

# Supporting Information

## Mechanistic insights into the rhodium-copper cascade catalyzed dual C-H annulation of indoles

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### 1. Complete reference for Gaussian 09

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski,

J.; and Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.

**2. M06/6-311+G(d,p)//B3-LYP/6-31G(d) calculated absolute energies, enthalpies, and free energies of all structures.**

**Table S1.** M06/6-311+G(d,p)//B3-LYP/6-31G(d) calculated absolute energies, enthalpies, and free energies of all structures.

Geometry	$E_{\text{(elec-B3-LYP)}}^1$	$H_{\text{(corr-B3-LYP)}}^2$	$G_{\text{(corr-B3-LYP)}}^3$	$E_{\text{(solv-M06)}}^4$	IF <sup>5</sup>
1	-1135.276114	0.231306	0.162496	-1134.960514	-
2	-607.670323	0.171365	0.119353	-607.449788	-
3	-1742.959804	0.407271	0.299815	-1742.431404	-
4-ts	-1742.939872	0.404732	0.298651	-1742.410370	-431.63
N <sub>2</sub>	-109.520718	0.008905	-0.012849	-109.485155	-
5	-1633.449004	0.391578	0.299064	-1632.948210	-
6	-403.120833	0.166988	0.125005	-402.926096	-
7-ts	-2036.557074	0.563888	0.446333	-2035.878676	-232.86
8	-2036.572484	0.565201	0.445182	-2035.900498	-
9-ts	-2036.541035	0.559494	0.442144	-2035.871866	-1262.75
10	-2036.561216	0.563091	0.449132	-2035.893160	-
11-ts	-2036.558841	0.562692	0.446366	-2035.878425	-253.36
12	-2036.607925	0.564756	0.444047	-2035.919120	-
13-ts	-2036.561487	0.558837	0.440755	-2035.876394	-1211.47
14	-2036.569739	0.563118	0.445231	-2035.887672	-
15	-650.836051	0.201300	0.145533	-650.604052	-
CH <sub>3</sub> COOH	-229.077610	0.067547	0.034687	-229.039420	-
16	-2458.337287	0.698098	0.555157	-2457.463151	-
17-threo-ts	-2458.309372	0.698104	0.561935	-2457.445592	-164.49
18-threo	-2458.339038	0.701150	0.565217	-2457.483800	-
19-threo-ts	-2687.407437	0.765156	0.616765	-2686.505962	-1073.02
20-threo	-1552.167435	0.534936	0.436138	-1551.578261	-
21-erythro-ts	-2458.308044	0.698349	0.563149	-2457.440266	-110.87
22-erythro	-2458.336797	0.701195	0.565126	-2457.481036	-
23-erythro-ts	-2687.408978	0.764982	0.615149	-2686.508678	-1350.41
24-erythro	-1552.173402	0.534978	0.435157	-1551.582195	-
25	-1733.265317	0.266291	0.187881	-1733.100685	-
C <sub>2</sub> H <sub>5</sub> OOCH <sub>3</sub>	-307.702009	0.127201	0.086631	-307.609674	-
26	-2977.735876	0.673622	0.536528	-2977.071030	-
27-ts	-2977.713449	0.666747	0.531262	-2977.045465	-478.57
HCl	-460.792269	0.009976	-0.011222	-460.797594	-
28	-2516.898539	0.657536	0.523091	-2516.229526	-
29-ts	-2516.883702	0.656370	0.526005	-2516.228983	-91.87
30	-2516.889605	0.657466	0.524869	-2516.238278	-
O <sub>2</sub>	-150.254027	0.007046	-0.015204	-150.298004	-

H <sub>2</sub> O <sub>2</sub>	-151.528502	0.029481	0.003487	-151.530620	-
31	-1550.981342	0.512054	0.414747	-1550.386121	-

<sup>1</sup>The electronic energy calculated by B3-LYP in gas phase. <sup>2</sup>The thermal correction to enthalpy calculated by B3-LYP in gas phase. <sup>3</sup>The thermal correction to Gibbs free energy calculated by B3-LYP in gas phase. <sup>4</sup>The electronic energy calculated by M06 in chloroform solvent. <sup>5</sup>The B3-LYP calculated imaginary frequencies for the transition states.

### 3. M06/6-311+G(d,p)//B3-LYP-D3/6-31G(d) calculated absolute energies, enthalpies, and free energies of the selected structures.

**Table S2.** M06/6-311+G(d,p)//B3-LYP-D3/6-31G(d) calculated absolute energies, enthalpies, and free energies of the selected structures.

Geometry	E <sub>(elec-B3-LYP-D3)</sub> <sup>1</sup>	H <sub>(corr-B3-LYP-D3)</sub> <sup>2</sup>	G <sub>(corr-B3-LYP-D3)</sub> <sup>3</sup>	E <sub>(solv-M06)</sub> <sup>4</sup>	IF <sup>5</sup>
1	-1135.309648	0.231315	0.163029	-1134.961078	-
2	-607.686878	0.171402	0.119381	-607.449798	-
N <sub>2</sub>	-109.520719	0.008905	-0.012849	-109.485155	-
6	-403.133315	0.167006	0.124743	-402.926118	-
14	-2036.669423	0.564751	0.446959	-2035.887606	-
15	-650.853629	0.201394	0.145758	-650.604014	-
CH <sub>3</sub> COOH	-229.080609	0.067538	0.034785	-229.039416	-
16	-2458.458398	0.699348	0.559444	-2457.464429	-
17-threo-ts	-2458.443100	0.698794	0.565632	-2457.448352	-127.39
18-threo	-2458.471298	0.702327	0.569470	-2457.485733	-
21-erythro-ts	-2458.445013	0.700066	0.569227	-2457.445565	-104.74
22-erythro	-2458.468366	0.702070	0.567733	-2457.483156	-

<sup>1</sup>The electronic energy calculated by B3-LYP-D3 in gas phase. <sup>2</sup>The thermal correction to enthalpy calculated by B3-LYP-D3 in gas phase. <sup>3</sup>The thermal correction to Gibbs free energy calculated by B3-LYP-D3 in gas phase. <sup>4</sup>The electronic energy calculated by M06 in chloroform solvent. <sup>5</sup>The B3-LYP-D3 calculated imaginary frequencies for the transition states.

### 4. M06/6-311+G(d,p)//B3-LYP/6-31+G(d) calculated absolute energies, enthalpies, and free energies of the selected structures.

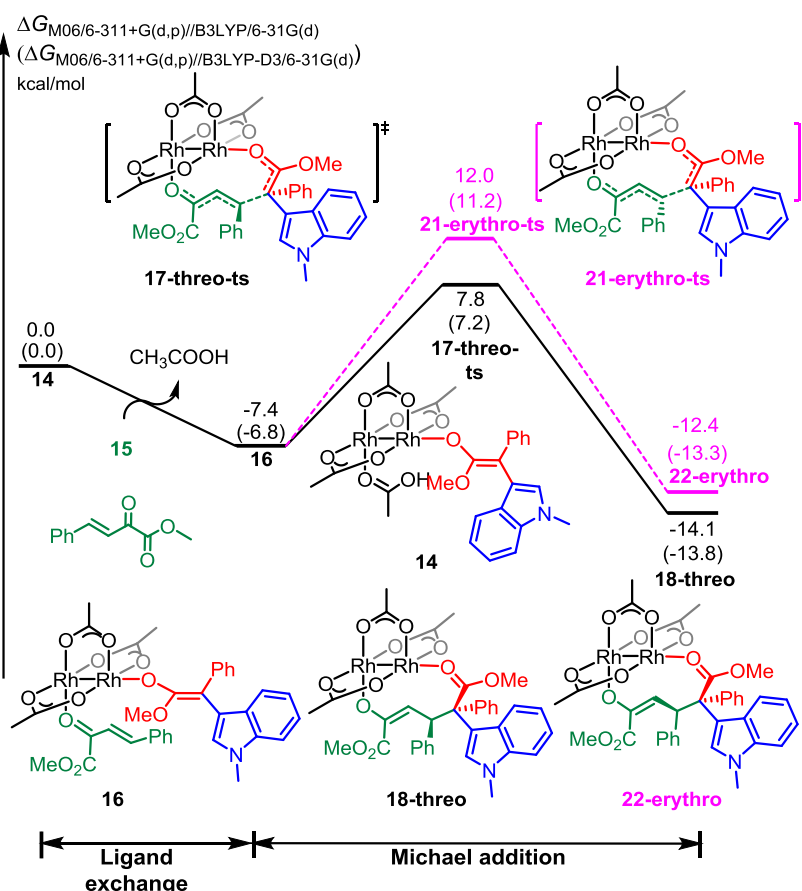
**Table S3.** M06/6-311+G(d,p)//B3-LYP/6-31+G(d) calculated absolute energies, enthalpies, and free energies of the selected structures.

Geometry	E <sub>(elec-B3-LYP/6-31+G(d))</sub> <sup>1</sup>	H <sub>(corr-B3-LYP/6-31+G(d))</sub> <sup>2</sup>	G <sub>(corr-B3-LYP/6-31+G(d))</sub> <sup>3</sup>	E <sub>(solv-M06)</sub> <sup>4</sup>	IF <sup>5</sup>
1	-1135.293056	0.231646	0.159349	-1134.961125	-
2	-607.694383	0.170979	0.118970	-607.449519	-
N <sub>2</sub>	-109.527021	0.008896	-0.012858	-109.485166	-

6	-403.136332	0.166721	0.124968	-402.925887	-
14	-2036.6155	0.563006	0.441885	-2035.886898	-
15	-650.863433	0.200857	0.144940	-650.603704	-
CH <sub>3</sub> COOH	-229.092588	0.067279	0.034309	-229.039374	-
16	-2458.396973	0.697021	0.553285	-2457.461868	-
17-threo-ts	-2458.368220	0.696612	0.559114	-2457.444800	-164.70
18-threo	-2458.396867	0.699730	0.562174	-2457.482886	-
21-erythro-ts	-2458.366421	0.696833	0.561023	-2457.439062	-114.77
22-erythro	-2458.395027	0.699745	0.563717	-2457.480117	-

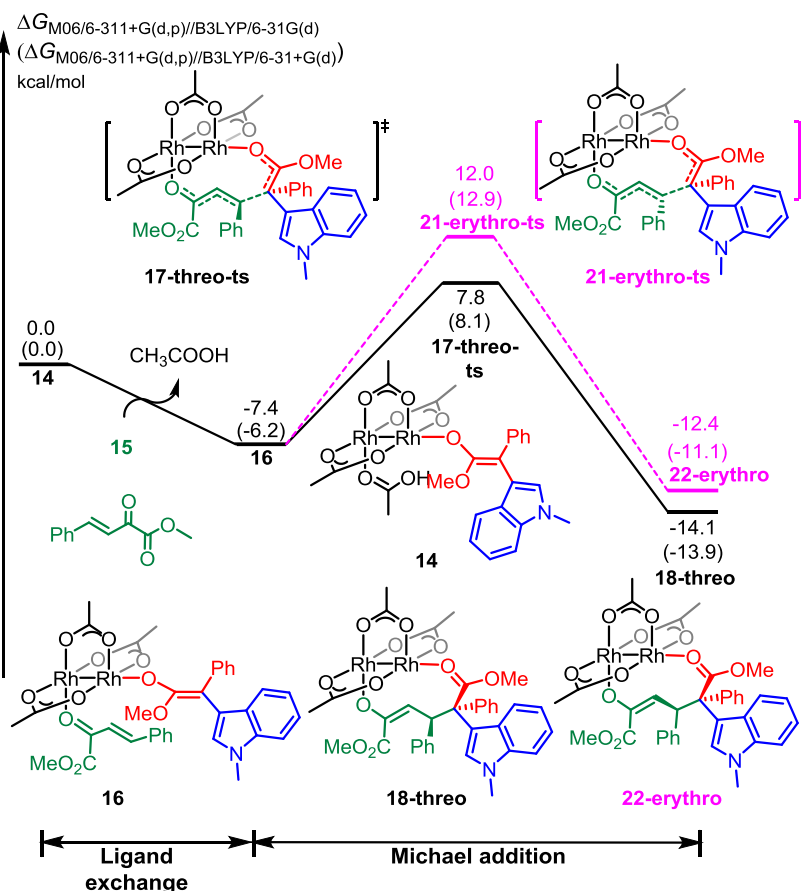
<sup>1</sup>The electronic energy calculated by B3-LYP/6-31+G(d) in gas phase. <sup>2</sup>The thermal correction to enthalpy calculated by B3-LYP/6-31+G(d) in gas phase. <sup>3</sup>The thermal correction to Gibbs free energy calculated by B3-LYP/6-31+G(d) in gas phase. <sup>4</sup>The electronic energy calculated by M06 in chloroform solvent. <sup>5</sup>The B3-LYP/6-31+G(d) calculated imaginary frequencies for the transition states.

## 5. Calculated energy profiles of key intermediates with and without dispersion corrections.



**Figure S1.** Gibbs free energy profiles for the Michael-type addition process in the Rh<sub>2</sub>(OAc)<sub>4</sub>-catalyzed reaction. The values given by kcal/mol are the relative free energies calculated by M06/6-311+G(d,p)//B3-LYP/6-31G(d) method in ethylacetate solvent. The values in parentheses are the free energies given by M06/6-311+G(d,p)//B3-LYP-D3/6-31G(d) method.

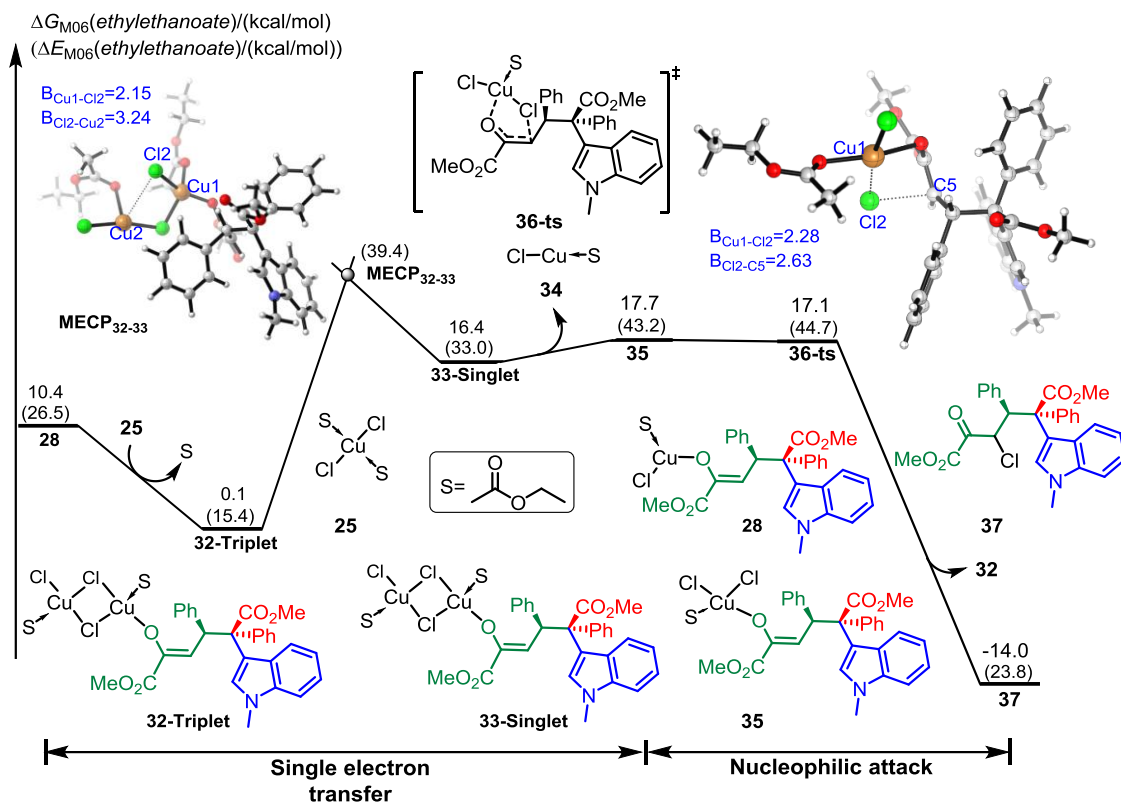
## 6. Calculated energy profiles of key intermediates with and without diffuse functions.



**Figure S2.** Gibbs free energy profiles for the Michael-type addition process in the  $\text{Rh}_2(\text{OAc})_4$ -catalyzed reaction. The values given by kcal/mol are the relative free energies calculated by M06/6-311+G(d,p)//B3-LYP/6-31G(d) method in ethylacetate solvent. The values in parentheses are the free energies given by M06/6-311+G(d,p)//B3-LYP/6-31+G(d) method.

## 7. Energy profiles of $\text{CuCl}_2$ -Catalyzed reaction to synthesize $\alpha$ -chloro carboxylate.

When copper(II) enolate intermediate **28** forms, ligand exchange between intermediate **28** and copper(II) chloride **25** then takes place with concomitant generation of a triplet cationic intermediate **32-Triplet**. An accurate structure of the crossing point is located as the minimum energy crossing point **MECP<sub>32-33</sub>**.<sup>1-2</sup> The CYLview structure shown in Figure S1 suggests that the Cu1–Cl2, Cu2–Cl2 bonds distance in **MECP<sub>32-33</sub>** is 2.15 Å and 3.24 Å. Through this structure, the singlet



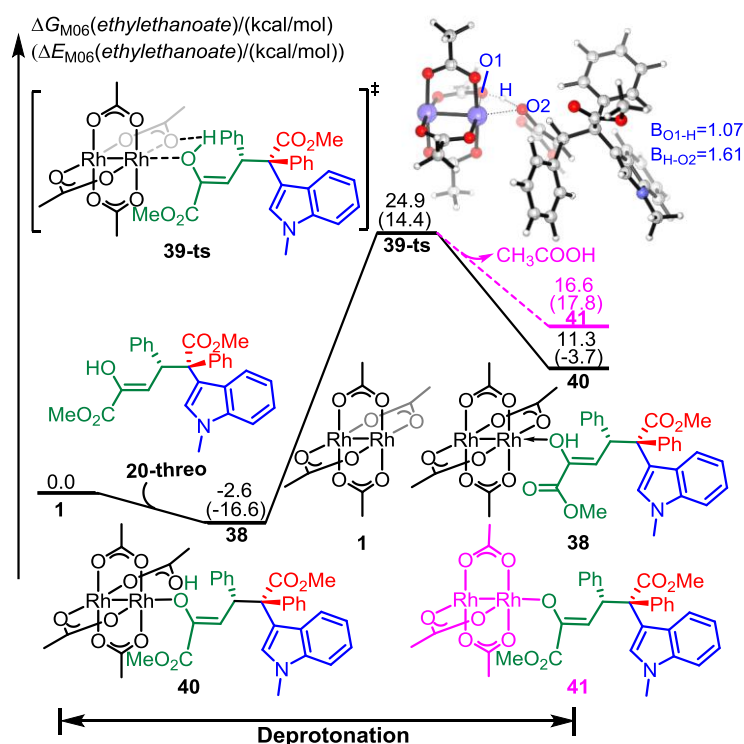
**Figure S3.** Gibbs energy profiles for the copper salt mediated  $\alpha$ -chlorocarboxylate synthesis. The values given by kcal/mol are the relative free energies calculated by M06/6-311+G(d,p)//B3-LYP/6-31G(d) method in ethylacetate solvent. The values in parentheses are the electronic energies given by M06/6-311+G(d,p)//B3-LYP/6-31G(d) method.

intermediate **33-Singlet** can be generated from triplet intermediate **32-Triplet**; and the energy span is 24.0 kcal/mol. Subsequent dissociation of copper(I) chloride **34** on the singlet potential energy surface afford copper(III) enolate intermediate **35**. The calculated free energy barrier of this step is 6.1 kcal/mol. Then, nucleophilic attack by coordinated chloride occurs via transition state **36-ts** to yield  $\alpha$ -chlorocarboxylate **37**. In the optimized geometry of transition state **36-ts** (Figure S3), the Cu1-Cl2 and Cl2-C5 bond lengths are 2.28 and 2.63 Å, respectively. Comparing with the pathway in Figure. 4, this results suggest that this results suggest that generation of singlet Cu(III) enolate via MECP is unfavorable, and intramolecular radical-type addition to the indole moiety can occur to give fused cyclic intermediate **30** in the presence of copper enolate **28**.

## References:

1. Koga, K. Morokuma, Determination of the lowest energy point on the crossing seam between two potential surfaces using the energy gradient, *Chem. Phys. Lett.* 1985, **119**, 371–374.
2. M. Lundberg, P. E. M. Siegbahn, Minimum energy spin crossings for an O–O bond formation reaction, *Chem. Phys. Lett.* 2005, **401**, 347–351.

## 8. Energy profiles of rhodium-catalyzed rhodium enolate generation.



**Figure S4.** Gibbs energy profiles of the rhodium-catalyzed rhodium enolate generation. The values given by kcal/mol are the relative free energies calculated by M06/6-311+G(d,p)//B3-LYP/6-31G(d) method in ethylacetate solvent. The values in parentheses are the electronic energies given by M06/6-311+G(d,p)//B3-LYP/6-31G(d) method.

The calculated free-energy profiles of rhodium enolate generation are shown in Figure S4. The dirhodium complex **1** is set to zero energy for the free-energy profile. Coordination of  $\alpha$ -oxo carboxylate **20-threo** to rhodium center results in the formation of intermediate **38** with a Gibbs free energy decrease of 2.6 kcal/mol. Then deprotonation by coordinated oxygen occurs via transition state **39-ts** with an energy



barrier of 27.5 kcal/mol to afford rhodium enolate **40**. The geometric structure shows that the length of the O1-H bond being formed in transition state **39-ts** is 1.07 Å and the O2-H bond being broken is 1.61 Å. Generation of an alternative rhodium enolate **41** with a dissociation of an acetic acid is also calculated, and its relative free energy is 5.3 kcal/mol higher than **40**. The calculated results show that rhodium mediated deprotonation of  $\alpha$ -oxo carboxylate is unfavorable compared with the copper mediated deprotonation pathway (Figure 4).

### 9. B3LYP/6-31G(d) geometries for all the optimized compounds and transition states.

<b>1</b>							
Rh	-0.00276000	0.00121500	1.19392300	H	-3.83779500	-2.52386900	0.58044400
Rh	0.00330300	0.00111900	-1.19393500	H	-3.29659600	-3.11951500	-1.01935900
C	1.90042300	1.83138000	0.00839200	<b>2</b>			
O	1.47806300	1.42769700	1.14098600	C	-0.50061500	0.40184600	0.00018600
O	1.48386000	1.42835500	-1.12733500	N	-0.84919600	1.67299300	0.00023600
C	-1.83072400	1.90060800	-0.00822900	N	-1.12119500	2.77829300	0.00067000
O	-1.42925100	1.48253200	1.12746600	C	0.94296800	0.07881200	0.00007300
O	-1.42346700	1.48169400	-1.14085300	C	1.38753800	1.25608400	0.00040900
C	-1.89949800	-1.82969800	-0.00832900	C	1.90470600	1.10722800	-0.00038900
O	-1.48427500	-1.42527200	1.12735800	C	2.75308200	-1.53950900	0.00028500
O	-1.47735200	-1.42579700	-1.14094900	H	0.66227500	-2.05850300	0.00073000
C	1.83044700	-1.89922600	0.00829400	C	3.26520300	0.81146000	-0.00048800
O	1.43079100	-1.47941800	-1.12739400	H	1.59531900	2.14884300	-0.00071700
O	1.42387000	-1.47965500	1.14091500	C	3.70023300	-0.51519900	-0.00014500
C	-2.88598900	2.98170500	-0.00183000	H	3.07437600	-2.57783400	0.00055300
C	-2.98313600	-2.88238900	-0.00176500	H	3.98605800	1.62469000	-0.00085800
C	2.99225500	2.87553700	0.00177200	H	4.76188800	-0.74546000	-0.00022000
C	2.87270000	-2.99290400	0.00175300	C	-1.62138800	-0.55102600	-0.00007400
H	-3.79860500	2.59363800	0.46292200	O	-1.51727900	-1.76305100	0.00015700
H	-2.54272200	3.82522800	0.60501600	O	-2.81575000	0.09392800	-0.00051300
H	-3.10365700	3.31403300	-1.01779700	C	-3.97071700	-0.75873600	-0.00025000
H	3.87810500	2.47093300	-0.49884400	H	-4.82725600	-0.08408000	0.00215800
H	2.66119000	3.74660900	-0.57243100	H	-3.98222600	-1.39162100	-0.89158200
H	3.24692700	3.17367500	1.01972100	H	-3.97952800	-1.39480600	0.88881000
H	2.46174100	-3.88198700	-0.48800800	<b>3</b>			
H	3.73955600	-2.66876100	-0.58254600	Rh	2.25397100	-0.96995900	0.32345400
H	3.17840700	-3.24035800	1.01924400	Rh	0.14131900	0.11849200	-0.10275300
H	-2.60777000	-3.78581300	0.49027500	C	2.28493000	0.86973200	-1.92117700

O	3.03842300	0.08115400	-1.26995400	C	-1.05459000	4.57174800	0.19404500
O	1.05084700	1.09280300	-1.68240600	H	-0.61590300	5.23149700	-0.55462000
C	1.90086500	1.52945500	1.74137800	H	-1.95335500	5.02000300	0.62457700
O	2.73256500	0.57954300	1.59360500	H	-0.33606800	4.35187700	0.98625200
O	0.76240300	1.62395800	1.17474700	<b>4-ts</b>			
C	0.14420700	-1.73046800	2.14532000	Rh	-2.41400600	-0.66838900	-0.27721100
O	1.36884000	-1.96626800	1.88852400	Rh	-0.10199200	0.06678600	0.05807000
O	-0.61402300	-0.93227700	1.50477900	C	-2.10812600	1.57188000	1.54989700
C	0.53069100	-2.39088300	-1.52255500	O	-2.99066800	0.82841100	1.02561100
O	-0.31539700	-1.44736600	-1.37193200	O	-0.84612600	1.49484800	1.36129600
O	1.66852000	-2.46741500	-0.96219800	C	-1.53124700	1.36318600	-2.13656200
C	2.30542900	2.66820900	2.65109700	O	-2.54251400	0.65187800	-1.85104900
C	-0.46219100	-2.43686800	3.33643000	O	-0.41072800	1.36215800	-1.52560900
C	2.89839000	1.63045900	-3.07525700	C	-0.45924400	-2.17790000	-1.78394200
C	0.12828500	-3.51681500	-2.44820800	O	-1.70802300	-2.11334700	-1.56539500
H	3.09085500	2.34655300	3.33745900	O	0.43898100	-1.43620500	-1.26136400
H	2.69217200	3.49337900	2.04122500	C	-1.05513200	-1.97032500	1.93745700
H	1.43768800	3.03379100	3.20586400	O	-0.02243500	-1.26874400	1.64982400
H	2.24576000	1.56783300	-3.95073500	O	-2.16212100	-1.95125300	1.32554600
H	2.98540500	2.68850000	-2.80352900	C	-1.64635300	2.27972000	-3.33499300
H	3.88834300	1.23680400	-3.31076300	C	0.02441300	-3.21478300	-2.77448700
H	-0.76377200	-4.01107100	-2.04915900	C	-2.58734300	2.67869000	2.46449100
H	-0.13230400	-3.11078600	-3.43077900	C	-0.92266600	-2.89470000	3.12852900
H	0.93787900	-4.24129600	-2.54703700	H	-2.67436700	2.63294900	-3.44318400
H	0.06946100	-3.36905100	3.53789700	H	-0.95432400	3.11930100	-3.24520800
H	-0.37125800	-1.78879600	4.21622100	H	-1.38316900	1.71441300	-4.23680900
H	-1.52372200	-2.62614500	3.16233300	H	-3.54531300	2.40981400	2.91417800
C	-2.13040800	1.13691800	-0.55693900	H	-1.84403000	2.88659900	3.23752400
N	-1.87862500	1.30815000	-1.87003600	H	-2.72865000	3.59110500	1.87291600
N	-1.64266300	1.40850700	-2.96807500	H	-0.04191100	-3.53336900	3.00851000
C	-3.15135100	0.08849500	-0.23987400	H	-0.77510200	-2.29926700	4.03613800
C	-3.67868400	-0.02536500	1.05732500	H	-1.81757700	-3.50916100	3.23653800
C	-3.59548000	-0.80313700	-1.23119800	H	0.26417400	-2.71771600	-3.72153900
C	-4.63534400	-1.00014200	1.33923300	H	0.94000400	-3.68664100	-2.40821300
H	-3.33981900	0.64751000	1.83219700	H	-0.74884900	-3.96416100	-2.95250100
C	-4.54929500	-1.77507300	-0.93753900	C	1.97516600	0.71543000	0.27260700
H	-3.19311400	-0.75364200	-2.23811000	N	1.98722500	1.02078300	2.01086000
C	-5.07810500	-1.87869700	0.34995900	N	1.70166800	0.85927500	3.07231800
H	-5.03549300	-1.06824600	2.34749800	C	3.10316100	-0.23496800	0.08660400
H	-4.87942000	-2.45034500	-1.72235700	C	4.31605300	0.15197800	-0.51949900
H	-5.82506000	-2.63403800	0.57798400	C	2.96622300	-1.56394200	0.53443400
C	-1.96182500	2.39771000	0.23109400	C	5.34806400	-0.76790700	-0.68570900
O	-2.29553900	2.53765000	1.38712000	H	4.43744300	1.16289500	-0.88828400
O	-1.38294500	3.36364900	-0.51303400	C	4.01175900	-2.47145200	0.38917900

