.698765	-1.838681	H	-1.702049	1.321969	-1.969220
H	1.292282	3.120573	-0.840711	H	-0.890794	1.924887	-0.529058
C	2.873209	-1.638244	1.372240	H	0.044371	1.447767	-1.993882
H	3.251882	-1.556662	2.394846	2b₂			
H	1.836737	-1.975474	1.399701	C	2.199268	0.180060	-0.030873
H	3.492531	-2.349599	0.815216	N	2.301181	1.429357	-0.570333
C	-1.202654	-1.452437	0.648766	C	3.613669	1.875523	-0.573864
O	-0.271391	-1.383358	1.468831	H	3.895974	2.842051	-0.962350
H	-1.448704	-2.406737	0.157648	C	4.361532	0.885518	-0.022267
C	-2.254484	-0.406949	0.556628	H	5.422483	0.821437	0.165025
C	-3.385644	-0.602327	-0.243391	N	3.484562	-0.138299	0.301356
C	-2.152237	0.756064	1.329719	C	1.163789	2.187901	-1.077556
C	-4.392493	0.355884	-0.282375	H	1.276666	2.377348	-2.149545
H	-3.462272	-1.502088	-0.843884	H	0.264171	1.595267	-0.906666
C	-3.156798	1.715161	1.286901	H	1.073317	3.140562	-0.547099
H	-1.278910	0.878559	1.959191	C	3.869637	-1.399780	0.920665
C	-4.279360	1.518216	0.480711	H	4.299009	-1.226970	1.912445
H	-5.265291	0.199458	-0.906512	H	2.968723	-2.007335	1.017747
H	-3.074071	2.613883	1.888636	H	4.597486	-1.926387	0.295711
H	-5.065143	2.265056	0.451760	C	-1.914027	-1.744699	-0.227343
Cu	0.336628	-0.716937	-0.800513	O	-0.764517	-1.893479	0.525366
C	-0.704976	-1.237720	-2.355461	H	-2.603499	-2.572485	0.022281
H	-1.229222	-2.200771	-2.263534	C	-2.692401	-0.451682	0.077538
H	-1.468542	-0.485292	-2.604223	C	-3.946900	-0.197743	-0.491363
H	-0.051091	-1.329512	-3.237310	C	-2.162338	0.500426	0.949799
2b₁				C	-4.640142	0.976136	-0.209637
C	2.120039	0.108458	0.070735	H	-4.392525	-0.931262	-1.156726
N	2.779622	1.246340	0.423621	C	-2.853512	1.677088	1.239385
C	4.077669	0.977942	0.831382	H	-1.216067	0.272567	1.425079
H	4.754447	1.752158	1.159295	C	-4.093318	1.924059	0.656336
C	4.242991	-0.365494	0.728367	H	-5.611746	1.150982	-0.660518
H	5.095880	-0.992419	0.939387	H	-2.426710	2.396921	1.931126
N	3.039541	-0.876575	0.267855	H	-4.635282	2.836349	0.881544
C	2.187520	2.579002	0.415032	Cu	0.675851	-0.842447	0.205115
H	2.820333	3.265819	-0.154996	C	-1.622625	-1.847396	-1.741665
H	1.208528	2.514936	-0.058352	H	-2.527125	-1.835160	-2.363513
H	2.077586	2.954002	1.437772	H	-0.986181	-1.006120	-2.052457
C	2.796952	-2.292635	0.002761	H	-1.078213	-2.778825	-1.935439
H	3.147987	-2.888911	0.849918	TS_{2e1}			
H	1.723301	-2.439538	-0.120825	Cu	-0.936114	1.326060	-0.410416
H	3.327990	-2.606626	-0.902214	C	0.337658	2.124293	1.415472
C	-1.305496	-1.242778	-0.595032	C	0.782065	0.861635	1.615048
O	-0.382157	-1.724335	0.171305	C	-3.360432	-0.157200	1.404624
H	-1.438757	-1.668537	-1.599862	C	-1.527832	-0.507055	-0.240615
C	-2.502575	-0.573805	-0.032959	N	-2.567696	-0.984682	0.508053
C	-3.505431	-0.081780	-0.878269	N	-1.087498	-1.611702	-0.911468
C	-2.661457	-0.445929	1.353227	C	-2.761621	-2.345138	0.313223
C	-4.634820	0.535265	-0.351918	C	-1.823791	-2.740955	-0.584016
H	-3.388497	-0.177216	-1.952902	C	0.038265	-1.601751	-1.837523
C	-3.792919	0.168489	1.878200	H	-3.540794	-2.899292	0.814103

H	-1.622731	-3.709539	-1.015797	H	3.777819	0.927132	2.305540
H	-0.209315	-2.188450	-2.727241	H	5.030010	2.177678	0.554780
H	0.937682	-2.007967	-1.365092	H	2.801524	0.082579	-2.441915
H	0.227231	-0.566741	-2.124932	C	-0.725759	-2.619556	1.282534
H	-3.071039	0.881919	1.240233	H	-0.736136	-1.956424	2.156719
H	-3.174550	-0.424618	2.450443	H	-0.368625	-3.595936	1.613471
H	-4.426930	-0.272504	1.187359	H	-1.753159	-2.763841	0.922173
H	-0.469079	2.518797	2.021276	2c₂			
H	0.908489	2.853161	0.857569	Cu	0.390963	0.576945	-0.394016
C	1.912392	0.237076	0.930994	C	-1.641268	2.731250	-0.136333
C	2.496323	0.798622	-0.220773	C	-1.361336	1.355624	-0.759722
C	3.572097	0.180465	-0.848099	C	3.563886	1.649067	-0.328274
C	4.088134	-1.018433	-0.355168	C	2.034807	-0.284241	-0.025015
C	2.435971	-0.978727	1.405375	N	3.288623	0.251156	-0.023404
C	3.510429	-1.596801	0.775382	N	2.236639	-1.589971	0.310076
H	2.087671	1.712447	-0.634438	C	4.246991	-0.695423	0.304705
H	3.901513	-2.529239	1.168408	C	3.580732	-1.860053	0.515671
H	0.251530	0.226500	2.318354	C	1.163605	-2.570392	0.441111
H	4.006967	0.633294	-1.732800	H	5.299591	-0.462811	0.358541
H	4.928261	-1.496162	-0.846507	H	3.940130	-2.840124	0.790001
H	1.994074	-1.433764	2.286330	H	1.125261	-2.958681	1.463422
C	-0.912469	3.081378	-1.250474	H	1.318505	-3.398877	-0.256789
H	0.096136	3.385143	-1.577967	H	0.220077	-2.074473	0.209330
H	-1.267627	3.883930	-0.584435	H	2.606007	2.132445	-0.527438
H ₁	-1.546950	3.127574	-2.149603	H	4.204867	1.731970	-1.211601
2c₁				H	4.049675	2.139109	0.521194
Cu	-0.728503	-1.268354	0.150419	H	-1.278475	3.497370	-0.831356
C	0.580596	-2.602758	-0.467360	H	-2.724699	2.907453	-0.043033
C	0.931181	-1.379757	-1.066456	C	-2.264096	0.231452	-0.373395
C	-3.475192	-0.064111	-1.291267	C	-3.094207	0.228688	0.764404
C	-1.479953	0.542966	0.065832	C	-3.896729	-0.866128	1.085597
N	-2.669937	0.870566	-0.516771	C	-3.915789	-2.001439	0.281260
N	-1.076866	1.706866	0.649643	C	-2.308767	-0.932670	-1.176709
C	-2.997576	2.202056	-0.303004	C	-3.114047	-2.018573	-0.863802
C	-1.993258	2.728965	0.440684	H	-3.119664	1.097324	1.411288
C	0.119883	1.848916	1.470646	H	-3.125159	-2.884036	-1.519956
H	-3.898561	2.648050	-0.695574	H	-1.411418	1.449238	-1.852378
H	-1.851373	3.722696	0.837030	H	-4.521248	-0.822676	1.973002
H	-0.138793	1.823225	2.534665	H	-4.544753	-2.848656	0.530568
