

## Supporting Information

# Mechanistic Study on Domino Rearrangement Promoted Meta C-H Activation in 2-methyl-N-methoxyaniline via Cu (NHC)<sup>+</sup>: The Motivation and Selectivity

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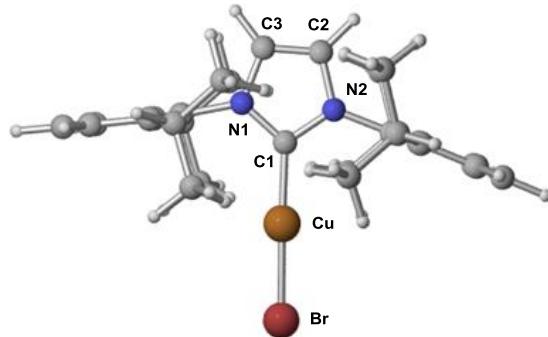
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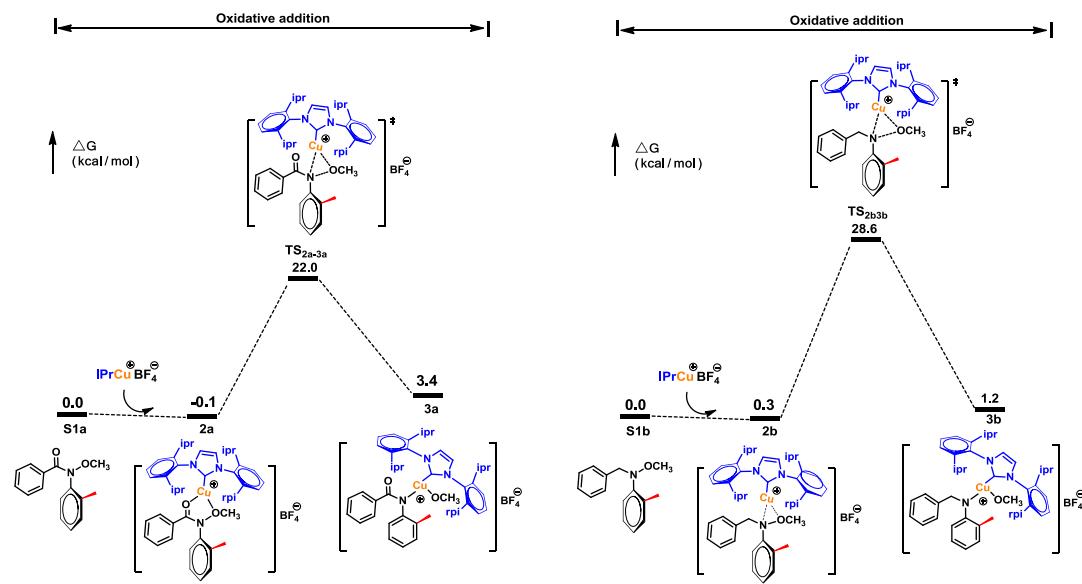
## Computational Details

All the calculations were carried out via density functional theory (DFT) calculation using Gaussian 09<sup>[1]</sup>. First, we calibrated our calculation by optimizing the structure of copper catalyst with four different methods and found that the geometry parameters calculated by M06-L<sup>[2]</sup> agreed well with the X-ray structure<sup>[3]</sup> (Table S1). We chose M06-L functional to do the geometry optimization and all species in this work were optimized in gas phase at T=298.15K and 1 atm pressure. Frequency calculation were performed to determine all the stationary points (no imaginary frequency) and transition state structures (only one imaginary frequency). The 6-31+G\*<sup>[4]</sup> basis set was used for the atoms (C、H、O、N、B、F). And the LANL2DZ basis set was used for Cu atoms<sup>[5]</sup> with the polarization functions added for Cu ( $f = 3.525$ )<sup>[6]</sup>. In addition, the intrinsic reaction coordinate (IRC) calculation<sup>[7]</sup> were applied to confirm the connection of each transition state to its corresponding appropriate intermediates, reactants, or products. Solvent effects were computed by using the SMD<sup>[8]</sup> model at the same level of theory while LANL2DZ basis set for Cu atoms and 6-311++G\*\* basis set for all other atoms. Toluene ( $\epsilon=2.3741$ ) was used as the solvent, corresponding to the experimental conditions, and Bondi atomic radii<sup>[9]</sup> used for the SMD calculation. All 3D molecular structures were generated by using the CYLview (Version) program<sup>[10]</sup>.