H	2.03747400	-1.86859400	1.00189400	H	0.91659200	-3.76510500	2.99040500
C	5.20295900	-2.07911100	-0.22652400	H	-0.73763600	-3.78033800	2.30777900
H	6.27100800	-0.45703000	-1.16727900	C	-1.94867900	0.59188800	0.03943900
H	3.89305400	-3.49059500	0.74684200	C	-3.09334000	-0.27443300	0.00908100
H	6.01431700	-2.79180600	-0.34902200	C	-4.36978100	0.16519500	0.46092400
C	2.12353300	2.09107800	-0.30274500	C	-2.97404200	-1.60069900	-0.48430700
O	2.43281200	2.25946500	-1.46500800	C	-5.46272500	-0.68715500	0.43624600
O	1.80011300	3.08779700	0.54320700	H	-4.47372000	1.16653500	0.86560400
C	1.73703100	4.39605100	-0.05069700	C	-4.08398900	-2.43487900	-0.53793900
H	1.48845400	5.07196600	0.76745300	H	-2.01146700	-1.93278200	-0.84846800
H	2.69894800	4.66413300	-0.49499500	C	-5.32318100	-1.98612500	-0.07039500
H	0.96223200	4.41930500	-0.82059500	H	-6.42635700	-0.34609700	0.80329000
<b>N<sub>2</sub></b>				H	-3.98621000	-3.44091600	-0.93554200
N	0.00000000	0.00000000	0.55265200	H	-6.18465800	-2.64818200	-0.10031700
N	0.00000000	0.00000000	-0.55265200	C	-2.21469400	2.03811000	0.25922200
<b>5</b>				O	-2.31592500	2.53424100	1.36521100
Rh	2.38999500	-0.52113000	0.02373800	O	-2.30988800	2.71349400	-0.89714900
Rh	-0.00307400	0.07652000	-0.00119600	C	-2.43214500	4.14215700	-0.77357100
C	1.79200000	2.00420100	-1.27224800	H	-2.50225200	4.51506100	-1.79516100
O	2.75968700	1.23926400	-0.98731100	H	-3.32766300	4.40573000	-0.20465000
O	0.55785000	1.80135000	-1.00302100	H	-1.55164400	4.55264300	-0.27317800
C	1.52544300	1.03196800	2.30401800	<b>6</b>			
O	2.55695200	0.47843400	1.81797200	C	-0.38913200	0.98546600	-0.00000700
O	0.35457100	1.03274900	1.79254600	C	0.15169700	-0.33266200	-0.00008900
C	0.65122200	-2.45367400	1.31755400	C	-0.66012100	-1.47342100	-0.00004300
O	1.86887400	-2.24193600	1.04406200	C	-2.03774800	-1.28157300	0.00000800
O	-0.33710300	-1.69920100	1.01445900	C	-2.59501500	0.01409300	0.00003100
C	0.94562100	-1.49697800	-2.29376700	C	-1.78594100	1.14382300	0.00004500
O	-0.10798400	-0.95893100	-1.80198700	C	0.72668300	1.88922200	0.00005800
O	2.10113700	-1.48542600	-1.77994300	C	1.86097400	1.12095200	-0.00004500
C	1.68762600	1.76717200	3.61656600	H	-0.23503300	-2.47337900	-0.00005500
C	0.32578400	-3.72684000	2.06998200	H	-2.69638400	-2.14592100	-0.00000800
C	2.10447600	3.29335700	-2.00199500	H	-3.67588500	0.1268500	0.00003500
C	0.76594700	-2.20558800	-3.61931900	H	-2.22547200	2.13820400	0.00011500
H	2.08778600	1.08084100	4.36967300	H	0.69063300	2.96997900	0.00005800
H	2.41606400	2.57491300	3.48977700	H	2.90165600	1.41712600	-0.00000900
H	0.73405700	2.17690100	3.95194000	N	1.53029200	-0.22406300	-0.00019400
H	1.50884600	3.35158500	-2.91840000	C	2.46052000	-1.33302600	0.00014800
H	1.82602200	4.14570000	-1.37312000	H	2.32883100	-1.95895800	0.89118600
H	3.16727400	3.34725500	-2.24253200	H	2.32752800	-1.96040200	-0.88966000
H	0.00010600	-2.98219000	-3.52301300	H	3.48058400	-0.94231800	-0.00093800
H	0.41404800	-1.49083700	-4.37051600	<b>7-ts</b>			
H	1.70709600	-2.65117900	-3.94465800	Rh	-2.73330700	-0.67258900	-1.00167500
H	0.61364200	-4.59048900	1.46105100	Rh	-0.66434400	0.18825900	0.04426200

C	-1.98083000	-2.04827600	1.43923900	H	-0.05617300	0.94653600	5.12689300
O	-2.84753700	-2.06477200	0.51971500	H	0.53562800	2.57318600	4.65348500
O	-0.94409700	-1.30285500	1.49891500	H	-1.05284800	2.01091600	4.07782200
C	-3.16364000	1.39077200	0.97966900	C	3.57936900	-0.73903200	0.75758700
O	-3.79541400	0.65456500	0.16421800	C	3.21277900	-2.08164300	0.52291000
O	-1.90151400	1.40893300	1.16652500	C	3.87969600	-2.90415400	-0.38024700
C	-1.57861900	1.60290200	-2.34847800	C	4.96640300	-2.34851200	-1.05986000
O	-2.53802700	0.78011100	-2.44465200	C	5.35704600	-1.01953700	-0.83578000
O	-0.66563800	1.60187300	-1.45704600	C	4.67014800	-0.20496800	0.06680900
C	-0.28533300	-1.88873000	-1.99472300	C	2.63873600	-0.20325500	1.73607900
O	0.36772400	-1.16188100	-1.16874900	C	1.83232400	-1.30240700	2.10684500
O	-1.54153300	-1.93466500	-2.12876100	H	3.58133700	-3.93440700	-0.54914900
C	-3.97528600	2.33263500	1.84529800	H	5.51788200	-2.95800800	-1.76998600
C	-1.50632900	2.71918100	-3.36863300	H	6.20723200	-0.61646600	-1.37850800
C	-2.20955100	-3.01242400	2.58988500	H	4.97256900	0.82573700	0.22208300
C	0.53619500	-2.76430000	-2.92134000	H	2.88773200	0.57995900	2.43576400
H	-4.97326000	2.47089100	1.42544500	H	1.01407200	-1.31716300	2.80695200
H	-4.07205600	1.90525500	2.85051100	N	2.13290200	-2.38301900	1.37167600
H	-3.45988800	3.29202500	1.93807000	C	1.38241100	-3.62630500	1.33441700
H	-3.15149600	-2.75637900	3.08632000	H	0.78444700	-3.67589800	0.41960600
H	-2.31546600	-4.03163600	2.20479700	H	2.07176400	-4.47478800	1.37116900
H	-1.39859900	-2.96862900	3.31979900	H	0.71798600	-3.66692000	2.19692200
H	0.60636900	-2.27381500	-3.89950400	<b>8</b>			
H	1.54610800	-2.90656100	-2.53130800	Rh	-2.82018500	-1.19690500	-0.20334300
H	0.03787900	-3.72582600	-3.07028600	Rh	-0.69114900	-0.01158100	0.04716100
H	-1.91853900	3.63269600	-2.92426400	C	-0.70322000	-2.77973200	0.99550600
H	-0.46542200	2.92016100	-3.63421700	O	-1.90194500	-2.87164600	0.58976700
H	-2.09026600	2.46470300	-4.25517600	O	0.04860200	-1.75333000	0.90945100
C	1.12684100	1.12334900	0.86841000	C	-2.50122900	0.16126500	2.32734700
C	2.03644100	1.86796800	-0.02948800	O	-3.31440900	-0.58973400	1.69989500
C	2.74873300	3.01686300	0.38895200	O	-1.37428200	0.57447300	1.90449300
C	2.23881600	1.42213600	-1.35330500	C	-2.88943300	1.53992500	-1.11436600
C	3.58863500	3.70167400	-0.48445600	O	-3.64372700	0.52554700	-0.96638500
H	2.61525500	3.39398700	1.39569700	O	-1.65188200	1.60627200	-0.82929900
C	3.08155800	2.10908900	-2.22519800	C	-1.08866300	-1.32253500	-2.54341400
H	1.72845600	0.52721400	-1.68399600	O	-0.21889600	-0.65829200	-1.88046200
C	3.75527500	3.25457800	-1.79926500	O	-2.21378200	-1.71618900	-2.11742300
H	4.11038000	4.59116600	-0.14065600	C	-2.89425100	0.58039400	3.72799700
H	3.21341600	1.74519600	-3.24100100	C	-3.53150600	2.79538400	-1.66554100
H	4.40854100	3.79315000	-2.48124800	C	-0.10057100	-3.99945000	1.66303900
C	0.70128500	1.84394800	2.10720800	C	-0.73340400	-1.64852300	-3.97980000
O	0.38386900	3.01927000	2.11818200	H	-3.98056900	0.66427700	3.80745300
O	0.58145300	1.05824800	3.21132100	H	-2.55799300	-0.18696600	4.43544000
C	-0.03865600	1.69829200	4.33620900	H	-2.41153700	1.52337000	3.99201900

H	-0.05571000	-3.82929400	2.74496000	H	6.13466500	0.80579300	1.04648600
H	-0.71004400	-4.88381600	1.46882600	H	6.71561300	0.88457200	-0.63912600
H	0.92331300	-4.15375900	1.31057500	H	5.89123900	2.29003500	0.08595000
H	-0.83527400	-0.74108900	-4.58646300	<b>9-ts</b>			
H	0.30752000	-1.97769300	-4.04938100	Rh	-2.61354400	-1.15739700	-0.93109600
H	-1.40145400	-2.41546400	-4.37540600	Rh	-0.78702800	0.08321300	0.18394000
H	-4.17725000	3.23162100	-0.89481600	C	-1.15942300	-2.70407700	1.04289300
H	-2.76893900	3.52444600	-1.94443600	O	-2.14290600	-2.78179900	0.24983000
H	-4.16280600	2.54737200	-2.52357200	O	-0.36655500	-1.71069000	1.17368000
C	1.41070000	1.16889100	0.27357500	C	-3.33083000	0.19685700	1.52462800
C	0.97565800	2.57713800	-0.01789400	O	-3.83385000	-0.46051000	0.55672100
C	0.38034500	3.39462200	0.97393200	O	-2.10632100	0.51290400	1.68068500
C	1.10241700	3.15055800	-1.30481000	C	-2.43181700	1.61384700	-1.70037100
C	-0.03785400	4.69093700	0.69195100	O	-3.02143200	0.53665700	-2.02597900
H	0.24014400	2.99005300	1.96506500	O	-1.50715600	1.73817300	-0.83400000
C	0.68032700	4.45294100	-1.58129800	C	0.02640900	-1.32188800	-2.32480300
H	1.51564300	2.58485400	-2.13240400	O	0.40028000	-0.38902400	-1.47005200
C	0.11030500	5.24018100	-0.58478100	O	-1.12930700	-1.77128100	-2.34577700
H	-0.49046600	5.28002900	1.48647600	C	-4.28569300	0.68243300	2.59354100
H	0.80311400	4.84521000	-2.58836500	C	-2.88953700	2.88352700	-2.38737700
H	-0.21438800	6.25575400	-0.79572000	C	-0.88743500	-3.90040000	1.93271300
C	1.78552500	0.84882700	1.67579700	C	1.07337400	-1.80670000	-3.29222000
O	1.36898300	1.37814200	2.69265000	H	-4.60955300	1.69943500	2.34243000
O	2.67719200	-0.19119100	1.76103700	H	-5.16654600	0.03874900	2.63922800
C	2.89590500	-0.69415100	3.08162000	H	-3.78033300	0.71983300	3.56102000
H	3.61858300	-1.50479900	2.96843600	H	-1.56053300	-4.72261100	1.68545000
H	3.29153200	0.08427100	3.74071500	H	0.15247000	-4.22486600	1.82176500
H	1.96262600	-1.07544800	3.50421000	H	-1.02983300	-3.61204500	2.97981900
C	2.96892900	-0.81099300	-0.82891100	H	1.46573600	-0.96320800	-3.87063800
C	4.34450100	-0.68413700	-0.58688000	H	1.90797000	-2.25079300	-2.73794100
C	5.22809800	-1.75403600	-0.53754200	H	0.64207000	-2.54689000	-3.96665800
C	4.68974100	-3.02268000	-0.77290700	H	-2.10483400	3.64170000	-2.35456600
C	3.32729900	-3.17571100	-1.05087100	H	-3.18492300	2.67018800	-3.41769400
C	2.45865700	-2.07703400	-1.08825200	H	-3.76838900	3.27212200	-1.85930500
C	2.35542300	0.57821100	-0.85110100	C	1.21463900	1.08106900	0.86928600
C	3.55881800	1.41864000	-0.64662300	C	1.07115400	2.55805500	0.56753100
H	6.28700300	-1.62061700	-0.33880300	C	1.07234000	3.55540800	1.56394100
H	5.34003300	-3.89218100	-0.75045900	C	0.97609300	3.00960700	-0.76812100
H	2.93226400	-4.16964000	-1.24211400	C	1.00256000	4.91152500	1.24059000
H	1.40562000	-2.20271200	-1.29410800	H	1.11371600	3.26594400	2.60478200
H	1.84533000	0.73294800	-1.80472300	C	0.92109800	4.36375900	-1.09273200
H	3.57547300	2.49731300	-0.56946000	H	0.92226100	2.28434700	-1.57333000
N	4.63903400	0.69781200	-0.41852300	C	0.93483400	5.33210300	-0.08720700
C	5.92525900	1.20045800	0.04769600	H	1.00859700	5.64475900	2.04375800

H	0.85214500	4.65973600	-2.13752100	C	-2.00615400	1.68274400	-3.75477600
H	0.88595100	6.38940700	-0.33438800	C	-1.47203500	-2.75669000	3.25512300
C	1.20708200	0.73544000	2.31724200	C	0.61948900	-3.64485800	-2.21022800
O	0.51701800	1.26333500	3.17474400	H	-3.91417800	3.17423000	1.06242900
O	2.05336600	-0.28608400	2.64191800	H	-4.95780800	1.92390400	1.78977300
C	1.96326100	-0.73747000	3.99546700	H	-3.47798800	2.49626100	2.63403400
H	2.68426700	-1.55311600	4.07991900	H	-2.10276200	-3.64662200	3.21332000
H	2.21307800	0.06600400	4.69409300	H	-0.44395800	-3.02614200	3.51146900
H	0.95324100	-1.09379900	4.21725900	H	-1.84834100	-2.09442900	4.04362100
C	2.99202600	-0.91427900	0.08200900	H	1.08799300	-3.26953600	-3.12788900
C	4.21348900	-0.82692000	-0.62541000	H	1.42131200	-3.91085800	-1.51186500
C	5.05976800	-1.91589400	-0.85613700	H	0.01373500	-4.52050800	-2.44408200
C	4.66084000	-3.14582500	-0.34770600	H	-1.08559200	1.59922800	-4.34167100
C	3.44823700	-3.26574200	0.35724000	H	-2.86132200	1.37301900	-4.35751300
C	2.61167600	-2.17441000	0.57136300	H	-2.11447400	2.73373300	-3.46755300
C	2.33493400	0.42531700	0.01241900	C	1.27782600	1.21220200	0.73106600
C	3.30974500	1.21358400	-0.65973300	C	1.04547100	2.64965200	0.30230800
H	5.98834300	-1.80707200	-1.40849500	C	0.81335700	3.70207700	1.21202800
H	5.28908900	-4.01926600	-0.49636900	C	1.08631900	3.00196300	-1.06474700
H	3.16054600	-4.23750200	0.74987100	C	0.64720300	5.01892200	0.78043900
H	1.68315800	-2.27354800	1.11543800	H	0.74912800	3.48856800	2.26946600
H	1.53223800	-0.02359800	-1.05153300	C	0.92416600	4.31687700	-1.49567900
H	3.26500000	2.27107700	-0.87485500	H	1.22711000	2.22632600	-1.80591200
N	4.37533900	0.49474000	-1.04667900	C	0.70409100	5.34255200	-0.57449700
C	5.49637400	0.98710300	-1.83282600	H	0.47635400	5.79792900	1.52001900
H	6.43568000	0.79671200	-1.30485700	H	0.96300300	4.53686800	-2.56053700
H	5.52962300	0.49162700	-2.80904900	H	0.57772000	6.36980700	-0.90712200
H	5.38183300	2.06219000	-1.98032600	C	1.18665100	1.00241700	2.21783500
<b>10</b>				O	0.37700800	1.50639000	2.97690400
Rh	-2.70000400	-1.19339700	-0.60507800	O	2.13641000	0.14504400	2.69475600
Rh	-0.62567700	0.06211700	0.05069500	C	2.03460700	-0.15560800	4.08877600
C	-1.51422500	-2.01048300	1.93800600	H	2.85198500	-0.84821600	4.29893300
O	-2.49181600	-2.24932100	1.16680300	H	2.13870800	0.75021300	4.69279000
O	-0.56183400	-1.18580400	1.72426100	H	1.06985400	-0.61900200	4.31400500
C	-3.10593500	1.19885100	0.96818300	C	2.95534400	-0.81270800	0.12123600
O	-3.73239700	0.25007900	0.39801800	C	4.14708000	-0.88410300	-0.66862100
O	-1.84266200	1.36493700	1.00511800	C	4.86694500	-2.06996500	-0.85703800
C	-1.89617300	0.83420900	-2.50440900	C	4.40421800	-3.22006800	-0.22727700
O	-2.78762300	-0.05221600	-2.32075000	C	3.25000500	-3.18133800	0.58118200
O	-0.90776200	1.08880200	-1.74137400	C	2.53504900	-1.99897900	0.76979700
C	-0.25272300	-2.57677800	-1.62055200	C	2.48382400	0.57245900	0.08665000
O	0.38276000	-1.48457700	-1.13745500	C	3.42579500	1.23003600	-0.68226100
O	-1.47525600	-2.63495300	-1.59190100	H	5.76699900	-2.08961600	-1.46516800
C	-3.92680700	2.25961200	1.66582800	H	4.94688000	-4.15355600	-0.34777200

H	2.92798800	-4.08428100	1.09406600	C	-3.75384600	0.50971400	3.10553900
H	1.67137200	-1.97508400	1.42410400	H	-2.93876400	2.17537900	2.04119700
H	1.35238300	-1.59848200	-0.94398100	C	-2.95284400	-1.67112000	2.45808300
H	3.47601800	2.27785800	-0.93551400	H	-1.47188900	-1.70265300	0.90236600
N	4.41293000	0.37804800	-1.13990700	C	-3.76668300	-0.87980900	3.26741800
C	5.53330700	0.75159300	-1.97945500	H	-4.38436900	1.13667300	3.73073200
H	6.48305800	0.48049300	-1.50429300	H	-2.95279100	-2.75192300	2.57616700
H	5.47867100	0.26172200	-2.95961300	H	-4.40656900	-1.33702600	4.01795400
H	5.51648300	1.83284300	-2.12949000	C	-0.97678000	2.38214200	0.38780200
<b>11-ts</b>				O	-0.82021800	2.98316000	1.43528200
Rh	3.19060100	-0.72404600	-0.09627100	O	-0.85378200	2.99579100	-0.81973300
Rh	0.85253900	0.06200100	0.01580100	C	-0.44727200	4.36936700	-0.76414000
C	1.98309200	-0.10182200	-2.68341900	H	-0.40228500	4.70101400	-1.80274200
O	3.06205600	-0.49524600	-2.15461300	H	-1.17059100	4.96828200	-0.20280300
O	0.89141100	0.16617900	-2.06766600	H	0.53206400	4.45150400	-0.29024200
C	2.93683400	2.13505100	0.16164400	C	-4.34482000	0.66472900	-1.06633500
O	3.81537300	1.22391200	0.08940900	C	-3.94127500	-0.68413200	-1.32989200
O	1.67312200	1.97073300	0.12111600	C	-4.85655300	-1.74930200	-1.26525500
C	2.11010200	-0.54408300	2.58328900	C	-6.16255600	-1.44411100	-0.91849900
O	3.16319800	-0.88265300	1.95883400	C	-6.57823800	-0.11607200	-0.63671100
O	1.02229800	-0.12582700	2.06516300	C	-5.68537700	0.93438400	-0.70240700
C	1.24172500	-2.85942500	-0.20155300	C	-3.21078900	1.46793300	-1.27336000
O	0.33201100	-1.96487800	-0.12378400	C	-2.10897100	0.61529100	-1.54799100
O	2.48916900	-2.65736800	-0.25053200	H	-4.55438400	-2.77059700	-1.47342500
C	3.42571400	3.56241500	0.29454800	H	-6.89377400	-2.24562500	-0.85782200
C	2.12730500	-0.64506200	4.09357000	H	-7.61366100	0.06628300	-0.36524300
C	1.97244800	0.09664100	-4.18507900	H	-6.00017600	1.95194100	-0.48904300
C	0.77359400	-4.30080900	-0.21070100	H	-3.14661500	2.54072600	-1.19090000
H	4.49959000	3.57991500	0.48777700	H	-1.21510400	0.86598500	-2.10190100
H	3.21978100	4.10715800	-0.63382300	N	-2.61628400	-0.68705300	-1.66222300
H	2.88785600	4.06432600	1.10419300	C	-1.90526700	-1.82589900	-2.21900400
H	2.05297700	1.16788500	-4.40370200	H	-1.92334200	-2.66874100	-1.52315500
H	2.81605700	-0.42124500	-4.64459900	H	-2.36484800	-2.12799900	-3.16849500
H	1.02996700	-0.25823800	-4.61149600	H	-0.86859300	-1.53918400	-2.38217000
H	0.51760100	-4.59879900	0.81289600	<b>12</b>			
H	-0.12467400	-4.41105900	-0.82453100	Rh	3.71204300	0.24916600	0.67052300
H	1.56544200	-4.95586900	-0.57815400	Rh	1.53589800	-0.09246800	-0.30908100
H	3.10795000	-0.96990400	4.44488000	C	2.37649800	-2.17092100	1.55888600
H	1.87478100	0.32728600	4.52795900	O	3.45383500	-1.51632800	1.70922400
H	1.36165400	-1.35666400	4.42024100	O	1.40010000	-1.84298100	0.80468800
C	-1.19914800	0.90335400	0.30151600	C	3.74925100	-1.23287200	-1.81830600
C	-2.09026700	0.31644100	1.32359400	O	4.52374600	-0.78747600	-0.91363800
C	-2.94129600	1.09744800	2.14341300	O	2.47954900	-1.11694700	-1.84102800
C	-2.12511400	-1.08290400	1.50173200	C	2.89596500	2.32135900	-1.17561800

O	3.85900400	1.99315700	-0.40813300	C	-7.72374000	-0.52831700	-0.80274100
O	1.81334700	1.67208300	-1.33694100	C	-6.53049300	-1.09191300	-1.27445900
C	1.53848100	1.41318500	2.18554800	C	-4.03953700	-1.63153400	-0.65733600
O	0.74698400	0.95159500	1.29989600	C	-3.36409500	-1.44687700	0.67229900
O	2.80258600	1.27387600	2.20575700	H	-6.74442500	0.39209500	2.34616400
C	4.38433000	-1.96007900	-2.98331800	H	-8.70979300	0.45577400	0.83824500
C	3.06578000	3.58147200	-1.99420500	H	-8.59872900	-0.49580900	-1.44508900
C	2.25394500	-3.47378400	2.31875800	H	-6.47142800	-1.49256000	-2.28365600
C	0.91990700	2.22941100	3.29952500	H	-3.86663300	-2.50893500	-1.26977200
H	5.45743600	-2.07696700	-2.82504200	H	-2.67195200	-2.16374200	1.10435900
H	3.91504700	-2.94080400	-3.10941400	N	-4.31847400	-0.86635100	1.55685600
H	4.20847900	-1.39179000	-3.90303900	C	-3.97686500	-0.30816000	2.84653100
H	2.74492300	-4.26851100	1.74444000	H	-3.74148500	0.76444400	2.79579700
H	2.76062200	-3.39567500	3.28342500	H	-4.80717800	-0.45287500	3.54688400
H	1.20483400	-3.74302700	2.45722900	H	-3.10497700	-0.83685000	3.24332800
H	0.79270100	3.26175000	2.95265500	<b>13-ts</b>			
H	-0.06602400	1.83650300	3.55929100	Rh	2.92689000	0.48375800	1.18513700
H	1.57210300	2.23642700	4.17494900	Rh	1.31068700	-0.27800900	-0.47347700
H	3.71729600	4.28745400	-1.47474600	C	1.75388400	-2.11357400	1.74358400
H	3.53434300	3.32183100	-2.95096400	O	2.57441600	-1.26617500	2.21972800
H	2.09319900	4.03260500	-2.20201500	O	1.08181300	-1.98665100	0.66701600
C	-2.86742700	-0.61645100	-0.56235800	C	4.04046400	-1.07054400	-0.98187900
C	-3.08528900	0.86804200	-0.64206600	O	4.37181700	-0.46180300	0.08502200
C	-3.86940400	1.41581000	-1.66515400	O	2.86377200	-1.15666400	-1.46779900
C	-2.46783100	1.73158200	0.27238200	C	2.52398100	2.31574600	-1.03818100
C	-4.04852500	2.79599900	-1.76463700	O	3.18593900	2.18508200	0.03945500
H	-4.34748900	0.75713500	-2.38360700	O	1.65247200	1.50348300	-1.49392800
C	-2.64744700	3.11225600	0.17492400	C	0.15284200	1.33082900	1.77938900
H	-1.81221500	1.32510900	1.03591600	O	-0.16754800	0.68511100	0.68350300
C	-3.44189000	3.64843600	-0.84055800	O	1.32669500	1.39436700	2.19687300
H	-4.66283600	3.20343100	-2.56324900	C	5.13626200	-1.78805100	-1.73738300
H	-2.15781500	3.77005100	0.88849000	C	2.82160900	3.54085900	-1.87718500
H	-3.58300800	4.72364000	-0.91463700	C	1.57639200	-3.40771200	2.50653700
C	-1.54542400	-1.09307100	-1.05180200	C	-0.95256900	2.00305400	2.54670600
O	-0.58045500	-0.35215700	-1.23391800	H	5.17247000	-2.83196700	-1.40403000
O	-1.50602000	-2.41845200	-1.25414600	H	4.92483500	-1.78156700	-2.80902100
C	-0.27780000	-2.98314200	-1.76470700	H	6.10410600	-1.32637100	-1.53186300
H	-0.54119100	-3.99598400	-2.07244000	H	2.26864400	-4.15520600	2.10100300
H	0.08370600	-2.39720300	-2.61150000	H	1.80910700	-3.26154200	3.56330300
H	0.47883000	-2.99496800	-0.98064300	H	0.55940800	-3.78632500	2.38282000
C	-5.41914300	-1.11641000	-0.44263500	H	-1.42516500	2.77752900	1.93381200
C	-5.50682200	-0.62201800	0.87810500	H	-1.73164900	1.27768200	2.79918900
C	-6.67948800	-0.02445300	1.34581000	H	-0.54554100	2.44903600	3.45457500
C	-7.78389600	0.00737000	0.48741900	H	1.95871900	3.80909800	-2.49076900



H	3.11738600	4.37695500	-1.23954400	O	2.52234900	-1.19920200	2.27318500
H	3.65815200	3.31230900	-2.54807200	O	1.01601200	-1.94548600	0.74442900
C	-2.36206200	-0.99474300	-0.83567900	C	4.00099700	-1.19828000	-0.92655000
C	-3.51309100	-1.82065400	-0.40617400	O	4.34313500	-0.55036100	0.11267100
C	-3.34572100	-2.97412700	0.38731200	O	2.82445500	-1.27207900	-1.41809300
C	-4.82895300	-1.48282000	-0.78381600	C	2.60423300	2.22183500	-1.15490400
C	-4.43692600	-3.74735800	0.78009600	O	3.24855600	2.12907600	-0.06082800
H	-2.34351200	-3.26184500	0.68699300	O	1.72030500	1.40922700	-1.58317100
C	-5.92206400	-2.25195200	-0.38551700	C	0.19376900	1.52169700	1.76307500
H	-4.99265100	-0.60701900	-1.40635100	O	-0.13644900	0.80538300	0.67459900
C	-5.73371400	-3.39075200	0.40057300	O	1.36271100	1.52442700	2.14797500
H	-4.27400500	-4.63117500	1.39280600	C	5.07660700	-1.98308500	-1.64091400
H	-6.92318600	-1.96513300	-0.69914100	C	2.93871500	3.39739900	-2.04785300
H	-6.58390900	-3.99260500	0.71110800	C	1.45646800	-3.29450800	2.64937400
C	-1.22726700	-1.54241400	-1.42565500	C	-0.89601700	2.27776100	2.45503800
O	-0.23915100	-0.84904800	-1.88883200	H	5.06544100	-3.01615300	-1.27389700
O	-1.19521700	-2.89877200	-1.57399100	H	4.88011900	-2.00319800	-2.71522100
C	-0.09379200	-3.43756400	-2.30650800	H	6.05873200	-1.55283500	-1.43574100
H	-0.26633300	-4.51617200	-2.32529400	H	2.09942500	-4.09190300	2.25811600
H	-0.06891500	-3.04751700	-3.32944500	H	1.72067700	-3.11906800	3.69405800
H	0.85862100	-3.21680600	-1.81819400	H	0.41933100	-3.62601700	2.56207400
C	-3.37443400	1.29397400	0.08142100	H	-1.32305900	3.03164800	1.78436100
C	-3.29395300	2.63194900	-0.37502900	H	-1.71630100	1.60576400	2.72785600
C	-3.99079500	3.68404500	0.22674000	H	-0.48689800	2.75880700	3.34350700
C	-4.80457900	3.37070200	1.31194300	H	2.07724000	3.67275400	-2.66009400
C	-4.90621300	2.04771600	1.78086500	H	3.27710300	4.24678400	-1.45048500
C	-4.19777800	1.00898100	1.18148200	H	3.75413500	3.10630800	-2.72061200
C	-2.43005200	0.49165800	-0.72747700	C	-2.41857100	-0.98613500	-0.87296700
C	-1.92278100	1.42390900	-1.67431800	C	-3.55234700	-1.83086800	-0.42738500
H	-3.90708800	4.70419500	-0.13612100	C	-3.37200600	-2.97967400	0.37119100
H	-5.36921000	4.15908100	1.80136700	C	-4.87555800	-1.49410600	-0.78159200
H	-5.55276600	1.83262500	2.62695500	C	-4.45720600	-3.74754900	0.78972600
H	-4.28742200	-0.00612700	1.55049100	H	-2.36656600	-3.26873000	0.65645400
H	-1.27899800	0.71107500	0.05856800	C	-5.96126900	-2.26099400	-0.36110900
H	-1.18312100	1.23051700	-2.43747400	H	-5.04824100	-0.61917300	-1.40216900
N	-2.39685000	2.67152300	-1.44317000	C	-5.76040500	-3.39455200	0.42940900
C	-1.95646300	3.88297700	-2.11614600	H	-4.28371700	-4.62633400	1.40692300
H	-2.81096900	4.39602700	-2.56916000	H	-6.96740800	-1.97463800	-0.65866600
H	-1.46580900	4.56438000	-1.41183500	H	-6.60514100	-3.99408300	0.75884100
H	-1.24761200	3.61127100	-2.89977400	C	-1.24946300	-1.53286600	-1.40345600
<b>14</b>				O	-0.26186100	-0.84380500	-1.87589100
Rh	2.94071600	0.49179800	1.16352900	O	-1.17391600	-2.89670600	-1.46314400
Rh	1.30508200	-0.30600000	-0.48722400	C	-0.07627900	-3.44996200	-2.18873800
C	1.67927000	-2.04304600	1.82966800	H	-0.23977100	-4.53012100	-2.17081100