H	0.614156	2.796432	1.240446	H	-1.698494	-0.961239	-2.076095
H	0.805564	1.034268	1.242238	C	-0.983709	2.993521	1.227759
H	-3.260685	-1.074770	-0.939914	H	-1.292593	2.258097	1.980625
H	-3.244877	0.009361	-2.359690	H	-1.232078	3.991515	1.614444
H	-4.535910	0.151345	-1.137157	H	0.109279	2.923255	1.142462
H	0.063297	-3.350334	-1.058614	TS_{3a}			
H	1.155253	-3.008812	0.357412	C	-2.797475	0.209126	-0.265670
C	2.035491	-0.506974	-0.639653	N	-4.040509	-0.353259	-0.235652
C	2.809686	-0.749202	0.511458	C	-4.939280	0.363453	-1.008633
C	3.832666	0.115364	0.887681	H	-5.975001	0.077094	-1.109495
C	4.125170	1.246719	0.126720	C	-4.249122	1.406676	-1.539026
C	2.351802	0.636490	-1.397116	H	-4.566966	2.205028	-2.192089
C	3.377502	1.497044	-1.024145	N	-2.947732	1.296873	-1.074871
H	2.611647	-1.623759	1.120031	C	-4.361675	-1.555837	0.526585
H	3.597509	2.365926	-1.635827	H	-4.646853	-2.370730	-0.146062
H	0.590442	-1.200428	-2.082266	H	-3.471680	-1.842324	1.088978
H	4.412500	-0.101378	1.778896	H	-5.181837	-1.354553	1.222067
H	4.927086	1.914848	0.419361	C	-1.863137	2.213383	-1.403318
H	1.776064	0.845611	-2.293483	H	-2.144683	3.239085	-1.145072
C	-1.877308	-2.300365	1.404524	H	-0.987562	1.920490	-0.821319
H	-1.470619	-2.205523	2.424145	H	-1.626780	2.161667	-2.471151
H	-1.932520	-3.376492	1.192499	O	1.221340	2.143762	0.409662
H	-2.910120	-1.922133	1.452289	O	3.375218	1.828786	1.125758
TS_{2c₂}				C	1.777683	3.466984	0.521374
Cu	-0.507341	-0.895447	-0.111197	C	3.266746	3.241554	0.888449
C	0.844300	-2.500753	0.050029	B	2.184066	1.242665	0.799005
C	1.271887	-1.419634	-0.847985	C	1.971275	-0.320656	0.815711
C	-3.876119	-0.895282	-0.635753	O	0.617133	-0.617469	1.170686
C	-1.849397	0.422347	-0.028001	H	2.605732	-0.781231	1.579287
N	-3.193576	0.333878	-0.262855	C	2.350263	-0.894846	-0.543031
N	-1.658868	1.744778	0.257679	C	3.662551	-1.302981	-0.798986
C	-3.818626	1.564911	-0.125279	C	1.410213	-0.970228	-1.575078
C	-2.848737	2.453516	0.208690	C	4.026205	-1.779984	-2.055992
C	-0.359119	2.326475	0.578637	H	4.399675	-1.254924	-0.004198
H	-4.877969	1.698896	-0.282484	C	1.770135	-1.453510	-2.829925
H	-2.899034	3.513240	0.406693	H	0.390010	-0.661153	-1.376876
H	-0.228097	2.416751	1.661851	C	3.080682	-1.858071	-3.076793
H	-0.278658	3.316095	0.121188	H	5.046267	-2.102424	-2.234553
H	0.421564	1.679241	0.176714	H	1.025280	-1.515565	-3.616273
H	-3.129946	-1.687678	-0.694711	H	3.361145	-2.236630	-4.053439
H	-4.359904	-0.785476	-1.611772	Cu	-1.300386	-0.409468	0.622302
H	-4.629028	-1.162829	0.112615	H	1.230912	4.013816	1.297249
H	0.585927	-3.419156	-0.468346	H	1.650371	3.989226	-0.432119
H	1.512377	-2.684640	0.888041	H	3.946470	3.515540	0.074430
C	2.285020	-0.453673	-0.451365	H	3.567961	3.779057	1.792447
C	2.591426	-0.176020	0.902070	C	0.323437	-1.741443	2.168869
C	3.567415	0.751117	1.254330	O	1.268193	-2.252526	2.709191
C	4.271289	1.454436	0.277828	O	-0.917497	-1.835960	2.176310
C	3.010687	0.271456	-1.419734	3a			
C	3.973487	1.197533	-1.062814	C	-1.798274	2.172214	0.541274
H	2.055028	-0.687574	1.695167	N	-1.010630	2.533296	1.592668
H	4.510312	1.727865	-1.843616	C	-1.435746	3.723874	2.159126
H	1.219461	-1.639799	-1.910269				

H	-0.939191	4.172942	3.005726	H	-1.107865	4.988556	-2.721660
C	-2.522096	4.126384	1.449123	C	-0.746435	-1.321831	-1.893910
H	-3.155856	4.993504	1.556180	O	0.458094	-1.772256	-1.953729
N	-2.727300	3.167721	0.468744	H	-1.189896	-0.896762	-2.815591
C	0.123417	1.738162	2.057559	C	-1.771058	-2.125181	-1.123691
H	-0.026458	1.439034	3.099133	C	-3.109697	-2.160296	-1.511546
H	0.195031	0.846445	1.435321	C	-1.367593	-2.870150	-0.012613
H	1.052238	2.309470	1.971068	C	-4.037283	-2.921467	-0.798308
C	-3.800668	3.192836	-0.515466	H	-3.426883	-1.599155	-2.385970
H	-3.698099	4.057387	-1.179182	C	-2.285951	-3.626513	0.702762
H	-3.727306	2.274113	-1.099647	H	-0.318915	-2.847176	0.260177
H	-4.774935	3.229377	-0.018452	C	-3.627226	-3.653493	0.311866
O	2.269618	-0.724506	2.050241	H	-5.075634	-2.944908	-1.111660
O	3.835622	-2.144003	1.165431	H	-1.962820	-4.198764	1.566064
C	3.083477	-1.127564	3.166474	H	-4.344713	-4.245933	0.869275
C	4.209652	-1.993515	2.545546	3b			
B	2.734814	-1.363088	0.931467	C	3.176926	0.482538	-0.011600
C	2.126190	-1.196654	-0.519021	N	4.417528	0.059193	0.369372
O	0.717338	-1.019994	-0.429152	C	5.049129	0.997996	1.170072
H	2.354993	-2.114657	-1.081785	H	6.039921	0.847144	1.570559
C	2.829947	-0.030340	-1.217426	C	4.186056	2.039384	1.297618
C	4.148606	-0.164045	-1.666703	H	4.278895	2.972196	1.832513
C	2.186048	1.199402	-1.378498	N	3.053392	1.709205	0.571624
C	4.808174	0.906565	-2.264477	C	4.985210	-1.222778	-0.025130
H	4.660334	-1.113722	-1.545635	H	5.178199	-1.846122	0.853672
C	2.844468	2.268660	-1.982807	H	4.254925	-1.717420	-0.667719
H	1.159589	1.296460	-1.043196	H	5.917529	-1.076386	-0.579342
C	4.157748	2.129126	-2.425866	C	1.869828	2.555485	0.438238
H	5.828702	0.784116	-2.611287	H	2.147689	3.524674	0.012914
H	2.325997	3.212989	-2.111461	H	1.160949	2.058196	-0.223729
H	4.668181	2.961554	-2.897431	H	1.397053	2.704920	1.413304
Cu	-1.623266	0.621610	-0.525167	O	-1.288867	2.882766	-0.979261
H	2.460426	-1.688523	3.871337	O	-3.487711	2.304837	-1.267042
H	3.464598	-0.233714	3.670155	C	-1.933043	4.081369	-1.443184
H	5.189782	-1.507065	2.593961	C	-3.438143	3.718116	-1.525571
H	4.286877	-2.984194	3.003333	B	-2.228312	1.885590	-0.923045
C	-1.459009	-1.029443	-1.554973	C	-1.918897	0.405092	-0.456926