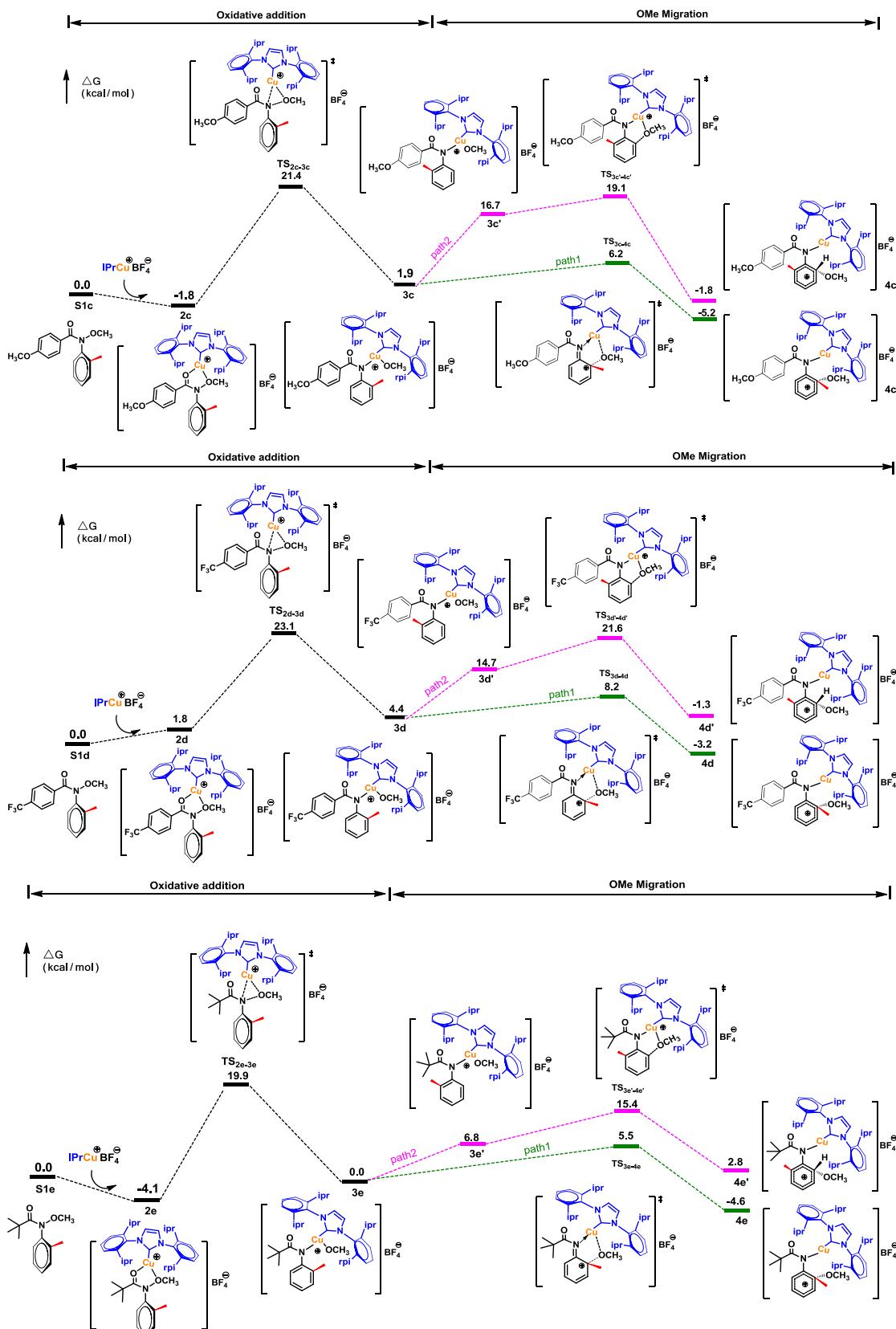
**Table S1.** The structure of copper catalyst obtained from DFT calculation by different density functionals.