H	-0.06509300	-3.09367600	-3.22423300	H	-5.27853300	-1.12180500	-0.88983400
H	0.88058400	-3.20848600	-1.71912100	H	-5.27735200	-1.12295900	0.89028500
C	-3.36193600	1.29533800	0.05931100	<b>CH<sub>3</sub>COOH</b>			
C	-3.26104600	2.65161000	-0.37093700	C	1.39758900	-0.10974700	-0.00002600
C	-3.85760800	3.70949400	0.32791600	H	1.68523500	-0.69299800	-0.88105700
C	-4.56792500	3.39948100	1.48362800	H	1.68543400	-0.68997700	0.88298400
C	-4.68177200	2.06640300	1.93011200	H	1.91753500	0.84844800	-0.00148100
C	-4.09112600	1.01741100	1.23281500	C	-0.09248500	0.12562400	-0.00009000
C	-2.59189500	0.47995100	-0.87894900	O	-0.64579600	1.20195400	0.00001000
C	-2.08410100	1.38808200	-1.80299200	O	-0.77860000	-1.04667400	-0.00000900
H	-3.77540500	4.73546800	-0.02023100	H	-1.72365400	-0.80297900	0.00024500
H	-5.04763000	4.19610300	2.04559400	<b>16</b>			
H	-5.25035700	1.85525100	2.83174000	Rh	-1.21883100	-2.01635800	-0.36135400
H	-4.19967200	-0.00516000	1.57779700	Rh	-2.90042800	-0.32059800	0.21681400
H	-1.07427000	0.85424800	0.31091300	C	-1.57683100	-1.56534200	2.48757600
H	-1.44314200	1.18983900	-2.64854300	O	-0.96078200	-2.31427400	1.66480000
N	-2.47688100	2.67801200	-1.50683900	O	-2.43008200	-0.65942300	2.19568400
C	-2.12019400	3.86460000	-2.25907800	C	-3.95340600	-3.01503400	-0.03217300
H	-3.00907600	4.33687700	-2.69392500	O	-2.79506800	-3.37929800	-0.37904200
H	-1.61238200	4.59771000	-1.62054600	O	-4.27089300	-1.82296900	0.29902300
H	-1.44376600	3.57865300	-3.06669400	C	-2.50188400	-0.71417200	-2.63788300
<b>15</b>				O	-1.61334600	-1.57075700	-2.34654700
C	0.72636200	0.72249900	-0.00016500	O	-3.23615600	-0.07414500	-1.80791500
C	-0.40692400	-0.01353700	-0.00031400	C	-5.06134400	-4.04280400	-0.03324600
H	0.59754400	1.80490800	-0.00012300	C	-2.69927400	-0.39379000	-4.10316100
H	-0.41036100	-1.09750400	-0.00034600	C	-1.23936100	-1.73297900	3.95141000
C	2.10514700	0.24455900	-0.00003900	H	-5.61471000	-3.96954800	-0.97689600
C	3.14681100	1.19213200	0.00027800	H	-4.64600400	-5.04884100	0.04989900
C	2.44612300	-1.12355000	-0.00022500	H	-5.76063700	-3.84843700	0.78367500
C	4.48145600	0.79269600	0.00041600	H	-0.41612400	-1.05066300	4.19484900
H	2.89734000	2.25034400	0.00041700	H	-2.09773000	-1.47476000	4.57563800
C	3.77819200	-1.52184100	-0.00009000	H	-0.90890400	-2.75446800	4.15089200
H	1.66271100	-1.87522700	-0.00048300	H	-2.03203500	0.43256800	-4.37605400
C	4.80106000	-0.56629000	0.00023400	H	-2.44193700	-1.25778100	-4.71946300
H	5.27026400	1.53971900	0.00066400	H	-3.72824800	-0.07960700	-4.29191700
H	4.02394200	-2.58019800	-0.00024000	C	2.62198500	-0.60522800	0.58498700
H	5.84062600	-0.88236400	0.00033800	C	2.38755800	0.61139000	1.37518600
C	-1.71667200	0.65305500	-0.00035200	C	1.11228900	0.98120600	1.87212800
O	-1.89409700	1.86083700	-0.00056300	C	3.46952100	1.45308400	1.73447400
C	-2.92208800	-0.31523300	-0.00009900	C	0.94506900	2.09492900	2.69470500
O	-2.80900500	-1.52515900	-0.00028800	H	0.25231400	0.38202600	1.60844700
O	-4.08517700	0.34195700	0.00036200	C	3.29456300	2.56948000	2.55022000
C	-5.25901500	-0.48754900	0.00062700	H	4.46285000	1.21113100	1.37186600
H	-6.10266600	0.20236400	0.00160900	C	2.03108000	2.90124600	3.04662100

H	-0.04987900	2.32949600	3.06818800	H	-0.61156200	6.19043300	-1.15711400
H	4.15628500	3.18478600	2.80092500	C	3.18368100	5.44146100	-0.80066600
H	1.89617000	3.76613400	3.69062500	H	2.59180300	3.44337600	-0.25414700
C	1.61657200	-1.27203800	-0.10361000	C	2.74679500	6.71480900	-1.17193200
O	0.44345800	-0.80187000	-0.40291800	H	1.03877800	7.96980900	-1.58944800
O	1.96796000	-2.53082900	-0.54445500	H	4.24521300	5.23493100	-0.70109700
C	1.12706700	-3.18452300	-1.46359800	H	3.46954700	7.50253400	-1.36664900
H	0.17136600	-3.51814800	-0.98662900	H	0.40569900	2.61793400	-0.24367900
H	1.64779100	-4.09842200	-1.75857100	<b>17-threo-ts</b>			
H	0.89522800	-2.57568100	-2.34204000	Rh	2.09157700	-1.28701200	-0.91153600
C	4.79372000	-1.37447200	-0.68332300	Rh	3.02217000	0.06514300	0.88149500
C	6.04752700	-1.90033000	-0.26608400	C	2.94477100	1.35150300	-1.73248900
C	7.06227800	-2.22532200	-1.17412900	O	2.57082400	0.23186100	-2.22010800
C	6.80875100	-2.01180900	-2.52586500	O	3.14329300	1.60007500	-0.50077300
C	5.57532800	-1.48487400	-2.96102500	C	4.95447900	-1.55058300	-0.56752000
C	4.57071800	-1.16704500	-2.05362600	O	3.94397800	-2.08307700	-1.14160500
C	3.99564200	-1.15599000	0.50445300	O	4.89507000	-0.58356500	0.24695200
C	4.79147100	-1.54758400	1.55731900	C	2.15985600	-2.56940300	1.69937500
H	8.01473600	-2.62912800	-0.84096800	O	1.67312900	-2.71423500	0.52507400
H	7.57509800	-2.25488700	-3.25738300	O	2.85515500	-1.58726300	2.10462500
H	5.41070400	-1.32657300	-4.02389500	C	6.30679900	-2.15124300	-0.86843900
H	3.62312300	-0.75769600	-2.39409900	C	1.85890000	-3.65790700	2.70387000
H	4.57040800	-1.54350300	2.61656100	C	3.16767600	2.49171500	-2.69844100
N	6.02566600	-1.99401600	1.11273000	H	6.47519700	-2.99883100	-0.19357500
C	7.09867300	-2.50016500	1.93925100	H	6.34136200	-2.52167500	-1.89543700
H	7.31478000	-3.55193400	1.71231800	H	7.09386300	-1.41404100	-0.69783600
H	8.01752600	-1.91818000	1.79416400	H	2.45220000	3.29026200	-2.47576300
H	6.80466000	-2.42571200	2.98869800	H	4.17296400	2.90091500	-2.55805300
C	-0.04441400	3.59544700	-0.40581900	H	3.04030500	2.15765200	-3.72940400
C	-1.40501300	3.67203600	-0.31159100	H	0.95455100	-3.38198900	3.25914200
H	-1.95323200	4.60013900	-0.42359700	H	1.68237200	-4.61111900	2.20109300
C	-2.18847200	2.50378600	-0.03911400	H	2.67906700	-3.74651000	3.41979100
O	-1.69713000	1.35873300	0.10821900	C	-2.11317300	0.22991800	-0.92441600
C	-3.69957700	2.72047500	0.07152000	C	-1.97876100	1.56816500	-1.56530600
O	-4.26423500	3.75067900	-0.21451900	C	-0.85281800	1.93432100	-2.33447200
O	-4.32102300	1.61993500	0.54833600	C	-3.00075600	2.53585400	-1.43802900
C	-5.76412300	1.67773200	0.64567500	C	-0.76783100	3.18193000	-2.95193000
H	-6.05760500	0.71043900	1.04939300	H	-0.03266900	1.23864200	-2.46276700
H	-6.05201900	2.49271700	1.31229000	C	-2.90723400	3.78507700	-2.04874100
H	-6.19080800	1.83581300	-0.34678100	H	-3.87132200	2.31246900	-0.83510700
C	0.87303400	4.68327300	-0.67459100	C	-1.79181400	4.11960100	-2.81772600
C	0.44766800	5.97787800	-1.04866500	H	0.10851900	3.41668700	-3.55111300
C	2.25693600	4.43133300	-0.55705700	H	-3.71509900	4.50138000	-1.91832800
C	1.37622900	6.97970000	-1.29638700	H	-1.72121100	5.09074800	-3.29960500

C	-0.97773600	-0.69475400	-1.12743300	C	-5.55616100	1.75880500	2.91711200
O	0.19815200	-0.41608500	-0.81670200	H	-5.22047500	3.79219400	2.27711700
O	-1.31977900	-1.85018200	-1.71288800	H	-5.57366000	-0.33227400	3.45228900
C	-0.35809800	-2.89353200	-1.92096300	H	-6.53754600	1.96417400	3.33666100
H	0.48255400	-2.53454700	-2.53167300	H	-1.27751000	-0.06232100	1.57278900
H	-0.89201600	-3.66227200	-2.48099400	<b>18-threo</b>			
H	-0.00091300	-3.29441100	-0.97103900	Rh	2.05266200	-1.11868400	-1.01418100
C	-3.79679500	-1.67360400	-0.24508700	Rh	2.82195500	0.11840900	0.94878300
C	-5.15388400	-1.94706000	-0.56456900	C	2.74104600	1.65576800	-1.54428900
C	-5.83783500	-3.06543200	-0.07498600	O	2.28647800	0.60934800	-2.12465800
C	-5.13851100	-3.93963400	0.74958000	O	3.08827000	1.73484600	-0.32585800
C	-3.78902900	-3.69906200	1.07579400	C	4.90695000	-1.27252600	-0.58988500
C	-3.11856600	-2.58333100	0.58565900	O	3.96659400	-1.64399500	-1.37698600
C	-3.43048400	-0.43700900	-0.92225300	O	4.74472600	-0.55518900	0.43433700
C	-4.57108900	-0.05359100	-1.60655200	C	2.12426000	-2.64772100	1.45703700
H	-6.87792500	-3.24790300	-0.33042600	O	1.84062900	-2.75472900	0.21412100
H	-5.63822600	-4.81980000	1.14464300	O	2.53698800	-1.60244900	2.04641300
H	-3.26403800	-4.39874500	1.72071500	C	6.29562100	-1.76688700	-0.92035500
H	-2.07871800	-2.42040500	0.85531700	C	1.98741900	-3.90185600	2.29104200
H	-4.71930300	0.78598200	-2.26877900	C	2.86134200	2.91847200	-2.36396500
N	-5.60198900	-0.94339400	-1.40173600	H	6.40762400	-2.79056600	-0.54427100
C	-6.94163700	-0.82931600	-1.93893100	H	6.44417100	-1.78903700	-2.00275800
H	-7.21858800	-1.73772800	-2.48641100	H	7.04615900	-1.13480600	-0.44232100
H	-7.67765100	-0.66180900	-1.14273100	H	2.24277800	3.69380100	-1.89903600
H	-6.97661800	0.01584600	-2.62966800	H	3.89842800	3.26896700	-2.34439600
C	-1.64817900	0.92893700	1.33488700	H	2.54852400	2.74907900	-3.39560100
C	-0.66210700	1.95324600	1.27071100	H	1.79114100	-3.64383500	3.33372500
H	-0.96028600	2.99051800	1.18220600	H	1.19429100	-4.53841600	1.89262400
C	0.69175000	1.73805600	1.44272300	H	2.92930400	-4.46166700	2.24581000
O	1.22700700	0.57247400	1.65709600	C	-2.18859000	0.36784800	-0.62255900
C	1.56975800	2.96724600	1.53098800	C	-2.73653200	1.57060900	-1.41281600
O	1.26277500	4.08366100	1.16639000	C	-1.89659500	2.35619600	-2.21905100
O	2.75838300	2.68059900	2.12281000	C	-4.06392600	1.99833600	-1.24914400
C	3.67979700	3.77833300	2.20458500	C	-2.37077200	3.49801100	-2.86499200
H	4.54792600	3.39189800	2.73920700	H	-0.85307400	2.08822600	-2.34547200
H	3.96114800	4.10775500	1.20094600	C	-4.54289600	3.13818500	-1.89906800
H	3.23103800	4.61373400	2.74777500	H	-4.72788400	1.45012800	-0.59234200
C	-2.99595300	1.23013900	1.83155600	C	-3.70093800	3.89134000	-2.71622800
C	-3.55408100	2.52771500	1.79158200	H	-1.69275200	4.08238500	-3.48105400
C	-3.75755700	0.21390800	2.44364000	H	-5.57686700	3.43958400	-1.75246700
C	-4.81673500	2.78376700	2.31992400	H	-4.07212000	4.77886500	-3.22148800
H	-2.99463000	3.34404800	1.34934000	C	-0.95369700	-0.23722300	-1.32813400
C	-5.01614200	0.47278800	2.98106500	O	0.04248300	-0.59624200	-0.69675000
H	-3.34821700	-0.78814000	2.50805600	O	-1.13264600	-0.43166300	-2.62739400

C	-0.16095700	-1.17808600	-3.38714300	H	-5.86656800	1.96744000	4.22498400
H	0.74716000	-0.58748400	-3.52094700	H	-1.22527900	-0.00445300	1.29061300
H	-0.63814000	-1.36358100	-4.34967600	<b>19-threo-ts</b>			
H	0.05729000	-2.13096100	-2.89368800	Rh	-4.08518700	-0.03821800	-1.05178200
C	-2.94307000	-2.10614600	0.09066400	Rh	-3.00239600	0.00155700	1.14063200
C	-4.02683000	-2.94924800	-0.28889600	C	-2.42011900	-2.34029500	-0.48770200
C	-4.18937900	-4.25017600	0.20046900	O	-3.22263300	-1.87678300	-1.36087300
C	-3.22621500	-4.73293500	1.07743800	O	-2.08716000	-1.77223100	0.60681300
C	-2.12627600	-3.93468400	1.44684900	C	-5.57838100	-1.34160300	1.06745700
C	-1.97232800	-2.63981700	0.96352100	O	-5.65493500	-0.98302000	-0.14959700
C	-3.13725100	-0.83865800	-0.59562200	O	-4.57770500	-1.11783300	1.81711900
C	-4.26597700	-1.00546200	-1.36838100	C	-4.73952800	2.26223100	0.58879100
H	-5.03594000	-4.86285100	-0.09621500	O	-4.92972100	1.77816600	-0.57521200
H	-3.32000500	-5.73851700	1.47778800	O	-4.06311200	1.72695400	1.52658800
H	-1.38154400	-4.33858500	2.12696100	C	-6.76472500	-2.05183500	1.67117200
H	-1.10237700	-2.06180500	1.25258100	C	-5.35437900	3.61242800	0.87740600
H	-4.72574100	-0.32101100	-2.06451400	C	-1.78928700	-3.67940900	-0.77914500
N	-4.81365700	-2.25415200	-1.18585500	H	-7.38184700	-1.31927500	2.20449400
C	-6.04724500	-2.73482700	-1.77448600	H	-7.37002700	-2.51702600	0.89098500
H	-5.88458700	-3.69203300	-2.28248400	H	-6.42824600	-2.79829600	2.39457500
H	-6.82606100	-2.86886700	-1.01382200	H	-0.79968100	-3.51573900	-1.21997700
H	-6.39765600	-2.00695200	-2.50940900	H	-1.66101800	-4.24696600	0.14590800
C	-1.74318500	0.84429200	0.84641300	H	-2.39951500	-4.23938200	-1.49084900
C	-0.75109600	1.97883700	0.80985000	H	-4.61466300	4.38844000	0.64780400
H	-1.08515900	2.96264300	0.50261400	H	-6.23332400	3.77530700	0.25040900
C	0.53142500	1.88257300	1.24083100	H	-5.61325200	3.69300500	1.93555300
O	1.08820500	0.77406500	1.71587200	C	2.96055700	-0.39668700	-0.59104900
C	1.33041000	3.16618900	1.26671600	C	2.59213300	-1.78403900	-1.14956500
O	1.08452100	4.16223000	0.60929700	C	1.79743500	-1.94132600	-2.29531100
O	2.35460700	3.10055600	2.14573700	C	3.00479600	-2.95282700	-0.48492000
C	3.19478200	4.26027400	2.19151900	C	1.46133500	-3.20747400	-2.77999700
H	3.93074800	4.05786100	2.97046200	H	1.42729300	-1.07464200	-2.82855900
H	3.68867800	4.40637600	1.22669700	C	2.66915100	-4.21997500	-0.96474400
H	2.61071800	5.15182900	2.43490500	H	3.59524800	-2.87405800	0.41906300
C	-2.92534700	1.17865100	1.76432700	C	1.90249400	-4.35616700	-2.12243800
C	-3.50803400	2.45570900	1.81337200	H	0.85415300	-3.28912700	-3.67788700
C	-3.42128900	0.20134400	2.64105100	H	3.01096300	-5.10100800	-0.42757800
C	-4.56076300	2.73570200	2.68627900	H	1.64862900	-5.34177200	-2.50367700
H	-3.13770100	3.24754000	1.17203200	C	2.77861400	0.71552400	-1.65598300
C	-4.47252000	0.47780400	3.51665500	O	2.20311400	1.77401900	-1.48039700
H	-2.97605600	-0.78840400	2.64456200	O	3.42853700	0.43467300	-2.80079400
C	-5.05130700	1.74713700	3.54056300	C	3.45629600	1.48344000	-3.78025300
H	-4.99034500	3.73428700	2.70315400	H	2.44660100	1.72012300	-4.12743400
H	-4.83161100	-0.30011600	4.18579500	H	4.05930500	1.09615300	-4.60200200

H	3.91023500	2.38495300	-3.36051300	O	-2.76096500	1.02192500	-2.21640400
C	5.15641000	0.89908400	0.23948600	C	-0.78803300	1.98030200	-3.12129700
C	6.54436500	0.57627300	0.25454800	H	0.06070900	2.35560000	-2.54259000
C	7.52904300	1.46532500	0.69974800	H	-0.38967800	1.51951700	-4.03348600
C	7.11700300	2.72317800	1.12270000	H	-1.46095600	2.79599000	-3.38837900
C	5.75525600	3.08054300	1.09546800	O	-0.83561200	-0.05864600	-1.82726700
C	4.77850700	2.19191600	0.65908500	H	-0.03963500	0.13721800	-1.00282900
C	4.45747600	-0.27429700	-0.26292800	<b>20-threo</b>			
C	5.43997200	-1.19272400	-0.55414700	C	-0.10558100	0.62853500	-0.64709700
H	8.57857400	1.18482700	0.71188300	C	0.09119200	2.15424500	-0.68895200
H	7.85457400	3.43918600	1.47486300	C	0.81281000	2.78082400	-1.71843200
H	5.45867300	4.07278400	1.42422900	C	-0.35033500	2.96226800	0.37329000
H	3.74242500	2.50948700	0.64618100	C	1.05462100	4.15538200	-1.70593600
H	5.35131000	-2.17547100	-0.99085100	H	1.19263000	2.19778300	-2.54974100
N	6.68911300	-0.70390300	-0.24052400	C	-0.11585100	4.33874300	0.38541800
C	7.93712600	-1.42951400	-0.35272400	H	-0.87193400	2.51248300	1.20913700
H	8.66388400	-0.86007200	-0.94346100	C	0.58435700	4.94519600	-0.65698700
H	8.37119100	-1.63392400	0.63394300	H	1.61425400	4.60534000	-2.52173600
H	7.75097300	-2.38082300	-0.85593600	H	-0.47565600	4.93285700	1.22157800
C	2.05826500	-0.00300800	0.66888400	H	0.76821000	6.01621800	-0.64838700
C	0.55033100	0.07406800	0.39786100	C	0.08799500	-0.02726000	-2.04162300
H	-0.00847700	-0.84719100	0.55140100	O	0.72361400	-1.03747300	-2.25912500
C	-0.19360500	1.21901200	0.70765200	O	-0.63251800	0.59649600	-2.99687100
O	-1.47063800	1.32217600	0.79153000	C	-0.61705900	-0.03338700	-4.28724200
C	0.47068500	2.59240300	0.82826000	H	0.40209900	-0.08906200	-4.67958900
O	1.32625400	2.87232000	1.64134600	H	-1.23999000	0.59506900	-4.92458900
O	-0.05822900	3.46502100	-0.04311000	H	-1.02816500	-1.04444500	-4.22294000
C	0.49866800	4.79014700	0.00385800	C	-2.05198200	-1.14642200	-0.20205000
H	-0.05838800	5.36495400	-0.73598700	C	-3.45052800	-1.04124300	0.04859200
H	0.37567000	5.22053600	1.00079500	C	-4.27920200	-2.15690900	0.21320200
H	1.56139100	4.76127800	-0.25057600	C	-3.69702900	-3.41403600	0.10256100
C	2.33039700	-0.84771200	1.92107200	C	-2.32266700	-3.54914800	-0.17439300
C	1.65053700	-2.04439500	2.20299700	C	-1.50059400	-2.43813300	-0.32966400
C	3.26215700	-0.39047100	2.86628400	C	-1.53595600	0.20973900	-0.29078200
C	1.90583800	-2.76264100	3.37300100	C	-2.62910900	1.03143500	-0.13879200
H	0.90897000	-2.42956700	1.51139100	H	-5.34105200	-2.04649200	0.41456100
C	3.52057500	-1.10566800	4.03684400	H	-4.31163600	-4.30204200	0.22199400
H	3.78539500	0.54349500	2.68879300	H	-1.89739700	-4.54399500	-0.27756300
C	2.84465600	-2.29854600	4.29547000	H	-0.45342300	-2.57191400	-0.57578900
H	1.36131900	-3.68413900	3.56401900	H	-2.68863400	2.10792700	-0.18613900
H	4.24499200	-0.72141300	4.75058000	N	-3.77710200	0.29931400	0.07570800
H	3.03819900	-2.85450800	5.20930300	C	-5.09555300	0.84201800	0.32977200
H	2.38910200	0.99845300	0.92512600	H	-5.82413600	0.44252700	-0.38515100
C	-1.51055500	0.92577700	-2.32105000	H	-5.43507400	0.60506000	1.34562300

H	-5.06011000	1.92780600	0.21821500	H	2.76586900	4.87544200	0.01534000
C	0.96986900	-0.03922800	0.34220300	H	1.36629500	4.45907600	1.01846300
C	2.37408700	0.26010500	-0.12075000	H	2.99082900	4.44878100	1.74560700
C	3.39245300	-0.58864900	-0.34827500	H	3.93933300	-4.18831500	-0.88340300
C	3.43871700	-2.07452900	-0.21017200	H	2.19319400	-4.32991800	-0.62890900
O	4.44454000	-2.68919900	-0.53959600	H	2.81939200	-3.94392000	-2.26032300
O	2.35337500	-2.66300300	0.30587300	C	-2.15222900	0.82086100	-0.71389700
C	2.42497600	-4.09525400	0.42552400	C	-2.17067400	2.26571700	-0.37054200
H	1.47145700	-4.39408200	0.86079000	C	-3.28903400	2.83842800	0.28078700
H	2.56326800	-4.55266500	-0.55722000	C	-1.11853800	3.14969800	-0.70967800
H	3.25464200	-4.38143000	1.07663800	C	-3.35819200	4.20245800	0.56180000
C	0.77635800	0.32481400	1.81892900	H	-4.11296500	2.20375800	0.57680900
C	1.49510800	1.35841000	2.43947800	C	-1.19724000	4.51333600	-0.43484000
C	-0.10978300	-0.42433800	2.60884800	H	-0.22942200	2.77567200	-1.19888900
C	1.32093200	1.64536400	3.79451100	C	-2.31547400	5.05616100	0.20335900
H	2.20594000	1.94281000	1.86515400	H	-4.23715600	4.59457100	1.06801200
C	-0.28820600	-0.13858800	3.96349900	H	-0.37659300	5.15892800	-0.73820800
H	-0.66118000	-1.24460700	2.16041800	H	-2.37217600	6.12082900	0.41319400
C	0.42492400	0.90075100	4.56300000	C	-0.93882200	0.30022100	-1.35787300
H	1.89280300	2.45031300	4.24938000	O	0.22036500	0.53767000	-0.95318400
H	-0.97940200	-0.73739700	4.55152900	O	-1.20133600	-0.42611100	-2.45214700
H	0.29216900	1.12105300	5.61914300	C	-0.15181600	-1.02414500	-3.22221100
H	0.80459300	-1.10888700	0.26394900	H	0.53129300	-0.25879900	-3.60633500
H	2.61602700	1.30380400	-0.30806000	H	-0.65918600	-1.51085900	-4.05602000
O	4.59544900	-0.10346300	-0.77776300	H	0.41048200	-1.74902400	-2.63590600
H	5.15994000	-0.89034200	-0.91739300	C	-3.70594500	-1.24637300	-1.24043100
<b>21-erythro-ts</b>				C	-5.03948900	-1.36545400	-1.71633500
Rh	2.29711600	0.49727800	-1.32130700	C	-5.66243200	-2.59939100	-1.93080400
Rh	3.05131400	-0.02769300	0.95126400	C	-4.92302500	-3.74772600	-1.66782200
C	2.55236000	2.78270200	0.45806600	C	-3.59590200	-3.65977700	-1.20426100
O	2.28805200	2.47882300	-0.75567200	C	-2.98393100	-2.42756100	-0.99433500
O	2.89504500	1.97528800	1.37729300	C	-3.41169400	0.17522200	-1.12380200
C	5.17255300	0.55655300	-0.95699600	C	-4.56738300	0.81496100	-1.54404300
O	4.24579700	0.66201100	-1.83027200	H	-6.68586000	-2.66142200	-2.29015600
O	4.98231000	0.28805800	0.26399800	H	-5.37443400	-4.72359700	-1.82444400
C	2.87324800	-2.32791700	-0.83430000	H	-3.03730700	-4.57130600	-1.00982900
O	2.42923400	-1.53193400	-1.72642400	H	-1.95915500	-2.38973500	-0.64108000
O	3.21716900	-2.00202800	0.34725400	H	-4.75971400	1.87241700	-1.64887700
C	6.58519500	0.80283100	-1.42898100	N	-5.54022100	-0.08879500	-1.90027600
C	2.96637900	-3.79266600	-1.18965500	C	-6.87604000	0.23464100	-2.35559600
C	2.42440500	4.23960600	0.83631600	H	-7.07432400	-0.21910000	-3.33363400
H	7.29795800	0.30711400	-0.76725600	H	-7.63407700	-0.11904400	-1.64574700
H	6.70860600	0.45705100	-2.45790200	H	-6.96640900	1.31882200	-2.45042400
H	6.78191800	1.88125100	-1.40828000	C	-1.62100000	0.02394700	1.63563600