C	0.009842	-1.379655	-1.653825	O	-0.627016	0.018159	-0.928948
C	-2.330504	-2.046790	-0.900593	H	-2.690706	-0.258884	-0.865104
C	-3.658596	-2.242486	-1.328025	C	-2.007368	0.333326	1.066641
C	-4.495788	-3.172003	-0.722262	C	-3.227038	0.560772	1.715752
C	-4.035672	-3.956034	0.336509	C	-0.872799	0.076653	1.838588
C	-2.722903	-3.785424	0.772217	C	-3.310222	0.524250	3.104726
C	-1.887038	-2.848793	0.169709	H	-4.116467	0.762792	1.126809
H	-1.829326	-0.838085	-2.569038	C	-0.956633	0.040166	3.229380
H	0.464784	-0.832402	-2.487490	H	0.062035	-0.108662	1.325457
H	0.188584	-2.456159	-1.814555	C	-2.173201	0.264396	3.869109
H	-4.032072	-1.648500	-2.157922	H	-4.265028	0.692874	3.591429
H	-5.511787	-3.294995	-1.085426	H	-0.067554	-0.172289	3.814109
H	-4.685785	-4.684531	0.808291	H	-2.238003	0.231737	4.951154
H	-2.344154	-4.386390	1.593730	Cu	1.921220	-0.394292	-1.047824
H	-0.877252	-2.711653	0.539159	H	-1.512194	4.353458	-2.417358
				H	-1.731161	4.892138	-0.735942
				H	-4.037876	4.236087	-0.769280
TS_{3b}				H	-3.870949	3.916140	-2.510855
C	3.062173	-0.460198	0.181579	C	-0.510423	-1.194355	-1.801372
N	3.944688	-1.502330	0.221501	O	0.767371	-1.265175	-2.182896
C	5.115015	-1.152245	0.874987	H	-1.202179	-1.017828	-2.648346
H	5.935629	-1.841162	1.005433	C	-0.988680	-2.430379	-1.034579
C	4.972685	0.143773	1.257278	C	-2.230696	-3.011080	-1.286337
H	5.644817	0.802056	1.786351	C	-0.154231	-3.020992	-0.081637
N	3.718886	0.548116	0.825949	C	-2.643589	-4.150028	-0.591745
C	3.669621	-2.808128	-0.369302	H	-2.877002	-2.579301	-2.045452
H	3.659055	-3.583065	0.403930	C	-0.558590	-4.151706	0.615481
H	2.691361	-2.757460	-0.851322	H	0.826063	-2.586391	0.080044
H	4.429771	-3.053538	-1.117306	C	-1.809853	-4.720145	0.364705
C	3.151134	1.873892	1.032679	H	-3.611891	-4.591843	-0.802156
H	3.828199	2.639445	0.640218	H	0.100126	-4.597450	1.353686
H	2.201112	1.920760	0.497844	H	-2.125309	-5.605225	0.906595
H	2.978246	2.057061	2.098345				
O	0.228889	2.935058	-0.693051	TS_{3c}			
O	-1.820978	3.394310	-1.607947	C	1.199452	-2.100943	-0.115873
C	0.334054	4.279177	-1.193093	N	0.424007	-3.224454	-0.038474
C	-1.091861	4.630083	-1.688026	C	1.193168	-4.376405	-0.024424
B	-1.027281	2.463160	-0.992570	H	0.758558	-5.362964	0.027893
C	-1.522155	1.004503	-0.639007	C	2.489034	-3.975855	-0.084091
O	-0.505030	0.079354	-1.013881	H	3.406674	-4.543996	-0.084233
H	-2.427669	0.795575	-1.222989	N	2.473140	-2.592073	-0.141394
C	-1.895735	0.946090	0.839182	C	-1.033704	-3.206816	-0.011943
C	-3.147365	1.397208	1.271588	H	-1.394911	-3.998674	0.650586
C	-0.976222	0.507631	1.794659	H	-1.363215	-2.240592	0.370867
C	-3.473633	1.405642	2.625368	H	-1.444867	-3.364915	-1.014681
H	-3.874468	1.736424	0.539939	C	3.672283	-1.763580	-0.186654
C	-1.301593	0.511588	3.148325	H	4.304570	-2.064005	-1.027531
H	-0.010409	0.149382	1.457931	H	3.372009	-0.725481	-0.319122
C	-2.550648	0.962262	3.571009	H	4.238848	-1.858446	0.744944
H	-4.453023	1.748939	2.941283	O	-2.089708	-0.574506	1.886081
H	-0.578085	0.157023	3.875103	O	-2.613945	1.462978	2.791669
H	-2.805097	0.961971	4.625179	C	-2.329153	-0.837920	3.279365
Cu	1.387733	-0.506807	-0.600449	C	-2.758492	0.528731	3.873456
H	1.074994	4.298371	-2.000096	B	-2.237475	0.776056	1.669056
H	0.676598	4.935349	-0.386698	C	-1.968934	1.467832	0.276243
H	-1.586333	5.372291	-1.051886				

O	-0.601867	1.224674	-0.037228	C	0.408518	0.000007	-0.002361
H	-2.111840	2.550673	0.412058	N	1.251228	-1.074124	0.003890
C	-2.952285	1.005337	-0.793440	N	1.251284	1.074096	0.004212
C	-4.235982	1.560738	-0.858476	C	2.580430	-0.679220	0.014289
C	-2.616403	0.001880	-1.705289	C	2.580464	0.679118	0.014499
C	-5.158658	1.122306	-1.804391	C	0.779810	-2.452351	-0.006707
H	-4.510522	2.350109	-0.164454	C	0.779685	-2.452363	-0.006538
C	-3.535150	-0.434918	-2.657233	H	1.137304	-2.989044	0.877943
H	-1.619147	-0.419933	-1.666336	H	3.396518	-1.385574	0.020753
C	-4.811705	0.120462	-2.709993	H	3.396590	1.385426	0.021096
H	-6.146120	1.569953	-1.842118	H	1.118421	2.969607	-0.909952
H	-3.250169	-1.207095	-3.364346	H	-0.311366	2.415893	0.004345
H	-5.525826	-0.216310	-3.453227	H	1.139072	2.989824	0.876617
Cu	0.617000	-0.326813	-0.270439	H	-0.311505	-2.415832	0.002597
H	-1.407611	-1.221733	3.730074	H	1.119917	-2.970473	-0.908675
H	-3.107723	-1.602415	3.368271	O	-3.219293	-0.000160	-0.071977
H	-3.801559	0.534042	4.207284	H	-3.659359	0.000919	0.786907
H	-2.123516	0.847249	4.705905				
C	1.487117	1.522114	-1.478847	3a₁'			
C	0.284950	2.213559	-1.247641	C	-1.225657	-0.028620	0.007929
C	2.702956	1.819747	-0.734700	N	-1.639112	1.269048	0.028240
C	3.981035	1.656401	-1.314687	C	-3.021498	1.355152	0.065653
C	5.145574	1.940740	-0.610200	H	-3.540920	2.300965	0.086180
C	5.087912	2.402291	0.705803	C	-3.493357	0.081554	0.068509
C	3.836310	2.561791	1.303546	H	-4.502782	-0.299497	0.091560
C	2.670289	2.264624	0.608373	N	-2.383423	-0.748664	0.032689
H	1.617318	1.060505	-2.454093	C	-0.734307	2.418502	0.012133
H	-0.453728	2.220630	-2.042827	H	-0.868292	3.012277	0.921456
H	0.294818	3.121298	-0.649272	H	0.294031	2.056017	-0.038734
H	4.046494	1.321525	-2.346074	H	-0.940859	3.042950	-0.862098
H	6.108109	1.815303	-1.097162	C	-2.427035	-2.203819	0.016475
H	5.995718	2.630271	1.252791	H	-2.960453	-2.564033	-0.868644
H	3.769233	2.908216	2.330490	H	-1.395200	-2.557370	-0.013799
H	1.709213	2.351905	1.103233	H	-2.917476	-2.585604	0.917332