Bond length and angle for copper catalyst					
Method/ (6-31+G*)	Cu(1)-C(1) (Å)	N(1)-C(1) (Å)	N(2)-C(1) (Å)	C(2)-C(3) (Å)	N(1)-C(1)-N(2) (°)
XRD	1.884	1.352	1.352	1.352	104.5
<b>M06L</b>	<b>1.883</b>	<b>1.368</b>	<b>1.375</b>	<b>1.353</b>	<b>104.4</b>
B3LYP	1.910	1.372	1.375	1.355	104.9
$\omega$ B97xd	1.902	1.360	1.364	1.350	104.8
BP86	1.876	1.384	1.388	1.366	104.5

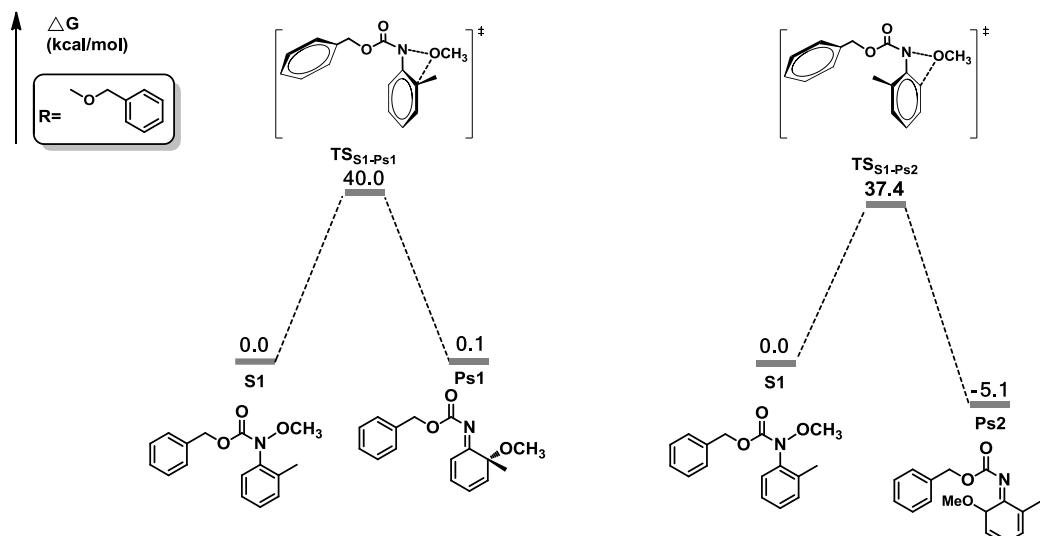


**Figure S1.** Energy profiles for oxidative addition process with different directing groups. All energies are in kcal/mol.

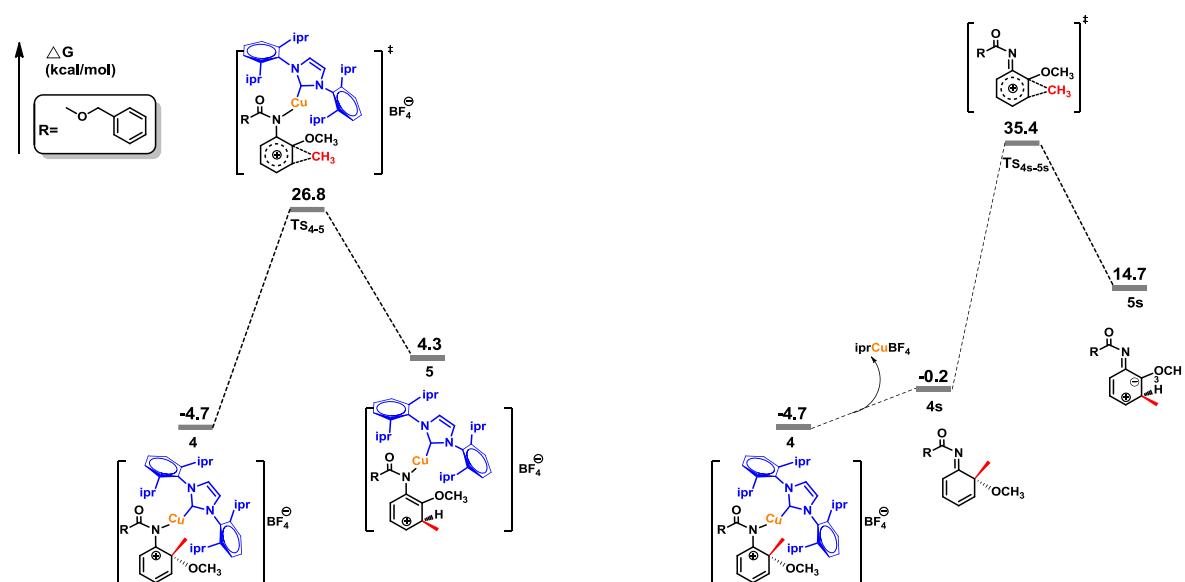


**Figure S2.** Energy profiles for the methoxy group migration with different directing groups. All energies are in kcal/mol. Experimental results: S1c ( $R_1=4$ -(methoxy)-benzoyl group: 33% yield);