C	-0.91497000	-1.19987400	1.63488300	H	3.30233600	-4.34429400	-0.58341800
H	-1.00480700	0.91548300	1.68225800	H	1.57271200	-4.23845600	-0.23566900
H	-1.45326800	-2.13840700	1.70439600	H	2.14781600	-4.07981700	-1.92679700
C	-2.95146800	0.13511200	2.22940600	C	-2.14366400	0.63600600	-0.43044800
C	-3.91891200	-0.89031300	2.15945600	C	-2.49408600	2.13686600	-0.65318600
C	-3.26319800	1.28966000	2.97903400	C	-3.64236700	2.69550700	-0.06270400
C	-5.14103500	-0.76142800	2.81238700	C	-1.66334500	3.00021000	-1.38543900
H	-3.71552700	-1.78434500	1.58080600	C	-3.95460900	4.04635600	-0.22000700
C	-4.48233400	1.40889900	3.64388200	H	-4.29827100	2.07491900	0.53344300
H	-2.52614800	2.08312800	3.05444700	C	-1.97490300	4.35281900	-1.54394200
C	-5.42847900	0.38526400	3.56052900	H	-0.74403200	2.64282000	-1.83601600
H	-5.87298900	-1.56164500	2.74072500	C	-3.12508200	4.88472800	-0.96500000
H	-4.69121500	2.30026700	4.22967700	H	-4.85020200	4.44143800	0.25232200
H	-6.38042600	0.47634000	4.07706800	H	-1.30766300	4.98628300	-2.12256300
C	0.46801300	-1.27037300	1.75172100	H	-3.36869800	5.93665300	-1.08665800
O	1.24109500	-0.23106500	1.83832300	C	-0.90719800	0.35135200	-1.31139100
C	1.03573900	-2.65804700	1.95909500	O	0.23472800	0.52785500	-0.88748200
O	0.62554300	-3.65930600	1.39796000	O	-1.20351400	-0.00878600	-2.54849000
O	2.01522600	-2.65865100	2.88049300	C	-0.14422600	-0.25667600	-3.49568700
C	2.65152900	-3.92430400	3.10907100	H	0.47975400	0.63672100	-3.61261100
H	3.33166400	-3.76191900	3.94542300	H	-0.65261200	-0.47488500	-4.43446500
H	1.91103300	-4.68988300	3.35425000	H	0.46036900	-1.10641000	-3.17487600
H	3.20847200	-4.22509400	2.21788200	C	-3.23993500	-1.73688300	-1.02972200
<b>22-erythro</b>				C	-4.50940000	-2.12926900	-1.54281000
Rh	2.27552700	0.44906000	-1.35373300	C	-4.84189300	-3.46065200	-1.81821900
Rh	2.90086700	0.02829200	0.96978400	C	-3.86816200	-4.42665800	-1.59527600
C	2.63949400	2.83071100	0.26903300	C	-2.59491800	-4.06688000	-1.11354500
O	2.36126600	2.45809000	-0.92442500	C	-2.27272800	-2.74326800	-0.83492400
O	2.93598000	2.07348400	1.24202300	C	-3.27319500	-0.28976300	-0.88059700
C	5.12552500	0.28212000	-0.94299100	C	-4.51547700	0.09711400	-1.33121900
O	4.23029000	0.44321000	-1.84569400	H	-5.82378600	-3.72995200	-2.19725600
O	4.88597300	0.09161800	0.28023400	H	-4.09218900	-5.47063500	-1.79668200
C	2.48402400	-2.36655000	-0.65883400	H	-1.84931100	-4.83849900	-0.94465600
O	2.19087100	-1.59547700	-1.63696800	H	-1.28868300	-2.50882100	-0.44517000
O	2.84377200	-1.99009100	0.50021600	H	-4.93306100	1.08664300	-1.43100900
C	6.56410800	0.36021900	-1.39667100	N	-5.26849700	-0.98941000	-1.71688600
C	2.36996100	-3.85533100	-0.88233800	C	-6.63101800	-0.94899900	-2.20550100
C	2.58701900	4.31795700	0.53537700	H	-6.70593000	-1.42827500	-3.18857200
H	7.20138900	-0.22530700	-0.73090100	H	-7.31663000	-1.45667100	-1.51592400
H	6.66107500	0.01245600	-2.42753600	H	-6.94309900	0.09308900	-2.30277300
H	6.89145100	1.40583300	-1.35598600	C	-1.67043200	0.47762900	1.10702800
H	3.01857100	4.86777200	-0.30525000	C	-1.02396700	-0.83443600	1.47037300
H	1.53817100	4.62160100	0.63280700	H	-0.90047100	1.24292100	1.22349800
H	3.11158300	4.55899800	1.46149200	H	-1.65110300	-1.71124100	1.57437800



C	-2.76173700	0.76531600	2.13572400	C	3.50468900	-0.30002800	-0.66067100
C	-3.86811900	-0.08161900	2.31441500	C	4.74569600	-1.24316900	-0.69836600
C	-2.63109200	1.87248700	2.98668200	C	5.59534100	-1.39106500	0.41385200
C	-4.82446500	0.19002800	3.29421100	C	5.03371900	-2.03268500	-1.82471900
H	-3.98318100	-0.95985600	1.68750300	C	6.69378300	-2.25142300	0.38460100
C	-3.58189400	2.14154400	3.97255800	H	5.39333900	-0.84940700	1.32758300
H	-1.77282100	2.52970300	2.87245300	C	6.12965200	-2.89717400	-1.85562900
C	-4.68764100	1.30381300	4.12595500	H	4.39636600	-1.99848500	-2.70086500
H	-5.67412000	-0.47766600	3.41395500	C	6.97355500	-3.00770100	-0.75281200
H	-3.45644100	3.00567700	4.62000900	H	7.32408100	-2.33459000	1.26624900
H	-5.43025300	1.51000100	4.89240300	H	6.31581100	-3.48635400	-2.74987400
C	0.27633000	-0.95274100	1.84487700	H	7.82813500	-3.67862200	-0.77513700
O	1.13149100	0.06063400	1.90758200	C	2.93903700	-0.30507200	-2.09991700
C	0.72189400	-2.31803000	2.31276100	O	2.05107800	-1.03109800	-2.50182900
O	0.23466700	-3.37470100	1.94593400	O	3.59369100	0.54589400	-2.90840300
O	1.71828800	-2.23976600	3.21733200	C	3.14788100	0.57948400	-4.27257400
C	2.23749100	-3.49666300	3.66897100	H	3.26343200	-0.40134200	-4.74265600
H	2.98677800	-3.24973400	4.42183000	H	3.78033000	1.31826500	-4.76517100
H	1.44332000	-4.11095300	4.10173200	H	2.09731900	0.87751200	-4.32401500
H	2.69676700	-4.03578600	2.83566200	C	3.06610600	2.33888000	-0.53689000
<b>23-erythro-ts</b>				C	3.81980500	3.44869800	-0.05910300
Rh	-3.83296000	0.06727400	1.20456300	C	3.36199900	4.76981100	-0.13128000
Rh	-3.00020200	0.04548500	-1.08149700	C	2.12515500	4.99251300	-0.72416000
C	-3.08235800	2.66462400	0.14291100	C	1.37094100	3.91918200	-1.23823900
O	-3.39025600	2.08232400	1.23766800	C	1.82715700	2.60827100	-1.15291000
O	-2.97898000	2.10946000	-0.99791400	C	3.86478800	1.14417400	-0.29942200
C	-5.88441200	0.33734100	-0.79761000	C	5.03659200	1.59933000	0.26065800
O	-5.68665600	0.47577600	0.45250000	H	3.95663400	5.59404200	0.25269900
O	-4.97589400	0.07632900	-1.64715900	H	1.74194100	6.00644700	-0.80156600
C	-3.69016700	-2.56071000	0.04869900	H	0.41689400	4.11646500	-1.71999700
O	-4.19164300	-1.94586500	1.04651300	H	1.21652600	1.80991000	-1.56018600
O	-3.12138000	-2.01842400	-0.95442000	H	5.92323100	1.05457400	0.54209000
C	-7.30083800	0.46439900	-1.30260400	N	5.01840300	2.96858100	0.42532700
C	-3.75288500	-4.06931600	0.05798900	C	6.08413200	3.77060800	0.98787800
C	-2.78559400	4.14430300	0.21034700	H	6.44056000	4.51381300	0.26442600
H	-7.72109800	-0.53924200	-1.43610000	H	5.75006800	4.29497900	1.89148500
H	-7.91599400	1.00760400	-0.58281200	H	6.91782900	3.11725500	1.25404400
H	-7.31097100	0.96638200	-2.27310500	C	2.38968300	-0.98090000	0.29457400
H	-3.23871700	4.59076800	1.09753000	C	1.04275200	-0.24708300	0.33166100
H	-1.69824800	4.27828800	0.25998600	H	2.22355200	-1.96093200	-0.15422300
H	-3.14394000	4.64077900	-0.69484600	H	1.11152500	0.82906600	0.49392600
H	-4.13563100	-4.43461300	-0.89965600	C	2.88219800	-1.23087500	1.71806900
H	-2.73497400	-4.45578000	0.18231500	C	3.11635800	-0.18862000	2.62908100
H	-4.38003000	-4.42538500	0.87675500	C	3.06904300	-2.54822300	2.15930600

C	3.55407500	-0.45769200	3.92680700	H	-0.86184000	1.32043300	4.12399300
H	2.94807700	0.83988100	2.32779500	C	-2.93077800	-0.58249500	-0.06693100
C	3.49891600	-2.82156000	3.45874300	C	-3.94509300	0.12395100	-0.76884800
H	2.87493100	-3.36855200	1.47324200	C	-5.27330800	-0.31544400	-0.82052100
C	3.75235800	-1.77495600	4.34643900	C	-5.58796600	-1.49084300	-0.14776400
H	3.72985900	0.36524500	4.61543600	C	-4.60091900	-2.20863700	0.55681200
H	3.63643900	-3.85251100	3.77504200	C	-3.28366600	-1.76737100	0.60283300
H	4.08933100	-1.98305600	5.35882300	C	-1.69836800	0.16340100	-0.23335200
C	-0.06087300	-0.57527200	-0.48848000	C	-2.02378000	1.25211700	-1.00731200
O	-0.99588600	0.27358900	-0.68786800	H	-6.03258200	0.23949000	-1.36468600
C	-0.21111200	-1.96877300	-1.08846700	H	-6.60948500	-1.86116400	-0.16686300
O	0.05464700	-3.00187300	-0.51011300	H	-4.87598100	-3.12568300	1.07107000
O	-0.67718000	-1.88884300	-2.34220900	H	-2.53548700	-2.33788700	1.14334700
C	-0.82217800	-3.14094700	-3.02739000	H	-1.40617700	2.06856300	-1.34687100
H	-1.11915200	-2.88268000	-4.04396200	N	-3.36591900	1.24271300	-1.33514400
H	0.12747200	-3.68154600	-3.02730200	C	-4.05056500	2.23086700	-2.14088900
H	-1.59403500	-3.74404800	-2.54428500	H	-4.45902400	1.78352400	-3.05568400
O	-1.98130600	-0.47387800	1.88893800	H	-4.87325900	2.69232700	-1.58136200
C	-1.84219300	0.72794800	3.98736700	H	-3.34218200	3.01315200	-2.42212400
H	-2.31546700	1.65112900	3.63436700	C	0.84055800	0.65119400	-0.31391800
H	-2.61818000	0.10984700	4.45183900	C	2.21403500	0.10693200	0.00604300
H	-1.07130200	0.96813000	4.72102800	C	3.14977200	-0.09019200	-0.93625400
C	-1.24641400	0.00082000	2.80452800	C	4.52078000	-0.59230900	-0.66753400
O	0.01897500	-0.13162300	2.76015900	O	5.31185700	-0.77263700	-1.58449100
H	0.42551300	-0.40445300	1.61329200	O	4.79976900	-0.82274700	0.62167800
<b>24-erythro</b>				C	6.12201300	-1.31721400	0.88891300
C	-0.33524000	-0.20970500	0.33926500	H	6.17176500	-1.43973600	1.97087900
C	-0.02689900	-1.69457400	-0.02194900	H	6.28220500	-2.27400900	0.38482600
C	0.48435700	-2.63620700	0.88135800	H	6.87478100	-0.60221200	0.54646700
C	-0.24908200	-2.10439000	-1.34653100	C	0.86224400	2.16799600	-0.06830500
C	0.75184300	-3.94666900	0.47333900	C	0.92210400	2.75533200	1.20516400
H	0.69148700	-2.35410700	1.90606800	C	0.93228500	3.01716500	-1.18590300
C	0.03132100	-3.40587400	-1.75656300	C	1.00076400	4.14197000	1.35049700
H	-0.65950300	-1.39777100	-2.06110100	H	0.93713400	2.13453100	2.09312500
C	0.53033900	-4.33873200	-0.84509300	C	1.01630700	4.40243800	-1.04261700
H	1.14151300	-4.65836500	1.19687100	H	0.93596300	2.58025800	-2.18179600
H	-0.14961600	-3.69259700	-2.78924600	C	1.04147700	4.97357600	0.23066000
H	0.74174700	-5.35709300	-1.16036800	H	1.04084600	4.57177100	2.34828300
C	-0.31026600	-0.02926500	1.87374400	H	1.06789700	5.03299800	-1.92670400
O	0.67156400	-0.20334100	2.57561200	H	1.10492300	6.05200100	0.34875100
O	-1.49061600	0.35117900	2.38440200	H	0.68882100	0.51794400	-1.38809400
C	-1.53154900	0.51467800	3.81083600	H	2.46506500	-0.09361600	1.03880400
H	-1.23397400	-0.40953900	4.31266600	O	2.93509600	0.14933400	-2.26240600
H	-2.56697000	0.76469300	4.04200300	H	3.76570700	-0.11136700	-2.70969200

**25**

Cl	0.00159100	-0.82511700	-2.15955600
Cl	-0.00156600	-0.80233700	2.16660500
Cu	0.00011600	-0.23444000	0.00044800
C	5.72372900	1.99656600	-0.00799600
H	5.84161300	3.08537400	-0.01376600
H	6.22185400	1.59139400	-0.89429000
H	6.22087500	1.60086800	0.88310200
C	4.24823900	1.64934700	-0.00702700
H	3.73047500	2.02151000	-0.89545400
H	3.72956900	2.03045600	0.87705900
O	4.14790800	0.19460600	0.00033400
C	2.93630600	-0.33505800	0.00235800
C	2.91611900	-1.83233600	0.00992200
H	3.92664900	-2.24236100	0.01259100
H	2.36362600	-2.16547500	0.89549100
H	2.36459000	-2.17455700	-0.87274100
O	1.92843700	0.38223000	-0.00168600
C	-5.72369000	1.99671700	-0.00562200
H	-5.84149900	3.08554200	-0.00911000
H	-6.22020100	1.59928300	0.88506000
H	-6.22251300	1.59334500	-0.89233500
C	-4.24822800	1.64937700	-0.00634600
H	-3.72891300	2.02886900	0.87806100
H	-3.73105900	2.02317200	-0.89442400
O	-4.14799000	0.19464600	-0.00176400
C	-2.93636500	-0.33510000	-0.00047100
C	-2.91641100	-1.83240800	0.00531800
H	-3.92702100	-2.24228700	0.00583700
H	-2.36351600	-2.17378200	-0.87681200
H	-2.36559400	-2.16664900	0.89149600
O	-1.92846900	0.38203800	-0.00356100

**C<sub>2</sub>H<sub>5</sub>OOCH<sub>3</sub>**

C	2.56827000	-0.39990500	-0.00003200
H	3.45499800	0.24352900	0.00000400
H	2.60686700	-1.03981500	-0.88758300
H	2.60689400	-1.03995000	0.88742000
C	1.31296700	0.45301500	0.00005000
H	1.25418700	1.09812700	-0.88271200
H	1.25422700	1.09800200	0.88290800
O	0.17868200	-0.44254400	0.00001500
C	-1.03855200	0.14699100	-0.00003700
C	-2.13861800	-0.89045300	0.00000200
H	-2.05069200	-1.53399600	-0.88172100

H	-2.05114100	-1.53340500	0.88220600
H	-3.10829900	-0.39155700	-0.00038800
O	-1.20261300	1.34769100	-0.00001900

**26**

C	2.67096300	-0.85883600	0.80485400
C	2.37948200	-0.13398600	2.15103800
C	1.10126600	-0.10209500	2.72687200
C	3.44744900	0.41686900	2.87791000
C	0.89187900	0.49941600	3.97053900
H	0.25157500	-0.54093400	2.21843500
C	3.23951800	1.01154800	4.12173900
H	4.44786400	0.38172900	2.46058900
C	1.95759000	1.06155000	4.67242200
H	-0.11194400	0.52307500	4.38601600
H	4.08307100	1.43743600	4.65891700
H	1.79247400	1.52926300	5.63940200
C	3.04137900	-2.27871100	1.31053300
O	2.23214600	-3.16002200	1.50966400
O	4.34724900	-2.41170200	1.62053400
C	4.69862700	-3.65100700	2.25988400
H	5.77399700	-3.59376900	2.43170300
H	4.16226600	-3.75575800	3.20659300
H	4.45350100	-4.49986700	1.61652200
C	3.94519300	1.24618800	-0.22909100
C	5.06008500	1.38397600	-1.10572700
C	5.51843100	2.62565200	-1.56127500
C	4.84101100	3.76013200	-1.13008200
C	3.73585500	3.65448200	-0.26240800
C	3.28598600	2.41968500	0.19063100
C	3.78243700	-0.17347200	0.02774500
C	4.77786000	-0.79564500	-0.68984000
H	6.37377700	2.70223200	-2.22678000
H	5.17057900	4.74016400	-1.46408300
H	3.22935800	4.55808900	0.06618700
H	2.43801700	2.36528100	0.86419700
H	-2.02794000	0.12976600	1.02116300
H	5.00750700	-1.84743700	-0.76825600
N	5.54737300	0.11964300	-1.37394200
C	6.70146000	-0.18292600	-2.19505100
H	6.57399900	0.21604800	-3.20804800
H	7.61753200	0.24043900	-1.76506200
H	6.81524800	-1.26696600	-2.26166400
C	1.35882100	-1.03708600	-0.08630200
C	0.71798100	0.27693800	-0.43911600

H	0.65629300	-1.61139200	0.51606400	C	0.68068700	-3.61902000	-1.79829600
H	1.30921900	1.01486500	-0.96562700	H	0.09478100	-1.58167000	-1.63424000
C	1.59115100	-1.85279700	-1.36533100	C	3.01594900	-4.10742200	-1.46718100
C	1.19614200	-3.19860800	-1.40554000	H	4.27361600	-2.42741800	-1.00803100
C	2.14417700	-1.29029100	-2.52740000	C	1.71989600	-4.54645000	-1.74947200
C	1.36117200	-3.96245900	-2.56206200	H	-0.33579200	-3.92873800	-2.02253600
H	0.76767000	-3.64946100	-0.51661900	H	3.83928600	-4.81652500	-1.43425600
C	2.30562200	-2.05194000	-3.68614400	H	1.52570300	-5.59968800	-1.93505200
H	2.44722700	-0.24850600	-2.53731800	C	3.01440100	0.09409500	-2.47275300
C	1.91701200	-3.39234900	-3.70829200	O	2.26171100	0.48039400	-3.34122600
H	1.04716200	-5.00317000	-2.56681300	O	4.32613700	-0.12773300	-2.69578500
H	2.73026300	-1.59211200	-4.57508700	C	4.75231800	0.06466400	-4.05593300
H	2.03894600	-3.98376200	-4.61209200	H	5.82099800	-0.15262300	-4.05820800
C	-0.57290900	0.58056000	-0.20097700	H	4.21849700	-0.61823100	-4.72185300
O	-1.43470500	-0.31314600	0.36731000	H	4.56494400	1.09257200	-4.37663200
C	-1.15165100	1.86996900	-0.64466300	C	3.73809900	-0.76719600	1.30939600
O	-2.35880500	2.14705100	-0.63231200	C	4.83061000	-0.15403900	1.98963600
O	-0.26330400	2.76016800	-1.07032600	C	5.23881900	-0.53773800	3.27224200
C	-0.78357000	4.01490800	-1.56106300	C	4.53474100	-1.56227900	3.89390900
H	0.09275500	4.56668800	-1.89900600	C	3.45330400	-2.19009100	3.24479600
H	-1.48102700	3.83928800	-2.38277400	C	3.05315900	-1.80863800	1.96924100
H	-1.29441200	4.54873100	-0.75656600	C	3.62666400	-0.11575200	0.01653500
Cl	-3.65406900	1.15175300	2.01055500	C	4.63009800	0.82517000	-0.01069300
Cl	-4.97929300	1.69324000	-2.17156800	H	6.07767200	-0.05437600	3.76527300
Cu	-4.05380300	1.11251300	-0.23149200	H	4.82602100	-1.88566700	4.88951100
C	-7.37390400	-4.03745300	0.06513100	H	2.92667000	-2.99694300	3.74759100
H	-6.86885000	-4.97608600	-0.18634500	H	2.22913000	-2.32106200	1.48497700
H	-8.20713700	-3.89743800	-0.63052200	H	-2.11520000	-0.54380700	-0.94470100
H	-7.77647800	-4.12377300	1.07921800	H	4.89398600	1.51856700	-0.79494300
C	-6.38566800	-2.89252100	-0.03286200	N	5.35575400	0.81699800	1.15992800
H	-5.97945500	-2.77416600	-1.04101300	C	6.50022900	1.65290600	1.45849900
H	-5.54918300	-3.00033700	0.66313300	H	6.33051800	2.23471100	2.37201700
O	-7.10644700	-1.67095300	0.31145700	H	7.40762300	1.05096000	1.59042200
C	-6.43537500	-0.53373900	0.26603500	H	6.65825700	2.34685000	0.63034100
C	-7.24103300	0.67772300	0.62104800	C	1.26342000	0.56466400	-0.73961500
H	-8.27144400	0.41362800	0.86137800	C	0.53258800	0.12103300	0.49924600
H	-6.76636700	1.17367800	1.47487900	H	0.59922900	0.44761300	-1.59601300
H	-7.20893900	1.37059400	-0.22706600	H	1.10880900	-0.16525400	1.37191900
O	-5.23962400	-0.51306500	-0.04938500	C	1.54550400	2.07102300	-0.62805600
<b>27-ts</b>				C	1.24422200	2.91242600	-1.70911100
C	2.55618700	-0.31038700	-1.04559100	C	2.05041000	2.65166700	0.54737700
C	2.22071500	-1.81533400	-1.25012200	C	1.45872700	4.28932300	-1.62594800
C	0.93089500	-2.26449800	-1.56228700	H	0.84536100	2.48127200	-2.62086500
C	3.26324100	-2.75758300	-1.22412600	C	2.26153100	4.02878400	0.63196900

H	2.27485800	2.02930900	1.40777300	H	-0.05466800	0.11256300	4.76431300
C	1.96970400	4.85332200	-0.45612400	H	3.98741100	-1.33604200	4.51984900
H	1.21454600	4.92113500	-2.47582600	H	2.08028000	-0.49937500	5.89009200
H	2.64882200	4.45695900	1.55332700	C	1.20885500	-2.53214800	0.44173300
H	2.12935000	5.92639900	-0.38887000	O	0.06500600	-2.93051000	0.56083500
C	-0.80914200	0.12860200	0.63219600	O	2.25581200	-3.37465500	0.38262400
O	-1.68774800	0.46735500	-0.35951500	C	1.93427300	-4.76953100	0.52344900
C	-1.48405800	-0.16015700	1.90676600	H	2.88637200	-5.29494700	0.44417900
O	-2.70507400	0.06739200	2.03992400	H	1.47100800	-4.95619400	1.49575800
O	-0.75260400	-0.64373300	2.89378500	H	1.24902200	-5.08820300	-0.26599800
C	-1.41940800	-0.88019200	4.15267400	C	3.77199100	0.43720100	-0.05396700
H	-0.64307200	-1.26023600	4.81513000	C	4.79735000	0.35614000	-1.03962000
H	-1.83835700	0.05217200	4.53808300	C	5.81419700	1.31057600	-1.15701500
H	-2.21562300	-1.61625800	4.02254200	C	5.80116200	2.37781200	-0.26671400
Cl	-2.81811900	-1.79794600	-1.50585700	C	4.79907700	2.48483800	0.71756400
Cl	-4.06614200	2.59719100	-0.92422300	C	3.79461200	1.53146900	0.83440600
Cu	-3.48172100	0.92808500	0.36957100	C	2.91868000	-0.72235800	-0.23786800
C	-7.48638100	-2.82785100	-0.88169200	C	3.45560400	-1.41467300	-1.29872200
H	-7.03164700	-3.81593500	-1.00802700	H	6.58553100	1.22405100	-1.91730900
H	-7.71551100	-2.42852700	-1.87447200	H	6.57312100	3.13959300	-0.33207200
H	-8.42226700	-2.94515200	-0.32571500	H	4.81001200	3.33065900	1.39911900
C	-6.51521600	-1.92663600	-0.14731800	H	3.03911600	1.63476000	1.60519800
H	-5.57887700	-1.78182100	-0.69153600	H	3.11778400	-2.33132900	-1.75795800
H	-6.27968700	-2.29513300	0.85537600	N	4.57872900	-0.78490700	-1.78726000
O	-7.17257200	-0.62267700	0.00624900	C	5.40115000	-1.24179500	-2.88775300
C	-6.45950800	0.37320500	0.48598900	H	5.44009700	-0.49019800	-3.68501400
C	-7.18382900	1.68359500	0.53763900	H	6.42503300	-1.45295000	-2.55580800
H	-8.22798400	1.57323500	0.24307900	H	4.97027900	-2.15835600	-3.29634400
H	-7.11266700	2.09357900	1.54986700	C	0.39426400	-0.24385500	-0.17877500
H	-6.66483300	2.37871700	-0.13221000	C	0.37225400	1.22840900	0.11415500
O	-5.29317100	0.20788800	0.87385700	H	-0.50637700	-0.66893900	0.26202700
<b>HCl</b>				H	1.25350900	1.83876900	-0.04204900
Cl	0.00000000	0.00000000	0.07163400	C	0.27245600	-0.47342200	-1.69202900
H	0.00000000	0.00000000	-1.21777400	C	-0.61177700	-1.44804600	-2.17992500
<b>28</b>				C	0.98828800	0.29706600	-2.62308400
C	1.61393100	-1.03285300	0.47453900	C	-0.76851600	-1.65590400	-3.55239200
C	1.73308400	-0.80951100	2.00947700	H	-1.17133600	-2.05627400	-1.47613700
C	0.65900100	-0.36506900	2.79342000	C	0.82800600	0.09430300	-3.99418900
C	2.92474100	-1.16961300	2.65930400	H	1.67038500	1.06748600	-2.27870700
C	0.78785500	-0.24847300	4.18004900	C	-0.04963200	-0.88413400	-4.46557100
H	-0.28552300	-0.09974500	2.33614300	H	-1.46073700	-2.41627000	-3.90536600
C	3.05064700	-1.05893600	4.04337800	H	1.38562400	0.70999800	-4.69521300
H	3.76022400	-1.53302200	2.07073500	H	-0.17880600	-1.03590600	-5.53394200
C	1.98251900	-0.59190400	4.81168700	C	-0.76631100	1.85987600	0.54089200

O	-1.88336600	1.21743300	0.82229500	C	-3.36111700	-1.95874500	0.30139500
C	-0.70535400	3.35411400	0.75297800	C	-2.57162500	-3.15020900	0.19564600
O	0.28685000	4.03326900	0.57245300	C	-3.15199400	-4.40296600	-0.01887500
O	-1.88827600	3.84891300	1.16240500	C	-4.54044300	-4.46478300	-0.10695300
C	-1.92957900	5.27447700	1.32621700	C	-5.33984300	-3.30575400	0.00516200
H	-2.95058000	5.50263000	1.63204800	C	-4.76810700	-2.05884000	0.19984800
H	-1.21525700	5.59311100	2.09055800	C	-2.45997700	-0.88260000	0.49228600
H	-1.69016500	5.77294600	0.38337400	C	-1.12941000	-1.43731400	0.47660700
Cl	-3.94581500	2.58113100	-1.99739900	H	-2.54486800	-5.29750100	-0.11383500
Cu	-3.29321300	1.28758800	-0.41191400	H	-5.01924200	-5.42702400	-0.26521000
C	-6.92090900	-3.60229900	0.03332000	H	-6.42006400	-3.39801000	-0.06137400
H	-7.72785900	-3.60663800	-0.70704100	H	-5.38654300	-1.17303000	0.30009300
H	-7.36865600	-3.64544000	1.03108900	H	-0.30120100	-1.08554900	1.08833800
H	-6.31269300	-4.50015200	-0.11445800	N	-1.24209100	-2.81573700	0.34154300
C	-6.08847800	-2.34701600	-0.13640700	C	-0.12684400	-3.75210400	0.33857900
H	-6.67096900	-1.43480100	0.01963400	H	0.11495300	-4.06320100	-0.68417400
H	-5.62061500	-2.28569500	-1.12292400	H	0.75390100	-3.28285000	0.78605700
O	-5.03201400	-2.39092900	0.86820500	H	-0.38337300	-4.63436300	0.93295000
C	-4.16657100	-1.38751900	0.89259200	C	-1.14828700	0.99372100	-0.28769500
C	-3.09514700	-1.54976600	1.92852300	C	-0.60580700	-0.22483400	-1.02905000
H	-3.45281200	-2.16785300	2.75442800	H	-0.54787800	1.08903700	0.62266100
H	-2.22806300	-2.04724500	1.47432200	H	-1.18467700	-0.59825600	-1.86623800
H	-2.77022800	-0.56777700	2.27354900	C	-0.97132200	2.30863200	-1.03620300
O	-4.26887400	-0.44388000	0.10244800	C	-0.43050300	3.40946600	-0.35252900
<b>29-ts</b>				C	-1.27754000	2.45919100	-2.39897300
C	-2.60818800	0.61326900	0.25780000	C	-0.22326900	4.62948900	-0.99721200
C	-2.94020000	1.42285900	1.51843100	H	-0.16610100	3.30595800	0.69640600
C	-3.21564300	2.79794400	1.44152700	C	-1.06749200	3.67836500	-3.04519300
C	-2.91562200	0.82282700	2.78339300	H	-1.68645100	1.62343700	-2.95386500
C	-3.45463100	3.54437500	2.59429800	C	-0.54389600	4.76908500	-2.34831600
H	-3.25170400	3.29022600	0.47599100	H	0.19658400	5.46596500	-0.44455600
C	-3.15650800	1.56892900	3.93965400	H	-1.31039700	3.77226300	-4.10057100
H	-2.71128200	-0.24028900	2.86804300	H	-0.37942500	5.71607200	-2.85580900
C	-3.42550900	2.93378400	3.85038400	C	0.81177300	-0.40061300	-1.11995200
H	-3.66722400	4.60689800	2.50888700	O	1.61249100	0.12221100	-0.29197800
H	-3.13399200	1.07723000	4.90860900	C	1.30763500	-1.36936900	-2.17438100
H	-3.61373800	3.51664500	4.74806100	O	0.57690500	-2.04333700	-2.87687100
C	-3.65491700	0.76502600	-0.87079100	O	2.64988000	-1.40224500	-2.23364300
O	-3.46933600	0.41377800	-2.01744200	C	3.20354200	-2.33666800	-3.17449200
O	-4.82954800	1.26970400	-0.44913100	H	2.86510600	-2.10282200	-4.18739200
C	-5.84605600	1.38638200	-1.46221100	H	4.28436200	-2.22666300	-3.09094800
H	-6.70961400	1.81749900	-0.95558700	H	2.90099800	-3.35569800	-2.92004800
H	-5.50451300	2.03822800	-2.26988500	Cl	3.28196200	-2.64980600	1.75865000
H	-6.08657100	0.40316900	-1.87468000	Cu	3.09583400	-0.78393500	0.64102200

