

Supplementary Information

Unraveling the Divergent Mode of Cu- or Zn-assisted Radical Addition of Imine: A Mechanistic Perspective on Lewis Acidic Metal-Induced enantioselectivity

Dongmin Fu,^a Ruopeng Bai,^c Jiang Wu,^c Kai Yang,^{*ac} Xiaokang Guo,^{*b} Yu Lan^{*abcd} and Tao Zhang^{*ab}

^{a.} College of Chemistry, and Pingyuan Laboratory, Zhengzhou University, Zhengzhou, Henan, 450001, P. R. China. E-mail: lanyu@cqu.edu.cn

^{b.} Institute of Intelligent Innovation, Henan Academy of Sciences, Zhengzhou, Henan, 451162, P. R. China. E-mail: zhangtao@hnas.ac.cn; xiaokang.guo@hnas.ac.cn

^{c.} School of Chemistry and Chemical Engineering, Chongqing Key Laboratory of Chemical Theory and Mechanism, Chongqing University, Chongqing, 401331, P. R. China. E-mail: lanyu@cqu.edu.cn

^{d.} Pingyuan Laboratory, Xinxiang, Henan, 453007, China

^{e.} Henan Sanmenxia Aoke Chemical Industry Co. Ltd., Sanmenxia 472000, China

These authors contributed equally

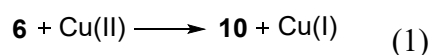
1. Complete reference for Gaussian 09

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian 09; Revision D.01; Gaussian, I. W., CT, 2013..

2. The barriers of the single electron transfer

The single electron transfer¹⁻³ (SET) activation energy was calculated using Marcus theory, and the barriers energy was calculated by the four-point model method. The reduction of electron acceptor oxidant **Cu(II)** (**7**) and the corresponding electron donors **6** was studied at 25 °C. This reaction involves a SET from a donor (Sub) to an acceptor (OX).

The Gibbs free energy of activation of the SET from **6** is calculated using Marcus theory and is shown below as an example (1). The same steps are taken to calculate the SET barrier for other substrate.



The activation Gibbs free energy is therefore given by

$$\Delta G^\ddagger = \frac{(\Delta G_0 + \lambda)^2}{4\lambda} \quad (2)$$

Here, λ is the reaction of internal reorganization energy, which calculated as

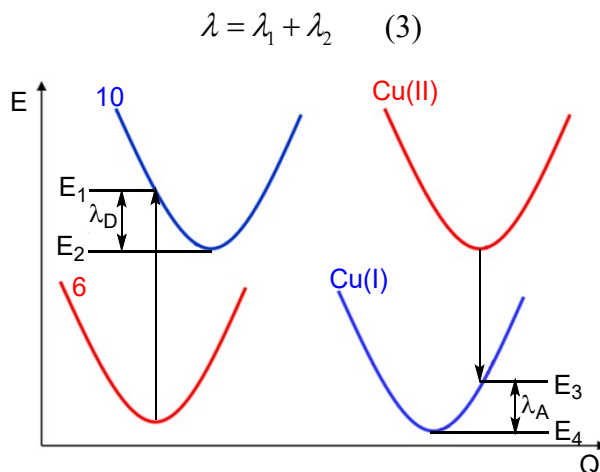


Figure. S1 Four-point model of internal reorganization energy

Then, λ_1 is the reorganization energy of substrate **6**, and λ_2 is the reorganization energy of photosensitizer **Cu(II)**.

$$\lambda_1 = E_1 - E_2 \quad (4)$$

$$\lambda_2 = E_3 - E_4 \quad (5)$$

As show in Figure S1, E_1 is the energy of **10** at non-equilibrium state with the same geometry and solvation state as reactant **6**, and E_2 is the energy of **10** at equilibrium state with minimum geometry and solvation. As well, E_3 is the energy of **Cu(I)** at non-equilibrium state with the same geometry and solvation state as reactant **Cu(II)**, and E_4 is the energy of **Cu(I)** at equilibrium state with minimum geometry and solvation

$$\lambda = \lambda_1 + \lambda_2 = 0.0484 \times 627.5 \text{ kcal/mol} + 0.0206 \times 627.51 \text{ kcal/mol} = 43.3 \text{ kcal/mol}$$

$\Delta G_0 = -25.7 \text{ kcal/mol}$ is the reaction driving energy of the SET.

Thus, the barrier of electron transfer is estimated by

$$\Delta G^\ddagger = \frac{(\Delta G_0 + \lambda)^2}{4\lambda} = \frac{(-25.7 \text{ kcal/mol} + 43.3 \text{ kcal/mol})^2}{4 \times 43.3 \text{ kcal/mol}} = 1.8 \text{ kcal/mol}$$

On the basis of the above computed method, the remaining energy barriers of single electron transfer can be calculated.

3. Non-covalent interaction

Non-covalent interaction (NCI) analysis includes intramolecular non-covalent interactions and intermolecular non-covalent interactions, belonging to the category of weak interactions, including such as hydrogen bond/halogen bond/dihydrogen bond / π - π stacking/ordinary van der Waals interaction. NCI analysis is a qualitative analysis, which mainly uses Multiwfn⁴ and VMD programs⁵. The combination of the two programs can realize the visualization of the region, type and strength of weak interaction. The Multiwfn program is a wave function analysis program with a powerful, flexible and efficient wave function topology analysis module. It can be used for topological analysis of various real space functions, such as electron density, electron density Laplace function, orbital wave function, etc. The VMD program is a molecular visualization program. In the process of theoretical calculation of organic reaction system, NCI analysis can show the influence of weak interaction in the structure on the stereoselectivity of reaction, so as to explain the origin of the stereoselectivity of reaction.

4. The energies of all the optimized structures

Table S1. The single-point energies (E), Gibbs free energy corrections (GFEC), and GFE (=E+GFEC) energies of the stationary points (SPs) involved in the reaction (unit: a.u.)

SP	GFEC	E	GFE	Imaginary Frequency
	(M06/def2-SVP/IEF-PCM)	(M06/def2-TZVP/IEF-PCM)		
1	0.212899	-1144.949157	-1144.736258	
*1	0.207405	-1144.843492	-1144.636087	
T2	0.206228	-1144.85126	-1144.645032	
3	0.096712	-271.438283	-271.341571	
T4ts	0.325814	-1416.300682	-1415.974868	1093.43 <i>i</i>
5	0.083948	-270.788005	-270.704057	
6	0.222323	-1145.535952	-1145.313629	
7	0.521695	-3929.560115	-3929.03842	
8ts	0.633124	-4200.358873	-4199.725749	266.33 <i>i</i>
9	0.635585	-4200.361144	-4199.725559	
10	0.224941	-1145.337065	-1145.112124	
11	0.52022	-3929.804199	-3929.283979	
12tsR	0.63184	-4200.602962	-4199.971122	285.30 <i>i</i>

12tsS	0.625779	-4200.594966	-4199.969187	284.63 <i>i</i>
13R	0.634755	-4200.635635	-4200.00088	
13S	0.633975	-4200.634826	-4200.000851	
14	0.648255	-4201.026313	-4200.378058	
15	0.139309	-1140.125434	-1139.986125	
16R	0.265565	-1411.596928	-1411.331363	
16S	0.265563	-1411.59693	-1411.331367	
17	0.54888	-4144.928974	-4144.380094	
18	0.546456	-4145.128793	-4144.582337	
19tsR	0.658483	-4415.7261	-4415.067617	256.66 <i>i</i>
19tsS	0.659053	-4415.73238	-4415.073327	274.47 <i>i</i>
20R	0.658833	-4415.730233	-4415.071400	
20S	0.659272	-4415.733238	-4415.073966	
21	0.662335	-4415.989913	-4415.327578	
22	0.677632	-4416.393805	-4415.716173	
23ts	0.769393	-5075.114265	-5074.344872	1230.14 <i>i</i>
24	0.536076	-3930.154332	-3929.618256	
25ts	0.800385	-5290.466686	-5289.666301	454.58 <i>i</i>
26	0.558727	-4145.509289	-4144.950562	

5. Supplementary data for the mechanism study

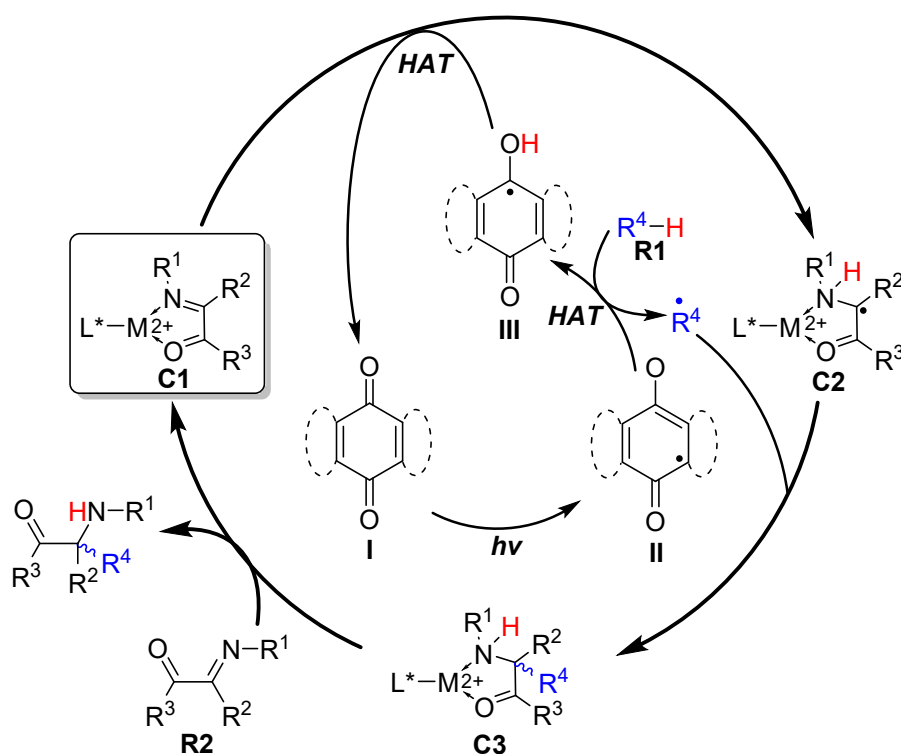


Figure. S2 Other possible pathway for Cu- or Zn-mediated radical addition of Imine

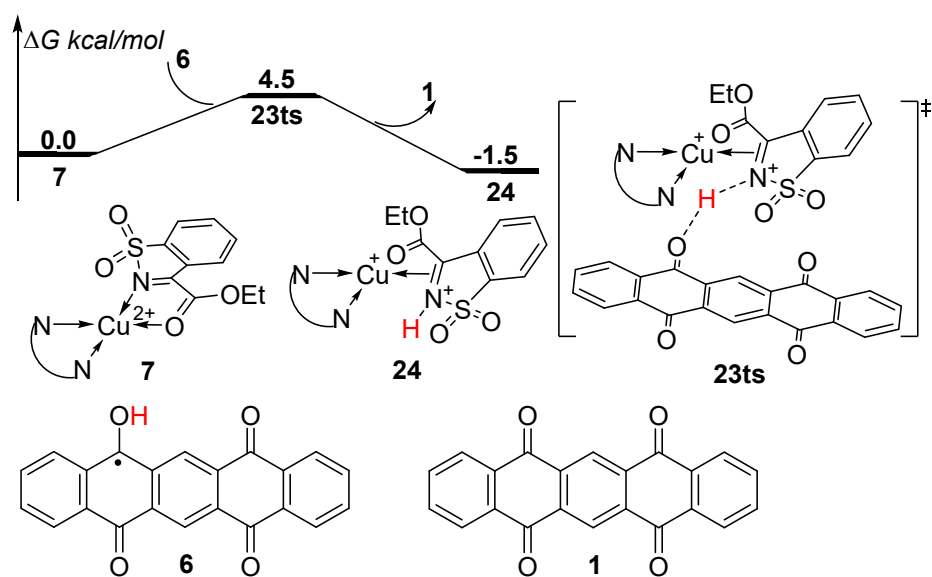


Figure. S3 Free energy profile for intermediate **7** undergoing HAT with semiquinone radical.

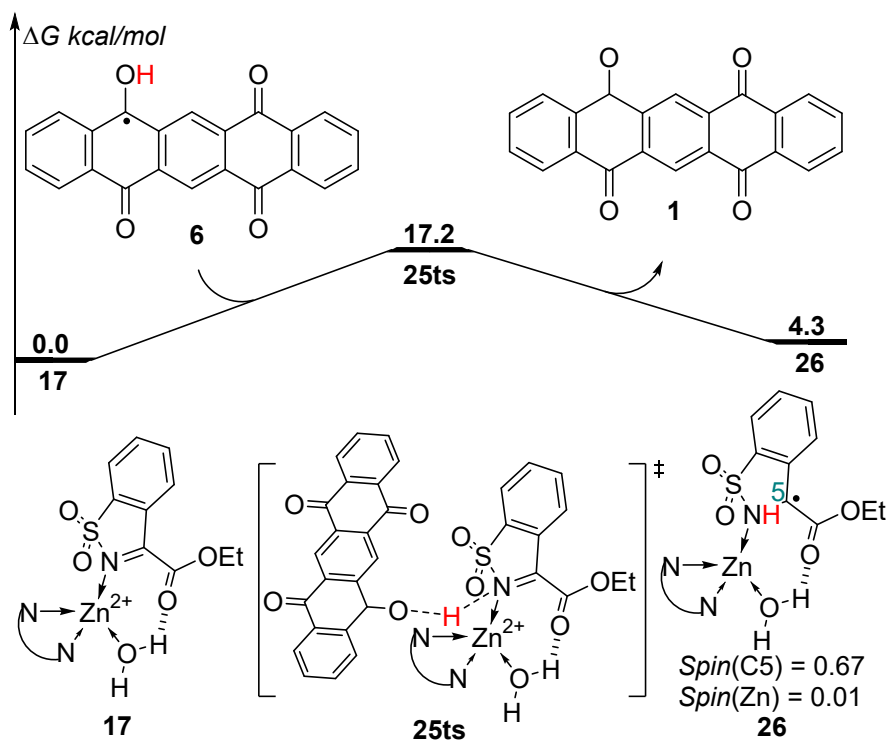


Figure. S4 Free energy profile for intermediate **17** undergoing HAT with semiquinone radical.

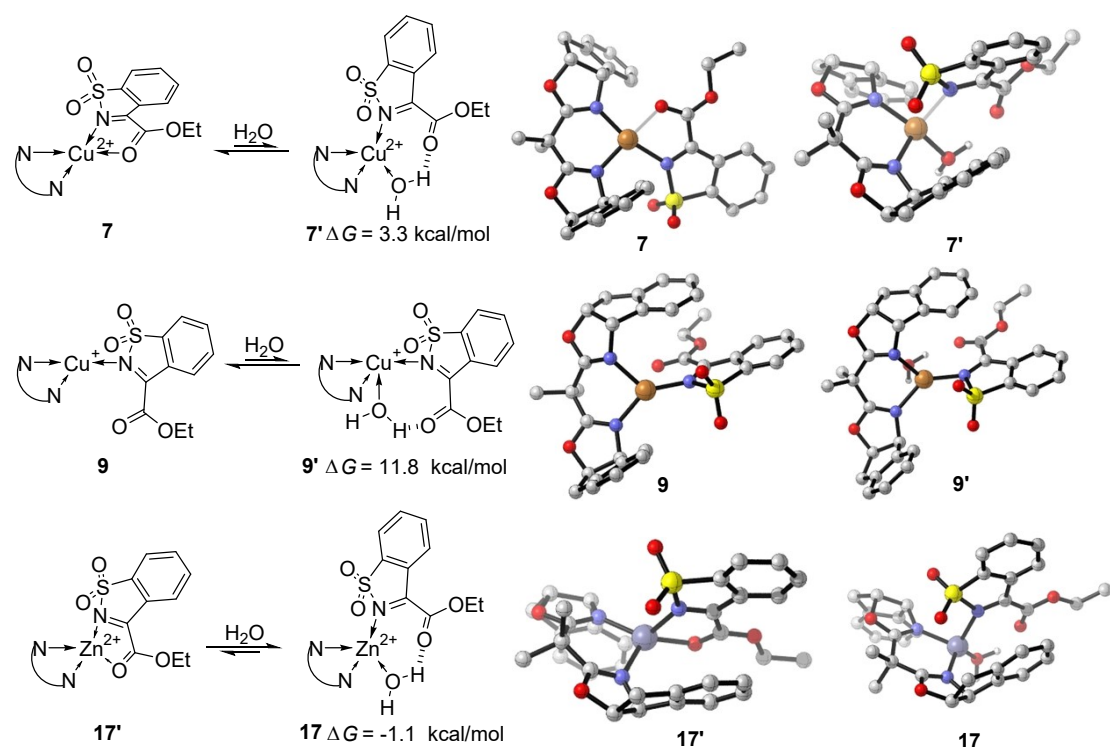


Figure. S5 The influence of H₂O molecule to intermediates. The oxygen atom of H₂O molecule has a pair of electrons that can coordinate with the metal, and the hydrogen atom of H₂O forms a hydrogen bond with the substrate α -carbonyl group.