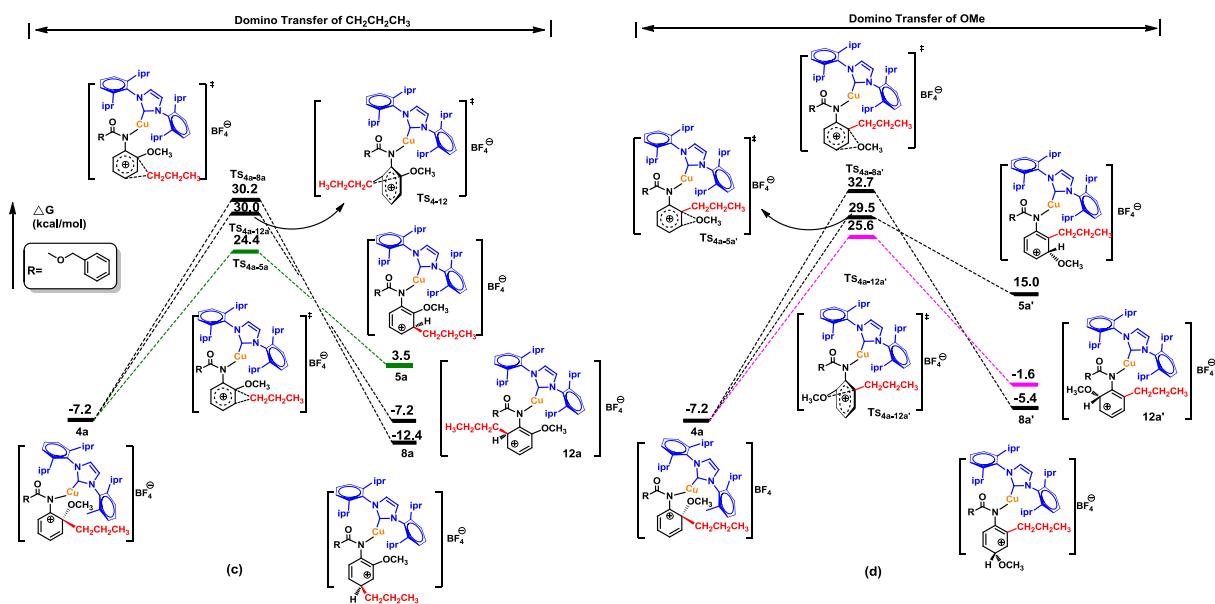
S1d ( $R_1=$ 4-(trifluoromethyl)-benzoyl group: 72% yield) and S1e ( $R_1=piv$ : 51%:25% low selectivity)



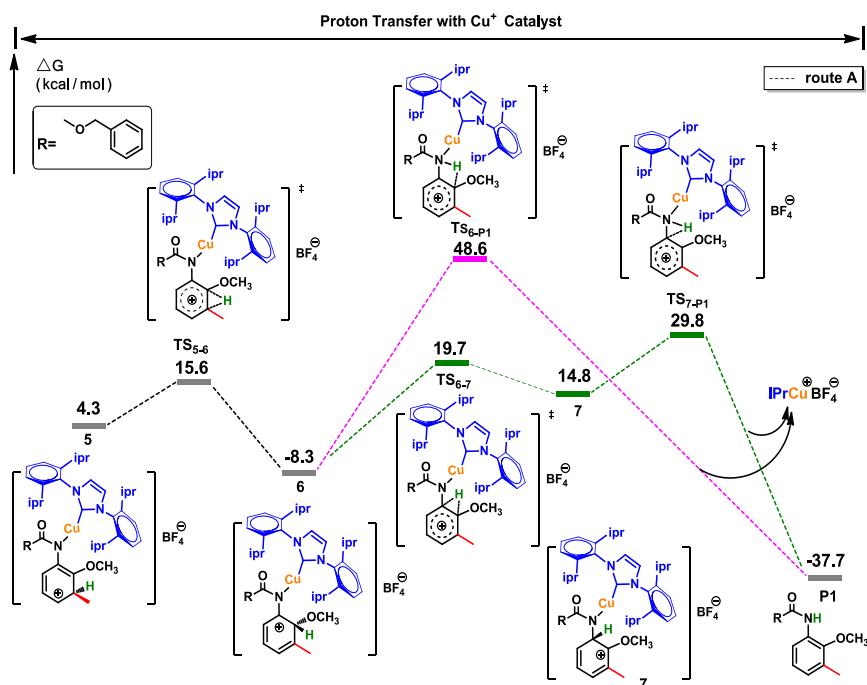
**Figure S3.** Energy profiles for the methoxy group migration without  $\text{Cu}^+$  catalyst. All energies are in kcal/mol.