				O	2.299495	-1.098180	-0.141661
3c				Cu	0.523587	-0.618161	-0.055356
C	-1.798274	2.172214	0.541274	C	3.242011	0.363377	0.014874
N	-1.010630	2.533296	1.592668	O	4.346005	0.070361	0.357028
C	-1.435746	3.723874	2.159126	O	2.478400	1.251379	-0.270548
H	-0.939191	4.172942	3.005726	H	2.773528	-1.827087	0.273574
C	-2.522096	4.126384	1.449123				
H	-3.155856	4.993504	1.556180	TS_{3a1'}			
N	-2.727300	3.167721	0.468744	C	-1.215231	-0.023606	0.000664
C	0.123417	1.738162	2.057559	N	-1.846133	1.184669	0.002491
H	-0.026458	1.439034	3.099133	C	-3.223798	1.034789	0.004144
H	0.195031	0.846445	1.435321	H	-3.898101	1.877515	0.005756
H	1.052238	2.309470	1.971068	C	-3.470937	-0.301149	0.003277
C	-3.800668	3.192836	-0.515466	H	-4.401447	-0.847883	0.003963
H	-3.698099	4.057387	-1.179182	N	-2.235090	-0.929425	0.001169
H	-3.727306	2.274113	-1.099647	C	-1.141381	2.464353	0.002516
H	-4.774935	3.229377	-0.018452	H	-1.402232	3.039597	0.896017
O	2.269618	-0.724506	2.050241	H	-0.069332	2.260908	0.001145
O	3.835622	-2.144003	1.165431	H	-1.404074	3.040664	-0.889747
C	3.083477	-1.127564	3.166474	C	-2.018622	-2.368703	-0.000488
C	4.209652	-1.993515	2.545546	H	-2.454848	-2.825652	-0.894252
B	2.734814	-1.363088	0.931467	H	-0.937813	-2.522762	-0.001290
C	2.126190	-1.196654	-0.519021	H	-2.453948	-2.827522	0.892761
O	0.717338	-1.019994	-0.429152	O	2.413961	-1.091343	-0.004261
H	2.354993	-2.114657	-1.081785	Cu	0.605316	-0.306920	-0.003374
C	2.829947	-0.030340	-1.217426	C	3.162925	0.239837	-0.000094
C	4.148606	-0.164045	-1.666703	O	4.364295	0.164012	0.018542
C	2.186048	1.199402	-1.378498	O	2.279680	1.113952	-0.017624
C	4.808174	0.906565	-2.264477	H	3.014956	-1.846980	0.024493
H	4.660334	-1.113722	-1.545635				
C	2.844468	2.268660	-1.982807	3a'			
H	1.159589	1.296460	-1.043196	C	-1.249471	0.026093	-0.000397
C	4.157748	2.129126	-2.425866	N	-2.346941	0.834620	0.000704
H	5.828702	0.784116	-2.611287	C	-3.519557	0.094875	0.001270
H	2.325997	3.212989	-2.111461	H	-4.495682	0.555153	0.002196
H	4.668181	2.961554	-2.897431	C	-3.151780	-1.212533	0.000356
Cu	-1.623266	0.621610	-0.525167	H	-3.745515	-2.113772	0.000332
H	2.460426	-1.688523	3.871337	N	-1.765914	-1.235142	-0.000469
H	3.464598	-0.233714	3.670155	C	-2.275530	2.290150	0.001374
H	5.189782	-1.507065	2.593961	H	-2.756363	2.698210	0.895635
H	4.286877	-2.984194	3.003333	H	-1.219766	2.565122	0.000041
C	-1.459009	-1.029443	-1.554973	H	-2.758892	2.699113	-0.891102
C	0.009842	-1.379655	-1.653825	C	-0.949872	-2.445859	-0.001495
C	-2.330504	-2.046790	-0.900593	H	-1.158643	-3.041923	-0.895139
C	-3.658596	-2.242486	-1.328025	H	0.100019	-2.147502	-0.000784
C	-4.495788	-3.172003	-0.722262	H	-1.159283	-3.043795	0.890740
C	-4.035672	-3.956034	0.336509	O	2.609799	-1.221755	0.003194
C	-2.722903	-3.785424	0.772217	Cu	0.538816	0.491232	-0.001141
C	-1.887038	-2.848793	0.169709	C	3.201470	0.066528	0.000452
H	-1.829326	-0.838085	-2.569038	O	4.410418	0.148839	0.000783
H	0.464784	-0.832402	-2.487490	O	2.314109	0.987481	-0.002103
H	0.188584	-2.456159	-1.814555	H	3.352284	-1.844712	0.005165
H	-4.032072	-1.648500	-2.157922				
H	-5.511787	-3.294995	-1.085426	TS_{3b'}			
H	-4.685785	-4.684531	0.808291	C	-2.332737	0.010211	0.073081
H	-2.344154	-4.386390	1.593730	N	-2.833550	1.225687	-0.293225
H	-0.877252	-2.711653	0.539159	C	-4.126728	1.402349	0.172147
				H	-4.693049	2.301722	-0.016243
3'				C	-4.455266	0.271338	0.849639
Cu	-1.433182	0.000047	-0.011435	H	-5.362242	-0.005258	1.365248

N	-3.350861	-0.564153	0.778335	H	3.347175	-1.126987	2.243254
C	-2.085165	2.197113	-1.087559	H	2.251353	0.923144	1.466781
H	-1.988261	3.138815	-0.538108	H	0.502183	3.147405	1.607468
H	-1.094475	1.782563	-1.286297				
H	-2.596804	2.383571	-2.036870	3c'			
C	-3.258000	-1.892538	1.364036	C	2.115086	-0.274475	0.021438
H	-4.021463	-2.555607	0.944884	N	3.074872	0.503088	-0.553998
H	-2.266463	-2.275914	1.115515	C	4.219283	-0.227335	-0.835201
H	-3.373490	-1.846770	2.451816	H	5.091358	0.213130	-1.294016
O	0.991743	-1.771482	-0.427858	C	3.976037	-1.500363	-0.428170
Cu	-0.656458	-0.627075	-0.352446	H	4.593825	-2.384652	-0.464601
C	1.753060	-0.615052	-1.313191	N	2.690158	-1.508331	0.090709
O	0.801699	0.181720	-1.663751	C	2.897009	1.924374	-0.833865
H	2.216646	-1.236414	-2.102336	H	3.062031	2.121881	-1.897569
C	2.819324	-0.085554	-0.362388	H	1.872686	2.196342	-0.569825
C	4.140542	-0.528249	-0.419206	H	3.599983	2.520225	-0.242511
C	2.468009	0.878388	0.585914	C	2.009009	-2.677779	0.630341
C	5.097893	-0.022492	0.461120	H	2.554754	-3.079333	1.490016
H	4.422551	-1.268141	-1.163061	H	1.015182	-2.355976	0.945768
C	3.415793	1.382910	1.468297	H	1.912385	-3.454067	-0.134960
H	1.442085	1.229488	0.591343	O	-0.659887	2.746577	-0.148913
C	4.736596	0.932243	1.408593	Cu	0.391232	0.257734	0.572661
H	6.124635	-0.368236	0.403307	C	-1.391480	0.807961	1.142571
H	3.132771	2.133045	2.199589	C	-1.444402	2.313548	1.004686
H	5.479232	1.329514	2.092087	C	-2.387327	0.047984	0.336728
H	1.519032	-2.053854	0.334280	C	-2.955401	-1.145423	0.824206
				C	-3.873730	-1.878729	0.081415
3b'				C	-4.273279	-1.441735	-1.182041
C	-2.290890	0.057026	-0.030953	C	-3.730753	-0.258981	-1.682006
N	-3.423019	-0.196592	-0.749618	C	-2.804534	0.470287	-0.941535
C	-4.394687	0.766216	-0.521610	H	-1.509368	0.550847	2.201666
H	-5.362631	0.738194	-0.998179	H	-1.027104	2.777093	1.907713
C	-3.863305	1.649865	0.362336	H	-2.472415	2.688946	0.870028