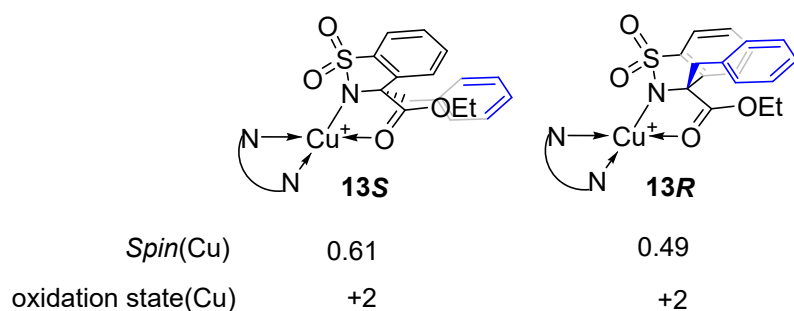


Figure. S6 The calculated spin and oxidation states for Cu in intermediate **13S** and **13R**

Energy difference	EWG (Cyano)	No substituent	EDG (Methoxyl)
$\Delta\Delta G^\ddagger$ (S-R)	1.8 kcal/mol	1.2 kcal/mol	3.7 kcal/mol

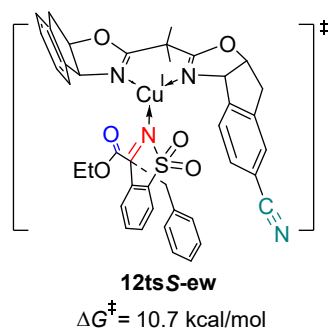
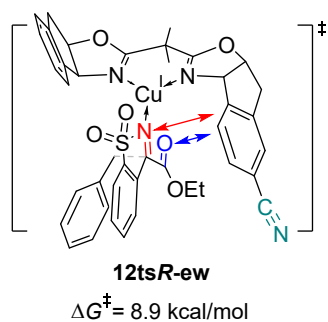
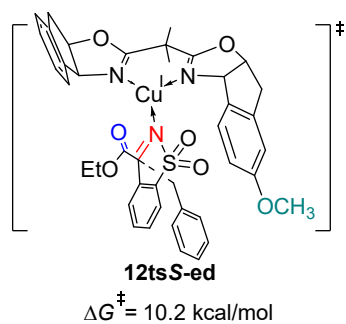
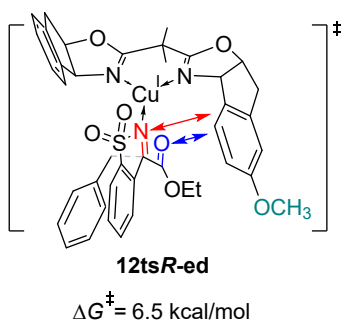
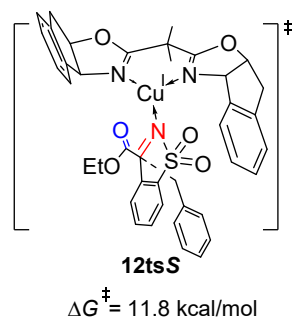
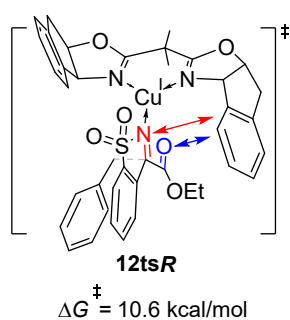


Figure. S7 Analysis of Ligand Substituent Effects.

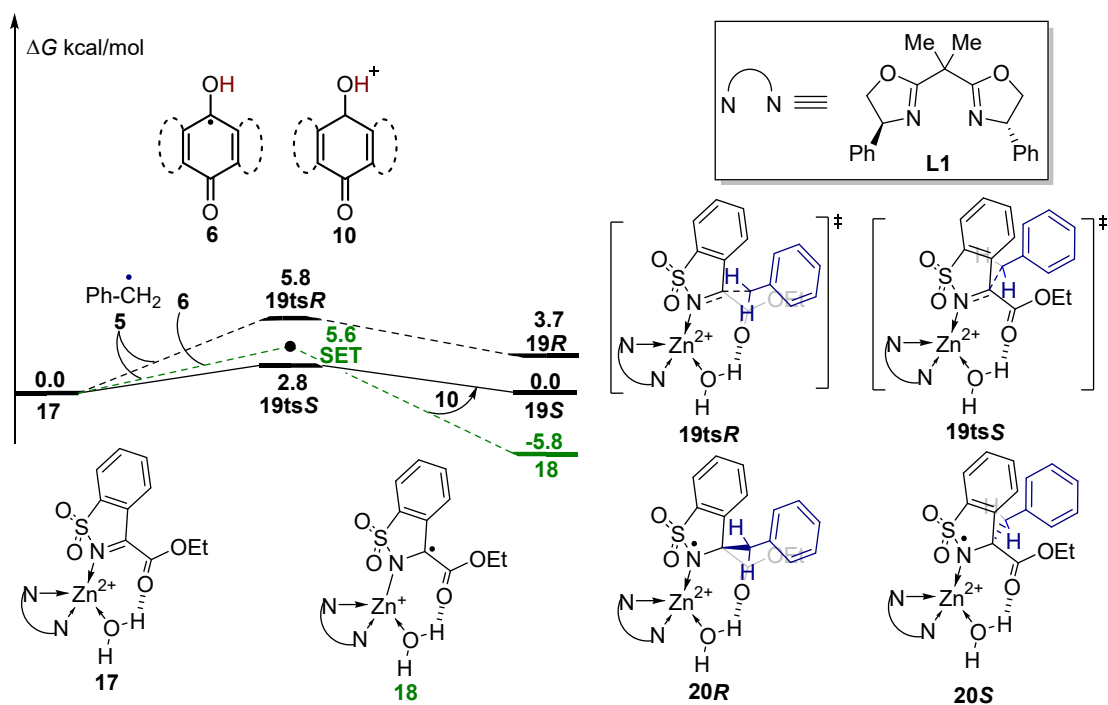


Figure. S8 Gibbs free energy profile in Zn-mediated hydroalkylation of α -carbonyl imines using Ligand L1.

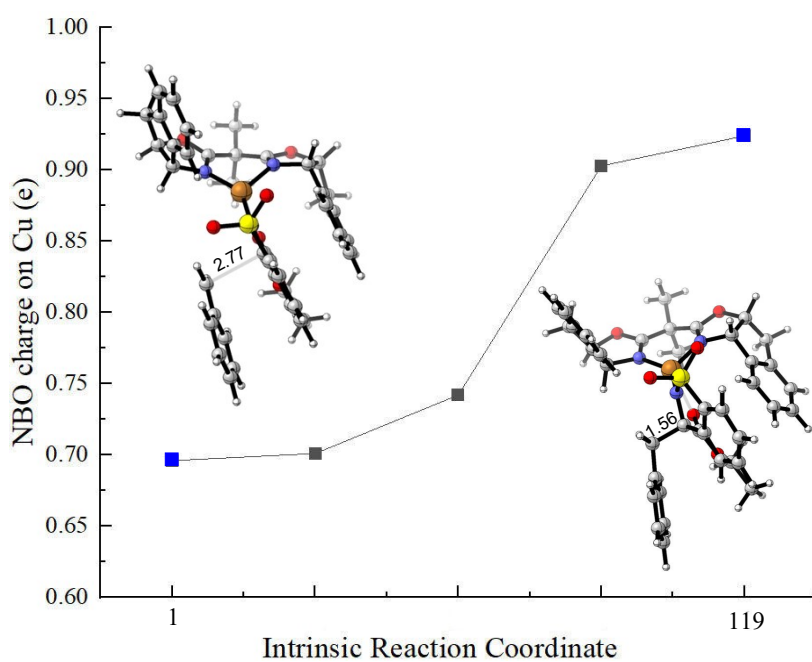


Figure. S9 NBO charge variation on the copper atom along the IRC pathway of transition state 12tsR.

6. Reference

- [1] R A Marcus, On the theory of oxidation-reduction reactions involving electron transfer. I, *J. Chem. Phys.*, 1956, **24**, 966-978.

- [2] R A Marcus, Electrostatic free energy and other properties of states having nonequilibrium polarization. I, *J. Chem. Phys.*, 1956, **24**, 979-989.
- [3] R A Marcus, Chemical and electrochemical electron-transfer theory. *Ann. Rev Phys. Chem.*, 1964, **15**, 155-196.
- [4] T Lu, F W Chen, Multiwfn: A multifunctional wavefunction analyzer, *J. Comput. Chem.*, 2012, **33**, 580-592.
- [5] W Humphrey, A Dalke, K Schulten, VMD: visual molecular dynamics, *J. Mol. Graphics*, 1996, **14**, 33-38.

7. Geometrical Coordinates of the Listed Compound

1				C	6.161476	0.698204	0.000023
C	-6.161476	0.698204	0.000029	H	4.931819	2.488372	0.000008
C	-4.958835	1.395773	0.000013	H	7.108354	-1.244607	0.000030
C	-3.745889	0.703560	-0.000003	H	7.108354	1.244607	0.000030
C	-3.745889	-0.703560	-0.000001				
C	-4.958835	-1.395773	0.000016	*1			
C	-6.161476	-0.698204	0.000030	C	6.143651	-0.698573	-0.001639
H	-7.108354	1.244608	0.000041	C	4.941294	-1.394574	-0.000623
H	-4.931819	2.488372	0.000010	C	3.726269	-0.703672	0.000458
H	-4.931819	-2.488372	0.000017	C	3.726280	0.703703	0.000524
H	-7.108354	-1.244607	0.000044	C	4.941305	1.394608	-0.000502
C	-2.481384	-1.480142	-0.000015	C	6.143659	0.698603	-0.001585
O	-2.473384	-2.695748	-0.000009	H	7.090216	-1.245693	-0.002491
C	-2.481384	1.480142	-0.000024	H	4.914996	-2.487206	-0.000646
O	-2.473384	2.695748	0.000002	H	4.915015	2.487241	-0.000408
C	-1.208808	-0.703134	-0.000017	H	7.090227	1.245716	-0.002390
C	-1.208808	0.703134	-0.000017	C	2.464735	1.488346	0.001738
C	0.000000	-1.394774	-0.000015	O	2.469388	2.707683	-0.000448
C	0.000000	1.394774	-0.000015	C	2.464720	-1.488319	0.001498
C	1.208808	-0.703134	-0.000012	O	2.469412	-2.707679	0.000952
H	0.000000	-2.487732	-0.000010	C	1.201799	0.710027	0.001225
C	1.208808	0.703134	-0.000015	C	1.201809	-0.710048	0.001157
H	0.000000	2.487732	-0.000021	C	-0.002719	1.394502	0.000888
C	2.481384	-1.480142	0.000014	C	-0.002763	-1.394493	0.000773
O	2.473384	-2.695748	-0.000061	C	-1.224342	0.707706	0.000470
C	2.481384	1.480142	-0.000038	H	-0.001090	2.488227	0.000972
O	2.473384	2.695748	0.000053	C	-1.224370	-0.707764	0.000426
C	3.745889	-0.703560	0.000002	H	-0.001260	-2.488220	0.000727
C	3.745889	0.703560	-0.000002	C	-2.463365	1.478159	0.000099
C	4.958835	-1.395773	0.000010	O	-2.476902	2.716913	0.000132
C	4.958835	1.395773	0.000012	C	-2.463409	-1.478421	0.000012
C	6.161476	-0.698205	0.000021	O	-2.476918	-2.717022	-0.000029
H	4.931819	-2.488372	0.000013	C	-3.713341	0.701623	-0.000316

C	-3.713325	-0.701624	-0.000360
C	-4.935133	1.396106	-0.000676
C	-4.935154	-1.395976	-0.000769
C	-6.132101	0.701262	-0.001075
H	-4.906127	2.489413	-0.000631
C	-6.132122	-0.701107	-0.001122
H	-4.906084	-2.489283	-0.000795
H	-7.077983	1.249276	-0.001354
H	-7.078025	-1.249085	-0.001437

T₂

C	6.135897	0.700465	-0.000001
C	4.936365	1.395588	-0.000026
C	3.717118	0.706470	-0.000028
C	3.717118	-0.706470	-0.000012
C	4.936365	-1.395588	0.000016
C	6.135897	-0.700465	0.000022
H	7.083172	1.246175	0.000004
H	4.908290	2.488049	-0.000034
H	4.908289	-2.488049	0.000022
H	7.083172	-1.246176	0.000041
C	2.467937	-1.500509	-0.000072
O	2.471807	-2.725898	0.000143
C	2.467937	1.500509	-0.000005
O	2.471807	2.725898	-0.000156
C	1.209692	-0.744418	-0.000011
C	1.209692	0.744418	-0.000026
C	0.000000	-1.426478	-0.000004
C	0.000000	1.426478	0.000003
C	-1.209692	-0.744418	0.000011
H	0.000000	-2.519750	-0.000010
C	-1.209692	0.744418	0.000023
H	0.000000	2.519750	0.000009
C	-2.467937	-1.500509	0.000047
O	-2.471807	-2.725898	-0.000087
C	-2.467937	1.500509	0.000027
O	-2.471807	2.725898	0.000100
C	-3.717118	-0.706470	0.000012
C	-3.717118	0.706470	0.000028
C	-4.936365	-1.395588	-0.000013
C	-4.936365	1.395588	0.000025
C	-6.135897	-0.700465	-0.000018
H	-4.908289	-2.488049	-0.000022
C	-6.135897	0.700465	0.000002

H	-4.908290	2.488049	0.000036
H	-7.083172	-1.246176	-0.000036
H	-7.083172	1.246175	-0.000003

3

C	1.195680	-1.204611	0.001920
C	-0.196935	-1.199844	-0.008461
C	-0.915337	0.002315	-0.010471
C	-0.193919	1.201506	-0.008461
C	1.199642	1.202482	0.001943
C	1.901028	-0.001710	0.008098
H	1.736179	-2.156177	0.001450
H	-0.745065	-2.148878	-0.017620
H	-0.739415	2.151919	-0.017787
H	1.742462	2.152703	0.001536
H	2.994816	-0.003492	0.013404
C	-2.413109	0.001160	0.007990
H	-2.800122	-0.116646	1.035105
H	-2.824996	0.942657	-0.386477
H	-2.826166	-0.829880	-0.584967