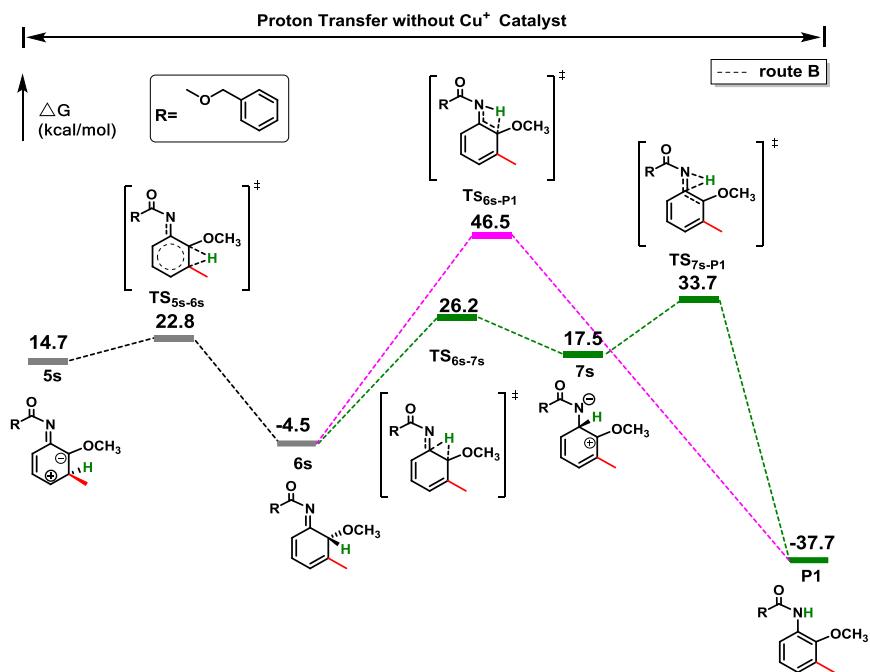
**Figure S4.** Energy profiles for [1.2]-methyl group transfer with or without  $\text{Cu}^+$  catalyst. All energies are in kcal/mol.



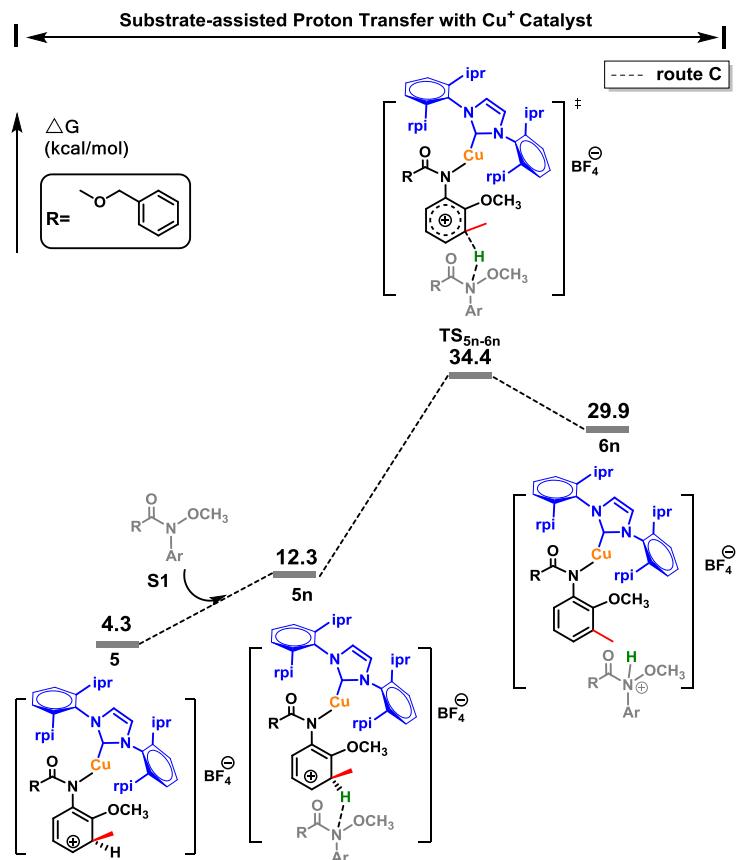
**Figure S5.** Energy profiles for domino transfer of propyl group (c) and methoxy group (d) process. All energies are in kcal/mol.



**Figure S6.** Energy profiles for proton transfer in the presence of  $\text{Cu}^+$  catalyst. All energies are in kcal/mol.