H	-4.278417	2.542377	0.805022	H	-2.666355	-1.495289	1.811755
N	-2.583564	1.202705	0.650250	H	-4.291390	-2.791535	0.495805
C	-3.572557	-1.341214	-1.637292	H	-4.992558	-2.009643	-1.761736
H	-3.746410	-1.011086	-2.666311	H	-4.028214	0.099245	-2.663136
H	-2.644279	-1.912782	-1.591968	H	-2.368670	1.371113	-1.358148
H	-4.404762	-1.973787	-1.312909	H	-0.901072	3.665470	-0.340520
C	-1.649971	1.862997	1.557834	TS1-CO₂-ins			
H	-2.087235	1.940726	2.558037	C	-2.797501	-0.209054	0.265761
H	-0.740456	1.260404	1.606651	N	-4.040609	0.353170	0.235679
H	-1.407076	2.864689	1.189171	C	-4.939287	-0.363558	1.008753
O	1.173891	-0.510120	1.944942	H	-5.975042	-0.077314	1.109587
Cu	-0.700039	-0.876410	0.036683	C	-4.248994	-1.406626	1.539276
C	1.819865	-1.286389	0.861428	H	-4.566734	-2.204933	2.192444
O	0.863396	-1.819369	0.091609	N	-2.947622	-1.296716	1.075101
H	2.430715	-2.068117	1.353511	C	-4.361957	1.555573	-0.526756
C	2.769501	-0.334556	0.121770	H	-4.647342	2.370510	0.145751
C	4.146121	-0.371578	0.337921	H	-3.471978	1.842144	-1.089130
C	2.257324	0.604333	-0.778286	H	-5.182029	1.354028	-1.222269
C	4.999430	0.515677	-0.321280	C	-1.862920	-2.213069	1.403631
H	4.557233	-1.108787	1.022583	H	-2.144315	-3.238819	1.145409
C	3.099203	1.492584	-1.435322	H	-0.987363	-1.920080	0.821657
H	1.188348	0.607359	-0.964248	H	-1.626617	-2.161282	2.471472
C	4.477224	1.452988	-1.207422	O	1.221284	-2.143699	-0.409542
H	6.069451	0.469582	-0.147240	O	3.375062	-1.828851	-1.125991
H	2.686870	2.214529	-2.133007	C	1.777535	-3.466953	-0.521287
H	5.135904	2.142401	-1.724517	C	3.266519	-3.241629	-0.888778
H	1.868089	-0.104397	2.488013	B	2.184004	-1.242661	-0.799024
				C	1.971319	0.320681	-0.815664
				O	0.617173	0.617582	-1.170585
TS_{sc}'				H	2.605786	0.781222	-1.579249
C	-1.737069	-0.312816	0.145094	C	2.350379	0.894831	0.543071
N	-3.048806	-0.143980	-0.207342	C	3.662718	1.302816	0.799011
C	-3.707972	-1.358049	-0.315740	C	1.410345	0.970351	1.575122
H	-4.750304	-1.431456	-0.585986	C	4.026440	1.779794	2.056008
C	-2.794050	-2.317847	-0.021923	H	4.399832	1.254662	0.004219
H	-2.884489	-3.392726	0.014449	C	1.770335	1.453612	2.829959
N	-1.603311	-1.665072	0.255619	H	0.390100	0.661419	1.376916
C	-3.658800	1.156924	-0.442757	C	3.080934	1.858012	3.076813
H	-4.532737	1.292664	0.202208	H	5.046542	2.102115	2.234555
H	-2.910622	1.915547	-0.206777	H	1.025488	1.515785	3.616306
H	-3.960944	1.260783	-1.489910	H	3.361448	2.236557	4.053450
C	-0.365610	-2.347398	0.620562	Cu	-1.300520	0.409644	-0.622326
H	-0.023133	-2.981153	-0.201318	H	1.230530	-4.013836	-1.296960
H	0.399731	-1.598705	0.822217	H	1.650458	-3.989100	0.432290
H	-0.526908	-2.959682	1.513492	H	3.946458	-3.515761	-0.074987
O	0.286535	2.785376	0.732282	H	3.567417	-3.779075	-1.792915
Cu	-0.493288	1.062778	0.300455	O	-0.917472	1.835727	-2.176487
C	1.544839	1.556829	-1.093770	C	0.323469	1.741258	-2.169019
C	1.619088	2.769405	-0.373868	O	1.268208	2.252237	-2.709501
C	2.124773	0.330966	-0.612814	Int1-CO₂-ins			
C	2.377865	-0.765748	-1.477420	C	2.956295	0.247662	0.334914
C	2.967290	-1.936440	-1.024837	N	4.279032	-0.036360	0.507383
C	3.336141	-2.087020	0.317007	C	4.708076	0.311765	1.778510
C	3.079871	-1.032710	1.194513	H	5.725499	0.165981	2.107652
C	2.468504	0.136043	0.753482	C	3.629088	0.828615	2.422001
H	1.204563	1.587661	-2.122814	H	3.523603	1.220560	3.421993
H	1.408512	3.677141	-0.929757	N	2.572337	0.782634	1.527567
H	2.429700	2.896374	0.345355	C	5.119127	-0.630438	-0.524364
H	2.123982	-0.664944	-2.528552	H	5.486699	-1.610651	-0.205386
H	3.159619	-2.740776	-1.729215	H	4.505684	-0.747363	-1.418938
H	3.810964	-2.997321	0.664537				

H	5.968450	0.021807	-0.749104	O	-1.066956	1.756293	-1.353122
C	1.215767	1.244681	1.813133	C	-0.811398	2.393539	0.882512
H	1.232328	2.297936	2.107841	C	-1.014695	2.926015	-0.548125
H	0.614058	1.134762	0.911461	B	-1.337545	0.642347	-0.497424
H	0.772389	0.646715	2.614834	C	-2.464748	-0.441654	-0.969992
O	-1.783463	2.175087	0.438772	O	-1.834005	-1.767432	-0.831682
O	-3.910846	1.609570	-0.197220	H	-2.654103	-0.317610	-2.040961
C	-2.610408	3.268818	0.875574	C	-3.770018	-0.413589	-0.228418
C	-4.060447	2.817977	0.566100	C	-4.749441	0.508749	-0.614987
B	-2.584374	1.266730	-0.205245	C	-4.031357	-1.248318	0.860878
C	-2.067995	-0.075212	-0.856860	C	-5.953146	0.604636	0.076909
O	-0.695534	0.065201	-1.245729	H	-4.564161	1.156919	-1.466173
H	-2.649182	-0.287135	-1.760862	C	-5.239887	-1.159126	1.547900
C	-2.236120	-1.240304	0.114448	H	-3.288050	-1.976359	1.159757
C	-3.514557	-1.624282	0.537960	C	-6.205226	-0.231598	-1.163056
C	-1.128925	-1.934508	0.607947	H	-6.699144	1.326495	-0.238521
C	-3.679822	-2.681472	1.427831	H	-5.427562	-1.819522	2.388022
H	-4.381860	-1.090267	0.164325	H	-7.145407	-0.164187	1.699331
C	-1.295782	-2.993879	1.498605	Cu	1.713333	-0.148788	-0.229629
H	-0.141635	-1.640020	0.273773	H	0.266264	2.332772	1.128440
C	-2.569907	-3.372266	1.913272	H	-1.296827	3.005868	1.651330
H	-4.678070	-2.971017	1.738380	H	-1.957562	3.487472	-0.632132
H	-0.425093	-3.528741	1.863387	H	-0.199455	3.581643	-0.882676
H	-2.699068	-4.199446	2.602461	O	-0.087766	-0.415863	-0.638404
Cu	1.895794	-0.042306	-1.153730	C	-0.514813	-1.689993	-0.678477
H	-2.322466	4.169506	0.322513	O	0.218536	-2.646073	-0.590446
H	-2.438307	3.442801	1.942423	1b₃			
H	-4.633481	2.594351	1.472622	C	-3.285627	-0.009170	-0.089268
H	-4.616515	3.548844	-0.028400	N	-4.329511	-0.180203	-0.948797