T_{4ts}

C	-6.197483	0.025959	-0.662605
C	-4.999742	0.656999	-0.948955
C	-3.772660	0.022095	-0.673331
C	-3.780487	-1.266960	-0.083238
C	-5.004262	-1.884485	0.205946
C	-6.203045	-1.251617	-0.082813
H	-7.143638	0.526517	-0.887255
H	-4.979404	1.653680	-1.396212
H	-4.978010	-2.875397	0.667268
H	-7.152228	-1.745505	0.142997
C	-2.529060	-1.969510	0.260876
O	-2.531001	-3.070670	0.806987
C	-2.523595	0.698229	-0.973386
O	-2.544155	1.908972	-1.423552
C	-1.281519	-1.276982	-0.095435
C	-1.297406	0.011300	-0.726450
C	-0.062528	-1.884927	0.180815
C	-0.063685	0.590476	-1.105075
C	1.151668	-1.279404	-0.149490
H	-0.056821	-2.861749	0.672672
C	1.139713	-0.023500	-0.825157
H	-0.055305	1.543882	-1.640636

C	2.411545	-1.958639	0.195624	H	-0.000029	-2.960128	0.938644
O	2.431372	-3.038816	0.768920				
C	2.395696	0.657661	-1.214241	6			
O	2.394846	1.737046	-1.785558	C	6.130001	0.668049	-0.001036
C	3.671261	-1.263487	-0.182383	C	4.937610	1.368507	0.000529
C	3.663709	-0.022119	-0.847878	C	3.706258	0.677422	0.000529
C	4.891777	-1.864645	0.138591	C	3.711545	-0.741424	-0.000851
C	4.875237	0.596266	-1.172190	C	4.930872	-1.427632	-0.002250
C	6.090000	-1.243165	-0.190338	C	6.131863	-0.735129	-0.002450
H	4.871651	-2.828954	0.652996	H	7.077602	1.213604	-0.001151
C	6.082284	-0.008709	-0.845818	H	4.933527	2.460433	0.001688
H	4.841689	1.558410	-1.690128	H	4.899037	-2.520270	-0.003100
H	7.040252	-1.720864	0.063862	H	7.079411	-1.280428	-0.003613
H	7.025947	0.479883	-1.103540	C	2.457362	-1.514433	-0.000242
H	-1.843207	2.744798	-0.543302	O	2.448290	-2.740669	-0.000536
C	1.912916	2.238303	1.524860	C	2.464499	1.388961	0.002194
C	0.935057	2.968159	0.880248	O	2.548492	2.718532	0.005127
C	-0.442619	2.699965	1.114958	C	1.207111	-0.730337	0.000367
C	-0.782634	1.647317	2.015176	C	1.221163	0.698166	0.000774
C	0.200857	0.915148	2.647397	C	-0.008783	-1.409157	0.000463
C	1.553880	1.204131	2.403880	C	-0.017542	1.376977	-0.000622
H	2.968967	2.454138	1.339024	C	-1.222145	-0.727796	0.000302
H	1.205874	3.759329	0.174592	H	-0.001097	-2.502427	0.000676
H	-1.841826	1.427748	2.190947	C	-1.215452	0.689811	-0.000709
H	-0.068857	0.108537	3.333571	H	-0.091419	2.470290	-0.002076
H	2.332540	0.619923	2.903478	C	-2.486909	-1.494598	0.001077
C	-1.467589	3.430903	0.423579	O	-2.497656	-2.713592	0.002350
H	-2.431264	3.502057	0.950868	C	-2.481320	1.472695	-0.001972
H	-1.148571	4.372708	-0.044567	O	-2.471530	2.690607	-0.003562
				C	-3.749465	-0.708029	0.000448
5				C	-3.746710	0.699489	-0.001151
C	0.000006	1.131873	1.210540	C	-4.965702	-1.394652	0.001418
C	0.000006	-0.252254	1.216802	C	-4.958445	1.395551	-0.001860
C	-0.000003	-0.993437	0.000000	C	-6.166295	-0.693832	0.000765
C	0.000006	-0.252254	-1.216802	H	-4.941109	-2.487344	0.002702
C	0.000006	1.131873	-1.210540	C	-6.163222	0.702891	-0.000911
C	0.000005	1.837056	0.000000	H	-4.927184	2.488118	-0.003134
H	0.000012	1.678986	2.158221	H	-7.114743	-1.237796	0.001557
H	0.000014	-0.800373	2.165162	H	-7.108591	1.252036	-0.001450
H	0.000014	-0.800373	-2.165162	H	1.676033	3.135761	0.011984
H	0.000012	1.678986	-2.158221				
H	-0.000004	2.930628	0.000000	7			
C	-0.000024	-2.397456	0.000000	C	3.188834	-0.244523	-0.134532
H	-0.000029	-2.960128	-0.938644	O	4.264643	-0.953165	0.096403

C	3.896903	-2.111410	0.906536	C	1.386168	5.168339	-0.308451
C	2.361044	-2.105422	0.791262	H	0.861334	6.028119	-0.758298
N	2.074886	-0.744361	0.285722	H	2.437136	5.475452	-0.185509
C	3.395772	0.993425	-0.956664	Cu	0.307581	0.037791	0.157852
C	1.277188	3.956465	-1.220523	C	-6.075645	-1.672463	-0.178734
O	2.512920	3.182276	-1.202262	C	-4.806612	-1.771495	0.392964
C	2.237847	1.947588	-0.869385	C	-3.823926	-0.873720	-0.029056
C	0.267356	2.978409	-0.587319	C	-4.137214	0.087313	-1.001808
N	1.003792	1.695039	-0.576693	C	-5.383069	0.201172	-1.576682
C	4.697263	1.692846	-0.556487	C	-6.359989	-0.708763	-1.145075
H	5.536128	0.991699	-0.652880	H	-6.859080	-2.364618	0.136424
H	4.881614	2.546498	-1.221120	H	-4.591733	-2.531133	1.145599
H	4.659785	2.056169	0.481693	H	-5.605232	0.956626	-2.333176
C	3.469236	0.517460	-2.427334	H	-7.361784	-0.657258	-1.577923
H	3.592942	1.387469	-3.088862	S	-2.718133	1.111761	-1.304386
H	4.337289	-0.145765	-2.554230	O	-2.140571	0.944561	-2.619014
H	2.556838	-0.028249	-2.715070	O	-2.887365	2.422531	-0.712610
C	2.078558	-3.167919	-0.242291	N	-1.714829	0.171326	-0.192335
C	4.407686	-3.389198	0.266927	C	-2.429873	-0.754970	0.359872
H	4.676838	-4.119680	1.048816	C	-1.645369	-1.618483	1.311327
H	5.325024	-3.202364	-0.313914	O	-0.435592	-1.419536	1.398179
C	3.247798	-3.867476	-0.556965	O	-2.299838	-2.516749	1.943688
C	0.876706	-3.468223	-0.880084	C	-1.569450	-3.426277	2.839073
H	-0.041161	-2.922086	-0.641512	H	-0.771204	-3.888124	2.234616
C	0.854470	-4.479134	-1.838773	H	-1.098034	-2.798487	3.611008
H	-0.079440	-4.723040	-2.352053	C	-2.554516	-4.407928	3.387183
C	2.021327	-5.181120	-2.150657	H	-3.023004	-4.994795	2.583819
H	1.990910	-5.971361	-2.905487	H	-2.032777	-5.105047	4.057571
C	3.222803	-4.881596	-1.511285	H	-3.340275	-3.902115	3.966891
H	4.134794	-5.432563	-1.759085				
H	4.290116	-1.917234	1.914753	8ts			
H	1.840813	-2.268286	1.747765	C	4.749369	-3.471307	0.706868
C	-0.668608	2.944623	1.845438	C	4.041169	-2.275987	0.838628
C	-0.697724	3.597188	3.076278	C	2.761772	-2.203189	0.289672
C	-0.021879	4.808043	3.248311	C	2.242218	-3.314457	-0.371620
C	0.688276	5.384191	2.196458	C	2.929177	-4.506416	-0.519840
C	0.723930	4.730561	0.966637	C	4.209641	-4.568983	0.034020
C	0.050264	3.518226	0.799773	H	5.750107	-3.546800	1.138872
H	-1.214680	2.004833	1.706736	H	4.484705	-1.422422	1.358029
H	-1.256969	3.164342	3.909904	H	2.485695	-5.361737	-1.035294
H	-0.054489	5.310813	4.218690	H	4.789976	-5.490287	-0.053731
H	1.210231	6.335383	2.335745	S	0.604711	-2.961662	-0.940589
H	1.084801	4.197269	-2.275438	O	-0.364233	-3.852117	-0.327138
H	-0.658350	2.882479	-1.173647	O	0.546515	-2.721626	-2.376536

N	0.553436	-1.424716	-0.171885	H	-5.519886	1.717631	-0.421754
C	1.811284	-1.068834	0.216304	C	-3.257673	-2.585007	0.544812
C	1.753920	0.052120	1.197272	C	-5.230345	-2.752425	-0.805536
O	0.704864	0.691860	1.309132	H	-5.457815	-3.729090	-1.264942
O	2.836336	0.310811	1.840536	H	-6.174037	-2.183172	-0.804168
C	2.864167	1.430503	2.783301	C	-4.614605	-2.917605	0.554260
H	2.098232	1.232330	3.548791	C	-2.475964	-2.717205	1.690379
H	2.560434	2.333615	2.226273	H	-1.403037	-2.496849	1.666088
C	4.251999	1.508200	3.336673	C	-3.077250	-3.173818	2.861440
H	4.517960	0.582930	3.868853	H	-2.481674	-3.287618	3.771183
H	4.316737	2.342171	4.049288	C	-4.436436	-3.499663	2.876792
H	4.988688	1.681561	2.537422	H	-4.894438	-3.860537	3.801983
C	2.506757	-0.032792	-1.359748	C	-5.211444	-3.380482	1.724931
H	2.202588	-0.791447	-2.091693	H	-6.272342	-3.646905	1.739833
H	1.814344	0.816218	-1.295227	H	-4.075809	-2.369384	-2.654317
C	3.903859	0.234051	-1.236575	H	-2.071192	-2.678276	-1.290008
C	4.844750	-0.694820	-1.748074	C	0.968901	3.532248	-0.240741
C	4.374670	1.401843	-0.584387	C	1.652751	4.536357	-0.923236
C	6.200936	-0.455958	-1.623027	C	1.150831	5.839675	-0.943944
H	4.481832	-1.599005	-2.248981	C	-0.039099	6.149989	-0.288677
C	5.731478	1.631849	-0.457457	C	-0.724865	5.143572	0.387188
H	3.655020	2.126839	-0.186628	C	-0.220588	3.839640	0.414845
C	6.645258	0.702115	-0.972999	H	1.354817	2.510475	-0.225911
H	6.924650	-1.166433	-2.028810	H	2.580454	4.305027	-1.454954
H	6.093213	2.536781	0.036709	H	1.692902	6.620333	-1.484217
H	7.717993	0.886077	-0.870858	H	-0.434013	7.169807	-0.310782
C	-3.423913	0.056379	-1.201109	H	-2.971219	3.607536	2.299536
O	-4.449607	-0.602133	-1.674331	H	-0.716560	2.544459	2.119462
C	-4.163263	-2.029148	-1.613176	C	-2.004937	5.245621	1.162986
C	-2.848530	-2.070166	-0.808373	H	-1.851998	5.741395	2.137069
N	-2.433376	-0.648609	-0.762521	H	-2.800515	5.806079	0.646885
C	-3.517415	1.555033	-1.290046	Cu	-0.819343	0.051823	0.106396
C	-2.402362	3.799371	1.377945				
O	-3.245866	3.343857	0.273923	9			
C	-2.774194	2.202181	-0.157386	C	4.580241	-3.699117	0.892749
C	-1.149711	2.927290	1.183078	C	4.010091	-2.428274	0.806456
N	-1.655775	1.808568	0.355079	C	2.708630	-2.314244	0.324869
C	-2.787175	1.990805	-2.581880	C	2.033938	-3.469427	-0.056852
H	-3.297415	1.556551	-3.454885	C	2.578974	-4.743727	0.018734
H	-2.818939	3.087959	-2.666659	C	3.880957	-4.842816	0.503005
H	-1.735758	1.664662	-2.579961	H	5.599382	-3.797744	1.274093
C	-4.973331	2.013801	-1.328875	H	4.582835	-1.547100	1.106831
H	-5.012665	3.107203	-1.416926	H	2.007747	-5.627204	-0.276990
H	-5.480384	1.577822	-2.199122	H	4.353673	-5.824273	0.584224

S	0.400805	-3.080916	-0.581946	C	-4.810059	2.325720	-1.106147
O	-0.602063	-3.687798	0.273334	H	-4.834229	3.422516	-1.141152
O	0.230100	-3.110383	-2.027660	H	-5.366629	1.936880	-1.968193
N	0.536743	-1.421486	-0.152991	H	-5.312825	1.993687	-0.185859
C	1.893804	-1.064204	0.069203	C	-3.629241	-2.354370	0.379936
C	1.867322	-0.003762	1.152907	C	-5.257299	-2.430936	-1.374995
O	0.831386	0.635678	1.348153	H	-5.347925	-3.390327	-1.912466
O	2.967579	0.200647	1.776175	H	-6.186981	-1.873290	-1.571623
C	3.038106	1.267778	2.781405	C	-4.963919	-2.645189	0.081355
H	2.287662	1.035104	3.552197	C	-3.129456	-2.532012	1.668575
H	2.735850	2.202831	2.279774	H	-2.076075	-2.347083	1.902376
C	4.439892	1.292552	3.301784	C	-3.990347	-2.991446	2.663158
H	4.700670	0.337962	3.782129	H	-3.615637	-3.138378	3.679741
H	4.536981	2.089232	4.052437	C	-5.326806	-3.274472	2.368676
H	5.160840	1.492636	2.494958	H	-5.990114	-3.635528	3.159508
C	2.403547	-0.333747	-1.322839	C	-5.820690	-3.108700	1.076583
H	2.064803	-1.028490	-2.105888	H	-6.865458	-3.338290	0.847296
H	1.821899	0.599232	-1.412096	H	-3.763868	-1.894165	-2.919005
C	3.863304	-0.117460	-1.378852	H	-2.110934	-2.489848	-1.201097
C	4.688151	-1.101014	-1.955808	C	1.258219	3.420559	-0.223847
C	4.451817	1.047549	-0.854680	C	2.001341	4.359355	-0.936654
C	6.062948	-0.923163	-2.009647	C	1.611550	5.700741	-0.951065
H	4.234537	-2.010447	-2.365892	C	0.474826	6.115496	-0.260002
C	5.827294	1.222441	-0.905359	C	-0.270573	5.175094	0.447557
H	3.822861	1.833717	-0.421002	C	0.124841	3.834131	0.471488
C	6.635415	0.234316	-1.476467	H	1.557730	2.369389	-0.220267
H	6.695974	-1.685933	-2.469148	H	2.888309	4.043896	-1.494117
H	6.277557	2.134670	-0.506166	H	2.199902	6.429310	-1.514986
H	7.719126	0.372226	-1.511569	H	0.166993	7.164918	-0.279290
C	-3.313302	0.338956	-1.177978	H	-2.590343	3.836510	2.423100
O	-4.294444	-0.233899	-1.825732	H	-0.429983	2.596436	2.201857
C	-4.046064	-1.670255	-1.880035	C	-1.517562	5.384722	1.256491
C	-2.918611	-1.836038	-0.845358	H	-1.299774	5.869055	2.223986
N	-2.421925	-0.448630	-0.667727	H	-2.276942	6.007786	0.758298
C	-3.360347	1.841386	-1.164715	Cu	-0.762939	0.126139	0.200664
C	-2.027491	3.977016	1.488671				
O	-2.927075	3.585682	0.403660	10			
C	-2.556163	2.410141	-0.034325	C	6.137040	0.688874	-0.028791
C	-0.853400	3.006955	1.272886	C	4.934726	1.381601	-0.002844
N	-1.465499	1.928892	0.463510	C	3.720222	0.671979	0.005430
C	-2.683966	2.349506	-2.460444	C	3.728153	-0.744434	-0.010323
H	-3.250482	1.991519	-3.332924	C	4.937654	-1.421177	-0.033354
H	-2.692026	3.450053	-2.467523	C	6.138528	-0.706253	-0.043863
H	-1.641335	2.004058	-2.539157	H	7.080405	1.238546	-0.037081