**Figure S7.** Energy profiles for proton transfer without Cu<sup>+</sup> catalyst. All energies are in kcal/mol.



**Figure S8.** Energy profiles for substrate-assisted proton transfer in the presence of Cu<sup>+</sup> catalyst. All

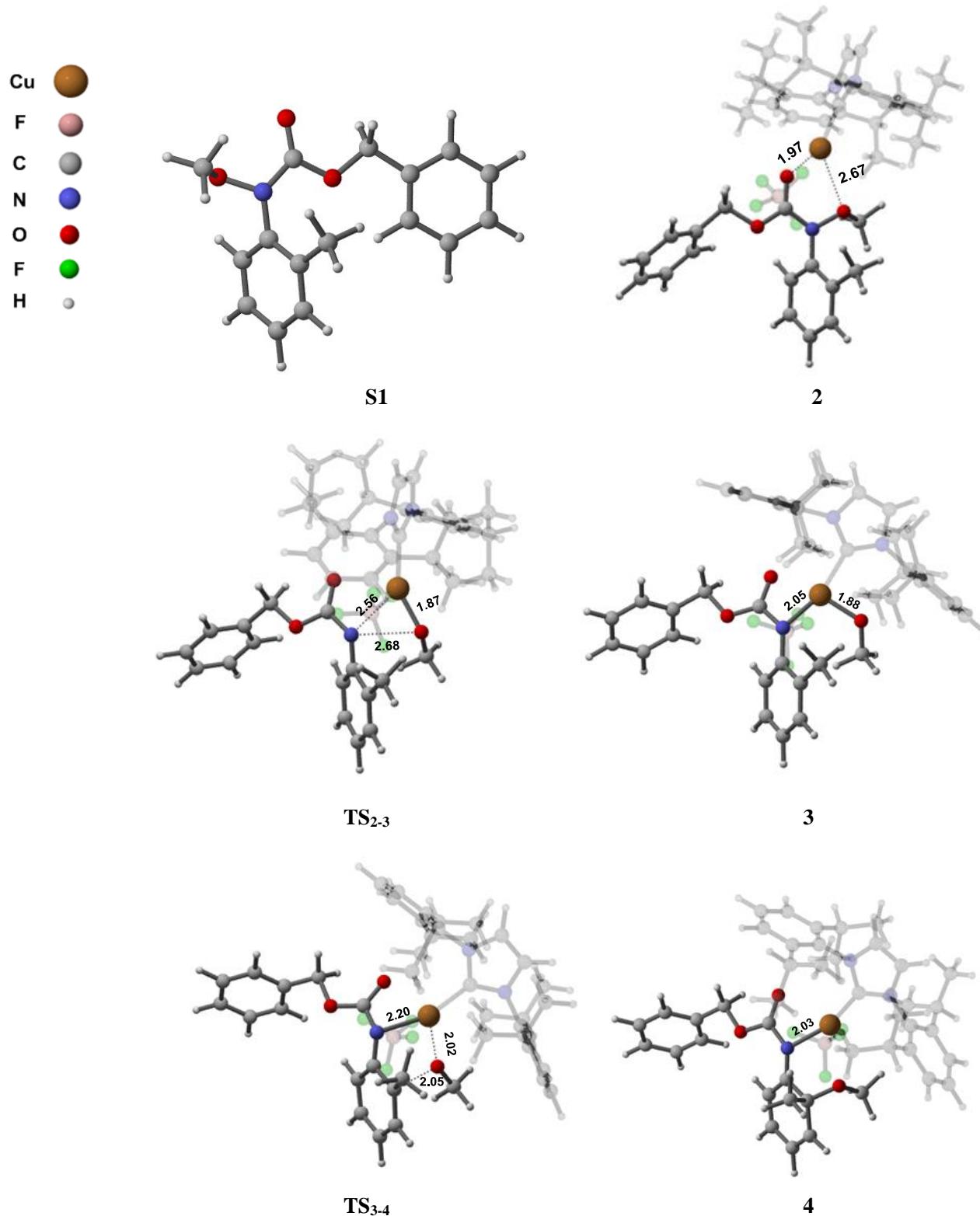
energies are in kcal/mol.