O	0.918350	-0.347067	-2.700455	C	-5.373275	0.679272	-0.648098
C	-0.352854	-0.327466	-2.578771	H	-6.293467	0.694917	-1.211335
O	-1.219502	-0.569975	-3.385746	C	-4.972431	1.406322	0.427874
TS2-CO₂-cyc				H	-5.473983	2.185627	0.980429
C	3.751444	-0.098563	-0.027554	N	-3.701826	0.970028	0.756573
N	4.666178	0.908312	-0.093745	C	-4.334416	-1.138638	-2.045223
C	5.948762	0.439008	0.146745	H	-4.424702	-0.622467	-3.005809
H	6.813788	1.084194	0.137715	H	-3.387143	-2.167879	-2.014565
C	5.835432	-0.896386	0.369141	H	-5.161457	-1.846550	-1.933236
H	6.583724	-1.641293	0.592527	C	-2.875789	1.537681	1.828074
N	4.489660	-1.206334	0.258535	H	-3.528211	2.069258	2.523835
C	4.321786	2.292392	-0.388236	H	-2.367642	0.728055	2.353838
H	4.819356	2.626502	-1.303786	H	-2.120482	2.209744	1.410892
H	3.240552	2.335954	-0.527973	O	1.875857	-1.258909	1.349289
H	4.608873	2.945726	0.441444	O	0.110697	-1.609801	-0.151337
C	3.921873	-2.544969	0.424376	C	1.144849	-2.382944	1.790377
H	4.112455	-2.910159	1.437899	C	0.385632	-2.841961	0.540813
H	2.844042	-2.492385	0.254876	B	1.129223	-0.565757	0.356136
H	4.369024	-3.232329	-0.299696	C	1.956217	0.211092	-0.817717
O	-1.644431	1.098631	1.289411	O	1.309721	1.521154	-0.871351
O	-1.603032	2.155241	-0.755754	H	1.773405	-0.249278	-1.794352
C	-1.158065	2.416698	1.547416	C	3.444057	0.363520	-0.619918
C	-1.377236	3.179863	0.218814	C	4.270126	-0.758640	-0.758279
B	-1.737786	0.954542	-0.081707	C	4.032357	1.588559	-0.299133
C	-2.417523	-0.311857	-0.770675	C	5.645143	-0.659945	-0.577493
O	-1.689479	-1.524848	-0.450230	H	3.829631	-1.719054	-1.005546
H	-2.368334	-0.177203	-1.857636	C	5.411272	1.687600	-0.114996
C	-3.864263	-0.479499	-0.367712	H	3.407404	2.467550	-0.206424
C	-4.828394	0.371565	-0.921060	C	6.224192	0.566680	-0.252493
C	-4.268378	-1.437038	0.565404	H	6.267301	-1.541807	-0.688932
C	-6.164960	0.272361	-0.546177	H	5.849235	2.648721	0.133041
H	-4.526366	1.116849	-1.650649	H	7.296472	0.645335	-0.110693
C	-5.607965	-1.538847	0.936061	Cu	-1.605393	-0.801036	-0.119975
H	-3.528569	-2.104821	0.986790	H	0.440580	-2.112708	2.594837
C	-6.561453	-0.685876	0.385443	H	1.829743	-3.147380	2.174077
H	-6.898498	0.939038	-0.987106	H	1.015904	-3.471014	-0.100648
H	-5.906835	-2.291471	1.658059	H	-0.547679	-3.373276	0.752484
H	-7.603293	-0.769030	0.674843	O	0.263814	0.572520	0.861638
Cu	1.917807	-0.076998	-0.263605	C	0.387031	1.663500	0.104863
H	-0.094348	2.366561	1.819007	O	-0.264000	2.670736	0.233756
H	-1.709570	2.850591	2.387840	TS1-CO₂-add			
H	-2.255749	3.836154	0.257302	C	-2.630310	-0.225585	0.252422
H	-0.509345	3.781560	-0.073977	N	-3.233729	0.823369	0.878420
O	0.070338	-0.152502	-0.490316	C	-4.515180	0.493557	1.291253
C	-0.347316	-1.384380	-0.347701	H	-5.155000	1.192244	1.808112
O	0.352639	-2.362131	-0.142315	C	-4.722688	-0.795133	0.915312
Int2-CO₂-cyc				H	-5.580038	-1.438711	1.039810
C	3.523808	-0.035990	0.152557	N	-3.563761	-1.217349	0.284978
N	4.324974	1.051312	0.316713	C	-2.596259	2.115772	1.096817
C	5.631402	0.674657	0.587998	H	-2.497626	2.317214	2.167974
H	6.419890	1.393368	0.750113	H	-1.606081	2.083159	0.642039
C	5.649399	-0.683731	0.592609	H	-3.181715	2.913676	0.629798
H	6.457561	-1.379119	0.759760	C	-3.359252	-2.553828	-0.273210
N	4.355367	-1.099575	0.324505	H	-4.066107	-2.732443	-1.089317
C	3.854925	2.427321	0.216191	H	-2.338656	-2.622832	-0.654571
H	4.387510	2.956660	-0.579437	H	-3.506823	-3.308132	0.505335
H	2.790575	2.395795	-0.020785	O	2.039114	-1.062077	1.394156
H	3.999749	2.952692	1.164925	O	4.057938	-0.597945	0.405175
C	3.925188	-2.494812	0.236092	C	3.020970	-1.691084	2.232531
H	4.082771	-2.999427	1.193747	C	4.385580	-1.247320	1.644100
H	2.862164	-2.515976	-0.011806	B	2.693964	-0.569305	0.293070
H	4.488525	-3.012408	-0.545613	C	1.932175	0.120877	-0.912709
O	-1.387808	1.100482	0.853693				

O	0.758779	-0.649666	-1.249052	C	2.579709	3.633697	1.978116
H	2.591413	0.107113	-1.789792	H	0.873081	4.043364	0.735247
C	1.498821	1.558664	-0.677206	C	2.749598	1.391539	2.823782
C	2.072280	2.351661	0.320313	H	1.145459	0.065427	2.269433
C	0.533263	2.137795	-1.514527	C	3.265520	2.680212	2.732025
C	1.689644	3.682659	0.486544	H	2.963991	4.646116	1.906366
H	2.834286	1.932183	0.967539	H	3.259959	0.643189	3.422050
C	0.153288	3.467181	-1.352804	H	4.182083	2.944141	3.248499
H	0.113103	1.545264	-2.317728	Cu	0.522000	-0.923317	0.200290
C	0.726439	4.245039	-0.346545	H	-0.500188	1.912065	-3.670572
H	2.148612	4.279720	1.267102	H	1.251410	2.213176	-3.519081
H	-0.583078	3.901274	-2.021067	H	0.878869	4.315197	-2.399739
H	0.433238	5.281660	-0.221973	H	-0.748881	4.223702	-3.115071
Cu	-0.930356	-0.361553	-0.478321	O	-2.234553	1.420175	-1.135792
H	2.882773	-2.776254	2.181055	C	-2.217056	0.209502	-0.855431
H	2.873147	-1.362877	3.266534	H	-1.497984	-0.457196	-1.350276
H	4.912601	-0.534394	2.289129	C	-3.333625	-0.463276	-0.159551
H	5.050183	-2.091573	1.438551	C	-3.314095	-1.851012	0.002258
C	0.965329	-2.265087	-1.319769	C	-4.420159	0.273142	0.322090
O	-0.132951	-2.756445	-1.465769	C	-4.366011	-2.500134	0.640409
O	2.132631	-2.554852	-1.197194	H	-2.464929	-2.414633	-0.371970
1b₃'				C	-5.471479	-0.374475	0.959943
C	-2.965551	-0.300228	-0.019464	H	-4.417540	1.347328	0.182787
N	-3.719891	0.829959	0.044535	C	-5.446709	-1.761037	1.120546
C	-5.043865	0.532048	0.326215	H	-4.347070	-3.577355	0.764559
H	-5.801571	1.294871	0.418802	H	-6.313417	0.197939	1.333380