H	4.921749	2.473200	0.009250	H	-2.662438	-3.449814	2.313586
H	4.925782	-2.513441	-0.042326	H	-1.622419	-4.364562	1.186241
H	7.087432	-1.247761	-0.063357	H	-1.052133	-2.803707	1.860055
C	2.462693	-1.521265	0.004744	C	-3.756895	-3.439634	-0.246416
O	2.452441	-2.731812	0.005914	H	-3.402593	-4.420571	-0.589172
C	2.472101	1.376824	0.033158	H	-4.506192	-3.596114	0.540936
O	2.544065	2.663698	0.075505	H	-4.244900	-2.928512	-1.090712
C	1.193343	-0.737267	0.013097	C	-3.766579	1.771213	0.467043
C	1.201854	0.679432	0.015995	C	-5.756692	0.680556	1.230942
C	-0.012275	-1.418837	0.013299	H	-6.376646	1.195654	1.984707
C	-0.011519	1.373520	0.001722	H	-6.410072	-0.065749	0.750318
C	-1.220500	-0.717182	0.008282	C	-5.143987	1.658020	0.267985
H	-0.021978	-2.512058	0.016054	C	-2.994787	2.647490	-0.290607
C	-1.219014	0.682620	-0.003091	H	-1.918503	2.745414	-0.111752
H	-0.089891	2.466737	-0.009421	C	-3.623240	3.413881	-1.270269
C	-2.505195	-1.489635	0.014008	H	-3.034038	4.106642	-1.877541
O	-2.483365	-2.702338	0.028472	C	-5.000874	3.302412	-1.478094
C	-2.490506	1.471354	-0.020795	H	-5.481814	3.909547	-2.250362
O	-2.451430	2.685092	-0.037233	C	-5.769854	2.429256	-0.709382
C	-3.759569	-0.705911	0.002392	H	-6.848984	2.350926	-0.873384
C	-3.753063	0.704139	-0.015952	H	-4.694980	-0.161814	2.975904
C	-4.975877	-1.391557	0.009510	H	-2.798917	1.298709	2.370820
C	-4.962110	1.402578	-0.027467	C	2.134605	-0.375301	-2.210562
C	-6.174449	-0.686339	-0.001392	C	3.488958	-0.288859	-1.884826
H	-4.958410	-2.484031	0.023878	C	4.163598	-1.397912	-1.365913
C	-6.167807	0.709607	-0.020326	C	3.500927	-2.611784	-1.174839
H	-4.933055	2.494859	-0.041503	C	2.147771	-2.698100	-1.494510
H	-7.123771	-1.227722	0.004755	C	1.475351	-1.581745	-2.001098
H	-7.111762	1.260237	-0.029114	H	1.597424	0.493877	-2.604770
H	1.683229	3.118296	0.106965	H	4.029196	0.651011	-2.042811
				H	5.226345	-1.315191	-1.117018
11				H	4.040825	-3.484020	-0.790790
C	-3.067005	-1.293487	0.825227	H	-0.158783	-3.963008	-3.085300
O	-4.304843	-1.292623	1.304249	H	-0.345542	-1.496352	-3.194599
C	-4.562369	0.005991	1.897080	C	1.221945	-3.871919	-1.359150
C	-3.293926	0.804499	1.517865	H	1.653321	-4.813363	-1.733339
N	-2.396798	-0.208293	0.947595	H	0.959948	-4.044438	-0.296824
C	-2.581430	-2.621813	0.301758	Cu	-0.633408	0.105873	0.109660
C	-0.036830	-3.441059	-2.126676	C	5.410031	2.675077	0.731641
O	-1.231714	-3.660651	-1.357193	C	4.534743	1.632005	1.037983
C	-1.527054	-2.498655	-0.770820	C	3.197832	1.752496	0.656858
C	0.032470	-1.907073	-2.241719	C	2.787775	2.916415	-0.003850
N	-0.868367	-1.469242	-1.157386	C	3.637405	3.957236	-0.320665
C	-1.933039	-3.354835	1.494382	C	4.976539	3.817664	0.059069

H	6.459917	2.591342	1.022204	H	-4.166778	4.175105	2.538778
H	4.887723	0.738669	1.554956	H	-4.795737	2.517877	2.347860
H	3.283580	4.847541	-0.846093	C	-1.920542	-1.434803	1.974131
H	5.687485	4.614198	-0.172477	H	-1.327447	-2.227680	1.506821
S	1.051863	2.801886	-0.340774	H	-1.370428	-0.713314	2.589490
O	0.275978	3.680774	0.514789	C	-3.304529	-1.646501	2.197216
O	0.754004	2.709794	-1.758469	C	-3.961143	-2.750960	1.598373
N	0.929438	1.196556	0.319724	C	-4.074347	-0.740202	2.967548
C	2.076359	0.811462	0.785001	C	-5.322512	-2.941457	1.770213
C	2.104790	-0.579959	1.355894	H	-3.372452	-3.458112	1.003613
O	1.116382	-1.275011	1.364449	C	-5.437159	-0.932914	3.126762
O	3.287015	-0.915996	1.814121	H	-3.575343	0.109887	3.445549
C	3.452663	-2.246141	2.347261	C	-6.065543	-2.031342	2.528794
H	2.845505	-2.323816	3.264265	H	-5.816390	-3.800959	1.308991
H	3.040136	-2.959088	1.613759	H	-6.022070	-0.230616	3.727088
C	4.916879	-2.453765	2.592753	H	-7.140650	-2.181065	2.660938
H	5.309767	-1.712824	3.305648	C	3.608244	0.537007	1.361411
H	5.090297	-3.455209	3.011713	O	4.697411	0.123591	1.993974
H	5.485533	-2.371106	1.652916	C	4.577239	-1.302389	2.222805
				C	3.240728	-1.651666	1.523305
				N	2.720048	-0.346915	1.092496
				C	3.503916	2.025874	1.148553
				C	1.841863	3.925845	-1.432120
				O	2.838186	3.685432	-0.421788
				C	2.758397	2.391964	-0.110540
				C	1.515608	2.513840	-1.952903
				N	2.031466	1.654745	-0.866469
				C	2.677583	2.578072	2.329862
				H	3.155846	2.295674	3.280906
				H	2.638482	3.676372	2.272193
				H	1.651176	2.178879	2.305939
				C	4.892967	2.669385	1.126878
				H	4.799732	3.755003	0.994524
				H	5.409141	2.479317	2.077539
				H	5.513070	2.267796	0.311200
				C	3.642350	-2.503661	0.352770
				C	5.692508	-2.068358	1.514150
				H	6.117950	-2.838705	2.179532
				H	6.523142	-1.391408	1.254755
				C	5.026042	-2.685899	0.317435
				C	2.816130	-3.031738	-0.634772
				H	1.728977	-2.913254	-0.582671
				C	3.398585	-3.740582	-1.683649
				H	2.764185	-4.158421	-2.470494
12tsR							
C	-5.187389	-0.870756	-1.438097				
C	-4.230068	-0.271576	-0.618993				
C	-2.899698	-0.679008	-0.734815				
C	-2.588801	-1.683113	-1.655937				
C	-3.523412	-2.297341	-2.470334				
C	-4.847376	-1.869882	-2.352043				
H	-6.229262	-0.549224	-1.359814				
H	-4.511596	0.513022	0.085400				
H	-3.234479	-3.075962	-3.180774				
H	-5.618983	-2.319410	-2.981665				
S	-0.856343	-2.028793	-1.556803				
O	-0.138135	-1.809383	-2.802034				
O	-0.626877	-3.270917	-0.822176				
N	-0.541876	-0.729674	-0.496603				
C	-1.687334	-0.227333	-0.028139				
C	-1.541490	1.011103	0.784144				
O	-0.456392	1.435607	1.124893				
O	-2.699691	1.556544	1.092314				
C	-2.698788	2.748842	1.894051				
H	-1.992244	3.469111	1.447972				
H	-2.314332	2.491378	2.897168				
C	-4.106727	3.265765	1.924070				
H	-4.450061	3.512474	0.906738				

C	4.783990	-3.920433	-1.730060	C	-3.513933	-4.520144	-1.140041
H	5.229365	-4.479482	-2.558053	H	-3.312133	-5.384288	-1.796150
C	5.604869	-3.401393	-0.729089	H	-4.586630	-4.564652	-0.890534
H	6.687921	-3.553307	-0.767096	C	-2.613807	-4.523755	0.063243
H	4.572581	-1.443838	3.312939	C	-0.717507	-3.325144	0.996724
H	2.500370	-2.138889	2.180668	H	0.005287	-2.503550	0.947175
C	-0.781538	1.571044	-2.730555	C	-0.725729	-4.196074	2.084800
C	-2.165004	1.752760	-2.706853	H	0.004111	-4.065844	2.888812
C	-2.723801	2.849661	-2.044769	C	-1.668212	-5.225443	2.157724
C	-1.910460	3.791230	-1.412272	H	-1.665214	-5.900943	3.017962
C	-0.529008	3.613556	-1.436896	C	-2.616345	-5.395941	1.149700
C	0.022918	2.504390	-2.084762	H	-3.355331	-6.200375	1.215643
H	-0.340160	0.704170	-3.234342	H	-3.155718	-3.314325	-2.955106
H	-2.818173	1.033368	-3.211889	H	-1.014070	-2.645091	-1.915719
H	-3.811159	2.975670	-2.032817	C	-0.462097	3.611948	-0.200394
H	-2.352037	4.663749	-0.918654	C	-0.066783	4.674576	-1.009863
H	2.285065	4.595020	-2.181676	C	-0.961192	5.710234	-1.297763
H	2.031066	2.234738	-2.888513	C	-2.256611	5.700211	-0.780763
C	0.540786	4.472477	-0.827036	C	-2.655399	4.635465	0.025761
H	0.397938	5.547827	-1.016024	C	-1.757544	3.604958	0.305718
H	0.567004	4.345750	0.272801	H	0.216763	2.793283	0.055558
Cu	1.178499	-0.022724	-0.107949	H	0.948187	4.703577	-1.418369

12tsS

C	-3.494395	-1.141439	-1.048646	H	-2.948736	6.517070	-1.006952
O	-4.145529	-2.186209	-1.550818	H	-4.272174	2.913816	2.312129
C	-3.176645	-3.220016	-1.859325	H	-1.867028	2.351962	2.088119
C	-1.881568	-2.655593	-1.234994	C	-3.970542	4.414647	0.718779
N	-2.231463	-1.273927	-0.884386	H	-4.127347	5.151196	1.525221
C	-4.356801	0.078657	-0.836561	H	-4.842325	4.497496	0.049124
C	-3.865846	3.004480	1.294261	Cu	-1.002831	0.033033	-0.023587
O	-4.589008	2.053902	0.473227	C	5.162902	-1.042867	2.128672
C	-3.735070	1.125682	0.054630	C	4.334701	-1.020742	1.004932
C	-2.401237	2.535171	1.139671	C	3.028922	-0.546764	1.144864
N	-2.508756	1.274381	0.392210	C	2.612311	-0.104319	2.405324
C	-4.536288	0.731982	-2.223200	C	3.421114	-0.105585	3.527255
H	-5.000350	0.013538	-2.915155	C	4.721936	-0.590036	3.372178
H	-5.190426	1.612306	-2.139529	H	6.184292	-1.418968	2.026769
H	-3.563908	1.046898	-2.634318	H	4.702108	-1.367156	0.036822
C	-5.716703	-0.341626	-0.268576	H	3.053944	0.251015	4.493018
H	-6.366809	0.537573	-0.170011	H	5.395628	-0.615015	4.232040
H	-6.196858	-1.062113	-0.943790	S	0.936715	0.453547	2.290087
H	-5.609685	-0.810144	0.722025	O	0.010564	-0.336929	3.084301
C	-1.665375	-3.500153	-0.008149	O	0.855184	1.910025	2.352619
				N	0.777050	-0.010768	0.654608

C	1.952775	-0.379135	0.146350	O	2.866390	0.791819	-1.334983
C	1.872848	-1.037670	-1.193642	C	2.946301	1.827141	-2.334672
O	0.880610	-0.990716	-1.882734	H	2.351599	2.687526	-1.979706
O	2.992367	-1.657922	-1.512580	H	2.473760	1.448959	-3.257869
C	3.045775	-2.347871	-2.775226	C	4.399138	2.151120	-2.515207
H	2.241995	-3.102255	-2.791383	H	4.840769	2.507918	-1.571181
H	2.825638	-1.622948	-3.577365	H	4.524335	2.937227	-3.273419
C	4.412128	-2.954126	-2.898311	H	4.961265	1.262269	-2.843008
H	4.595392	-3.679316	-2.090799	C	1.758657	-2.135045	-0.781941
H	4.508851	-3.480034	-3.858834	H	1.625780	-2.928756	-0.026773
H	5.191559	-2.177296	-2.850423	H	0.847178	-2.124023	-1.407794
C	2.710510	1.585620	-0.817700	C	2.982714	-2.377957	-1.606841
H	2.416837	2.111531	0.097505	C	4.035155	-3.151467	-1.105903
H	1.959066	1.530559	-1.613881	C	3.112925	-1.805951	-2.878083
C	4.089124	1.471671	-1.124364	C	5.200087	-3.331679	-1.848094
C	5.065221	1.799137	-0.149597	H	3.936685	-3.613528	-0.117072
C	4.524669	0.979893	-2.380442	C	4.276835	-1.980468	-3.621152
C	6.414504	1.640850	-0.421995	H	2.285109	-1.216938	-3.293041
H	4.734468	2.179967	0.823822	C	5.326765	-2.739541	-3.103320
C	5.874683	0.819584	-2.642512	H	6.013457	-3.941219	-1.444576
H	3.776593	0.736736	-3.143580	H	4.364095	-1.528346	-4.613466
C	6.822543	1.146162	-1.664319	H	6.241133	-2.879858	-3.686577
H	7.159775	1.900673	0.334327	C	-3.611410	0.299578	-1.245214
H	6.203516	0.445193	-3.616002	O	-4.631958	-0.274985	-1.850476
H	7.887820	1.020831	-1.876509	C	-4.316916	-1.678105	-2.061540
13R				C	-2.939816	-1.831097	-1.371753
C	5.103928	-0.537663	1.921028	N	-2.610284	-0.453539	-0.964402
C	4.242333	-0.550971	0.823952	C	-3.718986	1.791555	-1.077914
C	2.874416	-0.726459	1.041955	C	-2.003156	4.057533	1.166966
C	2.435046	-0.908060	2.350271	O	-3.111872	3.573223	0.376591
C	3.272287	-0.895306	3.457720	C	-2.821089	2.339985	-0.000308
C	4.630510	-0.699112	3.225790	C	-1.188214	2.781179	1.471951
H	6.174394	-0.392073	1.753713	N	-1.777316	1.809140	0.525797
H	4.637103	-0.408593	-0.184817	C	-3.210215	2.406961	-2.401494
H	2.873242	-1.028435	4.467038	H	-3.814775	2.035400	-3.242575
H	5.328447	-0.674142	4.066273	H	-3.305676	3.502550	-2.361176
S	0.688874	-1.187144	2.367734	H	-2.153601	2.142514	-2.570896
O	-0.034942	-0.231566	3.205145	C	-5.170866	2.199627	-0.818512
O	0.412219	-2.609806	2.560738	H	-5.243231	3.292209	-0.742531
N	0.487705	-0.747624	0.770651	H	-5.806135	1.866390	-1.649584
C	1.740732	-0.792279	0.028869	H	-5.555441	1.757403	0.113208
C	1.687247	0.365149	-0.970657	C	-3.204845	-2.723289	-0.193527
O	0.635544	0.780723	-1.415977	C	-5.309388	-2.580458	-1.332691
				H	-5.636121	-3.405504	-1.987947