C	7.30575000	1.18042700	-1.29992200	H	6.64471000	-2.96797600	-1.11901800
H	7.40324600	1.73440400	-2.24053200	H	5.40461000	-0.81033700	-1.11026500
H	6.60370700	0.35694300	-1.45816000	H	0.46415400	-1.24790000	-1.29627000
H	8.28594500	0.76768600	-1.04008600	N	1.47548000	-2.78677700	-0.28241900
C	6.80425700	2.11336500	-0.20850100	C	0.47837500	-3.84308000	-0.25629500
H	5.80926300	2.50109000	-0.43740000	H	0.48245500	-4.36748500	0.70671000
H	7.49224600	2.94533600	-0.04255900	H	-0.51969000	-3.42547400	-0.40785500
O	6.75788900	1.43799500	1.07815700	H	0.66320300	-4.57176000	-1.05611900
C	5.65932000	0.73569800	1.37121100	C	1.03279700	0.89129300	0.28408700
C	5.71978700	0.09253900	2.72836000	C	0.58520300	-0.52744100	0.73817700
H	5.36066700	-0.93925000	2.65599900	H	0.48493700	1.08361200	-0.64537600
H	6.72857700	0.13245500	3.14215900	H	1.06728400	-0.83598900	1.66453800
H	5.03396800	0.62431900	3.39841300	C	0.68868200	2.03736100	1.22089000
O	4.70591200	0.65779300	0.60000600	C	0.19873900	3.23298700	0.67001200
<b>30</b>				C	0.79191900	1.94766500	2.61870000
C	2.54293900	0.71025200	-0.20375200	C	-0.15796000	4.31160000	1.48057600
C	2.89760200	1.74605300	-1.27534800	H	0.09824500	3.31674100	-0.40896000
C	3.17276100	3.07721200	-0.92546100	C	0.42748800	3.02277100	3.43110600
C	2.89087900	1.40225200	-2.63227900	H	1.17569600	1.04233900	3.07304300
C	3.43411300	4.03364100	-1.90583300	C	-0.04483200	4.20974500	2.86783700
H	3.18807500	3.36876200	0.12005800	H	-0.52955300	5.22715900	1.02713000
C	3.15287100	2.35859600	-3.61607600	H	0.51537400	2.92974200	4.51055000
H	2.68686500	0.37416500	-2.91744500	H	-0.32593200	5.04482900	3.50434300
C	3.42529400	3.67850900	-3.25694800	C	-0.90895000	0.64505500	0.83794300
H	3.64883700	5.05798600	-1.61221200	O	-1.66289800	-0.23253800	-0.03507900
H	3.14777300	2.06678700	-4.66314600	C	-1.46036400	-1.42444700	2.04003500
H	3.63337700	4.42343700	-4.02049400	O	-0.77086100	-2.17276200	2.70089600
C	3.52416600	0.71153500	0.98712400	O	-2.76088900	-1.18939900	2.23464900
O	3.25169100	0.34209800	2.11126200	C	-3.40087800	-2.02324100	3.22231000
O	4.76986100	1.07426700	0.62339000	H	-2.84051400	-2.00043000	4.15954700
C	5.77151500	0.94578900	1.64843500	H	-4.39871100	-1.60525000	3.35160900
H	6.69718700	1.29983600	1.19405200	H	-3.45928000	-3.04567600	2.84162400
H	5.50998300	1.55387000	2.51781200	Cl	-3.35243800	-3.46616800	-0.45408500
H	5.86577000	-0.09900900	1.95503300	Cu	-3.74178300	-1.36485800	-0.58519500
C	3.48900500	-1.75003900	-0.73026800	C	-5.84697000	3.05228000	0.43460500
C	2.81508000	-3.00206700	-0.50335900	H	-5.41201500	3.84591700	1.05218200
C	3.51387600	-4.21077900	-0.50813300	H	-5.73524400	2.10562700	0.97051700
C	4.89366000	-4.17261200	-0.73504100	H	-6.91230300	3.26555000	0.30046600
C	5.57245100	-2.95764800	-0.94432900	C	-5.12889200	3.00797300	-0.90409500
C	4.88669600	-1.74792800	-0.93858500	H	-4.07408600	2.75058200	-0.79068500
C	2.50852200	-0.73690400	-0.67322600	H	-5.22206100	3.95127400	-1.44551300
C	1.16942800	-1.38232400	-0.45491700	O	-5.75005200	2.03845700	-1.80344300
H	3.00602700	-5.15277200	-0.32741200	C	-5.37070000	0.77190800	-1.71435000
H	5.45274200	-5.10444000	-0.74585800	C	-6.05278800	-0.13354500	-2.70025000

H -6.45960900 -1.00126100 -2.17189300  
H -6.84219800 0.39005000 -3.24112100  
H -5.30743400 -0.51049300 -3.40945000  
O -4.52363400 0.40328800 -0.89578300  
**31**  
C 0.78977400 0.76810600 0.16105300  
C 1.41974800 1.84652600 -0.71680800  
C 1.28894300 3.20427900 -0.38866200  
C 2.06514100 1.50861300 -1.91314900  
C 1.79791100 4.19470600 -1.22808800  
H 0.78654800 3.49207300 0.53033900  
C 2.57623900 2.49909900 -2.75470800  
H 2.16968900 0.46307200 -2.18602900  
C 2.44577000 3.84596600 -2.41527600  
H 1.68750600 5.24047800 -0.95311000  
H 3.07841100 2.21368000 -3.67547000  
H 2.84541600 4.61753800 -3.06806800  
C 0.99346600 1.01101700 1.66629600  
O 0.20763500 0.70517700 2.54054700  
O 2.22399200 1.49756800 1.92677000  
C 2.56494300 1.60230900 3.31868700  
H 3.57550100 2.01103600 3.34019400  
H 1.86898100 2.26770400 3.83623300  
H 2.53696400 0.61813200 3.79400600  
C 2.51484700 -1.40019000 -0.01578500  
C 2.12133600 -2.77489800 -0.02020900  
C 3.06017700 -3.81125900 -0.04094000  
C 4.40805000 -3.46358400 -0.03275100  
C 4.81457900 -2.11478000 -0.00943700  
C 3.88351400 -1.08247600 -0.00157800  
C 1.28992400 -0.65164400 -0.03100600  
C 0.25998400 -1.55139000 -0.00932000  
H 2.75441100 -4.85337300 -0.06237400  
H 5.15934400 -4.24846300 -0.04508800  
H 5.87552400 -1.87990200 0.00015300  
H 4.20162900 -0.04451700 0.01599300  
N 0.73005100 -2.84443300 0.00578700  
C -0.05217900 -4.06690400 -0.00229500  
H -1.05671900 -3.85633000 0.37039300  
H -0.12120200 -4.49820500 -1.00911100  
H 0.40937800 -4.80198000 0.66402700  
C -0.74569200 0.56145700 -0.23434900  
C -1.10330600 -0.92984200 0.11307500  
H -0.70588300 0.57461500 -1.32808600

H -1.48963100 -1.03726800 1.13034600  
C -1.76741000 1.60613400 0.17864300  
C -2.12571600 2.59259800 -0.75490000  
C -2.40432000 1.61898700 1.43031500  
C -3.07614400 3.56800900 -0.45027400  
H -1.65457700 2.59220400 -1.73434000  
C -3.36045600 2.58953200 1.73379500  
H -2.13542400 0.88337400 2.17846500  
C -3.69937600 3.56893000 0.79810900  
H -3.33341300 4.31953000 -1.19215400  
H -3.84063800 2.57916800 2.70903400  
H -4.44487300 4.32246700 1.03872200  
C -2.14211700 -1.45303500 -0.88033000  
O -2.03141500 -1.36128500 -2.08307800  
C -3.36032000 -2.17440400 -0.26820000  
O -3.30371500 -2.76361500 0.79390500  
O -4.43389200 -2.10147300 -1.05311400  
C -5.60590000 -2.78443300 -0.56769700  
H -5.89917600 -2.38850900 0.40792100  
H -6.37924200 -2.59550500 -1.31138600  
H -5.40818300 -3.85553900 -0.47663400  
**O<sub>2</sub>**  
O 0.00000000 0.00000000 0.60780600  
O 0.00000000 0.00000000 -0.60780600  
**H<sub>2</sub>O<sub>2</sub>**  
O -0.72030100 -0.14031200 -0.00002800  
H -1.03818800 0.77879800 0.00016900  
O 0.72030100 0.14031300 -0.00003600  
H 1.03818600 -0.77879800 0.00034500  
**32-Triplet**  
C -2.99904000 -0.32334600 -0.94231200  
C -3.89357500 0.86951900 -0.49849700  
C -3.35960400 2.11304700 -0.13007000  
C -5.29021300 0.74294800 -0.57300100  
C -4.20076400 3.18226000 0.18921800  
H -2.28828300 2.26622100 -0.08210500  
C -6.12799400 1.81211500 -0.25875900  
H -5.72118800 -0.20482500 -0.87669200  
C -5.58643500 3.03873700 0.12986400  
H -3.76270500 4.13262400 0.48430300  
H -7.20575700 1.68322400 -0.31706700  
H -6.23731000 3.87264200 0.37977900  
C -2.93498600 -0.08346200 -2.47591000  
O -2.11213200 0.62384300 -3.01885900



O	-3.95785400	-0.64805700	-3.15067900	H	0.80036700	2.81833300	5.38339800
C	-4.02719200	-0.31044200	-4.54648300	H	-0.79103500	2.01395900	5.59733600
H	-4.89497800	-0.84713400	-4.93162100	H	0.68630200	1.03004800	5.48771100
H	-4.15454500	0.76802000	-4.67193000	Cl	2.97454100	1.61726700	-1.65323400
H	-3.11704000	-0.62317200	-5.06459300	Cu	1.53875300	1.90210400	0.15883700
C	-4.18826300	-2.03890900	0.71992000	C	0.21756900	7.71225700	-1.47908000
C	-4.51837900	-3.42207600	0.63071200	H	0.09805700	7.89609900	-2.55206600
C	-5.11027400	-4.13028000	1.68291200	H	0.96429500	8.41212100	-1.09082400
C	-5.37241100	-3.43642500	2.85850300	H	-0.73871600	7.91482900	-0.98654900
C	-5.05320800	-2.06941800	2.97655500	C	0.65027000	6.27621300	-1.25892700
C	-4.47112400	-1.36870900	1.92696200	H	1.61030300	6.05216500	-1.73232600
C	-3.61304000	-1.65869200	-0.55747700	H	-0.08577700	5.55655600	-1.62794500
C	-3.62073200	-2.80209800	-1.32238100	O	0.79504900	6.08417000	0.17896700
H	-5.35573800	-5.18435100	1.58673200	C	1.16319200	4.87975200	0.59663200
H	-5.82838300	-3.95597300	3.69690900	C	1.28793000	4.76633000	2.08759400
H	-5.26461700	-1.55170000	3.90793000	H	0.96949000	5.68543200	2.58176000
H	-4.23748600	-0.31631600	2.04237400	H	0.69616300	3.91039000	2.42768700
H	-3.28060400	-2.94832400	-2.33634000	H	2.33583400	4.56184100	2.33669400
N	-4.15564300	-3.86448200	-0.62689800	O	1.38953200	3.96656700	-0.20038000
C	-4.35365200	-5.20389500	-1.13880000	Cl	5.02235500	-0.87766400	-2.55853100
H	-3.85435600	-5.94274400	-0.50102800	Cl	2.72198500	0.20621500	1.24443300
H	-5.42016500	-5.45534100	-1.19497300	Cu	3.83089900	-0.33709100	-0.75413700
H	-3.92661500	-5.26769800	-2.14196700	C	5.34748400	-5.72437600	1.78803000
C	-1.49848200	-0.19065300	-0.41778000	H	4.54325900	-6.46146400	1.88478300
C	-1.38576000	-0.05059800	1.07282300	H	5.78407900	-5.55985100	2.77811200
H	-1.11003200	0.72040400	-0.87389900	H	6.11842500	-6.13955500	1.13141000
H	-1.84523300	-0.79176500	1.71576700	C	4.78458900	-4.43684600	1.21984400
C	-0.58473300	-1.32890900	-0.89399800	H	4.02034600	-3.99322600	1.86389900
C	0.29266900	-1.11098300	-1.96730100	H	4.35510400	-4.56956700	0.22337300
C	-0.55052900	-2.57855900	-0.25272300	O	5.89239000	-3.49253700	1.11462200
C	1.17556400	-2.10802200	-2.39254900	C	5.63224500	-2.30293600	0.59803300
H	0.28168100	-0.15387900	-2.47817200	C	6.82581200	-1.39932300	0.51086500
C	0.32465700	-3.57848100	-0.68003900	H	7.72088000	-1.88692200	0.89878800
H	-1.20392600	-2.77362600	0.59107800	H	6.96218100	-1.11677900	-0.53853700
C	1.19157700	-3.34837800	-1.75057000	H	6.62429200	-0.48397800	1.07805100
H	1.85455600	-1.90931400	-3.21695900	O	4.49079200	-2.00234600	0.23440500
H	0.33092900	-4.53795300	-0.16797900	<b>MECP<sub>32-33</sub></b>			
H	1.87730100	-4.12452100	-2.08112300	C	-3.46831700	0.06434400	-1.01655900
C	-0.68387000	0.94536400	1.68928700	C	-3.65039600	1.58529900	-1.29089400
O	-0.11196200	1.96405100	1.07159600	C	-2.57045100	2.46857200	-1.41331800
C	-0.62611900	0.90743300	3.19545900	C	-4.94228900	2.07875200	-1.52733000
O	-1.15304500	0.06473300	3.89519600	C	-2.77968300	3.81774900	-1.72240500
O	0.09118600	1.93869200	3.70593000	H	-1.54964100	2.13130900	-1.27611400
C	0.19809200	1.94304300	5.13628700	C	-5.15259000	3.42093300	-1.84237400

H	-5.78889500	1.40513500	-1.45735500	H	-1.00904600	-5.53735600	0.46947700
C	-4.07085900	4.30054600	-1.93486400	C	-0.65862200	1.12231500	1.26220300
H	-1.92488400	4.48424500	-1.80057600	O	0.21310500	1.53160500	0.36557000
H	-6.16381200	3.77879700	-2.01141500	C	-0.53406500	1.62329400	2.67507100
H	-4.23282200	5.34805800	-2.17340100	O	-1.35908900	1.41572000	3.54061700
C	-3.39676400	-0.51053000	-2.45903900	O	0.57985100	2.36295200	2.85821600
O	-2.36299600	-0.63701800	-3.08338800	C	0.69471100	2.96624500	4.16041200
O	-4.60356600	-0.75933000	-2.99481600	H	1.63911000	3.51085900	4.14472300
C	-4.59138100	-1.14459400	-4.38204000	H	-0.14145300	3.65040400	4.33115900
H	-5.63438600	-1.33209100	-4.63986000	H	0.69676300	2.20414600	4.94417900
H	-4.18116700	-0.33872800	-4.99608700	Cl	2.44434100	-0.18291800	-2.22969200
H	-3.98800900	-2.04445100	-4.52538100	Cu	1.50718600	0.66120900	-0.48289100
C	-5.17941700	0.06476600	1.02469700	C	4.96251700	5.64985000	-1.63243300
C	-6.12765300	-0.88416400	1.50775200	H	4.83533200	6.10749800	-2.61863300
C	-6.88788700	-0.67361100	2.66761500	H	6.01512200	5.37573100	-1.51040800
C	-6.68927100	0.511129700	3.36050500	H	4.70415300	6.39198600	-0.87042900
C	-5.75681800	1.46855100	2.90518400	C	4.06794600	4.43208000	-1.51989700
C	-5.00995000	1.25952800	1.75263900	H	4.30577800	3.66418700	-2.26199700
C	-4.60943700	-0.49440200	-0.18997800	H	3.00840800	4.68200100	-1.61599500
C	-5.22618400	-1.70742900	-0.36739800	O	4.28465700	3.85998000	-0.19776300
H	-7.60736800	-1.41358600	3.01069900	C	3.50642500	2.84403500	0.15278100
H	-7.26016200	0.70598700	4.26446500	C	3.83769200	2.26730900	1.49579000
H	-5.62446500	2.38856900	3.46647700	H	4.51536900	2.92846200	2.04141000
H	-4.31418500	2.02072600	1.41737400	H	2.91569100	2.10935600	2.05962200
H	-5.08736500	-2.43783400	-1.14988700	H	4.32564200	1.29725000	1.34110800
N	-6.13352600	-1.95865700	0.64207600	O	2.61588000	2.44646800	-0.60580200
C	-6.98124700	-3.12712400	0.75526400	Cl	4.30681800	-4.09890200	-0.48149800
H	-6.82724700	-3.62868600	1.71838600	Cl	1.64092200	-1.05329400	0.83200400
H	-8.04202000	-2.86076300	0.66496300	Cu	3.07292400	-2.44338300	0.01086200
H	-6.72728800	-3.82810300	-0.04387200	C	8.91684800	-1.08317100	2.14151000
C	-2.04323400	-0.26580400	-0.38108700	H	8.99186900	-1.01809700	3.23234400
C	-1.77184600	0.38388600	0.93035000	H	9.54639900	-0.30077100	1.70484600
H	-1.29378200	0.05428700	-1.10594100	H	9.30661600	-2.05590700	1.82612200
H	-2.49802300	0.27049900	1.72995500	C	7.47055300	-0.91507300	1.71331400
C	-1.79036900	-1.76823000	-0.13676600	H	7.07338600	0.06563500	1.99167100
C	-0.89096200	-2.45522600	-0.96703100	H	6.82167100	-1.67938000	2.15289300
C	-2.39403100	-2.46013200	0.92895000	O	7.42614600	-1.05278800	0.27556400
C	-0.61876200	-3.80658600	-0.75574800	C	6.25737200	-0.76303300	-0.32560600
H	-0.40414200	-1.93004300	-1.78430700	C	6.28154900	-1.08336600	-1.79393400
C	-2.11678500	-3.81228600	1.13815700	H	7.28460300	-0.97417900	-2.21498500
H	-3.08636600	-1.95610200	1.59230400	H	5.96176700	-2.12650400	-1.90549900
C	-1.23084300	-4.48917100	0.29845700	H	5.56292800	-0.45108400	-2.31710400
H	0.08774600	-4.31923000	-1.40093700	O	5.29287600	-0.32158300	0.27686900
H	-2.59361700	-4.33217800	1.96425900				

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C	-3.48482900	-0.00170000	-1.02568100	C	-0.64584900	-3.83811000	-0.51063900
C	-3.66632400	1.49497100	-1.40643100	H	-0.43562000	-2.02311000	-1.64131400
C	-2.58188500	2.36845800	-1.57207000	C	-2.14574000	-3.74309300	1.37840300
C	-4.95417500	1.97140500	-1.70155700	H	-3.09992400	-1.85819400	1.73993500
C	-2.78717200	3.68877200	-1.98220700	C	-1.25822500	-4.46418200	0.57900800
H	-1.56656400	2.04139000	-1.38600900	H	0.05916800	-4.38407500	-1.13096100
C	-5.15679400	3.28703400	-2.11523000	H	-2.61403200	-4.21529000	2.23820900
H	-5.80324200	1.30410300	-1.60085800	H	-1.03175400	-5.50164500	0.80968900
C	-4.07238800	4.15588200	-2.25280700	C	-0.71822500	1.28558100	1.14174800
H	-1.93018500	4.34789900	-2.09379200	O	0.19387000	1.55799600	0.26570700
H	-6.16518000	3.63185900	-2.32870100	C	-0.63566700	1.93736900	2.50772800
H	-4.22834400	5.18295700	-2.57200000	O	-1.49314500	1.83696900	3.36297400
C	-3.40096000	-0.67032700	-2.42568700	O	0.49529800	2.65151900	2.66773000
O	-2.37034000	-0.80842900	-3.04803500	C	0.62526400	3.29004800	3.94912000
O	-4.60776800	-0.98775800	-2.93705900	H	1.57570100	3.82312300	3.91494800
C	-4.58829200	-1.45106300	-4.29998500	H	-0.20103600	3.98613900	4.11505500
H	-5.62932500	-1.65790000	-4.54994200	H	0.62911900	2.54462200	4.74867200
H	-4.17932000	-0.67944300	-4.95709900	Cl	2.42068300	-0.85306700	-2.00902100
H	-3.98017500	-2.35446800	-4.39056600	Cu	1.59066400	0.44158700	-0.36766100
C	-5.21202700	0.13747900	0.98870400	C	4.96012600	5.53640500	-1.99197100
C	-6.16430600	-0.77177600	1.53166000	H	4.83374000	5.91455200	-3.01211000
C	-6.92652700	-0.48089000	2.66665800	H	6.01527600	5.28370600	-1.84694100
C	-6.72387400	0.75249200	3.27888800	H	4.69581300	6.33616700	-1.29280100
C	-5.78780300	1.66997600	2.76577600	C	4.07670600	4.32080200	-1.78747000
C	-5.03848000	1.38011900	1.63064400	H	4.32939700	3.50355000	-2.46930800
C	-4.62993400	-0.50436100	-0.17272800	H	3.01532000	4.55180100	-1.91811100
C	-5.24369400	-1.73708900	-0.26402900	O	4.28169100	3.86189100	-0.42363400
H	-7.64874800	-1.19025800	3.06062200	C	3.59619100	2.78462700	-0.03862400
H	-7.29687600	1.00949100	4.16535500	C	3.87155700	2.37622100	1.38025600
H	-5.64848500	2.62433100	3.26517700	H	4.56139000	3.06872300	1.86575400
H	-4.33280500	2.10780700	1.24591200	H	2.92147300	2.33888300	1.92222000
H	-5.09434900	-2.52034700	-0.99132500	H	4.28938500	1.36349900	1.37949600
N	-6.16079300	-1.91008700	0.74400100	O	2.82651800	2.20241100	-0.79838500
C	-7.00216500	-3.07362200	0.94017800	Cl	4.10255600	-3.95799500	-0.62556900
H	-6.84364600	-3.50388900	1.93562400	Cl	1.89754300	-0.95102700	1.42711600
H	-8.06288400	-2.81672600	0.83348100	Cu	3.19855900	-2.03668700	-0.09392800
H	-6.74663800	-3.82646400	0.19180400	C	8.87980100	-0.91464900	2.25337200
C	-2.06942900	-0.28660600	-0.33805700	H	8.93682500	-0.80198000	3.34153900
C	-1.82449400	0.47935100	0.91448600	H	9.50898400	-0.14590200	1.79310200
H	-1.31844700	-0.00743700	-1.07678900	H	9.28261700	-1.89680500	1.98695100
H	-2.52301200	0.39078900	1.73817900	C	7.43803300	-0.78223900	1.79995400
C	-1.82422100	-1.76882000	-0.01001400	H	7.01678100	0.19661500	2.05149400
C	-0.92082700	-2.50113000	-0.79712200	H	6.79339200	-1.54911900	2.23899800
C	-2.42347200	-2.40501600	1.09262200	O	7.42335500	-0.93624800	0.35876900

C 6.22516400 -0.94832900 -0.23792600  
C 6.31590000 -1.22894300 -1.71122800  
H 7.31871900 -1.03260400 -2.09530100  
H 6.06484000 -2.28603900 -1.86205500  
H 5.56553400 -0.63921000 -2.24262700  
O 5.18128500 -0.77177000 0.38131300

**34**

Cu -1.47745900 -0.25892100 0.00007500  
Cl -3.57212900 -0.24008000 -0.00014400  
C 4.53400100 -0.81051600 -0.00030700  
H 4.93439300 -1.82968300 -0.00019500  
H 4.90866700 -0.29341600 0.88835400  
H 4.90810200 -0.29382900 -0.88944600  
C 3.01994100 -0.86731400 0.00018600  
H 2.61848300 -1.36592100 0.88656600  
H 2.61791000 -1.36625000 -0.88574400  
O 2.53589700 0.51242500 0.00011500  
C 1.23178000 0.70754700 0.00005300  
C 0.82547800 2.15269000 -0.00005900  
H 0.20626700 2.35138800 0.88113700  
H 1.69628300 2.80931200 -0.00024000  
H 0.20602100 2.35120300 -0.88113000  
O 0.44025100 -0.24582400 0.00010100

**35**

C 2.36193300 -0.53789800 0.93683100  
C 2.26089500 0.51301000 2.08049700  
C 1.03308600 0.87445600 2.65521700  
C 3.43796600 1.03383100 2.64306800  
C 0.98599600 1.76517100 3.73107700  
H 0.09661700 0.47657600 2.28441600  
C 3.38864900 1.91922500 3.71862900  
H 4.39881800 0.74467200 2.23217300

C 2.15970400 2.29475600 4.26521700  
H 0.01999100 2.03321500 4.14994300  
H 4.31440300 2.31474100 4.12870900  
H 2.11943200 2.98693700 5.10222300  
C 2.44303000 -1.86458600 1.73862500  
O 1.48404100 -2.54246700 2.03751900  
O 3.69140700 -2.13958700 2.17040000  
C 3.79074900 -3.25379100 3.07467200  
H 4.84951200 -3.33060700 3.32421500  
H 3.19545900 -3.06853000 3.97242100  
H 3.43744000 -4.17120700 2.59687700  
C 3.99113400 0.95169500 -0.54840500  
C 5.08947700 0.65042200 -1.40339700  
C 5.76235600 1.62722700 -2.14396700  
C 5.31891100 2.94089800 -2.02893600  
C 4.23626200 3.26824100 -1.19058900  
C 3.57590700 2.29481800 -0.44901600  
C 3.56329700 -0.29928900 0.04660100  
C 4.40416400 -1.26291100 -0.46878400  
H 6.59975800 1.37272500 -2.78750800  
H 5.81697500 3.72460300 -2.59280500  
H 3.91192600 4.30232600 -1.11886200  
H 2.75683900 2.57306200 0.20479300  
H 4.42439400 -2.32481400 -0.27582600  
N 5.31954000 -0.71228700 -1.33434600  
C 6.37060400 -1.42591200 -2.03075800  
H 6.28084200 -1.29115800 -3.11485500  
H 7.36114300 -1.07697700 -1.71495700  
H 6.28644700 -2.49089600 -1.80482200  
C 1.01051200 -0.62950800 0.08445800

C	0.63015000	0.63443900	-0.60245800	H	-7.43366900	0.88400400	0.93712000
H	0.22111800	-0.89516200	0.78609600	H	-7.39410100	1.02954300	-0.82920700
H	1.31572300	1.09013100	-1.30765800	O	-7.14486200	-0.89654300	-0.09258900
C	1.02318100	-1.72491300	-0.99521100	C	-5.82449100	-0.95787800	-0.05642800
C	0.27249400	-2.89286000	-0.78462300	C	-5.26489200	-2.34344100	-0.14298600
C	1.71102500	-1.58118200	-2.21279300	H	-4.69616100	-2.53793500	0.77325500
C	0.23662900	-3.90054400	-1.74721400	H	-6.05666500	-3.08315700	-0.26640500
H	-0.26290400	-3.01586700	0.15070900	H	-4.56460900	-2.38386400	-0.98417500
C	1.66758500	-2.58890700	-3.17867200	O	-5.14501400	0.07101700	0.04408500
H	2.27464700	-0.67878400	-2.42083900	Cl	-3.23613800	-0.48518300	2.32653600
C	0.93391600	-3.75255100	-2.94930300	<b>36-ts</b>			
H	-0.34101200	-4.80169000	-1.55857300	C	2.18129800	-0.12999900	1.03677400
H	2.20065100	-2.45478600	-4.11634000	C	2.19428600	1.32995300	1.57293200
H	0.89629100	-4.53395800	-3.70379600	C	1.11128300	1.82104900	2.32144000
C	-0.58715000	1.27491700	-0.43956100	C	3.33653600	2.13561800	1.45553600
O	-1.43032300	0.93455200	0.48306200	C	1.14809800	3.09898300	2.87999800
C	-0.85783200	2.48698600	-1.30402500	H	0.22479500	1.21764200	2.47392400
O	-0.10612800	2.87559300	-2.17609200	C	3.37314800	3.41336000	2.01660400
O	-2.00650800	3.09249200	-0.96760800	H	4.20591700	1.76429300	0.92777800
C	-2.36587500	4.21594900	-1.78645300	C	2.27680300	3.90468600	2.72530100
H	-1.58811300	4.98306800	-1.74718000	H	0.28751400	3.45652400	3.43810400
H	-2.50509800	3.89632300	-2.82261400	H	4.26771100	4.01987300	1.90123900
H	-3.30078600	4.59138800	-1.37061800	H	2.30486500	4.90012800	3.16053800
Cl	-2.93428100	-0.04777800	-2.01609700	C	2.21240300	-0.93165900	2.36907500
Cu	-3.14453400	0.18224400	0.18502000	O	1.23529700	-1.35858100	2.94533500
C	-9.26298700	0.21744700	-0.04919800	O	3.45187000	-0.99704100	2.89318400
H	-9.76515000	1.18839200	0.01832200	C	3.52485500	-1.54797500	4.22084600
H	-9.60318900	-0.40504300	0.78417400	H	4.58169800	-1.51860700	4.48729300
H	-9.56245600	-0.26076200	-0.98703500	H	2.93506200	-0.94342700	4.91446000
C	-7.76198700	0.42173300	0.00217700	H	3.14926700	-2.57434600	4.23434100