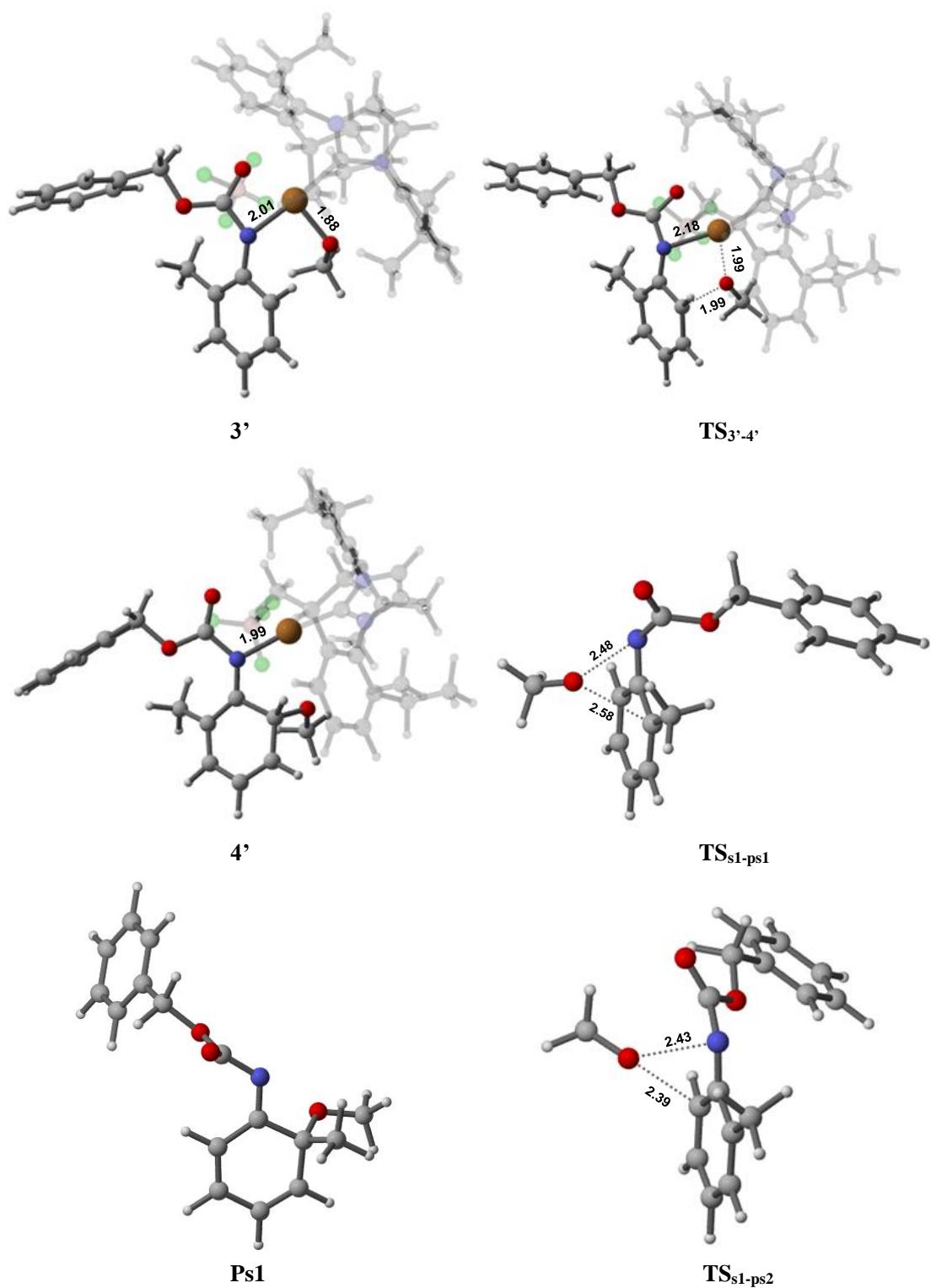
**Table S2.** The gas phase relative electronic energies ( $\Delta E_{\text{gas}}$ ), gas phase relative free energies ( $\Delta G_{\text{gas}}$ ) and solvation corrected relative electronic energies ( $\Delta E_{\text{sol}}$ ) calculated for species involved in the process of migration the methoxy group.