H	-6.220253	-2.018841	-1.066992	H	-5.626533	0.706932	-0.941736
C	-4.550061	-3.094010	-0.141476	C	-3.986382	-0.966744	1.662403
C	-2.301574	-3.129099	0.783919	H	-4.509543	-0.427871	2.467163
H	-1.245194	-2.846038	0.736309	H	-4.473629	-1.944256	1.521035
C	-2.767161	-3.904489	1.843666	H	-2.934628	-1.119097	1.955909
H	-2.068940	-4.216754	2.625146	C	-1.568426	-3.438776	-0.829355
C	-4.113607	-4.274404	1.906333	C	-3.528761	-4.121074	-2.019336
H	-4.467815	-4.884903	2.741887	H	-3.354029	-4.656556	-2.968811
C	-5.010539	-3.878789	0.914082	H	-4.563444	-4.348537	-1.716809
H	-6.061434	-4.179284	0.966132	C	-2.498415	-4.472189	-0.983971
H	-4.300979	-1.828905	-3.149838	C	-0.539110	-3.537175	0.104059
H	-2.143370	-2.207562	-2.036811	H	0.160274	-2.711769	0.265590
C	1.389511	2.467659	1.460530	C	-0.434131	-4.699056	0.866891
C	2.616196	2.993630	1.058477	H	0.363309	-4.789721	1.609358
C	2.665845	4.210014	0.370646	C	-1.349503	-5.740677	0.700446
C	1.497569	4.918916	0.087365	H	-1.258154	-6.643844	1.310258
C	0.271239	4.388510	0.483025	C	-2.388875	-5.633030	-0.222559
C	0.226368	3.162038	1.149357	H	-3.115403	-6.443099	-0.337282
H	1.326312	1.540074	2.034387	H	-3.575304	-2.270606	-3.235878
H	3.541268	2.455574	1.292935	H	-1.185845	-2.093471	-2.526188
H	3.633502	4.623164	0.070250	C	-0.616562	3.605153	-1.243557
H	1.547925	5.884885	-0.424219	C	-0.637769	4.526100	-2.289294
H	-2.429487	4.541699	2.055292	C	-1.652517	5.484698	-2.362697
H	-1.298657	2.376348	2.493287	C	-2.654222	5.539647	-1.394262
C	-1.099779	4.984136	0.340886	C	-2.636132	4.617795	-0.349275
H	-1.143823	6.028516	0.688197	C	-1.621647	3.660445	-0.282896
H	-1.438717	4.995410	-0.711286	H	0.174779	2.852785	-1.161893
Cu	-1.038778	0.042299	0.073924	H	0.143004	4.502683	-3.054561
13S				H	-1.658412	6.202004	-3.188254
C	-3.403927	-0.990642	-0.688375	H	-3.442577	6.295939	-1.456349
O	-4.166854	-1.873743	-1.299999	H	-3.178922	3.250586	2.600567
C	-3.329967	-2.631254	-2.225635	H	-0.977033	2.758534	1.609660
C	-1.920473	-2.274063	-1.725584	C	-3.573653	4.499922	0.818927
N	-2.144328	-1.049342	-0.943928	H	-3.458051	5.348855	1.514021
C	-4.081278	-0.144003	0.353016	H	-4.638219	4.475324	0.534120
C	-3.164522	3.201477	1.502660	Cu	-0.733324	0.076802	-0.196557
O	-4.061935	2.114992	1.132922	C	4.676579	-1.381908	2.561334
C	-3.341832	1.140203	0.616328	C	4.161645	-0.846356	1.381584
C	-1.817603	2.749415	0.896383	C	2.878124	-0.295190	1.398142
N	-2.083844	1.361241	0.480363	C	2.159310	-0.322562	2.585676
C	-5.539300	0.121989	-0.013485	C	2.653032	-0.845634	3.773599
H	-6.066420	-0.831282	-0.151920	C	3.938227	-1.378464	3.748360
H	-6.034434	0.675579	0.794776	H	5.681569	-1.811991	2.555838
				H	4.758197	-0.862833	0.465877

H	2.049793	-0.835858	4.685529	O	0.342639	-2.459278	-1.780429
H	4.370573	-1.800223	4.659370	O	1.024624	-3.774329	0.272283
S	0.549509	0.355662	2.324960	N	-0.400003	-1.579707	0.499840
O	-0.480145	-0.707091	2.342995	C	-1.868907	-1.345214	0.311274
O	0.298899	1.489814	3.213633	C	-1.970274	-0.355488	-0.842207
N	0.809237	0.808095	0.761573	O	-1.026964	0.390514	-1.114970
C	2.114327	0.371967	0.260558	O	-3.097773	-0.331305	-1.447934
C	1.855765	-0.621305	-0.861149	C	-3.333094	0.671570	-2.490040
O	0.721552	-0.808429	-1.309227	H	-2.628265	0.455875	-3.307950
O	2.900045	-1.228832	-1.318280	H	-3.068843	1.652468	-2.059497
C	2.768419	-2.147520	-2.433611	C	-4.769489	0.565988	-2.893475
H	1.976374	-2.872790	-2.186007	H	-4.994034	-0.429276	-3.303558
H	2.429120	-1.561792	-3.304402	H	-4.984323	1.312480	-3.670766
C	4.109601	-2.782012	-2.642255	H	-5.434917	0.756371	-2.037827
H	4.414515	-3.357811	-1.755468	H	-0.217955	-1.824097	1.483377
H	4.070692	-3.467883	-3.500166	C	-2.391623	-0.707872	1.629033
H	4.876217	-2.017499	-2.842402	H	-2.143823	-1.432172	2.424863
C	2.834464	1.634277	-0.313227	H	-1.778585	0.194137	1.821733
H	2.767261	2.370435	0.504788	C	-3.853724	-0.373880	1.712305
H	2.187799	2.008958	-1.127032	C	-4.705124	-1.170889	2.485078
C	4.247910	1.509606	-0.793774	C	-4.391009	0.732604	1.044689
C	5.314756	1.818085	0.057794	C	-6.067801	-0.892062	2.557650
C	4.533909	1.094401	-2.099578	H	-4.294800	-2.028085	3.030206
C	6.632988	1.680192	-0.370919	C	-5.753217	1.011079	1.110393
H	5.104031	2.164859	1.075682	H	-3.739806	1.396854	0.464566
C	5.849436	0.951702	-2.531959	C	-6.596229	0.192842	1.861525
H	3.709048	0.881981	-2.790567	H	-6.719805	-1.526588	3.163614
C	6.903470	1.236719	-1.664035	H	-6.156656	1.877532	0.578692
H	7.454406	1.923902	0.308709	H	-7.666303	0.409905	1.913720
H	6.054464	0.624958	-3.555908	C	3.187416	0.758438	1.206973
H	7.937734	1.128007	-2.002455	O	4.152149	0.376610	2.004223
14				C	4.010713	-1.054636	2.257842
				C	3.050030	-1.466390	1.131231
				N	2.416772	-0.177409	0.748294
C	-4.231325	-4.280538	-0.505973	C	3.127392	2.241477	0.971480
C	-3.855054	-2.988990	-0.136110	C	1.516381	3.906130	-1.860622
C	-2.498990	-2.678713	-0.062503	O	2.482738	3.741220	-0.771108
C	-1.580840	-3.664912	-0.415111	C	2.245401	2.593635	-0.187447
C	-1.927093	-4.956047	-0.790156	C	0.446500	2.879114	-1.462130
C	-3.285236	-5.259391	-0.815567	N	1.191714	1.958102	-0.579525
H	-5.294483	-4.527671	-0.552727	C	2.465661	2.892428	2.209000
H	-4.617737	-2.238167	0.080930	H	3.096851	2.725524	3.093945
H	-1.166336	-5.696300	-1.048593	H	2.371176	3.976820	2.046387
H	-3.609667	-6.265126	-1.091941	H	1.463281	2.474468	2.395338
S	0.043792	-3.008917	-0.466881				

C	4.543032	2.790338	0.773071	H	-0.173334	2.807823	-0.117769
H	4.501851	3.879967	0.645452	H	4.032205	0.083706	0.229002
H	5.156253	2.566160	1.655177	H	4.129758	2.589669	0.244405
H	5.027345	2.351433	-0.112354	S	1.451261	-1.633659	0.023488
C	3.974656	-2.006786	0.065851	O	1.917721	-2.272889	-1.193884
C	5.332200	-1.755690	2.021956	O	1.688973	-2.254161	1.314719
H	5.403582	-2.643295	2.673559	N	-0.238617	-1.357292	-0.129245
H	6.181019	-1.104704	2.284541	C	-0.462695	-0.095457	-0.149579
C	5.272036	-2.138766	0.572185	C	-1.876310	0.421254	-0.283422
C	3.684470	-2.341610	-1.254990	O	-2.125952	1.596812	-0.380712
H	2.672439	-2.256506	-1.661025	O	-2.756134	-0.556270	-0.287236
C	4.717460	-2.806039	-2.067499	C	-4.145915	-0.202598	-0.411374
H	4.509575	-3.072038	-3.107449	H	-4.233020	0.642285	-1.112093
C	6.014544	-2.934977	-1.565502	H	-4.615722	-1.085579	-0.866905
H	6.813016	-3.299488	-2.217658	C	-4.743406	0.120362	0.931607
C	6.300438	-2.605001	-0.242254	H	-4.285173	1.020764	1.368114
H	7.316095	-2.708689	0.151015	H	-5.822051	0.308696	0.825221
H	3.611150	-1.150648	3.278427	H	-4.610534	-0.716983	1.633218
H	2.294601	-2.200262	1.448652				
C	-1.566653	3.300155	0.161629	16R			
C	-2.356718	4.258946	0.793302	C	3.197735	2.144842	-1.194513
C	-2.120641	5.618863	0.576389	C	1.870776	1.855979	-0.875404
C	-1.084566	6.035839	-0.257332	C	1.568735	0.617050	-0.313531
C	-0.293011	5.077679	-0.885530	C	2.596872	-0.296646	-0.115817
C	-0.547641	3.716372	-0.690778	C	3.922122	-0.035980	-0.436167
H	-1.731596	2.235098	0.347735	C	4.216478	1.213815	-0.976012
H	-3.159220	3.948246	1.468711	H	3.444392	3.120916	-1.620973
H	-2.745971	6.362516	1.077476	H	1.082385	2.595132	-1.043844
H	-0.888744	7.101551	-0.406745	H	4.700545	-0.784197	-0.263417
H	2.061221	3.687513	-2.791096	H	5.249114	1.465993	-1.230687
H	0.005501	2.335408	-2.311837	S	1.926643	-1.816405	0.509126
C	0.882236	5.280210	-1.798354	O	2.557397	-2.263627	1.741934
H	0.568984	5.590277	-2.810254	O	1.783683	-2.750850	-0.600950
H	1.598749	6.038519	-1.445125	N	0.427711	-1.145633	0.861663
Cu	0.685378	0.131842	-0.119795	C	0.195971	0.070416	0.082469
				C	-0.544011	1.047792	0.993729
15				O	-0.758097	0.844512	2.160706
C	1.993839	2.834088	0.068503	O	-0.911510	2.133427	0.334037
C	0.743449	2.221699	-0.039914	C	-1.662492	3.120761	1.063233
C	0.691188	0.828628	-0.048459	H	-1.080997	3.417507	1.951526
C	1.875605	0.098704	0.051247	H	-2.589419	2.643230	1.425437
C	3.121843	0.683869	0.156084	C	-1.928824	4.270014	0.136814
C	3.165073	2.082151	0.162854	H	-0.987136	4.712077	-0.224320
H	2.055118	3.925085	0.077318	H	-2.495190	5.053730	0.660128

H	-2.517055	3.948855	-0.736682	C	0.628688	-0.243002	-1.185810
C	-0.628619	-0.243196	-1.185673	H	0.040127	-0.978138	-1.760961
H	-0.692608	0.673343	-1.793907	H	0.692651	0.673663	-1.793854
H	-0.040020	-0.978433	-1.760644	C	1.995544	-0.786235	-0.888548
C	-1.995458	-0.786439	-0.888327	C	2.170948	-2.147507	-0.611081
C	-3.113736	0.054782	-0.862355	C	3.113818	0.055002	-0.862515
C	-2.170842	-2.147695	-0.610736	C	3.434035	-2.652453	-0.313812
C	-4.378176	-0.448636	-0.562090	H	1.297560	-2.808275	-0.629809
H	-2.991357	1.118859	-1.094081	C	4.378265	-0.448435	-0.562310
C	-3.433924	-2.652621	-0.313406	H	2.991424	1.119098	-1.094166
H	-1.297443	-2.808453	-0.629407	C	4.540932	-1.804249	-0.286194
C	-4.540831	-1.804423	-0.285861	H	3.556423	-3.719185	-0.104202
H	-5.242741	0.221614	-0.551647	H	5.242823	0.221822	-0.551828
H	-3.556306	-3.719334	-0.103692	H	5.532812	-2.203136	-0.054272
H	-5.532710	-2.203297	-0.053908				
H	0.323832	-0.982220	1.868513				

16S

C	-3.197735	2.144734	-1.194295
C	-1.870752	1.855837	-0.875319
C	-1.568690	0.616918	-0.313443
C	-2.596830	-0.296731	-0.115570
C	-3.922109	-0.036037	-0.435781
C	-4.216488	1.213749	-0.975646
H	-3.444393	3.120800	-1.620772
H	-1.082358	2.594970	-1.043861
H	-4.700528	-0.784228	-0.262907
H	-5.249143	1.465952	-1.230209
S	-1.926606	-1.816487	0.509345
O	-2.557086	-2.263553	1.742351
O	-1.784059	-2.751055	-0.600674
N	-0.427526	-1.145836	0.861473
C	-0.195918	0.070319	0.082405
C	0.544064	1.047666	0.993685
O	0.758609	0.844150	2.160535
O	0.911130	2.133488	0.334054
C	1.662122	3.120890	1.063136
H	1.080768	3.417572	1.951542
H	2.589167	2.643459	1.425176
C	1.928167	4.270137	0.136645
H	0.986368	4.712084	-0.224343
H	2.494526	5.053935	0.659841
H	2.516283	3.949007	-0.736943
H	-0.323253	-0.982636	1.868318

17

C	-1.115457	-2.428376	-1.054400
O	-0.631323	-3.628433	-1.279915
C	0.591299	-3.487171	-2.040411
C	0.553358	-2.016750	-2.500623
N	-0.534953	-1.450479	-1.669519
C	-2.370158	-2.407360	-0.211639
C	-3.608843	0.124764	2.122326
O	-3.464039	-1.192909	1.515667
C	-2.609356	-1.112475	0.523819
C	-2.860859	1.027872	1.119288
N	-2.164904	0.065287	0.244408
C	-3.547718	-2.541184	-1.207243
H	-3.440173	-3.470023	-1.787171
H	-4.496537	-2.585618	-0.652481
H	-3.576436	-1.684845	-1.899165
C	-2.369684	-3.574568	0.778742
H	-3.308595	-3.578181	1.346491
H	-2.288354	-4.526736	0.239581
H	-1.528435	-3.491336	1.483664
C	1.905780	-1.476551	-2.146971
C	1.825839	-3.653098	-1.144389
H	2.422430	-4.536211	-1.421789
H	1.508039	-3.799067	-0.098170
C	2.594587	-2.376062	-1.326052
C	2.470611	-0.264534	-2.529473
H	1.935927	0.413377	-3.203591
C	3.736872	0.065636	-2.043700
H	4.219858	0.996573	-2.358278