C	-5.121274	-0.819437	0.442682	H	-6.268699	-2.263986	1.618141
H	-5.959963	-1.463594	0.657904	1b₄			
N	-3.843930	-1.310300	0.228272	C	-2.724609	-0.858910	0.933523
C	-3.193577	2.174585	-0.164387	N	-3.187630	-0.084503	1.950856
H	-3.410037	2.804121	0.703329	C	-4.535619	-0.306521	2.173411
H	-2.113077	2.100635	-0.288676	H	-5.086489	0.214876	2.940928
H	-3.635373	2.623004	-1.059460	C	-4.934522	-1.239699	1.270116
C	-3.474099	-2.724966	0.266339	H	-5.900886	-1.685023	1.090525
H	-4.024672	-3.278181	-0.500175	N	-3.814078	-1.565444	0.522601
H	-2.402467	-2.810001	0.076339	C	-2.352538	0.834068	2.729522
H	-3.698647	-3.145446	1.250758	H	-1.942847	0.322066	3.605914
O	3.282851	-0.256841	1.191597	H	-1.537948	1.210594	2.102483
O	4.239765	-0.790011	-0.857250	H	-2.969189	1.673859	3.059455
C	4.650601	-0.549376	1.445877	C	-3.803697	-2.513652	-0.583041
C	5.307065	-0.537337	0.047737	H	-4.481702	-2.183729	-1.375721
B	3.017539	-0.705841	-0.136659	H	-2.788193	-2.553191	-0.977803
C	1.765412	0.025721	-0.911437	H	-4.101492	-3.508271	-0.237103
O	0.649431	-0.928364	0.740646	O	-0.049196	2.201880	0.794876
H	1.968177	0.065351	-1.984551	O	2.200432	2.508667	0.239261
C	1.294967	1.363141	-0.423035	C	0.371375	3.428250	1.372576
C	0.809525	1.513122	0.885815	C	1.676808	3.761772	0.626858
C	1.338181	2.489742	-1.249304	B	1.170969	1.490448	0.391924
C	0.380125	2.753848	1.345254	C	1.014368	0.476289	-0.908762
H	0.840577	0.665879	1.558727	O	0.874477	-0.868291	-0.262035
C	0.914390	3.736174	-0.787866	H	1.964831	0.444866	-1.453952
H	1.711025	2.388725	-2.263368	C	-0.110796	0.607004	-1.904560
C	0.429015	3.871641	0.510126	C	-0.673279	1.853326	-2.202386
H	0.029217	2.856178	2.366780	C	-0.577112	-0.517015	-2.607208
H	0.964458	4.598958	-1.443307	C	-1.673912	1.971063	-3.164661
H	0.105682	4.840662	0.874503	H	-0.340205	2.722682	-1.653455
Cu	-1.151604	-0.511164	-0.356777	C	-1.582750	-0.399293	-3.564276
H	4.748960	-1.537811	1.920404	H	-0.112530	-1.479070	-2.425173
H	5.069924	0.202571	2.125262	C	-2.137538	0.847522	-3.846293
H	5.759729	0.440837	-0.176374	H	-2.096917	2.946695	-3.379467
H	6.084465	-1.304914	-0.056918	H	-1.918485	-1.278721	-4.104466
C	1.090052	-2.197363	-0.225563	H	-2.915479	0.944071	-4.595858
O	0.225463	-3.023151	-0.048509	Cu	-0.986574	-0.855650	0.261749
O	2.344158	-2.203432	-0.044410	H	0.560281	3.306756	2.452205
TS1-PhCHO-add				H	-0.407531	4.191460	1.243488
C	1.736092	-2.209021	-0.373168	H	1.473671	4.387296	-0.260087
N	2.533428	-2.158581	-1.477142	H	2.393619	4.303569	1.259014
C	3.335744	-3.283791	-1.572984	O	1.546795	0.465901	1.467271
H	4.037374	-3.426286	-2.380534	C	1.736942	-0.774070	0.957355
C	3.037733	-4.067399	-0.504728	H	1.340931	-1.552057	1.624240
H	3.427580	-5.026357	-0.199486	C	3.166214	-1.126774	0.569617
N	2.060764	-3.397138	0.214556	C	3.479718	-2.438735	0.203271
C	2.550874	-1.048369	-2.426564	C	4.173872	-0.162252	0.595697
H	2.340386	-1.417900	-3.435042	C	4.782221	-2.784444	-0.142627
H	1.786760	-0.325156	-2.134512	H	2.697179	-3.191414	0.185541
H	3.531009	-0.561539	-2.415974	C	5.478688	-0.508769	0.246403
C	1.463649	-3.885333	1.450747	H	3.917787	0.853689	0.870781
H	2.227517	-4.000194	2.225998	C	5.786622	-1.816468	-0.121047
H	0.726330	-3.150753	1.777368	H	5.016343	-3.805025	-0.426057
H	0.968316	-4.846820	1.283713	H	6.256630	0.246913	0.262219
O	0.325847	1.467520	-1.820809	H	6.803571	-2.083062	-0.388084
O	-0.576111	3.496502	-1.179986	TS1-B₂cg₂-coord			
C	0.288552	2.277443	-2.999417	Cu	-1.194546	-0.230504	0.053655
C	-0.026160	3.697897	-2.481092	B	1.233521	-2.218718	0.330003
B	-0.434351	2.151075	-0.845141	O	1.594998	-3.186092	1.240097
C	-0.430841	1.650875	0.685413	O	0.621132	-2.748320	-0.786857
O	-0.761608	0.276395	0.765333	C	-3.011850	-0.598607	0.110131
H	-1.210370	2.218619	1.217224	N	-4.009620	0.204823	0.575923
C	0.881204	1.996912	1.387790	N	-3.669326	-1.697271	-0.364543
C	1.402300	3.297785	1.317687	C	-5.253787	-0.376738	0.394414
C	1.570956	1.055513	2.157618	C	-5.040499	-1.580175	-0.197561
				C	1.217161	-4.469652	0.724529

C	0.707330	-4.179764	-0.708242	C	-1.796609	0.596047	0.434881
C	-3.001362	-2.838630	-0.974132	H	-1.860579	0.404609	1.511841
C	-3.795463	1.534643	1.142093	C	-3.178733	0.455131	-0.173031
O	0.598359	0.165378	-0.042159	C	-4.262810	1.094924	0.439205
H	-6.168203	0.108808	0.699351	C	-3.398047	-0.263489	-1.348933
H	-5.730873	-2.350562	-0.505325	C	-5.538274	1.026442	-0.115255
H	0.440516	-4.896989	1.369950	H	-4.108898	1.643697	1.364689
H	2.085698	-5.135312	0.738670	C	-4.675035	-0.336112	-1.901108
H	-0.278334	-4.614599	-0.906383	H	-2.566377	-0.784501	-1.802542
H	1.402246	-4.531919	-1.478841	C	-5.748856	0.310151	-1.292092
H	-3.371785	-2.997084	-1.992043	H	-6.367911	1.524456	0.375574
H	-1.932475	-2.620752	-1.007896	H	-4.832399	-0.907991	-2.809555
H	-3.174496	-3.744774	-0.383564	H	-6.741838	0.248966	-1.724054
H	-2.732827	1.665981	1.347864	TS2-metathesis			
H	-4.113333	2.304338	0.432692	Cu	-1.114284	0.179432	0.196693
H	-4.366887	1.632607	2.070019	B	-1.716961	-1.869600	-0.318096
B	0.375669	2.477537	0.822519	C	-2.189196	1.600972	0.782119
O	-0.538679	2.283033	1.855909	N	-3.437395	2.001126	0.408204
O	1.631070	2.768839	1.302139	N	-1.844464	2.478497	1.768359
C	0.192795	2.216411	3.091522	C	-3.860901	3.095845	1.147030
C	1.608241	2.721998	2.733724	C	-2.854690	3.395537	2.008448
H	2.396335	2.053012	3.086283	C	-0.564083	2.436378	2.466778
H	1.801465	3.726620	3.123804	C	-4.219915	1.368152	-0.646205