C	3.75784700	0.21379500	-1.08899200	H	-0.46459100	-5.03167500	0.80459900
C	4.78760300	-0.57864100	-1.67297700	H	1.74137500	-3.98720000	-2.73763400
C	5.43166200	-0.22927200	-2.86359000	H	0.59407600	-5.70597400	-1.34767100
C	5.02362200	0.94056400	-3.49710700	C	-0.47608200	1.55833100	-0.50132300
C	4.00534300	1.74098000	-2.94712500	O	-1.24976400	1.62676800	0.48232400
C	3.38009700	1.39805500	-1.75251500	C	-0.50857300	2.61292000	-1.59468000
C	3.33848000	-0.46427100	0.12393900	O	0.35720200	2.72417500	-2.44302800
C	4.11447500	-1.60250800	0.19561400	O	-1.57969300	3.40334100	-1.48993200
H	6.21912900	-0.84874100	-3.28342700	C	-1.68047200	4.44225900	-2.47844900
H	5.49931500	1.23922900	-4.42705000	H	-0.81590200	5.10863800	-2.41866500
H	3.69915500	2.64771900	-3.46017200	H	-1.73156200	4.00886200	-3.48080900
H	2.61470100	2.04978300	-1.34946600	H	-2.59878000	4.97845100	-2.24125200
H	4.11061000	-2.38484000	0.93900600	Cl	-1.95425100	-0.51910100	-1.52094000
N	4.98576800	-1.68146400	-0.86205900	Cu	-3.05289000	0.46386500	0.22081800
C	5.96082300	-2.72942900	-1.08670700	C	-8.91938700	-0.94665500	-1.20104100
H	5.79099000	-3.21795500	-2.05302100	H	-9.44829600	-0.26464000	-1.87540900
H	6.98118400	-2.32836800	-1.06992300	H	-9.41020700	-0.91365800	-0.22329600
H	5.86575200	-3.47777700	-0.29732100	H	-9.00668100	-1.96228500	-1.59993200
C	0.74937900	-0.53979400	0.33200400	C	-7.46633900	-0.52702100	-1.09283000
C	0.37211000	0.42295000	-0.73577100	H	-7.35227600	0.48006900	-0.68209200
H	0.01793600	-0.45165400	1.13541500	H	-6.95029900	-0.56166600	-2.05692300
H	0.87514900	0.38959300	-1.69511500	O	-6.81317600	-1.46391900	-0.19151300
C	0.74715800	-1.98954700	-0.15622000	C	-5.52965500	-1.24939800	0.07888000
C	0.09539200	-2.96394000	0.61286900	C	-4.94530000	-2.23002000	1.05290100
C	1.33789000	-2.38108800	-1.36626900	H	-4.64872600	-1.67482900	1.95031300
C	0.04500200	-4.29360200	0.19035700	H	-5.66000600	-3.01340600	1.30869700
H	-0.36376400	-2.67756200	1.55280700	H	-4.04025200	-2.66795500	0.61959400
C	1.28376700	-3.70922100	-1.79161400	O	-4.90928700	-0.31831100	-0.43512600
H	1.84095300	-1.65130900	-1.99252500	Cl	-3.75378600	1.05329500	2.22227800
C	0.63889000	-4.67238300	-1.01426000	<b>37</b>			

C	-0.38244400	0.12270300	-1.06093200	H	-1.19807000	-0.64298800	2.22038000
C	0.92505200	0.77237300	-1.64187300	H	-1.28130800	2.75341800	-1.75890200
C	1.51387900	0.32291100	-2.83535800	N	-2.06646400	3.20923900	0.16141100
C	1.59666900	1.77399500	-0.92075300	C	-2.53828300	4.55799500	-0.07560600
C	2.71150800	0.87008500	-3.29779900	H	-3.62044300	4.62996900	0.08553400
H	1.04479800	-0.46919000	-3.40528300	H	-2.03729300	5.27071500	0.59000000
C	2.80361000	2.31096800	-1.37776700	H	-2.32000600	4.83401900	-1.10940900
H	1.18061200	2.14322100	0.00889200	C	0.06273600	-1.23093000	-0.35208800
C	3.36469200	1.86801500	-2.57434300	H	0.67644200	-1.72443700	-1.10951400
H	3.13699100	0.50356400	-4.22825200	C	-1.05721100	-2.24011100	-0.07237900
H	3.29672400	3.08126400	-0.79043200	C	-2.40338200	-1.90571400	0.12224700
H	4.29913800	2.28913700	-2.93544600	C	-0.71549000	-3.60245800	-0.09815000
C	-1.23636100	-0.36106100	-2.27385400	C	-3.36981600	-2.89902300	0.30943400
O	-0.93558900	-1.31307100	-2.96521100	H	-2.71710000	-0.86898200	0.12258300
O	-2.33232000	0.37990200	-2.51476900	C	-1.67399600	-4.59386400	0.09729200
C	-3.12987900	-0.06111600	-3.62743300	H	0.31776000	-3.88604500	-0.27908800
H	-3.96934300	0.63330800	-3.67424800	C	-3.01054500	-4.24516600	0.30561100
H	-2.54939100	-0.03085700	-4.55316900	H	-4.40694100	-2.61015800	0.45963500
H	-3.48063600	-1.08246400	-3.46048500	H	-1.37803900	-5.63942500	0.07516300
C	-1.57766700	1.23016200	1.17050100	H	-3.76270100	-5.01566700	0.45344000
C	-2.15547900	2.52399600	1.35575300	C	2.52271000	-0.96639000	0.37243700
C	-2.70013900	2.95935900	2.56873200	O	2.93862300	-1.64261600	-0.53773100
C	-2.67344000	2.07943400	3.64230100	C	3.46868200	-0.10538900	1.23921500
C	-2.12042300	0.79360900	3.49450800	O	3.07712300	0.75436100	1.99961700
C	-1.58421400	0.36492900	2.28668600	O	4.74625700	-0.42414300	1.02479300
C	-1.12643800	1.16806100	-0.21317600	C	5.70353900	0.34021000	1.77848300
C	-1.45184800	2.39390300	-0.75426700	H	6.67814400	-0.06012000	1.50045800
H	-3.12967200	3.95250100	2.66619300	H	5.63165800	1.39987000	1.51916500
H	-3.08541500	2.38434500	4.60019100	H	5.52577200	0.22141200	2.85054400
H	-2.11424400	0.11437100	4.34238700	C	1.05201300	-0.92399800	0.81011800

H	0.84372800	0.01452900	1.31669300	H	7.90214100	1.30911400	-1.63799800
Cl	1.06018400	-2.15296300	2.17907400	H	7.34945300	3.64993200	-1.00828700
<b>38</b>				H	5.27032900	4.16103600	0.24053700
C	2.86518500	-0.74760500	0.81492600	H	3.69942400	2.37176100	0.88345100
C	2.67235000	0.05037300	2.13912400	H	-0.88667900	2.55841400	0.27676000
C	1.40794500	0.45012000	2.59616500	H	4.93041500	-2.49341600	-0.45452100
C	3.77905100	0.27258700	2.97505600	N	6.16196100	-0.83200700	-0.95182200
C	1.26574800	1.09598200	3.82715300	C	7.25378100	-1.52245500	-1.60643900
H	0.51596100	0.26531000	2.01248400	H	7.40745100	-1.13530700	-2.62041400
C	3.63504900	0.91149900	4.20614500	H	8.18893500	-1.41086500	-1.04392500
H	4.76163000	-0.05600100	2.65536400	H	7.01173500	-2.58516400	-1.67457300
C	2.37602100	1.33412400	4.63635400	C	1.68341200	-0.48742100	-0.23757700
H	0.27466700	1.40646400	4.14773600	C	1.64818000	0.94493500	-0.70209300
H	4.51088700	1.07742900	4.82822200	H	0.75493000	-0.72788200	0.27814400
H	2.26185500	1.83611800	5.59363100	H	2.48652400	1.29466100	-1.29143500
C	2.68816400	-2.19950900	1.33153000	C	1.75332700	-1.41461700	-1.45974000
O	1.62191200	-2.77335500	1.40575900	C	0.87194700	-2.50299100	-1.54575700
O	3.82926400	-2.73840400	1.80801700	C	2.64514700	-1.20278300	-2.52385900
C	3.67843600	-4.00960500	2.46244900	C	0.89745300	-3.36611200	-2.64285500
H	4.68218800	-4.29172400	2.78190900	H	0.16397600	-2.66794300	-0.74216200
H	3.01217200	-3.91743700	3.32415600	C	2.66773100	-2.06098500	-3.62553100
H	3.26869100	-4.75240900	1.77314100	H	3.32924500	-0.36122300	-2.50534400
C	4.88425400	0.79154000	-0.01550300	C	1.79784000	-3.15021900	-3.68830900
C	6.08827700	0.52952400	-0.73052300	H	0.21030000	-4.20810100	-2.67917900
C	6.98802000	1.53739100	-1.09699900	H	3.36584800	-1.87226500	-4.43740500
C	6.67238800	2.84323400	-0.74078700	H	1.81656900	-3.81917800	-4.54496600
C	5.48871500	3.13216000	-0.03292800	C	0.68368000	1.85812200	-0.51669600
C	4.59997800	2.12775900	0.33157900	O	-0.46803200	1.66879300	0.21833700
C	4.22905400	-0.48708600	0.19481700	C	0.76256000	3.25940100	-1.00812300
C	5.05042000	-1.42263200	-0.39138600	O	-0.09087100	4.07758300	-0.69242300



O	1.82343300	3.53153700	-1.77358400	H	-2.17820300	-4.33832000	1.58582300
C	1.93472500	4.89455500	-2.22019600	H	-0.68900400	-3.36928900	1.88201700
H	2.86006800	4.93410100	-2.79419300	H	-3.76446100	0.98504000	4.44794200
H	1.07850900	5.16018100	-2.84541500	H	-4.09820500	2.55361100	3.70522300
H	1.98047900	5.57346800	-1.36495800	H	-5.42554500	1.36731700	3.92970000
Rh	-2.42614700	0.39619700	-0.01560900	<b>39-ts</b>			
Rh	-4.54633700	-0.73183400	-0.01830300	C	3.26668300	-0.62303400	0.95806600
C	-2.93590800	-1.21686900	-2.37457700	C	3.29562300	0.40073300	2.12936300
O	-2.05531200	-0.45457800	-1.85671600	C	2.12677300	0.90868600	2.71485000
O	-4.05182900	-1.53290600	-1.84867200	C	4.53104500	0.74823300	2.70020700
C	-4.59246900	1.91014400	-1.21686400	C	2.20053300	1.76660900	3.81570000
O	-3.34745300	1.99023300	-0.95097700	H	1.14826100	0.65561800	2.32376500
O	-5.34730900	0.91976200	-0.95956800	C	4.60169000	1.60128500	3.80087800
C	-4.05901100	0.90213100	2.33178000	H	5.44434000	0.34745400	2.27375600
O	-2.93108800	1.20508500	1.81817900	C	3.43368500	2.11987500	4.36286100
O	-4.93086800	0.13560700	1.81413600	H	1.28036100	2.15455900	4.24576500
C	-2.39325500	-2.23670100	1.21189900	H	5.57208800	1.85939900	4.21756100
O	-3.63215400	-2.31573900	0.93203800	H	3.48506600	2.78712800	5.21959800
O	-1.63015600	-1.25248400	0.93134500	C	3.31309700	-1.95803800	1.74804500
C	-5.21570600	3.10799700	-1.89776200	O	2.33376500	-2.52745800	2.18161800
C	-4.36891300	1.49423500	3.68857500	O	4.56821000	-2.38123500	2.01613500
C	-2.62561900	-1.77517000	-3.74465000	C	4.65298100	-3.51163300	2.89875400
C	-1.77667600	-3.39378600	1.96281900	H	5.71887900	-3.71662600	3.00648200
H	-5.10589300	3.98892900	-1.25672300	H	4.20715600	-3.27309500	3.86809300
H	-4.68356700	3.31554500	-2.83164200	H	4.13437800	-4.37458600	2.47292100
H	-6.27213500	2.92833100	-2.10246100	C	4.95098400	0.81757500	-0.53155200
H	-3.33395100	-2.56265300	-4.00782800	C	5.98215000	0.47719600	-1.45453200
H	-2.69477500	-0.96784300	-4.48276100	C	6.70834400	1.43699000	-2.16923600
H	-1.60038000	-2.15495400	-3.76557500	C	6.39315400	2.77393400	-1.95597000
H	-2.05746900	-3.31378700	3.02003900	C	5.37807200	3.13990200	-1.04980200

C	4.66094200	2.18352100	-0.34029000	O	-0.53621700	1.04414100	0.72424300
C	4.44369200	-0.42750900	0.01580500	C	0.15879400	2.76539700	-0.72777600
C	5.17131200	-1.42199800	-0.59492000	O	-0.81156900	3.44677800	-0.40400900
H	7.49151100	1.14967200	-2.86550000	O	1.06972400	3.18759700	-1.61791300
H	6.93778300	3.54521200	-2.49407600	C	0.85853300	4.49648900	-2.16371400
H	5.15452400	4.19277200	-0.89887600	H	1.69709400	4.66801700	-2.83894500
H	3.88511300	2.48819500	0.35284300	H	-0.08806600	4.53805800	-2.71009100
H	-1.72240800	2.12546300	0.79314600	H	0.84575300	5.24817800	-1.36952500
H	5.10688200	-2.49181600	-0.46656900	Rh	-2.43951500	-0.05953400	0.18048700
N	6.09412800	-0.89899400	-1.47571200	Rh	-4.82193500	-0.19879300	-0.21072300
C	7.03713900	-1.65688300	-2.27018700	C	-3.35982400	-2.62165100	-0.73833300
H	6.89041100	-1.46803500	-3.34047500	O	-2.28798800	-1.97522400	-0.50263500
H	8.07132200	-1.40059500	-2.00901300	O	-4.54967600	-2.16384100	-0.66609800
H	6.88408600	-2.72178000	-2.08241300	C	-3.28894800	0.59965800	-2.53111800
C	1.87950700	-0.61330300	0.16236500	O	-2.27219700	0.63390900	-1.76264600
C	1.55143400	0.73747100	-0.41309500	O	-4.47323600	0.28329500	-2.18617600
H	1.11108900	-0.86470000	0.89387200	C	-3.84744200	2.54534900	0.54084000
H	2.24375400	1.18760100	-1.11238300	O	-2.76069300	1.86989000	0.90799500
C	1.81420300	-1.69672400	-0.92285500	O	-4.86172300	1.92208000	0.19787000
C	1.17469100	-2.91639100	-0.65295500	C	-3.98074600	-0.88991500	2.48502700
C	2.35127300	-1.50557900	-2.20675800	O	-5.02583600	-0.68563500	1.78318100
C	1.09041700	-3.91687500	-1.62409700	O	-2.77610900	-0.75151300	2.09530900
H	0.74662500	-3.08062000	0.32966800	C	-3.05538900	0.94409700	-3.98400900
C	2.26281000	-2.50161100	-3.18091800	C	-3.79178000	4.03766000	0.62646600
H	2.83979300	-0.56911600	-2.45495000	C	-3.20621800	-4.07669300	-1.11319100
C	1.63476900	-3.71522100	-2.89332600	C	-4.18804200	-1.36860300	3.90407300
H	0.59641900	-4.85586500	-1.38445100	H	-2.62483100	0.07065000	-4.48747400
H	2.68502600	-2.32598600	-4.16760000	H	-3.99506900	1.20671600	-4.47327100
H	1.56719000	-4.49181700	-3.65134600	H	-2.33524300	1.76196600	-4.06621100
C	0.41242200	1.41648400	-0.13206300	H	-4.00584800	-4.37993600	-1.79261000

H	-2.22644400	-4.24526000	-1.56443300	C	-6.49183600	-1.72785000	-2.39430000
H	-3.27947600	-4.68546200	-0.20417300	C	-5.97197300	-3.01495200	-2.46044300
H	-5.15233200	-1.02552700	4.28485400	C	-4.85971300	-3.38437200	-1.67817400
H	-4.18644000	-2.46506600	3.90972700	C	-4.24820000	-2.48230600	-0.81557800
H	-3.37296600	-1.02445300	4.54418700	C	-4.39878600	0.01518200	0.04538300
H	-3.64450800	4.33428100	1.67139500	C	-5.29677800	0.98432700	-0.33929400
H	-2.92716500	4.39496700	0.05911600	H	-7.34881600	-1.43721400	-2.99565200
H	-4.71959400	4.46693000	0.24765000	H	-6.42928000	-3.74426900	-3.12356600
<b>40</b>				H	-4.47370000	-4.39786300	-1.74778300
C	-3.21592400	0.21723000	0.98022100	H	-3.39298000	-2.79020500	-0.22510000
C	-2.95377000	-1.03254600	1.87121400	H	0.32702500	3.03949800	0.19231300
C	-1.66277600	-1.44527900	2.23335700	H	-5.38459600	2.00707400	-0.00353000
C	-4.05099500	-1.71183100	2.42501100	N	-6.18426300	0.49989600	-1.27524800
C	-1.48129100	-2.52918600	3.09659500	C	-7.27307000	1.23791000	-1.88009500
H	-0.78285200	-0.94587600	1.84544200	H	-7.15830900	1.28493400	-2.96964200
C	-3.86728000	-2.79032100	3.28980900	H	-8.24004600	0.77404700	-1.65046600
H	-5.05641600	-1.39532600	2.16812000	H	-7.27345400	2.25681300	-1.48694700
C	-2.57859700	-3.20753300	3.62701300	C	-1.92218700	0.65843400	0.16488500
H	-0.47090900	-2.83892400	3.35027800	C	-1.39516600	-0.45321800	-0.70231100
H	-4.73408200	-3.30423600	3.69730700	H	-1.15731100	0.88590500	0.90836400
H	-2.43177700	-4.05024600	4.29750600	H	-2.08170300	-0.99652600	-1.33706700
C	-3.46248800	1.27757000	2.08248300	C	-2.12990900	1.95002000	-0.64738100
O	-2.57470400	1.88318400	2.65693200	C	-1.97318900	3.21766000	-0.05326900
O	-4.75223100	1.40042200	2.44232100	C	-2.42743200	1.91217400	-2.01872600
C	-4.99907200	2.23573000	3.58709600	C	-2.09513400	4.39433400	-0.80300300
H	-6.07939300	2.21404300	3.73270500	H	-1.80701500	3.28494200	1.01717100
H	-4.48332700	1.83912100	4.46530700	C	-2.55420200	3.08361700	-2.76686700
H	-4.65465200	3.25621400	3.40106800	H	-2.54329000	0.95367200	-2.51219500
C	-4.74859100	-1.16765200	-0.72038100	C	-2.38208800	4.33250600	-2.16619900
C	-5.87153600	-0.82168500	-1.52620300	H	-1.96821400	5.35759400	-0.31441300

H	-2.78066300	3.01747600	-3.82807900	H	6.82971900	-1.81943100	-2.53329800
H	-2.47102600	5.24307700	-2.75245700	H	7.77106700	-0.78956300	-1.40257800
C	-0.08132300	-0.79870000	-0.74105800	H	2.19452200	3.35435000	-2.86188900
O	0.87748500	-0.26690700	0.00208800	H	3.95568300	3.46942200	-3.05300000
C	0.35713200	-1.89017000	-1.65990500	H	3.01104100	2.27986500	-4.01210100
O	1.55360400	-2.18804100	-1.79027800	H	-0.28302100	2.31256900	2.64054000
O	-0.59310300	-2.53581000	-2.33230600	H	1.16125100	2.73100300	3.59208700
C	-0.15294300	-3.57529300	-3.22672400	H	0.40950000	3.93819900	2.51057900
H	-1.06488200	-3.96767200	-3.67631800	H	2.81990500	-2.33290300	3.94152100
H	0.51153500	-3.16351500	-3.99041600	H	3.38562000	-3.65537100	2.89468800
H	0.37337600	-4.35592500	-2.67202900	H	4.55795600	-2.57808900	3.72506100
Rh	2.77015700	-0.78242300	-0.60751100	<b>41</b>			
Rh	4.09627600	0.84594300	0.69225600	C	2.98307600	-0.11504400	-1.10182500
C	3.26800500	1.75995900	-1.93719600	C	2.67302000	-1.59527000	-1.46854500
O	2.69003400	0.63911400	-2.10772900	C	1.36665900	-2.09145800	-1.58756700
O	3.94780600	2.12064800	-0.92194700	C	3.74068100	-2.44906700	-1.79077900
C	5.66934700	-0.93623400	-0.95611200	C	1.14379200	-3.41223900	-1.98796100
O	4.58328700	-1.45729600	-1.34386600	H	0.50701900	-1.47064600	-1.36512900
O	5.76082200	0.02470400	-0.12506700	C	3.51552200	-3.76420400	-2.19465600
C	3.55873500	-1.68079800	2.04362900	H	4.75700300	-2.07615500	-1.71985800
O	2.93633700	-2.07175700	1.00475300	C	2.21221000	-4.25512900	-2.29184700
O	4.14306200	-0.56041700	2.20606100	H	0.12213300	-3.77655800	-2.06321100
C	1.55915100	2.40948000	1.52583600	H	4.36135500	-4.40448200	-2.43190900
O	2.58659200	1.78253300	1.78500800	H	2.03282700	-5.28073800	-2.60396200
O	1.24558400	2.70947000	0.27324500	C	3.17833700	0.50054700	-2.51341100
C	6.95926000	-1.51404000	-1.49219200	O	2.27143200	0.92355000	-3.19945800
C	3.58978400	-2.63375200	3.22097700	O	4.44835500	0.42612900	-2.96574200
C	3.10958300	2.77883100	-3.04534400	C	4.63224300	0.83094900	-4.33271900
C	0.65661100	2.87812600	2.63675700	H	5.69758900	0.70762400	-4.53105300
H	7.21909600	-2.40534900	-0.90909900	H	4.04035900	0.19921600	-5.00022700

H	4.33098400	1.87260400	-4.47038100	C	2.25641100	4.90797000	0.19927900
C	4.52621100	-0.82551700	0.95298000	H	1.14820900	5.13668600	-1.63856300
C	5.71177800	-0.28318000	1.52771500	H	3.32214800	4.34490200	1.98849600
C	6.32056400	-0.82676100	2.66507500	H	2.36864700	5.97625800	0.36643200
C	5.72490400	-1.94133000	3.24378700	C	-0.07207400	-0.33251400	0.99566200
C	4.55140000	-2.49816200	2.69740300	O	-1.01391800	-0.28573900	0.04727300
C	3.95154700	-1.95663000	1.56646700	C	-0.55825400	-0.76511900	2.32921700
C	4.20846000	-0.01427600	-0.20800300	O	-1.77565500	-0.85559900	2.57832400
C	5.18912600	0.94870100	-0.26559100	O	0.35540900	-1.03884800	3.25265900
H	7.22692000	-0.39538300	3.08104800	C	-0.13319000	-1.39986200	4.55994400
H	6.17175400	-2.38924000	4.12733400	H	0.76100800	-1.57119600	5.15850600
H	4.10872700	-3.37231700	3.16746900	H	-0.73185300	-0.58694200	4.97808600
H	3.05045900	-2.40335500	1.16165500	H	-0.74046500	-2.30606600	4.50041600
H	5.32296000	1.74580600	-0.98104400	Rh	-2.88779900	-0.25954200	0.78960400
N	6.09312700	0.80361500	0.76546300	Rh	-3.86938900	0.42236400	-1.33650200
C	7.26687300	1.62058700	0.99045200	C	-2.87122200	2.60061300	0.29764200
H	7.24496400	2.06864700	1.99094400	O	-2.62788800	1.74668500	1.20720500
H	8.18680700	1.03095100	0.89220700	O	-3.41722500	2.35749300	-0.83462300
H	7.28708000	2.42450600	0.25151900	C	-5.78350000	0.17577700	0.76064600
C	1.73035600	0.62973000	-0.46289700	O	-4.85578300	-0.19606400	1.52275500
C	1.22854400	0.00139200	0.81031600	O	-5.65125900	0.50604900	-0.47900300
H	0.93534200	0.56229100	-1.20486200	C	-3.69338400	-2.44997200	-0.94444800
H	1.90670100	-0.12415100	1.64431300	O	-3.18401000	-2.22226900	0.19541000
C	1.96201600	2.12977100	-0.23024300	O	-4.09303300	-1.56904400	-1.78292800
C	1.42481100	3.06280000	-1.13131800	C	-7.19029700	0.24056900	1.30736600
C	2.64485200	2.62009100	0.89549300	C	-3.83055200	-3.89921200	-1.35423300
C	1.57072900	4.43666300	-0.92172600	C	-2.45306800	4.02666100	0.56399000
H	0.90215600	2.70399500	-2.01204900	H	-7.52746300	-0.77438900	1.54379000
C	2.79247100	3.99210800	1.10683200	H	-7.19119700	0.81534700	2.23805100
H	3.05605400	1.92779400	1.62257100	H	-7.87103700	0.69146600	0.58391600

H	-1.39981000	4.13850400	0.27876200	H	-2.83251100	-4.32667000	-1.50087700
H	-3.05276500	4.72021700	-0.02900200	H	-4.31392800	-4.46470700	-0.55206300
H	-2.54060100	4.25302900	1.62919800	H	-4.40370300	-3.98776400	-2.27832600

**10. B3-LYP-D3/6-31G(d) geometries for selected the optimized compounds and transition states**

**1**

Rh	-0.00395800	0.00159200	1.19660400	H	3.62627100	-2.80748000	-0.58140300
Rh	0.00474200	0.00112000	-1.19656000	H	3.04237200	-3.36309700	1.01926400
C	1.96840700	1.75231400	0.01026100	H	-2.74635200	-3.67488100	0.49186400
O	1.53140100	1.36607100	1.14336400	H	-3.92741300	-2.36624500	0.58134000
O	1.53788600	1.36808600	-1.12683600	H	-3.41247400	-2.98622600	-1.01935300
C	-1.75183700	1.96829000	-0.01011300	<b>2</b>			
O	-1.36836400	1.53708600	1.12696200	C	-0.50034200	0.40006100	0.00023600
O	-1.36216500	1.53433500	-1.14323700	N	-0.84788500	1.67125600	0.00049500
C	-1.96699500	1.75059900	-0.01022900	N	-1.11688500	2.77695800	0.00103300
O	-1.53970700	-1.36274100	1.12683500	C	0.94236100	0.07702000	0.00007900
O	-1.52858000	-1.36593300	-1.14333300	C	1.38804100	-1.25757800	0.00079100
C	1.75108300	-1.96710600	0.01014800	C	1.90328200	1.10662600	-0.00076700
O	1.37195600	-1.53203400	-1.12690100	C	2.75394500	-1.53957000	0.00065400
O	1.36058800	-1.53390300	1.14326900	H	0.66536900	-2.06203400	0.00140400
C	-2.76394700	3.08826200	-0.00236500	C	3.26405800	0.81210300	-0.00086200
C	-3.08948000	-2.75995500	-0.00227000	H	1.59360100	2.14820400	-0.00141400
C	3.09959800	2.75186700	0.00223900	C	3.70038000	-0.51436000	-0.00014400
C	2.74806500	-3.10059000	0.00218300	H	3.07610900	-2.57758400	0.00122200
H	-3.68849700	2.73278600	0.46464100	H	3.98422600	1.62591700	-0.00153400
H	-2.38591200	3.91576800	0.60571900	H	4.76221400	-0.74368500	-0.00021800
H	-2.97013500	3.42922900	-1.01786400	C	-1.62243500	-0.55038600	-0.00022400
H	3.96441100	2.31251200	-0.50554800	O	-1.52112400	-1.76269400	-0.00024100
H	2.79791500	3.63565400	-0.56860100	O	-2.81567100	0.09726500	-0.00059100
H	3.37068500	3.03640200	1.01984400	C	-3.97051400	-0.75672100	-0.00024600
H	2.30036500	-3.96913600	-0.49197900	H	-4.82810200	-0.08323800	0.00442400