C	4.413992	-0.811439	-1.189596	H	5.655693	5.032468	-1.398423
H	5.408941	-0.543772	-0.821011	H	5.422972	4.491173	0.281413
C	3.852864	-2.037694	-0.830969	Zn	-0.654470	0.422740	-0.988694
H	4.404975	-2.730040	-0.188365	O	-0.830219	1.933030	-2.253678
H	0.541392	-4.216888	-2.858514	H	-0.023303	2.485419	-2.231743
H	0.293561	-1.875153	-3.563773	H	-1.165222	1.873923	-3.159633
C	-3.846560	2.612793	-0.699566				
C	-5.007983	3.156780	-1.245272	18			
C	-6.257489	2.846445	-0.701681	C	-4.861716	-0.558720	2.866919
C	-6.365018	1.993305	0.395182	C	-4.194653	-1.242909	1.856510
C	-5.206427	1.446397	0.942615	C	-2.872831	-0.880375	1.542266
C	-3.959685	1.755909	0.392479	C	-2.289715	0.151206	2.296175
H	-2.866835	2.852668	-1.125927	C	-2.937993	0.842808	3.304892
H	-4.943125	3.832977	-2.102171	C	-4.253479	0.477910	3.585959
H	-7.160333	3.281046	-1.139801	H	-5.893050	-0.836129	3.101887
H	-7.345371	1.759334	0.820895	H	-4.695141	-2.039129	1.304102
H	-3.142850	0.055190	3.115310	H	-2.436515	1.645869	3.852108
H	-2.118468	1.691234	1.593950	H	-4.808405	0.999706	4.369550
C	-5.068676	0.550363	2.139779	S	-0.645822	0.414535	1.729590
H	-5.294219	1.093256	3.073415	O	-0.452536	1.773508	1.202454
H	-5.736098	-0.326226	2.122811	O	0.350918	-0.031803	2.704470
C	4.874668	0.395675	2.983426	N	-0.767749	-0.683298	0.460209
C	4.227062	1.046183	1.932367	C	-1.967755	-1.342307	0.505835
C	2.915859	0.674998	1.626167	C	-2.236715	-2.360585	-0.490545
C	2.304142	-0.325450	2.393291	O	-1.475769	-2.667239	-1.405526
C	2.921553	-0.978012	3.438562	O	-3.421955	-2.941625	-0.345408
C	4.239410	-0.599575	3.724020	C	-3.821010	-3.910655	-1.322596
H	5.903154	0.671375	3.226544	H	-3.705142	-3.468742	-2.327845
H	4.740962	1.815418	1.355333	H	-3.133063	-4.771480	-1.270902
H	2.414949	-1.754666	4.015962	C	-5.242578	-4.290169	-1.025672
H	4.772910	-1.094565	4.538864	H	-5.905485	-3.412694	-1.091973
S	0.661792	-0.586460	1.795449	H	-5.596308	-5.040969	-1.746675
O	0.464949	-1.915984	1.241201	H	-5.333880	-4.716294	-0.014627
O	-0.347604	-0.013502	2.664267	O	0.756661	-1.797052	-2.338586
N	0.874388	0.537962	0.455101	H	0.826190	-1.614893	-3.285342
C	2.022235	1.124542	0.551841	C	2.634876	1.111817	0.483940
C	2.305614	2.246854	-0.430768	O	3.444380	1.141670	1.522640
O	1.494882	2.587796	-1.257811	C	3.528930	-0.201614	2.080411
O	3.470466	2.789717	-0.234593	C	2.837461	-1.047695	0.993791
C	3.877659	3.888432	-1.093461	N	2.212487	-0.045816	0.117745
H	3.727483	3.569662	-2.138214	C	2.399010	2.442325	-0.186515
H	3.193405	4.729838	-0.899403	C	-0.575818	3.615970	-1.931385
C	5.307311	4.198783	-0.773004	O	0.669288	3.715128	-1.205594
H	5.953699	3.329864	-0.972104	C	1.138359	2.497124	-1.022437

C	-0.607260	2.139460	-2.381351	C	-4.065959	-1.279569	3.273358
N	0.527987	1.547673	-1.645812	C	-3.559850	-1.492761	1.990693
C	2.373909	3.550051	0.870099	C	-2.402095	-0.814335	1.604937
H	3.310046	3.537643	1.442853	C	-1.809931	0.055260	2.521953
H	2.273920	4.530621	0.387815	C	-2.298560	0.290290	3.796063
H	1.530782	3.402697	1.561839	C	-3.454607	-0.397394	4.165520
C	3.579065	2.652735	-1.161494	H	-4.967426	-1.815177	3.581114
H	3.472815	3.623797	-1.668516	H	-4.068137	-2.176080	1.307718
H	4.526434	2.655269	-0.601522	H	-1.797483	0.978397	4.481532
H	3.615513	1.854293	-1.918958	H	-3.879099	-0.247691	5.161016
C	3.969328	-1.761039	0.306887	S	-0.352988	0.752073	1.818639
C	4.976134	-0.661469	2.180498	O	-0.477610	2.172922	1.518978
H	5.126479	-1.242500	3.106504	O	0.848124	0.289744	2.504044
H	5.661855	0.199233	2.241531	N	-0.503476	-0.119487	0.354457
C	5.179852	-1.513316	0.959247	C	-1.690884	-0.778514	0.294039
C	3.914390	-2.543693	-0.843140	C	-1.705789	-1.927153	-0.688164
H	2.961333	-2.716136	-1.355403	O	-0.939997	-1.995233	-1.627543
C	5.098627	-3.089367	-1.335699	O	-2.640856	-2.796550	-0.426608
H	5.080400	-3.708971	-2.236757	C	-2.813441	-3.927429	-1.318878
C	6.311960	-2.850550	-0.684190	H	-2.906420	-3.535601	-2.345517
H	7.233637	-3.285599	-1.081405	H	-1.893462	-4.532145	-1.276784
C	6.361273	-2.062130	0.464645	C	-4.028936	-4.675044	-0.862208
H	7.314699	-1.877182	0.969071	H	-4.925385	-4.036055	-0.905552
H	2.987871	-0.167273	3.036135	H	-4.196437	-5.545669	-1.511708
H	2.054998	-1.716963	1.391251	H	-3.905558	-5.037234	0.169599
C	-2.539362	0.404504	-2.196422	O	0.704379	-0.297324	-2.843599
C	-3.802621	0.138258	-1.668214	H	0.086212	-1.055473	-2.846042
C	-4.451557	1.090349	-0.878276	H	1.418749	-0.484978	-3.470653
C	-3.852506	2.320871	-0.609885	C	-2.826610	0.489517	-0.769861
C	-2.593848	2.591136	-1.141887	H	-2.276536	0.369476	-1.712391
C	-1.946353	1.634340	-1.927209	H	-2.527731	1.372859	-0.190977
H	-2.024757	-0.350841	-2.803532	C	-4.205342	0.115283	-0.742760
H	-4.290964	-0.820666	-1.871515	C	-5.062751	0.642485	0.253410
H	-5.440633	0.867985	-0.466659	C	-4.725957	-0.813703	-1.676307
H	-4.368204	3.066042	0.003445	C	-6.390617	0.256781	0.307474
H	-0.519608	4.336872	-2.757755	H	-4.662127	1.361122	0.977276
H	-0.440865	1.992456	-3.462940	C	-6.051322	-1.203753	-1.610261
C	-1.776755	3.841393	-1.006249	H	-4.067874	-1.215725	-2.454757
H	-2.342940	4.748617	-1.270243	C	-6.883892	-0.671725	-0.616628
H	-1.421184	3.970472	0.030711	H	-7.053522	0.672335	1.069923
Zn	0.571246	-0.344833	-0.985966	H	-6.451646	-1.918644	-2.333365
H	-0.073918	-2.317297	-2.170700	H	-7.931524	-0.980281	-0.567544
				C	3.388599	0.061065	0.898730
				O	4.058515	-0.593903	1.824498

19tsR

C	3.553865	-1.953144	1.896206	C	1.320522	4.953098	-0.269265
C	2.493335	-1.984081	0.772022	H	1.458512	6.044835	-0.278273
N	2.506811	-0.611893	0.249578	H	1.448520	4.626062	0.780724
C	3.767932	1.515145	0.773640	Zn	1.069664	0.132536	-0.917198
C	2.329817	4.216237	-1.159779				
O	3.341818	3.544177	-0.377084	19tsS			
C	2.971739	2.283385	-0.249984	C	-3.403021	-0.139115	0.804088
C	1.564332	3.054472	-1.816263	O	-4.113041	0.404140	1.770075
N	1.982165	1.906289	-0.984661	C	-3.629170	1.752111	2.006846
C	3.522362	2.197657	2.135510	C	-2.489431	1.900584	0.975180
H	4.080888	1.670720	2.921205	N	-2.499337	0.608214	0.273343
H	3.872441	3.238225	2.094204	C	-3.783070	-1.562703	0.477301
H	2.452583	2.182974	2.396357	C	-1.913027	-4.174686	-1.241367
C	5.257982	1.593944	0.395922	O	-2.954670	-3.600777	-0.417351
H	5.570275	2.644753	0.326708	C	-2.809962	-2.291493	-0.423077
H	5.862527	1.102822	1.170631	C	-1.311850	-2.947973	-1.961802
H	5.453206	1.102348	-0.569680	N	-1.935251	-1.816887	-1.242121
C	3.016818	-2.973471	-0.224751	C	-3.934002	-2.331612	1.799058
C	4.633031	-2.977653	1.546112	H	-4.698290	-1.849116	2.421572
H	4.665945	-3.783744	2.297699	H	-4.246878	-3.363531	1.594978
H	5.630794	-2.508459	1.557863	H	-2.981408	-2.351173	2.351132
C	4.239824	-3.500470	0.192581	C	-5.129967	-1.523073	-0.275510
C	2.440113	-3.335522	-1.438762	H	-5.464393	-2.549388	-0.486074
H	1.474832	-2.908737	-1.741103	H	-5.887541	-1.030457	0.350783
C	3.113287	-4.247813	-2.249244	H	-5.040711	-0.974906	-1.226378
H	2.682722	-4.554307	-3.206589	C	-2.905668	3.043378	0.096537
C	4.338668	-4.781431	-1.837876	C	-4.690573	2.803970	1.685033
H	4.856144	-5.498961	-2.480586	H	-4.832998	3.493718	2.532932
C	4.908184	-4.415592	-0.618892	H	-5.669337	2.325334	1.512951
H	5.865500	-4.842773	-0.305883	C	-4.163585	3.520154	0.472999
H	3.143158	-2.071647	2.908448	C	-2.214643	3.595216	-0.980550
H	1.473662	-2.217862	1.128791	H	-1.221501	3.227270	-1.269889
C	-0.982574	2.843173	-2.277388	C	-2.808082	4.636011	-1.692235
C	-2.247130	3.374757	-2.015330	H	-2.283922	5.087134	-2.539113
C	-2.389069	4.458404	-1.145490	C	-4.068546	5.113482	-1.322717
C	-1.275271	5.036134	-0.534351	H	-4.521979	5.933145	-1.886904
C	-0.013416	4.513107	-0.799474	C	-4.751761	4.563247	-0.239204
C	0.120945	3.421859	-1.662188	H	-5.734032	4.949092	0.049353
H	-0.856473	2.009978	-2.978832	H	-3.291424	1.772077	3.052058
H	-3.130723	2.953594	-2.505785	H	-1.492353	2.028972	1.437166
H	-3.384008	4.871566	-0.956774	C	1.195891	-2.314238	-2.305384
H	-1.394205	5.892659	0.135244	C	2.510494	-2.558055	-1.907518
H	2.850620	4.873399	-1.867776	C	2.784704	-3.546695	-0.958023
H	1.848765	2.845826	-2.863261	C	1.758528	-4.319490	-0.415878

C	0.445141	-4.079260	-0.814368	C	4.011251	2.395992	1.913176
C	0.169490	-3.066353	-1.735651	C	3.304974	3.487918	-0.152886
H	0.969623	-1.542820	-3.052438	C	5.266412	2.963095	1.777743
H	3.332987	-1.982634	-2.344077	H	3.777945	1.761822	2.774655
H	3.819030	-3.725831	-0.649473	C	4.560971	4.052766	-0.281145
H	1.983579	-5.107416	0.309210	H	2.524067	3.694408	-0.893301
H	-2.400668	-4.894277	-1.911604	C	5.546012	3.784433	0.678837
H	-1.578940	-2.869283	-3.030784	H	6.036458	2.779242	2.530632
C	-0.801471	-4.794689	-0.386341	H	4.785071	4.711200	-1.124078
H	-0.728437	-5.884274	-0.528749	H	6.538713	4.230700	0.574752
H	-1.013805	-4.623858	0.683015				
Zn	-1.132189	0.010411	-1.039784	20R			
C	4.567993	-1.555686	2.072940	C	-4.214987	-1.002595	3.245800
C	3.997128	-0.699987	1.128566	C	-3.745350	-1.163037	1.942747
C	2.607563	-0.590727	1.082436	C	-2.526631	-0.584708	1.588461
C	1.850616	-1.326215	1.997180	C	-1.840482	0.140502	2.557162
C	2.393513	-2.179502	2.940977	C	-2.283926	0.315320	3.862092
C	3.785322	-2.288640	2.966001	C	-3.498238	-0.274400	4.198130
H	5.655346	-1.657143	2.106369	H	-5.167282	-1.459857	3.525213
H	4.627407	-0.145450	0.430765	H	-4.330863	-1.733352	1.217976
H	1.759943	-2.750864	3.623647	H	-1.701359	0.886773	4.588735
H	4.262014	-2.956567	3.687091	H	-3.890566	-0.167943	5.212015
S	0.136306	-1.000000	1.726589	S	-0.346524	0.776183	1.893671
O	-0.634714	-2.205137	1.452642	O	-0.372012	2.211041	1.651479
O	-0.409259	-0.044776	2.687349	O	0.833829	0.185920	2.511110
N	0.424105	-0.156626	0.269461	N	-0.558312	0.015311	0.365161
C	1.725689	0.217006	0.190510	C	-1.850431	-0.559204	0.229330
C	2.124928	0.702078	-1.179419	C	-1.701220	-1.901618	-0.509318
O	1.311213	1.170862	-1.947522	O	-0.998668	-2.013715	-1.491860
O	3.407604	0.613881	-1.394514	O	-2.416412	-2.846301	0.016771
C	3.944592	1.096821	-2.650476	C	-2.457309	-4.150602	-0.625252
H	3.500860	0.493409	-3.461131	H	-2.489713	-3.995083	-1.715363
H	3.608589	2.138394	-2.788057	H	-1.508747	-4.659205	-0.388087
C	5.435076	0.972927	-2.561418	C	-3.662598	-4.866087	-0.097049
H	5.738919	-0.076049	-2.422324	H	-4.583564	-4.318019	-0.351180
H	5.902067	1.346821	-3.483336	H	-3.725909	-5.868791	-0.542796
H	5.819262	1.564011	-1.713956	H	-3.610482	-4.978840	0.996031
O	-1.080233	0.748860	-2.898265	O	0.314593	-0.142738	-2.796609
H	-0.187198	1.048438	-3.143363	H	0.870357	-0.184312	-3.588970
H	-1.504736	0.332340	-3.661242	H	-0.221747	-0.961578	-2.738564
C	1.723986	2.022934	1.060576	C	-2.661132	0.419517	-0.779304
H	0.903450	2.442493	0.464917	H	-2.077079	0.425387	-1.714070
H	1.423053	1.650188	2.046968	H	-2.580890	1.413370	-0.311504
C	3.006740	2.644928	0.946534	C	-4.068748	0.007728	-0.981513