H	0.201878	1.180244	3.444249	C	-3.709618	-3.015334	-0.164973
H	-0.306790	2.837567	3.839239	O	-2.464525	-2.718941	0.481636
B	-0.084079	2.561179	-0.794689	C	-3.551369	-2.454215	-1.590528
O	-1.373728	2.269875	-1.215590	O	-2.398961	-1.597491	-1.511036
O	0.727601	2.917584	-1.845857	H	-4.822655	3.560984	0.993626
C	-1.440124	2.429744	-2.643449	H	-2.770696	4.169859	2.755596
C	0.018468	2.694879	-3.074173	H	-0.132124	3.439789	2.515392
H	0.121872	3.574366	-3.713620	H	-0.686433	2.041265	3.480112
H	0.461196	1.833858	-3.582823	H	0.102912	1.783743	1.901637
H	-2.104936	3.268125	-2.873174	H	-4.461117	2.096964	-1.426558
H	-1.854334	1.520761	-3.086430	H	-3.625387	0.560513	-1.075695
C	1.546529	-0.684980	0.554538	H	-5.149615	0.960315	-0.236030
H	1.589422	-0.526004	1.650296	H	-3.878876	-4.094284	-0.150159
C	2.971340	-0.434428	0.045668	H	-4.521731	-2.529181	0.387030
C	4.061612	-1.110312	0.611058	H	-4.417086	-1.875015	-1.923533
C	3.208416	0.468682	-0.991459	H	-3.354076	-3.239081	-2.327382
C	5.355806	-0.891148	0.147810	O	0.721783	-0.491841	-0.153109
H	3.890552	-1.813885	1.420060	B	0.111249	-1.854337	-0.052860
C	4.505383	0.689262	-1.453567	B	1.814738	1.126014	-1.614657
H	2.371532	1.015670	-1.402432	C	1.970258	-0.208046	-0.784959
C	5.583862	0.010358	-0.891720	O	0.906837	2.107084	-1.304525
H	6.187581	-1.421365	0.600696	O	2.588007	1.429310	-2.705376
H	4.672829	1.405285	-2.251810	C	1.035696	3.163318	-2.271478
H	6.591872	0.186141	-1.252217	C	2.230554	2.742692	-3.165600
Int1-B₂eg₂-coord				C	1.124447	-3.913841	-0.485967
Cu	0.985015	0.163183	-0.095632	O	0.520072	-2.779397	-1.102867
B	-1.184485	2.036465	0.196526	C	0.651836	-3.855107	0.976206
O	-0.638749	2.795764	1.209066	O	0.448752	-2.475862	1.217379
O	-1.116614	2.645028	-1.027441	H	1.213805	4.107087	-1.747932
C	2.710518	0.861877	-0.027211	H	0.098505	3.245553	-2.831460
N	3.316604	1.449890	1.041727	H	3.095291	3.404934	-3.051567
N	3.672069	0.847382	-0.991629	H	1.969436	2.688401	-4.226986
C	4.627776	1.790185	0.751577	H	2.221457	-3.834524	-0.550376
C	4.850980	1.414807	-0.535197	H	0.814199	-4.828829	-1.001748
C	-0.114412	4.003122	0.630535	H	-0.288950	-4.409101	1.107115
C	-0.536696	3.945780	-0.859985	H	1.392769	-4.255158	1.676252
C	3.459421	0.338245	-2.343677	H	2.190241	-1.032240	-1.475584
C	2.677016	1.616641	2.345723	C	3.128203	-0.096279	0.210497
O	-0.837484	-0.335388	-0.121237	C	4.386764	0.343883	-0.222087
H	5.278363	2.257247	1.474860	C	2.960091	-0.432047	1.556651
H	5.729299	1.503786	-1.155866	C	5.450265	0.448848	0.670494
H	0.974690	4.009402	0.755219	H	4.533427	0.602428	-1.265403
H	-0.531646	4.863872	1.161979	C	4.027265	-0.322821	2.448104
H	0.309971	4.053409	-1.545651	H	2.004101	-0.821197	1.882413
H	-1.287971	4.701550	-1.113568	C	5.273836	0.120660	2.013646
H	4.338000	-0.228959	-2.663061	H	6.418119	0.787305	0.315423
H	2.588093	-0.318823	-2.331141	H	3.882874	-0.598210	3.487862
H	3.288347	1.161987	-3.044184	H	6.101365	0.201914	2.710130
H	1.596667	1.665280	2.200635	1+egB-O-CHPh-Beg			
H	2.913816	0.773231	3.001008	Cu	-2.059696	0.336219	0.328648
H	3.025687	2.545423	2.804618	B	-1.410341	2.189451	0.074543
B	-0.647697	-1.751805	0.537972	C	-2.850871	-1.403667	0.599818
O	-0.623617	-1.564565	1.988747	N	-4.186912	-1.687606	0.588451
O	-1.751268	-2.655415	0.252835	N	-2.264354	-2.616815	0.789467
C	-1.446674	-2.563590	2.565410	C	-4.423961	-3.042145	0.759707
C	-2.457661	-2.904899	1.459514	C	-3.204855	-3.628971	0.883115
H	-3.347889	-2.261316	1.523984	C	-0.818669	-2.831271	0.808936
H	-2.787842	-3.949020	1.491150	C	-5.222348	-0.676027	0.425541
H	-1.921934	-2.182224	3.476506	C	-1.111512	4.321470	-0.818593
H	-0.845678	-3.446441	2.831127	O	-1.781656	3.055029	-0.958975
B	0.810456	-2.417022	-0.166310	C	-0.186885	4.147826	0.401094
O	1.629626	-3.279661	0.540824	O	-0.499939	2.839714	0.915741
O	1.233195	-2.330205	-1.499761	H	-5.418386	-3.460892	0.786791
C	2.664747	-3.775120	-0.317806	H	-2.929483	-4.662179	1.030140
C	2.234027	-3.338583	-1.729084	H	-0.583863	-3.626444	1.522049
H	1.782610	-4.157681	-2.297581	H	-0.463689	-3.105141	-0.187609
H	3.053159	-2.917866	-2.318673	H	-0.324522	-1.909163	1.113769
H	2.740176	-4.859541	-0.211707	H	-5.864518	-0.634443	1.311291
H	3.619801	-3.327788	-0.018960	H	-4.722181	0.285070	0.293961

H	-5.834674	-0.891761	-0.455871
H	-0.558442	4.538424	-1.736536
H	-1.860500	5.105512	-0.670415
H	-0.372601	4.893661	1.179347
H	0.873231	4.175936	0.134411
O	1.226000	-0.794339	-0.927958
B	0.319830	-0.300181	-1.804466
B	1.910120	0.607550	1.004698
C	2.284527	0.046789	-0.431681
O	1.057676	-0.019054	1.866863
O	2.478860	1.746063	1.501970
C	0.907278	0.832346	3.022586
C	1.970016	1.942023	2.836199
C	-0.715024	1.051666	-3.305210
O	0.394911	0.936604	-2.397530
C	-1.575115	-0.206404	-3.032741
O	-0.748739	-1.060577	-2.226079
H	1.068537	0.234518	3.924057
H	-0.107479	1.235619	3.017372
H	2.803738	1.856824	3.541811
H	1.538276	2.942889	2.902965
H	-0.324927	1.079753	-4.329958
H	-1.253692	1.971451	-3.080116
H	-2.475548	0.043360	-2.464924
H	-1.857558	-0.735877	-3.945588
H	2.416892	0.895030	-1.111968
C	3.593756	-0.727011	-0.384585
C	4.778197	-0.055615	-0.054523
C	3.648283	-2.095251	-0.654752
C	5.988945	-0.738451	-0.002527
H	4.744924	1.005610	0.167971
C	4.863488	-2.777855	-0.602472
H	2.736172	-2.615631	-0.915098
C	6.037524	-2.105024	-0.276935
H	6.897214	-0.202087	0.250357
H	4.889975	-3.840426	-0.819987
H	6.981529	-2.637182	-0.238445