H	-3.98169300	-1.38924300	-0.89245300	O	0.98460400	-2.04656800	0.61504400
H	-3.97663200	-1.39557400	0.88742700	C	3.94694600	-1.08447100	-0.97129400
<b>N<sub>2</sub></b>				O	4.25958300	-0.49413100	0.11065800
N	0.00000000	0.00000000	0.55265200	O	2.77873800	-1.16563100	-1.48099700
N	0.00000000	0.00000000	-0.55265200	C	2.39762000	2.29631900	-0.97812200
<b>6</b>				O	3.06130300	2.15211400	0.09778700
C	-0.38829100	0.98706200	0.00001200	O	1.54963300	1.47654800	-1.46429700
C	0.15236100	-0.33077900	-0.00009200	C	0.05463400	1.33239800	1.85582300
C	-0.65665000	-1.47286900	-0.00007600	O	-0.25029600	0.62812700	0.75304700
C	-2.03464300	-1.28219000	-0.00001400	O	1.22026200	1.35657400	2.25240500
C	-2.59270300	0.01372600	0.00004600	C	5.05236700	-1.78938200	-1.71984300
C	-1.78476900	1.14476600	0.00005900	C	2.64487500	3.55529400	-1.77946300
C	0.72756800	1.89052100	0.00004200	C	1.43880000	-3.48854700	2.44040400
C	1.86228100	1.12199800	-0.00005400	C	-1.06107400	2.04472200	2.54678800
H	-0.22649800	-2.47054800	-0.00009000	H	5.09862200	-2.83026200	-1.37872600
H	-2.69294000	-2.14675200	-0.00000400	H	4.84310700	-1.78962700	-2.79168900
H	-3.67366500	0.12546400	0.00009500	H	6.01266500	-1.31366400	-1.51094600
H	-2.22378100	2.13922300	0.00012600	H	2.11338800	-4.23836600	2.01048600
H	0.69046900	2.97113900	0.00006200	H	1.67952600	-3.37056700	3.49868100
H	2.90317200	1.41716900	-0.00007700	H	0.41371300	-3.84306300	2.31024900
N	1.52982100	-0.22253600	-0.00020400	H	-1.47088100	2.82635700	1.89678800
C	2.45138700	-1.33794600	0.00018300	H	-1.88604100	1.35554700	2.74954300
H	2.31085900	-1.96171600	0.89135300	H	-0.68706800	2.48352000	3.47158400
H	2.30878700	-1.96379200	-0.88918200	H	1.70088300	3.93975100	-2.17496500
H	3.47560300	-0.95817100	-0.00148900	H	3.14244200	4.31027800	-1.16836200
<b>14</b>				H	3.28595200	3.30826500	-2.63344000
Rh	2.81891600	0.43084700	1.21754800	C	-2.37720000	-0.96862100	-0.99418700
Rh	1.22605300	-0.32714500	-0.49456900	C	-3.51996900	-1.75534600	-0.48227100
C	1.63588800	-2.18395700	1.70393600	C	-3.34555100	-2.83664800	0.40491900
O	2.44471700	-1.34253400	2.21007600	C	-4.83917300	-1.41281300	-0.83961900

C	-4.43910100	-3.53651700	0.91123600	C	-1.44387800	3.85460700	-2.10946500
H	-2.33798200	-3.12191000	0.68886700	H	-2.19477100	4.58958400	-2.41889900
C	-5.93381300	-2.10926600	-0.32903200	H	-0.75931400	4.32997200	-1.39477000
H	-4.99889000	-0.58125800	-1.52072200	H	-0.87263000	3.54143000	-2.98512100
C	-5.74139700	-3.17654300	0.55156900	<b>15</b>			
H	-4.27461300	-4.36442300	1.59727500	C	-0.72659900	-0.72750000	-0.00017000
H	-6.93975200	-1.82025500	-0.62419300	C	0.40585200	0.00943600	-0.00034700
H	-6.59301000	-3.72107800	0.95112000	H	-0.59713600	-1.81002300	-0.00012000
C	-1.22700600	-1.57411400	-1.49626300	H	0.40702500	1.09338100	-0.00039500
O	-0.20679600	-0.93617900	-1.97045700	C	-2.10408300	-0.24717300	-0.00003200
O	-1.19576600	-2.93938300	-1.51206800	C	-3.14845500	-1.19194000	0.00029800
C	-0.04578200	-3.54356200	-2.10715400	C	-2.44101700	1.12216500	-0.00022200
H	-0.24050200	-4.61809600	-2.07242400	C	-4.48201000	-0.78838400	0.00044100
H	0.08082700	-3.21890100	-3.14510200	H	-2.90317800	-2.25117400	0.00044100
H	0.86264100	-3.30739500	-1.54714300	C	-3.77191300	1.52440700	-0.00008200
C	-3.21838900	1.35600200	-0.08777900	H	-1.65578100	1.87179300	-0.00048900
C	-2.93350900	2.70965900	-0.44331200	C	-4.79775500	0.57170000	0.00025200
C	-3.43491500	3.79990800	0.27857300	H	-5.27299700	-1.53306900	0.00069700
C	-4.24309000	3.52768500	1.37902100	H	-4.01452200	2.58346400	-0.00023700
C	-4.54386100	2.19948800	1.74720900	H	-5.83638600	0.89076000	0.00036000
C	-4.04409800	1.11757100	1.02962500	C	1.71575700	-0.65689700	-0.00038400
C	-2.47403500	0.49938500	-1.01146800	O	1.89331800	-1.86480400	-0.00063400
C	-1.80542000	1.38029200	-1.85684500	C	2.92036800	0.31377200	-0.00010700
H	-3.20022100	4.82095700	-0.00875100	O	2.80621300	1.52382100	-0.00038400
H	-4.65110200	4.35080200	1.95888500	O	4.08487900	-0.34136700	0.00044500
H	-5.18215000	2.01892300	2.60774800	C	5.25547500	0.49435200	0.00069700
H	-4.28685700	0.10238500	1.32134400	H	6.10300600	-0.19098100	0.00168800
H	-1.17429700	0.71258800	0.36207900	H	5.27106900	1.12992800	-0.88952000
H	-1.10547800	1.14709700	-2.64307200	H	5.26988900	1.13109900	0.89009200
N	-2.08126400	2.69171900	-1.52683800	<b>CH3COOH</b>			



C	1.39678000	-0.10890900	-0.00000100	H	-2.23968000	0.18456100	-4.69920600
H	1.68215500	-0.69176800	-0.88201500	H	-3.51042700	1.30812700	-4.10411600
H	1.68225700	-0.69099300	0.88249300	C	2.26396100	-0.71741800	0.81503200
H	1.91617300	0.84960300	-0.00044800	C	1.89603400	0.36920800	1.74331000
C	-0.09343900	0.12661500	-0.00000400	C	0.61056500	0.44917400	2.31743100
O	-0.64647400	1.20305200	0.00000100	C	2.82296600	1.37167100	2.10446500
O	-0.77578700	-1.04822600	-0.00000500	C	0.26401900	1.47374900	3.19374800
H	-1.72254200	-0.81168300	0.00002700	H	-0.12185400	-0.29513600	2.04888700
<b>16</b>				C	2.47630300	2.39948700	2.97892500
Rh	-1.54654700	-1.71730200	-0.58995200	H	3.81752400	1.34958200	1.67086000
Rh	-3.03501400	0.02845100	0.29024700	C	1.19337500	2.46106700	3.53184100
C	-2.00712700	-1.83205300	2.27361600	H	-0.74152700	1.49578100	3.60779800
O	-1.41287400	-2.44845700	1.33099900	H	3.21099400	3.16397500	3.22104000
O	-2.73964400	-0.79338200	2.15701500	H	0.92486200	3.26261700	4.21515300
C	-4.40266100	-2.38180300	-0.55015100	C	1.32854800	-1.26500500	-0.04772600
O	-3.27600900	-2.83243700	-0.90782000	O	0.21483500	-0.69218000	-0.39576800
O	-4.59702600	-1.24464800	-0.00474300	O	1.66757800	-2.46245600	-0.63659600
C	-2.49647400	0.20431400	-2.56229000	C	0.88251100	-2.89575500	-1.72603600
O	-1.77399400	-0.83176300	-2.44599300	H	-0.14663400	-3.18943800	-1.40359000
O	-3.18944500	0.75369500	-1.63659500	H	1.36067600	-3.80003700	-2.10718900
C	-5.62392200	-3.22974500	-0.81521300	H	0.79701900	-2.14073000	-2.51424900
C	-2.52177400	0.88493800	-3.91089800	C	4.49388500	-1.34446400	-0.41195000
C	-1.77010900	-2.33928700	3.67552500	C	5.80416900	-1.66585900	0.03977500
H	-6.05437600	-2.93474900	-1.77941700	C	6.87066700	-1.87825500	-0.84048400
H	-5.34853000	-4.28494800	-0.86619500	C	6.61567700	-1.75115300	-2.20306000
H	-6.37676800	-3.06356700	-0.04123600	C	5.32665400	-1.42557200	-2.67439000
H	-0.91435100	-1.79301300	4.09033400	C	4.26767500	-1.22918200	-1.79307900
H	-2.64145300	-2.14527400	4.30481900	C	3.66406500	-1.16456400	0.76111000
H	-1.52807700	-3.40376600	3.66067700	C	4.49640100	-1.38227500	1.83854500
H	-1.79729500	1.70807300	-3.89681200	H	7.86303700	-2.12802700	-0.47518600

H	7.42208400	-1.90793700	-2.91445900	H	5.03497400	1.77680000	-1.84207300
H	5.15832100	-1.33699700	-3.74454000	H	5.57317900	4.21200900	-2.04244200
H	3.27480400	-0.99570600	-2.16523900	H	0.66455700	1.51115400	-0.35023500
H	4.26765700	-1.32365500	2.89388900	<b>17-threo-ts</b>			
N	5.78098500	-1.68504400	1.42088100	Rh	2.06663300	-1.13180900	-1.00751700
C	6.91092900	-1.98796100	2.27073000	Rh	2.91852500	-0.11582100	1.04008300
H	7.25361700	-3.01979000	2.12282900	C	3.08344800	1.54699100	-1.35636900
H	7.74759600	-1.31014900	2.06130600	O	2.66855000	0.54913200	-2.03517500
H	6.61656700	-1.86414600	3.31531400	O	3.33127200	1.54961600	-0.10742900
C	0.74701300	2.59245400	-0.43910000	C	4.84922800	-1.70694100	-0.44609000
C	-0.39369900	3.29945800	-0.17409400	O	3.88504800	-2.00793500	-1.22830000
H	-0.48739000	4.37279600	-0.29277900	O	4.76386900	-0.91200600	0.53502000
C	-1.56374000	2.56315300	0.19707800	C	1.69311000	-2.70611000	1.41431600
O	-1.50630100	1.35038400	0.50751900	O	1.40718800	-2.69405100	0.16606100
C	-2.90929700	3.27960300	0.17311600	O	2.40731200	-1.85619900	2.02663500
O	-3.07627100	4.40245600	-0.24574700	C	6.17358000	-2.38276900	-0.70236100
O	-3.88337700	2.49930900	0.68744000	C	1.08691300	-3.82568000	2.22615600
C	-5.22408000	3.02895500	0.61013000	C	3.26673800	2.86193000	-2.07068200
H	-5.85588300	2.27691800	1.08064100	H	6.18451600	-3.34355200	-0.17446900
H	-5.27988300	3.98187600	1.14125400	H	6.30277600	-2.57625200	-1.76950500
H	-5.50170500	3.17184300	-0.43710200	H	6.99056900	-1.76862700	-0.31830300
C	2.03552300	3.09048000	-0.86643600	H	2.57496900	3.58268200	-1.61975100
C	2.35170000	4.46107500	-0.97754800	H	4.28368400	3.23266400	-1.90865200
C	3.02640100	2.13660900	-1.18417600	H	3.06771900	2.75905000	-3.13839500
C	3.61636400	4.85552700	-1.39799700	H	0.04663300	-3.55998300	2.45096600
H	1.60775800	5.21132000	-0.72603000	H	1.08318100	-4.75515900	1.65124200
C	4.29126400	2.53240700	-1.60506300	H	1.62602900	-3.95340200	3.16641200
H	2.79613500	1.08229500	-1.07236500	C	-2.07975500	0.37957400	-1.06222000
C	4.58691600	3.89439100	-1.71440000	C	-2.00553600	1.79100700	-1.47472700
H	3.85383800	5.91261300	-1.47920400	C	-0.79019000	2.37527400	-1.90994200

C	-3.12476600	2.65014400	-1.38423100	C	-6.89960300	-1.11416800	-1.26053500
C	-0.70929900	3.72466900	-2.23817000	H	-7.26340900	-2.05971100	-1.67628400
H	0.10918400	1.77698000	-1.97900200	H	-7.38955500	-0.93890300	-0.29440500
C	-3.03610700	4.00107200	-1.71591000	H	-7.17198500	-0.30759000	-1.94510000
H	-4.06141600	2.27395700	-1.00040600	C	-1.66839100	0.86559800	1.30246600
C	-1.83007900	4.55258900	-2.14926100	C	-0.71891400	1.91507200	1.25417000
H	0.24602800	4.13283600	-2.55631800	H	-1.03676400	2.93752800	1.09059500
H	-3.92084000	4.62666000	-1.62314000	C	0.63441200	1.71806300	1.44141700
H	-1.76182800	5.60640500	-2.40399900	O	1.15980300	0.56695300	1.75028500
C	-0.89319200	-0.44117800	-1.36597300	C	1.51335300	2.94718500	1.39150800
O	0.22889900	-0.22374300	-0.86997900	O	1.31071100	3.91863000	0.68723200
O	-1.13444500	-1.41945900	-2.24436300	O	2.55047700	2.84576400	2.24897400
C	-0.15536600	-2.42283700	-2.55134600	C	3.52345700	3.89589400	2.15423300
H	0.79201600	-1.96657700	-2.88125700	H	4.25473800	3.68945700	2.93629200
H	-0.57345700	-2.98249000	-3.38870900	H	3.99600600	3.86611800	1.16850800
H	0.00106700	-3.07978800	-1.69388100	H	3.05610800	4.87243700	2.30758000
C	-3.39324400	-1.73544700	-0.40652200	C	-3.05602700	1.07197900	1.69122200
C	-4.74931500	-2.14759900	-0.47742000	C	-3.68107300	2.33886300	1.65208500
C	-5.19841300	-3.35424400	0.06957500	C	-3.83035900	-0.02648300	2.12406900
C	-4.25742400	-4.17214200	0.68789100	C	-5.02433800	2.48509900	1.99012300
C	-2.90235400	-3.79049600	0.76017200	H	-3.11495900	3.21169300	1.35007200
C	-2.46445500	-2.58536700	0.21943200	C	-5.17163000	0.12227700	2.46381400
C	-3.30751900	-0.41318500	-1.01088800	H	-3.36782200	-1.00435300	2.19386500
C	-4.59520800	-0.11819300	-1.42087800	C	-5.77967300	1.37854200	2.38950400
H	-6.24486000	-3.64114000	0.02029300	H	-5.48241900	3.47002300	1.94765700
H	-4.57256500	-5.11697300	1.12176300	H	-5.74065100	-0.74537500	2.78711500
H	-2.18782400	-4.44809400	1.24840100	H	-6.82694800	1.49825700	2.65503200
H	-1.41725700	-2.30983200	0.30788900	H	-1.26800600	-0.12733500	1.47822200
H	-4.96939900	0.74101000	-1.95461600	<b>18-threo</b>			
N	-5.45955400	-1.15096400	-1.11780700	Rh	2.06663300	-1.13180900	-1.00751700

Rh	2.91852500	-0.11582100	1.04008300	C	-1.83007900	4.55258900	-2.14926100
C	3.08344800	1.54699100	-1.35636900	H	0.24602800	4.13283600	-2.55631800
O	2.66855000	0.54913200	-2.03517500	H	-3.92084000	4.62666000	-1.62314000
O	3.33127200	1.54961600	-0.10742900	H	-1.76182800	5.60640500	-2.40399900
C	4.84922800	-1.70694100	-0.44609000	C	-0.89319200	-0.44117800	-1.36597300
O	3.88504800	-2.00793500	-1.22830000	O	0.22889900	-0.22374300	-0.86997900
O	4.76386900	-0.91200600	0.53502000	O	-1.13444500	-1.41945900	-2.24436300
C	1.69311000	-2.70611000	1.41431600	C	-0.15536600	-2.42283700	-2.55134600
O	1.40718800	-2.69405100	0.16606100	H	0.79201600	-1.96657700	-2.88125700
O	2.40731200	-1.85619900	2.02663500	H	-0.57345700	-2.98249000	-3.38870900
C	6.17358000	-2.38276900	-0.70236100	H	0.00106700	-3.07978800	-1.69388100
C	1.08691300	-3.82568000	2.22615600	C	-3.39324400	-1.73544700	-0.40652200
C	3.26673800	2.86193000	-2.07068200	C	-4.74931500	-2.14759900	-0.47742000
H	6.18451600	-3.34355200	-0.17446900	C	-5.19841300	-3.35424400	0.06957500
H	6.30277600	-2.57625200	-1.76950500	C	-4.25742400	-4.17214200	0.68789100
H	6.99056900	-1.76862700	-0.31830300	C	-2.90235400	-3.79049600	0.76017200
H	2.57496900	3.58268200	-1.61975100	C	-2.46445500	-2.58536700	0.21943200
H	4.28368400	3.23266400	-1.90865200	C	-3.30751900	-0.41318500	-1.01088800
H	3.06771900	2.75905000	-3.13839500	C	-4.59520800	-0.11819300	-1.42087800
H	0.04663300	-3.55998300	2.45096600	H	-6.24486000	-3.64114000	0.02029300
H	1.08318100	-4.75515900	1.65124200	H	-4.57256500	-5.11697300	1.12176300
H	1.62602900	-3.95340200	3.16641200	H	-2.18782400	-4.44809400	1.24840100
C	-2.07975500	0.37957400	-1.06222000	H	-1.41725700	-2.30983200	0.30788900
C	-2.00553600	1.79100700	-1.47472700	H	-4.96939900	0.74101000	-1.95461600
C	-0.79019000	2.37527400	-1.90994200	N	-5.45955400	-1.15096400	-1.11780700
C	-3.12476600	2.65014400	-1.38423100	C	-6.89960300	-1.11416800	-1.26053500
C	-0.70929900	3.72466900	-2.23817000	H	-7.26340900	-2.05971100	-1.67628400
H	0.10918400	1.77698000	-1.97900200	H	-7.38955500	-0.93890300	-0.29440500
C	-3.03610700	4.00107200	-1.71591000	H	-7.17198500	-0.30759000	-1.94510000
H	-4.06141600	2.27395700	-1.00040600	C	-1.66839100	0.86559800	1.30246600

C	-0.71891400	1.91507200	1.25417000	O	4.27026700	0.90105600	-1.68613000
H	-1.03676400	2.93752800	1.09059500	O	4.96629500	0.40093200	0.39928000
C	0.63441200	1.71806300	1.44141700	C	3.10581000	-2.26948700	-0.87552400
O	1.15980300	0.56695300	1.75028500	O	2.70261100	-1.45764100	-1.77009500
C	1.51335300	2.94718500	1.39150800	O	3.33535500	-1.98496200	0.34456000
O	1.31071100	3.91863000	0.68723200	C	6.57684900	1.16660600	-1.18398000
O	2.55047700	2.84576400	2.24897400	C	3.27117100	-3.71427600	-1.27616400
C	3.52345700	3.89589400	2.15423300	C	2.01038100	4.13933000	1.04091200
H	4.25473800	3.68945700	2.93629200	H	7.30122200	0.64347500	-0.55667000
H	3.99600600	3.86611800	1.16850800	H	6.74738400	0.94672100	-2.24017400
H	3.05610800	4.87243700	2.30758000	H	6.70139600	2.24549400	-1.03440800
C	-3.05602700	1.07197900	1.69122200	H	2.42187700	4.84535000	0.31403200
C	-3.68107300	2.33886300	1.65208500	H	0.92272700	4.26992600	1.04752900
C	-3.83035900	-0.02648300	2.12406900	H	2.41192900	4.33515900	2.03638000
C	-5.02433800	2.48509900	1.99012300	H	3.32507100	-3.81356600	-2.36168500
H	-3.11495900	3.21169300	1.35007200	H	4.16500800	-4.13516200	-0.80780900
C	-5.17163000	0.12227700	2.46381400	H	2.39876500	-4.26057000	-0.89887100
H	-3.36782200	-1.00435300	2.19386500	C	-2.08268200	0.70660200	-0.79839800
C	-5.77967300	1.37854200	2.38950400	C	-1.99763500	2.18406100	-0.64261100
H	-5.48241900	3.47002300	1.94765700	C	-3.01413500	2.89779900	0.03157700
H	-5.74065100	-0.74537500	2.78711500	C	-0.93569500	2.94426500	-1.17721000
H	-6.82694800	1.49825700	2.65503200	C	-2.96216200	4.28266300	0.18006800
H	-1.26800600	-0.12733500	1.47822200	H	-3.85128900	2.35903200	0.45249900
<b>21-erythro-ts</b>				C	-0.88975100	4.32952300	-1.03525300
Rh	2.33937300	0.51079500	-1.26339900	H	-0.13187100	2.45786400	-1.70843300
Rh	3.03623500	-0.04851900	1.01480700	C	-1.89752700	5.01284700	-0.35009800
C	2.31592400	2.72522000	0.61288500	H	-3.76086600	4.78839300	0.71723900
O	2.11397200	2.44848300	-0.61774500	H	-0.05355800	4.87339200	-1.46672700
O	2.73351900	1.92231600	1.50576800	H	-1.85674600	6.09311000	-0.23878300
C	5.17235500	0.78395500	-0.78809000	C	-0.89232100	0.00372700	-1.26734000

O	0.27055600	0.32201700	-0.93644500	C	-3.11102400	1.56895500	2.77039400
O	-1.16219200	-1.03457300	-2.05994600	C	-5.16103800	-0.31566700	2.69854400
C	-0.15157300	-2.01840300	-2.33799200	H	-3.79888700	-1.56068900	1.61229100
H	0.64361200	-1.59735900	-2.95262600	C	-4.33094100	1.84863600	3.38171300
H	-0.67717200	-2.80717800	-2.87758400	H	-2.31140300	2.30296000	2.79620500
H	0.26053000	-2.41097600	-1.40692200	C	-5.36558600	0.91064300	3.33960500
C	-3.84161800	-1.26840500	-1.08454300	H	-5.95880800	-1.05277600	2.66369900
C	-5.21016000	-1.27556100	-1.47015200	H	-4.47447600	2.79935800	3.88833300
C	-5.99141200	-2.43506300	-1.50341500	H	-6.32128000	1.12931100	3.80876700
C	-5.38165900	-3.63216100	-1.14551200	C	0.40798400	-1.32834400	1.61535500
C	-4.02325500	-3.66055500	-0.77346400	O	1.22678200	-0.34432200	1.84995400
C	-3.25398500	-2.50188100	-0.74708900	C	0.93377900	-2.74222600	1.57642600
C	-3.39134600	0.11899800	-1.12863100	O	0.57378400	-3.57799400	0.76059900
C	-4.49464400	0.84056000	-1.56099800	O	1.82605100	-2.97013200	2.54929600
H	-7.03672500	-2.39992000	-1.79702200	C	2.48396800	-4.24630700	2.51610600
H	-5.95666900	-4.55387500	-1.15926500	H	3.04568500	-4.30989500	3.44820400
H	-3.56236400	-4.60809100	-0.50791200	H	1.75440500	-5.05734700	2.44516600
H	-2.21090600	-2.56108400	-0.46900100	H	3.16195400	-4.27862500	1.65972200
H	-4.57583900	1.89809700	-1.76202000				
N	-5.57760100	0.02358100	-1.76843200	<b>22-erythro</b>			
C	-6.89997200	0.44315400	-2.18065900	Rh	2.24776900	0.37767100	-1.33527900
H	-6.88684500	1.51504800	-2.38899800	Rh	2.84019600	0.15786100	1.02572300
H	-7.20789200	-0.08811600	-3.08857400	C	2.32335900	2.87200600	0.13458600
H	-7.63666600	0.24605600	-1.39225700	O	2.15896400	2.40812900	-1.04951600
C	-1.58346700	0.09663400	1.51170400	O	2.68274500	2.21456400	1.15677200
C	-0.96265800	-1.17732400	1.50850200	C	5.08370700	0.43078000	-0.86592900
H	-0.89350600	0.93466200	1.53360300	O	4.20692200	0.46502500	-1.79953500
H	-1.56214600	-2.07935700	1.51143600	O	4.82553600	0.31360600	0.36324800
C	-2.88990900	0.33999800	2.11331900	C	2.57057000	-2.36022500	-0.44217000
C	-3.93720200	-0.60481100	2.10226600	O	2.26276200	-1.67620000	-1.47855300
				O	2.91679600	-1.88641900	0.68561000

C	6.52462700	0.57400900	-1.29181300	H	0.43385300	-1.31223100	-3.05069200
C	2.47553900	-3.86103700	-0.54401000	C	-3.03934100	-1.83052100	-0.99376300
C	2.02347700	4.34126100	0.31255200	C	-4.28469100	-2.35802300	-1.43413300
H	7.18727300	0.16613800	-0.52632200	C	-4.49133900	-3.72275600	-1.66555700
H	6.68830200	0.07635900	-2.25068000	C	-3.41198400	-4.57737400	-1.47092900
H	6.74890800	1.63938200	-1.41991200	C	-2.15867900	-4.07854200	-1.06237600
H	2.47579700	4.91811500	-0.49906000	C	-1.96117200	-2.72261300	-0.83008200
H	0.93672800	4.47697900	0.25477100	C	-3.20747800	-0.39261600	-0.87752900
H	2.38114200	4.69407400	1.28102500	C	-4.49840100	-0.13304300	-1.27448900
H	3.37424500	-4.31766700	-0.11912100	H	-5.45745500	-4.09824300	-1.99057900
H	1.62028500	-4.17921600	0.06302600	H	-3.53677300	-5.64373900	-1.63769000
H	2.34209100	-4.17618000	-1.58018400	H	-1.33097200	-4.76526300	-0.91097700
C	-2.12368000	0.59236000	-0.47109700	H	-0.99060800	-2.37732300	-0.49231400
C	-2.45148900	2.07994300	-0.75143200	H	-5.01357700	0.80813100	-1.38113900
C	-3.64983600	2.65616200	-0.29703100	N	-5.15855400	-1.30098200	-1.59543300
C	-1.50695400	2.93102800	-1.34968200	C	-6.53616500	-1.41444700	-2.02492900
C	-3.91036700	4.01537700	-0.47579200	H	-6.59757500	-1.90774500	-3.00216400
H	-4.37318500	2.05226900	0.23481800	H	-7.12649700	-1.99278200	-1.30387300
C	-1.76647000	4.29164800	-1.52672600	H	-6.96860900	-0.41514700	-2.10974100
H	-0.53794600	2.55973500	-1.66562400	C	-1.68738800	0.50830800	1.08116000
C	-2.97409600	4.84139100	-1.09779300	C	-1.06279900	-0.78969500	1.50610000
H	-4.84660600	4.42784600	-0.10937800	H	-0.91670800	1.27508700	1.18506400
H	-1.01403400	4.91765600	-1.99925700	H	-1.68711300	-1.67024600	1.59041100
H	-3.17741000	5.89993400	-1.23462900	C	-2.83280200	0.85792200	2.01844900
C	-0.88784100	0.26674600	-1.31939900	C	-3.93381700	0.00501900	2.19413400
O	0.24233000	0.36022200	-0.84564800	C	-2.79702000	2.05899300	2.73896400
O	-1.15949400	-0.04987800	-2.57204800	C	-4.98052400	0.36069000	3.04581800
C	-0.08907700	-0.44312300	-3.45507800	H	-3.97586500	-0.93709600	1.65804400
H	0.60741800	0.39006700	-3.60800500	C	-3.83908000	2.41410100	3.59675100
H	-0.57750500	-0.68869000	-4.39745900	H	-1.94820500	2.72603400	2.61303000

C	-4.93981000	1.56852300	3.74723300	O	0.27098800	-3.31200100	1.89416500
H	-5.82716500	-0.31065900	3.16598400	O	1.67420400	-2.17964600	3.25923100
H	-3.79166600	3.35241200	4.14331100	C	2.28570700	-3.42629000	3.61393000
H	-5.75468200	1.84288300	4.41216400	H	2.98022900	-3.19306900	4.42171100
C	0.23294500	-0.89388200	1.89029100	H	1.53495800	-4.14956900	3.94421700
O	1.07325700	0.13195800	1.95573200	H	2.82572900	-3.82897000	2.75186900
C	0.70646300	-2.25645000	2.32706400				

### 11. B3-LYP/6-31+G(d) geometries for selected the optimized compounds and transition states

**1**

Rh	-0.00094800	-0.00337200	1.19547800	H	-2.85032700	3.61566000	-0.50096900
Rh	-0.00155200	0.00362000	-1.19545600	H	-3.99813100	2.27609100	-0.56719800
C	-2.01322000	1.71250100	0.00818900	H	-3.48028300	2.91980400	1.02191100
O	-1.56713200	1.33186900	1.14022500	H	3.62290000	2.83883700	-0.48464700
O	-1.57027600	1.33665800	-1.12730200	H	2.28764200	3.98939300	-0.58267000
C	-1.71260400	-2.01275100	-0.00804800	H	2.90880400	3.48773800	1.02109800
O	-1.33692100	-1.56963800	1.12742200	H	4.03149200	-2.21820500	0.48500000
O	-1.33460900	-1.56446400	-1.14010800	H	2.90012200	-3.56979500	0.58215600
C	2.01168400	-1.71141100	-0.00813300	H	3.43229700	-2.97359800	-1.02122900
O	1.56565100	-1.33920600	1.12733900	<b>2</b>			
O	1.56668100	-1.32951100	-1.14016900	C	-0.50034200	0.40006100	0.00023600
C	1.71150200	2.01198700	0.00807500	N	-0.84788500	1.67125600	0.00049500
O	1.33167200	1.57238900	-1.12738300	N	-1.11688500	2.77695800	0.00103300
O	1.33430700	1.56302500	1.14012500	C	0.94236100	0.07702000	0.00007900
C	-2.68285500	-3.17089000	-0.00281400	C	1.38804100	-1.25757800	0.00079100
C	3.16805100	-2.68382300	-0.00276000	C	1.90328200	1.10662600	-0.00076700
C	-3.16175500	2.69411800	0.00276300	C	2.75394500	-1.53957000	0.00065400
C	2.69529100	3.15868800	0.00266100	H	0.66536900	-2.06203400	0.00140400
H	-2.20406100	-4.04225200	0.45761800	C	3.26405800	0.81210300	-0.00086200
H	-3.55604800	-2.91673200	0.60668600	H	1.59360100	2.14820400	-0.00141400
H	-2.99345300	-3.41761300	-1.01955400	C	3.70038000	-0.51436000	-0.00014400