C	-5.096572	0.656058	-0.278799	C	-0.979789	3.095493	-2.144380
C	-4.391889	-1.046145	-1.852910	C	-2.207604	3.644412	-1.769260
C	-6.418024	0.259002	-0.441669	C	-2.261909	4.664094	-0.816525
H	-4.844286	1.478285	0.400094	C	-1.095787	5.161452	-0.233087
C	-5.711275	-1.451342	-2.005086	C	0.129531	4.617344	-0.605724
H	-3.598995	-1.536007	-2.430077	C	0.178036	3.587667	-1.549467
C	-6.725394	-0.802378	-1.294496	H	-0.927000	2.306770	-2.903698
H	-7.214712	0.775932	0.099137	H	-3.131676	3.281687	-2.231039
H	-5.958136	-2.267658	-2.688713	H	-3.229490	5.090392	-0.537053
H	-7.763987	-1.121701	-1.414514	H	-1.146377	5.969529	0.502300
C	3.338427	-0.044386	0.777846	H	2.968375	4.921953	-1.777998
O	3.980602	-0.739684	1.690290	H	1.838199	2.999532	-2.846670
C	3.373068	-2.054646	1.797995	C	1.503111	4.972402	-0.115568
C	2.331181	-2.040458	0.656454	H	1.686197	6.056505	-0.071362
N	2.408884	-0.665500	0.137740	H	1.663421	4.582096	0.907713
C	3.796439	1.390975	0.670363	Zn	1.027887	0.226955	-0.964380
C	2.442242	4.248946	-1.089289				
O	3.449770	3.487417	-0.383838	20S			
C	3.020403	2.243893	-0.302323	C	-3.365885	-0.078639	0.833749
C	1.597372	3.164023	-1.781177	O	-4.096530	0.480327	1.774119
N	1.989934	1.955021	-1.022168	C	-3.595249	1.818213	2.031416
C	3.619695	2.042029	2.059231	C	-2.415826	1.940028	1.042723
H	4.167908	1.462122	2.813912	N	-2.421958	0.646998	0.340077
H	4.020794	3.064631	2.042884	C	-3.769643	-1.492896	0.500273
H	2.556609	2.073863	2.344818	C	-2.046338	-4.131308	-1.329215
C	5.280115	1.400893	0.261517	O	-3.030697	-3.529672	-0.455352
H	5.645509	2.436072	0.217353	C	-2.825091	-2.230649	-0.421181
H	5.872926	0.855152	1.008158	C	-1.328970	-2.911762	-1.953430
H	5.430527	0.930828	-0.722205	N	-1.923868	-1.772720	-1.219691
C	2.834519	-3.051956	-0.328729	C	-3.896830	-2.266836	1.823358
C	4.379530	-3.162676	1.499406	H	-4.643348	-1.781056	2.464618
H	4.298593	-3.969047	2.247241	H	-4.222055	-3.295273	1.620920
H	5.411626	-2.781848	1.570213	H	-2.932570	-2.297229	2.354239
C	4.011416	-3.648910	0.126027	C	-5.133450	-1.439254	-0.219899
C	2.280795	-3.376449	-1.563066	H	-5.478372	-2.462400	-0.427036
H	1.351417	-2.898097	-1.892268	H	-5.873425	-0.944872	0.425281
C	2.929496	-4.320847	-2.356212	H	-5.063739	-0.889302	-1.171344
H	2.515194	-4.597342	-3.329656	C	-2.782369	3.077434	0.142065
C	4.109757	-4.922357	-1.908741	C	-4.620367	2.895007	1.670519
H	4.609117	-5.663245	-2.539128	H	-4.766727	3.594985	2.509257
C	4.656295	-4.594983	-0.668439	H	-5.606693	2.441707	1.475246
H	5.577296	-5.075710	-0.325689	C	-4.039363	3.587182	0.468916
H	2.938966	-2.106279	2.806476	C	-2.041656	3.585677	-0.920331
H	1.297637	-2.235676	0.998044	H	-1.058444	3.159486	-1.158205

C	-2.580662	4.626715	-1.673870	H	3.621259	1.977969	-2.899349
H	-2.018325	5.048862	-2.511081	C	5.441377	0.808177	-2.637527
C	-3.839976	5.142757	-1.352734	H	5.735599	-0.231951	-2.427859
H	-4.252414	5.962743	-1.946849	H	5.891277	1.103867	-3.595723
C	-4.574720	4.630845	-0.283607	H	5.854360	1.457373	-1.849129
H	-5.556961	5.046496	-0.040546	O	-1.095304	0.733055	-2.970150
H	-3.298514	1.831667	3.089011	H	-0.218911	1.122321	-3.144018
H	-1.435944	2.061201	1.539872	H	-1.770124	1.319736	-3.342743
C	1.225110	-2.383573	-2.072603	C	1.653479	1.849736	0.946786
C	2.494802	-2.714401	-1.592913	H	0.834579	2.362098	0.415063
C	2.653948	-3.778723	-0.702483	H	1.335916	1.655266	1.983007
C	1.557612	-4.546322	-0.308813	C	2.919021	2.623479	0.874855
C	0.290402	-4.219354	-0.787246	C	3.884017	2.509348	1.886879
C	0.125986	-3.126738	-1.639698	C	3.176166	3.462786	-0.220792
H	1.099373	-1.576198	-2.802972	C	5.080864	3.211796	1.799356
H	3.371070	-2.146206	-1.922635	H	3.682452	1.875756	2.757061
H	3.651030	-4.023923	-0.324666	C	4.372367	4.163941	-0.308470
H	1.692980	-5.397077	0.365584	H	2.416983	3.578944	-1.003406
H	-2.601668	-4.744067	-2.051029	C	5.331331	4.031766	0.698451
H	-1.520005	-2.770406	-3.031139	H	5.822526	3.125626	2.597638
C	-1.008514	-4.922839	-0.527607	H	4.558647	4.824378	-1.159434
H	-0.971446	-5.978009	-0.843336	H	6.273040	4.583052	0.631510
H	-1.278001	-4.927445	0.542241	21			
Zn	-1.148802	0.064439	-1.070490	C	-3.296829	-0.102987	0.808966
C	4.622377	-1.551955	2.019226	O	-3.892747	0.555418	1.783943
C	4.040207	-0.624445	1.151260	C	-3.341220	1.897916	1.834218
C	2.651842	-0.535080	1.096546	C	-2.494947	1.957431	0.545231
C	1.909602	-1.369358	1.933365	N	-2.507433	0.572079	0.054797
C	2.461833	-2.300153	2.800875	C	-3.665970	-1.560869	0.723285
C	3.851714	-2.384269	2.831820	C	-1.919850	-4.359047	-0.802246
H	5.711743	-1.627972	2.055378	O	-2.908541	-3.687142	0.007660
H	4.670464	0.004911	0.520794	C	-2.761252	-2.386718	-0.163578
H	1.830870	-2.942334	3.420569	C	-1.402410	-3.241157	-1.729109
H	4.337150	-3.105410	3.493109	N	-1.958702	-2.019953	-1.103750
S	0.193482	-1.068387	1.709830	C	-3.674094	-2.144354	2.143326
O	-0.574485	-2.267447	1.421345	H	-4.403718	-1.601953	2.758602
O	-0.354064	-0.107068	2.662563	H	-3.957649	-3.204211	2.113208
N	0.455088	-0.172461	0.259612	H	-2.677479	-2.051137	2.599701
C	1.766957	0.379213	0.260392	C	-5.076679	-1.641220	0.102406
C	2.152716	0.669985	-1.190142	H	-5.407832	-2.689685	0.072962
O	1.324671	1.051682	-1.990429	H	-5.783277	-1.067625	0.719938
O	3.424708	0.547005	-1.416759	H	-5.085510	-1.233254	-0.920627
C	3.951526	0.943212	-2.710027	C	-3.246052	2.901667	-0.353839
H	3.491412	0.295488	-3.474626	C	-4.436883	2.950724	1.726542

H	-4.252077	3.773433	2.437904	C	2.502144	0.313984	-1.230974
H	-5.417984	2.526080	1.995738	O	1.923693	0.494789	-2.287066
C	-4.359963	3.428704	0.304490	O	3.785195	0.067376	-1.163637
C	-2.962016	3.243804	-1.674068	C	4.585212	0.146703	-2.358512
H	-2.086373	2.824735	-2.181427	H	4.317004	-0.695514	-3.016809
C	-3.816486	4.124822	-2.335447	H	4.320635	1.072742	-2.895633
H	-3.612273	4.406603	-3.372396	C	6.022509	0.114149	-1.931315
C	-4.933528	4.652201	-1.681739	H	6.246611	-0.807448	-1.372316
H	-5.594901	5.342247	-2.213415	H	6.681441	0.151850	-2.810476
C	-5.210826	4.310417	-0.359176	H	6.257049	0.977339	-1.287714
H	-6.083578	4.729980	0.150515	O	-0.622302	0.918133	-2.629428
H	-2.750016	1.948539	2.759214	H	0.366508	0.878168	-2.705125
H	-1.445087	2.249856	0.725954	H	-1.008406	0.783011	-3.505404
C	1.047560	-2.678904	-2.404159	C	1.588942	2.021627	0.301356
C	2.394848	-2.874582	-2.103620	H	0.929134	2.318015	-0.534814
C	2.770812	-3.711321	-1.050559	H	1.011016	2.129106	1.235607
C	1.808544	-4.387381	-0.300784	C	2.824621	2.867860	0.328804
C	0.463053	-4.204873	-0.607098	C	3.410240	3.233992	1.545488
C	0.091489	-3.336426	-1.636413	C	3.453169	3.256061	-0.860510
H	0.751646	-2.012341	-3.222191	C	4.609346	3.942437	1.574639
H	3.164010	-2.378944	-2.702595	H	2.920138	2.947400	2.482813
H	3.832027	-3.851656	-0.824533	C	4.656159	3.958084	-0.836001
H	2.108337	-5.054818	0.512698	H	2.986054	3.008213	-1.821210
H	-2.438260	-5.172677	-1.327005	C	5.241959	4.295389	0.383895
H	-1.775815	-3.299127	-2.766552	H	5.054303	4.219999	2.534478
C	-0.732235	-4.836009	0.043004	H	5.135991	4.250762	-1.774797
H	-0.662861	-5.934450	0.083547	H	6.185064	4.848785	0.405267
H	-0.848171	-4.473809	1.078697				
Zn	-1.034340	-0.233474	-1.047491	22			
C	4.472033	-0.474438	2.808422	C	-3.295292	-0.035561	0.898995
C	3.979135	0.097701	1.635962	O	-3.964528	0.579452	1.846371
C	2.630116	-0.069374	1.311571	C	-3.460971	1.935834	1.979441
C	1.835467	-0.788484	2.196465	C	-2.482897	2.049388	0.790162
C	2.298538	-1.363600	3.371633	N	-2.429907	0.673152	0.258560
C	3.648142	-1.203239	3.669943	C	-3.687245	-1.481060	0.719991
H	5.530888	-0.352912	3.052422	C	-2.164898	-4.219856	-1.124679
H	4.652235	0.652715	0.979772	O	-3.097946	-3.558531	-0.238659
H	1.624575	-1.923679	4.025745	C	-2.847124	-2.268487	-0.256951
H	4.063812	-1.646354	4.578710	C	-1.532249	-3.050789	-1.905472
S	0.170079	-0.771554	1.620493	N	-1.982178	-1.867043	-1.129621
O	-0.434595	-2.112616	1.544881	C	-3.628048	-2.173793	2.092458
O	-0.612010	0.190679	2.422012	H	-4.269401	-1.639578	2.804913
N	0.546185	-0.217023	0.131480	H	-3.987832	-3.206952	2.002318
C	1.829171	0.483015	0.133468	H	-2.597514	-2.190786	2.477589

C	-5.131999	-1.495837	0.173201	H	4.242083	-2.016166	4.481005
H	-5.470776	-2.534107	0.051014	S	0.312679	-1.096083	1.647566
H	-5.799711	-0.993231	0.886719	O	-0.271704	-2.420972	1.518275
H	-5.197652	-0.980626	-0.798066	O	-0.454363	-0.041415	2.291305
C	-3.149061	3.010385	-0.154799	N	0.719969	-0.531338	0.016293
C	-4.574881	2.954551	1.771841	C	1.969299	0.300932	0.138289
H	-4.497542	3.764483	2.516508	C	2.670674	0.304641	-1.226363
H	-5.562930	2.490049	1.922575	O	2.067274	0.490715	-2.265187
C	-4.354278	3.473302	0.379846	O	3.959632	0.180626	-1.143371
C	-2.708267	3.427177	-1.408412	C	4.783456	0.456740	-2.306494
H	-1.751761	3.075698	-1.811543	H	4.771486	-0.441467	-2.944739
C	-3.506269	4.305509	-2.139274	H	4.309521	1.277057	-2.868149
H	-3.179531	4.648769	-3.124703	C	6.148700	0.808342	-1.798367
C	-4.721216	4.757669	-1.616421	H	6.592048	-0.024507	-1.231903
H	-5.337704	5.445797	-2.201292	H	6.814920	1.042085	-2.640701
C	-5.149775	4.350327	-0.354434	H	6.096569	1.693772	-1.143548
H	-6.094614	4.719637	0.055460	O	-0.461283	1.079455	-2.492999
H	-2.984337	1.988113	2.968444	H	0.511864	0.945729	-2.629460
H	-1.465244	2.358622	1.085701	H	-0.902870	1.182554	-3.348007
C	0.967550	-2.595755	-2.446288	C	1.562148	1.772931	0.431633
C	2.289788	-2.875724	-2.094013	H	0.826290	2.065119	-0.340278
C	2.568358	-3.841172	-1.120879	H	1.042821	1.782141	1.405028
C	1.539158	-4.557382	-0.509075	C	2.718411	2.730029	0.424263
C	0.219061	-4.276169	-0.854760	C	3.435080	3.002982	1.594054
C	-0.055556	-3.280800	-1.796052	C	3.118591	3.337198	-0.772332
H	0.742476	-1.855107	-3.220601	C	4.545369	3.843793	1.562655
H	3.108346	-2.348655	-2.593582	H	3.117996	2.550127	2.540168
H	3.607378	-4.051629	-0.852965	C	4.227493	4.178837	-0.805363
H	1.766883	-5.326353	0.234384	H	2.542486	3.157636	-1.687823
H	-2.752919	-4.908197	-1.744929	C	4.947903	4.427330	0.362357
H	-1.887817	-2.943157	-2.944289	H	5.095984	4.051425	2.484208
C	-1.039718	-4.909199	-0.340714	H	4.525388	4.651861	-1.745349
H	-1.044153	-6.000022	-0.491325	H	5.816967	5.090367	0.340083
H	-1.168505	-4.740090	0.742377	H	0.976403	-1.401926	-0.482027
Zn	-1.132849	-0.063053	-1.027598				
C	4.612005	-0.743138	2.773899	23ts			
C	4.104359	-0.125701	1.630094	C	-2.867876	-2.244875	2.197599
C	2.762364	-0.309060	1.292439	O	-2.619446	-3.043736	3.214417
C	1.989775	-1.089236	2.153808	C	-1.208371	-2.938461	3.510237
C	2.466676	-1.713923	3.298794	C	-0.627028	-2.255326	2.257117
C	3.813000	-1.536012	3.598657	N	-1.850856	-1.717956	1.606726
H	5.667094	-0.604227	3.021991	C	-4.333162	-1.985360	1.938390
H	4.760389	0.482331	1.006718	C	-5.905760	-1.530697	-1.340187
H	1.811333	-2.321183	3.928033	O	-5.746064	-2.073640	0.003893