H	3.07610900	-2.57758400	0.00122200	H	2.32954100	-1.95847000	0.89265300
H	3.98422600	1.62591700	-0.00153400	H	2.32765600	-1.96042800	-0.89063700
H	4.76221400	-0.74368500	-0.00021800	H	3.48268100	-0.94357800	-0.00137600
C	-1.62243500	-0.55038600	-0.00022400	<b>14</b>			
O	-1.52112400	-1.76269400	-0.00024100	Rh	2.96485500	0.49330100	1.15497300
O	-2.81567100	0.09726500	-0.00059100	Rh	1.31830400	-0.30039700	-0.48549900
C	-3.97051400	-0.75672100	-0.00024600	C	1.72803100	-2.06243600	1.80739800
H	-4.82810200	-0.08323800	0.00442400	O	2.56856200	-1.21475200	2.25036900
H	-3.98169300	-1.38924300	-0.89245300	O	1.05180800	-1.95489700	0.73048000
H	-3.97663200	-1.39557400	0.88742700	C	4.01595100	-1.16934100	-0.96628500
<b>N<sub>2</sub></b>				O	4.36327500	-0.52869900	0.07665600
N	0.00000000	0.00000000	0.55256300	O	2.83345500	-1.24643200	-1.44362700
N	0.00000000	0.00000000	-0.55256300	C	2.58671100	2.24803400	-1.14333300
<b>6</b>				O	3.24380300	2.14689300	-0.05665000
C	-0.38936900	0.98617500	0.00000700	O	1.70609900	1.43025400	-1.56971900
C	0.15270100	-0.33258800	-0.00009000	C	0.21057300	1.48715400	1.79861100
C	-0.65979200	-1.47490700	-0.00005700	O	-0.12376800	0.78167700	0.70287500
C	-2.03957100	-1.28324000	0.00000300	O	1.38563300	1.50088100	2.16498600
C	-2.59800100	0.01415000	0.00004800	C	5.09307000	-1.93327300	-1.70073300
C	-1.78755200	1.14530000	0.00005400	C	2.89715500	3.44176400	-2.02073900
C	0.72658700	1.89109600	0.00003200	C	1.52640500	-3.32371800	2.61736400
C	1.86327200	1.12104000	-0.00006100	C	-0.88141200	2.20836300	2.52307700
H	-0.23595700	-2.47575200	-0.00005600	H	5.21050600	-2.91843100	-1.23305500
H	-2.69825700	-2.14791500	0.00002600	H	4.81400600	-2.07788300	-2.74666500
H	-3.67916400	0.12677600	0.00009200	H	6.04736700	-1.40635900	-1.62394800
H	-2.22751200	2.13985100	0.00010700	H	2.25913300	-4.07223200	2.29114000
H	0.69108700	2.97240700	0.00005200	H	1.69473300	-3.12571100	3.67872000
H	2.90398400	1.41846000	-0.00009300	H	0.52629400	-3.73041300	2.45176700
N	1.53174700	-0.22385400	-0.00019900	H	-1.40460900	2.89789900	1.85142600
C	2.46234300	-1.33442000	0.00017000	H	-1.62979600	1.49370100	2.88349300

H	-0.45136900	2.75432500	3.36330700	C	-2.10623400	1.39077200	-1.79099100
H	2.05620200	3.66566200	-2.68088900	H	-3.83587600	4.73151300	-0.02513200
H	3.15142400	4.31006900	-1.40742600	H	-5.12095400	4.18596600	2.03278500
H	3.76808900	3.20264100	-2.64322500	H	-5.30373500	1.84361000	2.82775100
C	-2.43217400	-0.98415000	-0.86050000	H	-4.21911900	-0.00916100	1.59230100
C	-3.56835600	-1.83191500	-0.42285500	H	-1.06679800	0.82478500	0.35889500
C	-3.39139200	-2.97510300	0.38564700	H	-1.46255800	1.19584800	-2.63602900
C	-4.88921900	-1.50598200	-0.79797500	N	-2.51035600	2.67920800	-1.50000900
C	-4.47801800	-3.74841300	0.79633900	C	-2.16006000	3.86660200	-2.25573100
H	-2.38786300	-3.25490800	0.68843500	H	-3.05641700	4.34723500	-2.66606300
C	-5.97734400	-2.27863000	-0.38803600	H	-1.62862300	4.59245900	-1.62739600
H	-5.06032000	-0.63555300	-1.42634200	H	-1.50777500	3.57709200	-3.08215100
C	-5.78041400	-3.40679300	0.41457200	<b>15</b>			
H	-4.30691600	-4.62230000	1.42167500	C	0.73001700	0.72962700	-0.00001900
H	-6.98133300	-2.00057200	-0.70154200	C	-0.40576500	-0.00664200	-0.00009700
H	-6.62590300	-4.01017500	0.73598900	H	0.60803100	1.81297200	0.00007300
C	-1.26235400	-1.52978600	-1.39317500	H	-0.40603000	-1.09090500	-0.00018800
O	-0.27151800	-0.84133500	-1.85712100	C	2.10839200	0.24645900	-0.00003300
O	-1.19389300	-2.89499900	-1.47000700	C	3.15304400	1.19282200	0.00011000
C	-0.07991900	-3.45235500	-2.17073100	C	2.44703000	-1.12362100	-0.00017400
H	-0.26639500	-4.52898500	-2.18646800	C	4.48884600	0.79045900	0.00011900
H	-0.02466900	-3.06682600	-3.19418100	H	2.90706900	2.25220000	0.00021800
H	0.86103100	-3.24115100	-1.65635700	C	3.77987100	-1.52500800	-0.00016600
C	-3.38444600	1.29379600	0.07132400	H	1.66372200	-1.87574300	-0.00029100
C	-3.29584500	2.65019100	-0.36476100	C	4.80626700	-0.57057000	-0.00001800
C	-3.90885000	3.70535000	0.32586800	H	5.27914300	1.53635600	0.00023300
C	-4.62679900	3.39224800	1.47853900	H	4.02331700	-2.58422200	-0.00027600
C	-4.72896200	2.05820300	1.93038800	H	5.84541400	-0.88904100	-0.00001100
C	-4.11948300	1.01287800	1.24117800	C	-1.71786300	0.65538300	-0.00003800
C	-2.60745700	0.48220900	-0.86329600	O	-1.90040200	1.86383400	0.00004500

C	-2.92577500	-0.31573800	-0.00012200	C	-1.44268000	-1.77285600	3.89158100
O	-2.80644600	-1.52723600	-0.00034100	H	-5.97028900	-3.52706900	-1.02506700
O	-4.09017400	0.33417700	0.00026900	H	-4.98662500	-4.77788100	-0.22471000
C	-5.27246900	-0.48925400	0.00033700	H	-5.94901700	-3.61120500	0.74157200
H	-6.10824200	0.21019000	0.00087900	H	-0.55695600	-1.18531200	4.16286100
H	-5.29319500	-1.12040700	-0.89223200	H	-2.28026500	-1.44056100	4.50966600
H	-5.29261500	-1.12111500	0.89241600	H	-1.22164600	-2.82744800	4.07286100
<b>CH<sub>3</sub>COOH</b>				H	-2.04920700	0.61251900	-4.41540100
C	1.39787400	-0.11940000	-0.00000300	H	-2.50090700	-1.06249100	-4.78489500
H	1.68083000	-0.70461100	-0.88172900	H	-3.75864600	0.14492000	-4.34888800
H	1.68105100	-0.70173700	0.88357500	C	2.53479100	-0.80125500	0.60923300
H	1.92539600	0.83512300	-0.00152400	C	2.35847500	0.37015800	1.47844100
C	-0.08899000	0.12534400	-0.00005700	C	1.09314000	0.84230100	1.91340700
O	-0.63590900	1.20794700	-0.00008100	C	3.49116400	1.06102800	1.98169300
O	-0.78953900	-1.04038600	0.00006400	C	0.97799100	1.90707200	2.80810000
H	-1.73699900	-0.80493100	0.00017500	H	0.19844700	0.36342500	1.54162700
<b>16</b>				C	3.36964500	2.13256300	2.86664100
Rh	-1.37303300	-1.95733800	-0.42809700	H	4.48162500	0.73897100	1.67626900
Rh	-2.95156400	-0.17006000	0.16525000	C	2.11113900	2.56620900	3.29778600
C	-1.73660100	-1.54183100	2.42734700	H	-0.01434300	2.22150700	3.12697200
O	-1.16702800	-2.31667900	1.59428400	H	4.26889500	2.63079300	3.22395800
O	-2.51479600	-0.56776200	2.14196300	H	2.01606500	3.39555300	3.99427400
C	-4.16937500	-2.78989000	-0.14005200	C	1.51289600	-1.37258300	-0.13746600
O	-3.03540100	-3.21409400	-0.50139400	O	0.35714400	-0.84138100	-0.40077100
O	-4.40943100	-1.58909100	0.22589400	O	1.82795900	-2.59878200	-0.69101000
C	-2.56046700	-0.54455500	-2.69565500	C	0.92098700	-3.19273200	-1.58972000
O	-1.71305100	-1.44456700	-2.40920500	H	-0.01977700	-3.50990900	-1.07331900
O	-3.26758000	0.11753500	-1.85876800	H	1.39801200	-4.11202500	-1.93817500
C	-5.33868900	-3.74678000	-0.15602000	H	0.67153800	-2.54641000	-2.43547100
C	-2.73949200	-0.20030800	-4.15780700	C	4.78798300	-1.32539500	-0.63373600

C	5.97354700	-2.03512800	-0.28806400	C	0.97231600	5.85039600	-0.84175200
C	7.05829700	-2.15112400	-1.16813100	C	2.59374800	4.05520600	-0.59373900
C	6.94567100	-1.53813400	-2.41526500	C	2.00827700	6.74869700	-1.06980800
C	5.78010300	-0.82711400	-2.77674000	H	-0.05463000	6.20334400	-0.85906400
C	4.70516300	-0.71742400	-1.89812900	C	3.62975500	4.95989000	-0.81848000
C	3.88788900	-1.40690600	0.49388200	H	2.81597800	3.01113100	-0.39032400
C	4.55443200	-2.14292700	1.44597800	C	3.33978800	6.30622000	-1.05848300
H	7.95726100	-2.69843000	-0.89555600	H	1.78515500	7.79531700	-1.25857300
H	7.76896400	-1.61073900	-3.12171700	H	4.65973100	4.61489400	-0.80430600
H	5.72412300	-0.36233500	-3.75826800	H	4.14617500	7.01289900	-1.23681300
H	3.80678400	-0.17422700	-2.18226300	H	0.55723000	2.46387000	-0.27962600
H	4.22635300	-2.43355600	2.43605500				
N	5.80967200	-2.52456700	0.99361700	<b>17-ts-threo</b>			
C	6.77240100	-3.32515100	1.72003000	Rh	2.08263900	-1.27999600	-0.90703200
H	6.95506900	-4.28306000	1.21551800	Rh	3.02123200	0.05543600	0.89558200
H	7.72805100	-2.79511600	1.82081500	C	2.99493700	1.34603900	-1.71894800
H	6.38252500	-3.52852700	2.72039500	O	2.59618800	0.23520400	-2.20812400
C	0.21661500	3.49424600	-0.36508400	O	3.19218600	1.58718400	-0.48475200
C	-1.12545100	3.71386600	-0.22495400	C	4.93857100	-1.60176500	-0.53148900
H	-1.57183400	4.70061600	-0.26810300	O	3.92374700	-2.10742800	-1.12222900
C	-2.02020900	2.61647000	0.00613700	O	4.88639500	-0.63793700	0.28829700
O	-1.64073200	1.42518700	0.08418700	C	2.09204200	-2.56397900	1.70620900
C	-3.50483700	2.96572800	0.16723300	O	1.61983000	-2.69995100	0.52397200
O	-3.96734000	4.07168700	-0.00515800	O	2.79825300	-1.59240300	2.11857900
O	-4.22338600	1.88842700	0.53753900	C	6.28402500	-2.22452000	-0.81731200
C	-5.65420600	2.06601600	0.69036300	C	1.76198100	-3.64844900	2.70590500
H	-6.02987600	1.08398000	0.97314800	C	3.25861200	2.47876400	-2.68341500
H	-5.84700500	2.80682200	1.46913000	H	6.49366200	-2.97990600	-0.05011100
H	-6.08303500	2.39522300	-0.25833500	H	6.28441000	-2.71288700	-1.79425700
C	1.24819100	4.48462100	-0.60109800	H	7.06804400	-1.46490200	-0.76513700
				H	2.62188400	3.33032900	-2.42109400

H	4.29997800	2.80451500	-2.58773500	C	-3.42667700	-0.44958600	-0.91549700
H	3.06155000	2.16724700	-3.71089300	C	-4.58746300	-0.08604000	-1.57992100
H	2.57555000	-3.75649000	3.42751400	H	-6.80623400	-3.33668800	-0.27647300
H	0.86031400	-3.35420100	3.25699700	H	-5.50772400	-4.88598100	1.17385600
H	1.56717600	-4.59681800	2.19978700	H	-3.13112100	-4.41565200	1.71115100
C	-2.12141700	0.23842400	-0.93417300	H	-2.00375600	-2.40833100	0.83377000
C	-2.00795500	1.57289900	-1.58460100	H	-4.76530100	0.75165700	-2.23785700
C	-0.89197600	1.94396100	-2.36758400	N	-5.59724800	-0.99717800	-1.35911100
C	-3.03660500	2.53367600	-1.45262500	C	-6.94500000	-0.91654300	-1.88600400
C	-0.82066100	3.18988600	-2.99276500	H	-7.18337400	-1.80378700	-2.48518300
H	-0.06590000	1.25484400	-2.49844900	H	-7.68005800	-0.82951600	-1.07620500
C	-2.95919900	3.78116900	-2.07175800	H	-7.02373100	-0.03398700	-2.52479900
H	-3.89927100	2.30970100	-0.83802900	C	-1.64671400	0.95557400	1.32240000
C	-1.85208900	4.12102600	-2.85416400	C	-0.66436700	1.98369100	1.24398700
H	0.05133100	3.43004000	-3.59668200	H	-0.96861200	3.01852300	1.14308100
H	-3.77071200	4.49285600	-1.93544900	C	0.69212500	1.77630000	1.41755900
H	-1.79259600	5.09136100	-3.33992900	O	1.22849500	0.61411900	1.64629300
C	-0.97379400	-0.67173300	-1.15370000	C	1.56764800	3.01049000	1.49538300
O	0.19558500	-0.39354000	-0.82294100	O	1.26462800	4.11867900	1.09511000
O	-1.30010800	-1.80951300	-1.78204800	O	2.74112800	2.73973600	2.11554600
C	-0.32465400	-2.83208800	-2.03791500	C	3.66763500	3.83482800	2.20311400
H	0.52022900	-2.42851500	-2.61398800	H	4.52742700	3.44427600	2.74883900
H	-0.84512600	-3.56916600	-2.65102100	H	3.96082700	4.15800200	1.20060300
H	0.01704200	-3.28725400	-1.10648800	H	3.21662400	4.67336500	2.74073900
C	-3.75645900	-1.69496300	-0.23714100	C	-2.99371700	1.25469500	1.82464300
C	-5.11364800	-1.99565200	-0.53563000	C	-3.55197400	2.55337600	1.79761400
C	-5.76606200	-3.13090900	-0.03795700	C	-3.75372400	0.23386100	2.43367700
C	-5.03363700	-3.99367900	0.77351200	C	-4.81224500	2.80738200	2.33665200
C	-3.68240900	-3.72485200	1.07807000	H	-2.99455700	3.37504300	1.36186300
C	-3.04464700	-2.59147300	0.58044200	C	-5.01054000	0.48913700	2.98131000

H	-3.34406600	-0.76896300	2.49048000	C	-2.19497300	0.37290400	-0.63066400
C	-5.55088700	1.77755600	2.93069400	C	-2.73420400	1.58433000	-1.41572200
H	-5.21430700	3.81730100	2.30469100	C	-1.89337800	2.35544400	-2.23582500
H	-5.56555700	-0.31941800	3.45049200	C	-4.05258600	2.03417100	-1.23473200
H	-6.52956900	1.98067000	3.35845300	C	-2.35754800	3.50490900	-2.87854300
H	-1.27288400	-0.03404200	1.56341900	H	-0.85490600	2.07319600	-2.37501200
<b>18-threo</b>				C	-4.52317700	3.18192100	-1.87962700
Rh	2.05464600	-1.13573600	-1.00177800	H	-4.71767500	1.49964400	-0.56714500
Rh	2.83452400	0.13194700	0.93784100	C	-3.68021600	3.92109900	-2.71149500
C	2.77189500	1.62509400	-1.58412000	H	-1.67765900	4.07832700	-3.50341600
O	2.32204600	0.56615000	-2.14656500	H	-5.54977800	3.50113100	-1.71660200
O	3.08953800	1.73232400	-0.35929500	H	-4.04380100	4.81479200	-3.21211900
C	4.91043100	-1.30149600	-0.57697100	C	-0.96085100	-0.23766800	-1.33831200
O	3.96227500	-1.69609800	-1.34392600	O	0.04519600	-0.57720800	-0.71310100
O	4.75557400	-0.54622500	0.42160400	O	-1.15104800	-0.45496800	-2.63338900
C	2.12486000	-2.62453500	1.49668000	C	-0.17676700	-1.19817500	-3.39549500
O	1.81849200	-2.74422000	0.26001800	H	0.73202200	-0.60702300	-3.52488600
O	2.56005900	-1.57439000	2.06190400	H	-0.65414500	-1.37812400	-4.35906700
C	6.29570700	-1.81114600	-0.89819000	H	0.03751800	-2.15311000	-2.90439700
C	1.97931800	-3.85721500	2.36109400	C	-2.96186900	-2.10093700	0.06409200
C	2.92549900	2.86183300	-2.43735000	C	-4.06406700	-2.92843800	-0.30046600
H	6.41761200	-2.80888800	-0.45920100	C	-4.23044600	-4.23358100	0.18028700
H	6.42955200	-1.90082600	-1.97935000	C	-3.25055400	-4.73726900	1.02986200
H	7.05101700	-1.14887200	-0.46972800	C	-2.13094600	-3.95477400	1.37989400
H	2.28088000	3.65086400	-2.03370800	C	-1.97631500	-2.65475900	0.90794000
H	3.95856900	3.22082500	-2.37953500	C	-3.15630600	-0.82392300	-0.60324800
H	2.66334800	2.65541100	-3.47680700	C	-4.30531900	-0.96908900	-1.35201700
H	1.51973800	-3.59045100	3.31713100	H	-5.09033100	-4.83517600	-0.10194800
H	1.38943400	-4.62033700	1.84957000	H	-3.34532300	-5.74686200	1.42076700
H	2.97616800	-4.26126200	2.57444400	H	-1.37036800	-4.37667600	2.03128000

H	-1.09295600	-2.08940700	1.18213700	H	-1.21945500	-0.00873200	1.27679400
H	-4.77170600	-0.27463600	-2.03431000	<b>21-ts-erythro</b>			
N	-4.86347600	-2.21439200	-1.17078300	Rh	2.28834900	0.51177700	-1.32582300
C	-6.11390300	-2.67653700	-1.74173700	Rh	3.05125600	-0.03226200	0.93851100
H	-5.96613100	-3.61720200	-2.28483200	C	2.58364800	2.78988800	0.45844800
H	-6.87044100	-2.83315500	-0.96273100	O	2.28745000	2.49010000	-0.74940100
H	-6.48340100	-1.92437600	-2.44247200	O	2.93597800	1.97427200	1.36740600
C	-1.74225800	0.84192400	0.84117700	C	5.16966100	0.52608600	-0.98404600
C	-0.75609300	1.98300000	0.80622400	O	4.23541900	0.67174900	-1.84391300
H	-1.09943200	2.96670600	0.50773300	O	4.98249800	0.24957800	0.23631200
C	0.53043600	1.89265800	1.23018600	C	2.82427600	-2.32717500	-0.85205000
O	1.09350700	0.78487400	1.69658800	O	2.40143100	-1.51701700	-1.74287100
C	1.32426200	3.18106800	1.27038400	O	3.16857300	-2.01058100	0.33233600
O	1.06785900	4.18908800	0.63226600	C	6.58743300	0.66985800	-1.48273500
O	2.35787000	3.10159600	2.13510700	C	2.89133300	-3.79103500	-1.21708700
C	3.19801700	4.26201800	2.21355400	C	2.48686700	4.24733100	0.84458500
H	3.94686800	4.02697600	2.97133400	H	7.25639900	0.91468300	-0.65499000
H	3.67460100	4.44809500	1.24675100	H	6.90870300	-0.28322400	-1.92034200
H	2.61534800	5.14002500	2.50656900	H	6.64164700	1.43405400	-2.26220100
C	-2.92008400	1.16500800	1.77025800	H	2.73532800	4.88595900	-0.00704400
C	-3.49762000	2.44373800	1.84698700	H	1.45343900	4.46017200	1.14305400
C	-3.41550200	0.17377500	2.63317000	H	3.14322500	4.46027200	1.69129500
C	-4.54608900	2.71274500	2.73104500	H	2.80831500	-3.92586900	-2.29739300
H	-3.12884500	3.24747500	1.21908500	H	3.82628300	-4.22635900	-0.85179300
C	-4.46225400	0.43745200	3.52070300	H	2.06362600	-4.30985200	-0.71875100
H	-2.97348400	-0.81759300	2.61828600	C	-2.16389100	0.81768300	-0.70682800
C	-5.03764200	1.70960400	3.57066800	C	-2.20322100	2.26186000	-0.36250500
H	-4.97060600	3.71333300	2.76851800	C	-3.33946100	2.82452100	0.26827100
H	-4.81979800	-0.35179100	4.17791100	C	-1.15169300	3.15684700	-0.67878700
H	-5.84842500	1.92064700	4.26374600	C	-3.42859700	4.18922400	0.54579900

H	-4.16209100	2.18281200	0.55457800	H	-7.03189400	-0.30574800	-3.39266900
C	-1.24765600	4.52098300	-0.40579600	H	-7.61986500	-0.25149400	-1.71012000
H	-0.24613200	2.79195400	-1.14534700	C	-1.62759200	0.03466700	1.64177800
C	-2.38621300	5.05466600	0.20684000	C	-0.91802300	-1.18864800	1.66630800
H	-4.32106500	4.57268500	1.03565300	H	-1.01489700	0.92943400	1.67802700
H	-0.42445700	5.17332000	-0.68803900	H	-1.45465700	-2.12589400	1.76627800
H	-2.45781700	6.11922500	0.41454200	C	-2.95881300	0.14724000	2.23736200
C	-0.94196800	0.32687300	-1.36580900	C	-3.92761200	-0.87794300	2.16819900
O	0.21323100	0.54655900	-0.94344400	C	-3.26798000	1.30057700	2.99078200
O	-1.19615100	-0.34599100	-2.49667800	C	-5.14947800	-0.75045500	2.82546500
C	-0.13994100	-0.88238200	-3.30674900	H	-3.72725900	-1.77212800	1.58779200
H	0.52849700	-0.08234200	-3.64396200	C	-4.48595500	1.41931400	3.66132900
H	-0.64627100	-1.32134800	-4.16744300	H	-2.53080200	2.09463500	3.06542600
H	0.43067600	-1.63654400	-2.76648700	C	-5.43452800	0.39560100	3.57893700
C	-3.67216400	-1.27325800	-1.24623600	H	-5.88188700	-1.55084400	2.75384000
C	-4.99735000	-1.42300100	-1.73935400	H	-4.69201600	2.30993900	4.24998200
C	-5.58930500	-2.67306700	-1.95785300	H	-6.38475300	0.48562900	4.09951700
C	-4.82466200	-3.80500000	-1.68387700	C	0.46651700	-1.25298100	1.78147000
C	-3.50329000	-3.68499200	-1.20522400	O	1.23675700	-0.20930400	1.82625200
C	-2.92472900	-2.43627300	-0.98875400	C	1.04054100	-2.62946500	2.04949800
C	-3.41067100	0.15332500	-1.12770300	O	0.61836400	-3.66178800	1.55399600
C	-4.57529500	0.76838800	-1.56403500	O	2.04526800	-2.58031900	2.94085500
H	-6.60707100	-2.76187100	-2.32872600	C	2.69033300	-3.82987500	3.23522400
H	-5.25128300	-4.79188000	-1.84335700	H	3.43064300	-3.59902800	4.00200600
H	-2.92523900	-4.58261100	-1.00115300	H	1.96401400	-4.55880700	3.60527900
H	-1.90618200	-2.37215800	-0.62041800	H	3.17653800	-4.21800600	2.33627100
H	-4.79026200	1.82117100	-1.67656400				
N	-5.52441800	-0.15813800	-1.93056800	<b>22-erythro</b>			
C	-6.86248100	0.13590300	-2.40325000	Rh	2.27781700	0.45240700	-1.35858000
H	-6.98152600	1.21907000	-2.48024400	Rh	2.90064000	0.01142100	0.96245600
				C	2.63896500	2.82357600	0.28474000



O	2.35208800	2.45906300	-0.90956700	H	-1.29951300	5.00673800	-2.09638300
O	2.93789000	2.05590300	1.24949500	H	-3.33633100	5.96440600	-1.01439800
C	5.12959200	0.28684800	-0.94633300	C	-0.91240600	0.35911700	-1.32633800
O	4.23375900	0.45982400	-1.84657200	O	0.23163700	0.51740700	-0.90218500
O	4.88668900	0.07880000	0.27413900	O	-1.21247500	0.01798400	-2.56929200
C	2.50028500	-2.37160100	-0.69107300	C	-0.15554400	-0.22479100	-3.52284300
O	2.20812000	-1.59010500	-1.66199300	H	0.46526500	0.67101000	-3.63634200
O	2.84043100	-2.00409800	0.47726200	H	-0.66960000	-0.43800200	-4.45986800
C	6.56929100	0.36787000	-1.39588900	H	0.44951900	-1.07712700	-3.20897900
C	2.41319700	-3.85839800	-0.93979200	C	-3.26497500	-1.71107200	-1.06433400
C	2.59708100	4.30885200	0.56409500	C	-4.54748600	-2.09105600	-1.55605900
H	7.19483800	-0.27540200	-0.77237300	C	-4.89079400	-3.41889500	-1.84254400
H	6.66108400	0.09253300	-2.44911700	C	-3.91451700	-4.39248800	-1.65272000
H	6.91832200	1.40101700	-1.27789400	C	-2.62750900	-4.04291700	-1.19492300
H	2.98906000	4.86774800	-0.29017800	C	-2.29619700	-2.72256100	-0.90558000
H	1.55310600	4.60972600	0.71381100	C	-3.28696700	-0.26750800	-0.89344900
H	3.16160200	4.54282600	1.46905500	C	-4.53704000	0.13291700	-1.31372600
H	3.33623400	-4.34320500	-0.60621400	H	-5.88099500	-3.68164200	-2.20538600
H	1.59116600	-4.26430800	-0.33876500	H	-4.14656700	-5.43335400	-1.86261000
H	2.23977500	-4.06846000	-1.99692600	H	-1.88087100	-4.81948600	-1.05348300
C	-2.14564100	0.64120100	-0.43790000	H	-1.30048100	-2.49239100	-0.54258500
C	-2.48520300	2.14910300	-0.63553300	H	-4.95323100	1.12551400	-1.39052900
C	-3.61874800	2.71182900	-0.01993800	N	-5.30496700	-0.94545700	-1.69688000
C	-1.66072100	3.01423000	-1.37437200	C	-6.67472100	-0.88984700	-2.16773600
C	-3.92334700	4.06796800	-0.15667500	H	-6.75881300	-1.31471100	-3.17542400
H	-4.27035200	2.09266000	0.58313900	H	-7.34506700	-1.44067900	-1.49637400
C	-1.96324100	4.37262500	-1.51396600	H	-6.99624500	0.15366900	-2.20198100
H	-0.75057900	2.65571900	-1.84318300	C	-1.66624400	0.45549400	1.09578100
C	-3.09972300	4.90881500	-0.90861600	C	-1.02495400	-0.86427600	1.44740200
H	-4.80672300	4.46486700	0.33755600	H	-0.89215900	1.21558800	1.22068800

H	-1.65613000	-1.73936200	1.54809400
C	-2.74769000	0.73268700	2.13884500
C	-3.86522600	-0.10265700	2.30739400
C	-2.59017900	1.81319800	3.02038300
C	-4.80888800	0.15604800	3.30492200
H	-4.00134100	-0.96302700	1.65948400
C	-3.52782300	2.07096800	4.02407500
H	-1.72092200	2.45843900	2.91767600
C	-4.64714800	1.24619700	4.16618000
H	-5.66672600	-0.50327700	3.41566800
H	-3.38128700	2.91444100	4.69456400
H	-5.37880500	1.44264800	4.94604000
C	0.27330000	-0.98145700	1.83344200
O	1.12535300	0.03427400	1.89527700
C	0.71706400	-2.33815300	2.33151400
O	0.22307900	-3.40359900	1.99547300
O	1.72034000	-2.23983500	3.22510100
C	2.23529100	-3.48082100	3.72871300
H	3.00912700	-3.20327900	4.44584800
H	1.44394200	-4.05574700	4.21829300
H	2.66180100	-4.07138800	2.91287000