C	-4.600392	-1.660286	0.491309	C	-2.996379	2.478671	-0.076260
C	-4.494214	-0.985823	-1.631341	C	-2.656524	2.956141	1.197122
N	-3.856263	-0.966779	-0.304500	C	-3.443880	3.824182	1.927025
C	-5.178527	-3.182034	2.377962	C	-4.632491	4.253722	1.328252
H	-5.001650	-3.392092	3.440204	H	-5.929655	4.150672	-0.387314
H	-6.243596	-2.953971	2.241680	H	-4.484742	2.578102	-1.651636
H	-4.939235	-4.084768	1.796584	H	-3.144566	4.166268	2.920932
C	-4.712266	-0.742981	2.775593	H	-5.280187	4.952377	1.862466
H	-5.768926	-0.487373	2.602471	S	-1.185547	2.183293	1.804055
H	-4.581797	-0.975228	3.844061	O	-0.043040	3.057120	1.932268
H	-4.080856	0.126660	2.533172	O	-1.540916	1.213264	2.818711
C	0.292802	-1.212808	2.806602	N	-0.952824	1.299505	0.237907
C	-0.956416	-1.990174	4.689006	C	-1.979785	1.564808	-0.610148
H	-0.666392	-2.522621	5.607918	C	-1.720844	1.263765	-2.074094
H	-1.886920	-1.439608	4.925601	O	-0.668379	0.813482	-2.440248
C	0.100773	-1.055728	4.179633	O	-2.766008	1.531560	-2.817523
C	1.223079	-0.449624	2.114302	C	-2.658222	1.292150	-4.249961
H	1.382385	-0.611846	1.044750	H	-1.861159	1.947942	-4.634606
C	1.946540	0.516811	2.810784	H	-2.333195	0.247720	-4.390546
H	2.682119	1.135968	2.286670	C	-3.996191	1.575175	-4.860618
C	1.751750	0.686717	4.184077	H	-4.308986	2.613430	-4.672476
H	2.332738	1.441021	4.721801	H	-3.941045	1.430085	-5.948587
C	0.837131	-0.104010	4.879065	H	-4.769287	0.894469	-4.470788
H	0.701953	0.024676	5.956998	H	0.173730	1.233946	-0.151045
H	-0.836784	-3.957531	3.678638	C	7.683051	-5.076194	-0.523890
H	-0.135329	-2.938802	1.543865	C	6.453480	-4.428184	-0.565786
C	-2.560501	-2.140688	-2.947279	C	6.395784	-3.033272	-0.589010
C	-2.201692	-3.215223	-3.759568	C	7.588702	-2.284231	-0.568929
C	-3.158815	-4.157034	-4.145951	C	8.818677	-2.944462	-0.528670
C	-4.482400	-4.043662	-3.723694	C	8.865496	-4.333968	-0.506108
C	-4.843695	-2.971495	-2.911134	H	7.723929	-6.168101	-0.505373
C	-3.886321	-2.025740	-2.535841	H	5.516080	-4.989752	-0.580719
H	-1.800093	-1.415023	-2.635266	H	9.730767	-2.342329	-0.514687
H	-1.165833	-3.323894	-4.091455	H	9.830793	-4.845614	-0.473462
H	-2.863969	-4.996507	-4.781429	C	7.577629	-0.802594	-0.587167
H	-5.225105	-4.789046	-4.022316	O	8.596548	-0.142994	-0.574089
H	-6.695321	-0.768520	-1.269635	C	5.069947	-2.376509	-0.634359
H	-4.495082	0.029692	-2.060650	O	4.028995	-3.004177	-0.661763
C	-6.192569	-2.637959	-2.341326	C	6.239406	-0.134292	-0.619205
H	-6.883912	-2.272641	-3.119802	C	5.054088	-0.883953	-0.641607
H	-6.694508	-3.490105	-1.855553	C	6.180229	1.259307	-0.628185
Cu	-2.127498	-0.302804	0.256998	C	3.823082	-0.234187	-0.664235
C	-4.995918	3.801422	0.059107	C	4.952190	1.909999	-0.655755
C	-4.191430	2.915584	-0.656408	H	7.103264	1.844945	-0.614298

C	3.760839	1.157977	-0.663981
H	2.912772	-0.837603	-0.687050
C	4.920270	3.397641	-0.676807
O	5.939259	4.052797	-0.632761
C	2.446651	1.822502	-0.637345
O	1.440517	1.109679	-0.484172
C	3.580179	4.037913	-0.777895
C	2.390858	3.277231	-0.775703
C	3.513585	5.424014	-0.887228
C	1.160143	3.929144	-0.913576
C	2.280901	6.060137	-1.011971
H	4.447113	5.991832	-0.878911
C	1.104140	5.311677	-1.032894
H	0.240376	3.343230	-0.946530
H	2.236781	7.148265	-1.100613
H	0.139004	5.810931	-1.146037

24

C	0.838053	-2.557894	0.663849
O	1.642834	-3.597144	0.694319
C	2.637729	-3.399816	-0.342246
C	2.019314	-2.304100	-1.229498
N	0.997864	-1.736447	-0.316296
C	-0.116402	-2.434753	1.828794
C	-3.433886	-0.868484	1.849878
O	-2.433076	-1.894456	2.141894
C	-1.331944	-1.603032	1.494742
C	-2.798793	-0.145202	0.648666
N	-1.395067	-0.582378	0.702518
C	-0.542628	-3.823081	2.311559
H	0.341863	-4.401301	2.607350
H	-1.202265	-3.723471	3.183230
H	-1.080203	-4.379526	1.529505
C	0.638448	-1.695983	2.956434
H	-0.023188	-1.583503	3.828594
H	1.513822	-2.290445	3.260102
H	0.981506	-0.700316	2.632120
C	3.165305	-1.396972	-1.548995
C	3.941134	-2.815182	0.213099
H	4.740289	-3.565394	0.309665
H	3.762486	-2.408880	1.227572
C	4.265389	-1.704867	-0.745184
C	3.229780	-0.388326	-2.507682
H	2.380165	-0.194166	-3.174948

C	4.415905	0.334080	-2.641674
H	4.495258	1.123130	-3.394327
C	5.516859	0.031142	-1.835252
H	6.445239	0.595352	-1.957976
C	5.452145	-0.991836	-0.889556
H	6.323342	-1.230242	-0.272570
H	2.771334	-4.365327	-0.846532
H	1.496690	-2.675746	-2.128017
C	-3.220567	-0.579779	-1.890735
C	-4.040847	-1.200098	-2.831172
C	-5.145220	-1.949416	-2.416954
C	-5.438041	-2.100427	-1.062613
C	-4.621112	-1.479415	-0.120525
C	-3.530537	-0.712905	-0.539138
H	-2.339022	-0.019435	-2.226055
H	-3.815495	-1.106940	-3.896758
H	-5.780212	-2.431965	-3.164673
H	-6.293854	-2.703415	-0.745695
H	-3.525300	-0.265174	2.764668
H	-2.858009	0.955971	0.708149
C	-4.734557	-1.494241	1.377392
H	-5.590077	-0.892326	1.728451
H	-4.867809	-2.501241	1.804047
Cu	0.132356	-0.001562	-0.284729
C	-0.600329	3.738939	2.888074
C	-0.898480	3.223736	1.627388
C	0.128440	2.644029	0.877099
C	1.422956	2.613185	1.421093
C	1.734905	3.102586	2.674541
C	0.691380	3.677133	3.409102
H	-1.396094	4.200548	3.476295
H	-1.911878	3.277659	1.227954
H	2.751905	3.061254	3.072371
H	0.898635	4.089443	4.399106
S	2.606230	1.848336	0.350764
O	3.492703	2.767530	-0.311284
O	3.026426	0.568899	0.869878
N	1.239137	1.508341	-0.863554
C	0.054124	2.036619	-0.447524
C	-0.975058	2.254135	-1.535953
O	-0.689420	2.031723	-2.682788
O	-2.125075	2.637855	-1.050012
C	-3.209646	2.924607	-1.984656
H	-2.952461	3.867696	-2.492428

H	-3.226013	2.124964	-2.741727
C	-4.479715	3.001607	-1.196117
H	-4.419024	3.771053	-0.411529
H	-5.310327	3.266168	-1.865507
H	-4.718387	2.030443	-0.732866
H	1.455763	1.489248	-1.874788

25ts

C	4.222352	0.238246	-0.602746
O	5.069877	1.245927	-0.632475
C	4.763734	2.146742	0.463081
C	3.815792	1.289922	1.324594
N	3.420255	0.198384	0.408994
C	4.325236	-0.660906	-1.810915
C	2.855500	-3.887141	-2.624154
O	3.711184	-2.731586	-2.779332
C	3.558149	-1.958631	-1.723807
C	2.372095	-3.778623	-1.161107
N	2.829302	-2.427809	-0.770081
C	3.822575	0.155985	-3.018728
H	4.468874	1.034050	-3.155978
H	3.869820	-0.458840	-3.928578
H	2.784483	0.486487	-2.871591
C	5.806456	-1.038035	-2.012723
H	5.906266	-1.648880	-2.919701
H	6.410928	-0.129755	-2.132233
H	6.194646	-1.610660	-1.156268
C	4.687537	0.834966	2.467958
C	6.010789	2.439447	1.279957
H	5.990994	3.480992	1.644263
H	6.918339	2.345321	0.662301
C	5.936040	1.462407	2.416854
C	4.378693	-0.064013	3.485530
H	3.399774	-0.549317	3.527028
C	5.345186	-0.341191	4.450632
H	5.121809	-1.044171	5.257878
C	6.597529	0.276271	4.397087
H	7.345872	0.050476	5.161750
C	6.899258	1.183971	3.383623
H	7.876918	1.673743	3.350175
H	4.303877	3.038731	0.008724
H	2.910697	1.820354	1.663742
C	-0.028445	-4.106649	-0.204535
C	-1.377293	-4.283449	-0.511322

C	-1.798499	-4.300157	-1.842569
C	-0.882292	-4.147649	-2.882945
C	0.465922	-3.978482	-2.579209
C	0.883424	-3.949910	-1.246202
H	0.314374	-4.118745	0.837314
H	-2.108286	-4.411072	0.292502
H	-2.859052	-4.442276	-2.070841
H	-1.218295	-4.172160	-3.924037
H	3.479778	-4.768421	-2.822010
H	2.840782	-4.507477	-0.476673
C	1.618064	-3.810462	-3.524121
H	1.632763	-4.571295	-4.319788
H	1.575631	-2.824503	-4.019825
Zn	1.991890	-1.200390	0.568632
O	2.065756	-2.136901	2.336772
H	1.227999	-2.012468	2.835310
H	2.434586	-3.014458	2.507285
C	-4.274249	-1.328033	-1.551538
C	-3.433842	-1.511919	-0.459482
C	-2.096450	-1.077505	-0.549049
C	-1.681488	-0.495177	-1.758293
C	-2.500308	-0.315129	-2.860048
C	-3.825445	-0.737402	-2.741094
H	-5.317451	-1.648834	-1.476603
H	-3.802388	-1.979822	0.456752
H	-2.126000	0.147383	-3.777385
H	-4.515479	-0.604073	-3.577425
S	0.015283	-0.052906	-1.644836
O	0.869455	-0.963467	-2.399561
O	0.247181	1.379017	-1.843296
N	0.129147	-0.395764	0.052148
C	-1.054643	-1.047645	0.441594
C	-1.136952	-1.504822	1.824236
O	-0.304196	-1.189662	2.665804
O	-2.169264	-2.284119	2.057495
C	-2.413527	-2.715166	3.409413
H	-1.571629	-3.354617	3.722815
H	-2.419702	-1.825273	4.058083
C	-3.725912	-3.439549	3.407521
H	-3.694751	-4.324867	2.753560
H	-3.979995	-3.772581	4.423801
H	-4.528067	-2.773016	3.052058
H	0.305172	0.917631	0.705984
C	2.297495	5.525567	-0.489285

C	1.728292	4.414439	0.120056	H	4.952931	1.344985	1.132662
C	0.430833	4.015952	-0.225795	H	2.414287	-2.134361	3.715080
C	-0.292476	4.734804	-1.205614	H	4.896915	-1.910693	3.964090
C	0.302750	5.824219	-1.830243	S	0.630500	-0.565108	1.894544
C	1.588872	6.223533	-1.468128	O	0.377799	-1.742384	1.077048
H	3.302156	5.849051	-0.206366	O	-0.302696	-0.202902	2.942249
H	2.273110	3.859693	0.887944	N	0.734987	0.863936	0.812722
H	-0.258608	6.354000	-2.603556	C	2.110940	1.252893	0.715437
H	2.044237	7.089167	-1.955334	C	2.412109	2.422824	-0.110564
C	-1.665060	4.328203	-1.614111	O	1.578157	2.989113	-0.801104
O	-2.244030	4.853287	-2.539362	O	3.661470	2.810560	-0.018961
C	-0.152745	2.817228	0.330601	C	4.087376	3.937866	-0.816560
O	0.584881	1.960499	0.912447	H	3.814629	3.735831	-1.866188
C	-2.319220	3.278260	-0.783540	H	3.513085	4.821423	-0.493555
C	-1.589987	2.602494	0.217303	C	5.564862	4.094299	-0.619717
C	-3.659690	2.979622	-0.974556	H	6.105249	3.193176	-0.950055
C	-2.241618	1.736770	1.092275	H	5.932482	4.946778	-1.207848
C	-4.302366	2.068899	-0.130251	H	5.805779	4.279083	0.438024
H	-4.219956	3.464712	-1.779027	O	-0.600480	2.141672	-1.907541
C	-3.602575	1.481396	0.931039	H	-0.713769	2.190798	-2.867292
H	-1.717266	1.260652	1.926952	C	-2.703412	-1.140450	0.467341
C	-5.735116	1.726441	-0.389533	O	-3.633275	-1.287740	1.378023
O	-6.300987	2.158570	-1.372212	C	-3.821974	-0.021908	2.074628
C	-4.271532	0.564784	1.900108	C	-3.005217	0.950889	1.199606
O	-3.629162	0.056058	2.800682	N	-2.224047	0.052084	0.325515
C	-6.404109	0.841775	0.593367	C	-2.440411	-2.376499	-0.357145
C	-5.712040	0.306314	1.698242	C	0.574982	-3.326702	-2.173143
C	-7.755193	0.540864	0.412340	O	-0.663317	-3.525010	-1.447735
C	-6.389551	-0.501955	2.614150	C	-1.161705	-2.347115	-1.157987
C	-8.418663	-0.272386	1.325648	C	0.537392	-1.828311	-2.533952
H	-8.271285	0.964028	-0.453232	N	-0.570731	-1.329044	-1.692381
C	-7.737984	-0.788872	2.429496	C	-2.490858	-3.621682	0.530751
H	-5.839982	-0.889066	3.476278	H	-3.453240	-3.666129	1.055787
H	-9.477764	-0.500458	1.181997	H	-2.390481	-4.523617	-0.086406
H	-8.265479	-1.417787	3.150844	H	-1.680904	-3.611310	1.274747

26

C	5.046135	-0.271238	2.559269	H	-3.456760	-3.306340	-2.045931
C	4.394407	0.593730	1.691236	H	-4.550575	-2.496618	-0.891672
C	2.992922	0.494436	1.542004	H	-3.578152	-1.518835	-2.037916
C	2.334476	-0.499149	2.298778	C	-4.050547	1.712795	0.428669
C	2.969178	-1.376268	3.156589	C	-5.279005	0.406880	2.016359
C	4.354387	-1.246393	3.287926	H	-5.565258	0.901914	2.960013
H	6.129225	-0.187533	2.674829	H	-5.944022	-0.465068	1.909977
				C	-5.333004	1.363255	0.860197

C	-3.861082	2.624967	-0.606546
H	-2.854149	2.897218	-0.942187
C	-4.982610	3.187110	-1.213821
H	-4.858049	3.907925	-2.026484
C	-6.267184	2.837560	-0.788693
H	-7.137471	3.286461	-1.275354
C	-6.451278	1.927194	0.250494
H	-7.459125	1.660621	0.582154
H	-3.433545	-0.170961	3.091962
H	-2.325753	1.595371	1.783400
C	2.455969	-0.077170	-2.444242
C	3.761105	0.180376	-2.021225
C	4.468533	-0.783570	-1.298466
C	3.891357	-2.016028	-0.989757
C	2.594528	-2.283251	-1.423373
C	1.888150	-1.312372	-2.139658
H	1.894424	0.670449	-3.017964
H	4.244451	1.128178	-2.277730
H	5.496100	-0.575830	-0.985152
H	4.460529	-2.770226	-0.437413
H	0.544755	-3.998090	-3.040835
H	0.292606	-1.622484	-3.590264
C	1.796281	-3.546626	-1.272635
H	2.367722	-4.444535	-1.553595
H	1.463129	-3.692413	-0.229773
Zn	-0.705828	0.459735	-0.895114
H	0.207312	2.651880	-1.641753
H	0.195264	1.606298	1.288208