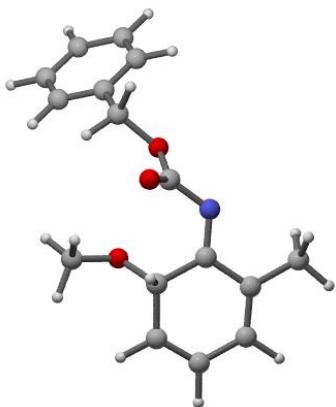
species	$\Delta G_{\text{gas}}$	$\Delta E_{\text{gas}}$	$\Delta E_{\text{sol}}$
<b>S1</b>	0.0	0.0	0.0
<b>2</b>	-3.6	-21.7	-15.9
<b>TS<sub>2-3</sub></b>	17.3	0.6	6.9
<b>3</b>	-1.8	-20.0	-13.3
<b>TS<sub>3-4</sub></b>	0.4	-17.9	-11.3
<b>4</b>	-11.2	-30.8	-24.4
<b>3'</b>	2.5	-14.8	-8.1
<b>TS<sub>3'-4'</sub></b>	12.2	-5.4	1.4
<b>4'</b>	-3.0	-22.6	-15.8
<b>S1a</b>	0.0	0.0	0.0
<b>2a</b>	-5.0	-22.4	-17.5
<b>TS<sub>2a-3a</sub></b>	17.5	2.0	6.6
<b>3a</b>	-2.5	-18.3	-12.4
<b>S1b</b>	0.0	0.0	0.0
<b>2b</b>	-5.0	-12.5	-17.2
<b>TS<sub>2b-3b</sub></b>	24.2	10.1	4.6
<b>3b</b>	-2.3	-16.5	-12.9
<b>S1c</b>	0.0	0.0	0.0
<b>2c</b>	-6.7	-22.6	-17.7
<b>TS<sub>2c-3c</sub></b>	16.7	1.4	6.1
<b>3c</b>	-4.2	-21.2	-15.1
<b>TS<sub>3c-4c</sub></b>	0.8	-16.4	-11.0
<b>4c</b>	-10.8	-27.3	-21.6
<b>3c'</b>	9.9	-6.8	0.1
<b>TS<sub>3c'-4c'</sub></b>	13.2	-4.1	1.8
<b>4c'</b>	-6.4	-24.2	-19.6
<b>S1d</b>	0.0	0.0	0.0
<b>2d</b>	-2.7	-20.6	-16.2
<b>TS<sub>2d-3d</sub></b>	18.0	1.3	6.4
<b>3d</b>	-2.2	-20.8	-14.2
<b>TS<sub>3d-4d</sub></b>	2.7	-15.9	-10.4
<b>4d</b>	-9.1	-27.5	-21.6
<b>3d'</b>	7.5	-10.6	-3.4
<b>TS<sub>3d'-4d'</sub></b>	15.3	-3.8	2.5
<b>4d'</b>	-6.1	-23.7	-18.9
<b>S1e</b>	0.0	0.0	0.0
<b>2e</b>	-8.8	-27.3	-22.6

<b>TS<sub>2e-3e</sub></b>	14.4	0.8	6.2
<b>3e</b>	-6.5	-23.2	-16.8
<b>TS<sub>3e-4e</sub></b>	-0.2	-17.7	-12.0
<b>4e</b>	-10.6	-29.8	-23.8
<b>3e'</b>	1.3	-16.7	-11.2
<b>TS<sub>3e'-4e'</sub></b>	9.8	-8.0	-2.4
<b>4e'</b>	-3.2	-21.0	-14.9
<b>TS<sub>s1-ps1</sub></b>	41.4	45.0	43.5
<b>TS<sub>s1-ps2</sub></b>	38.1	41.2	40.5
<b>Ps1</b>	1.3	2.5	1.4
<b>Ps2</b>	-5.0	-5.3	-5.3

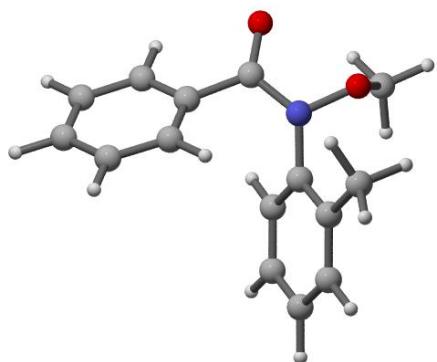
**Figure S9.** Optimized geometries with partial structural parameters (distances in Å) for the species involved in the process of migration of the methoxy group. Unimportant hydrogen and carbon atoms are transparent for clarity.



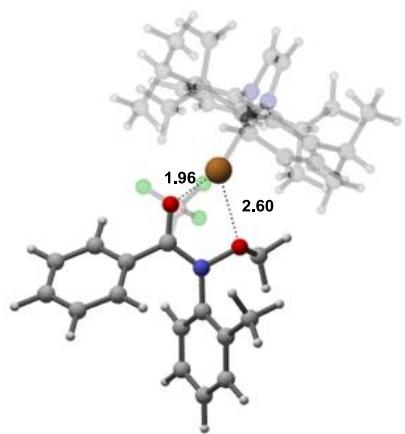




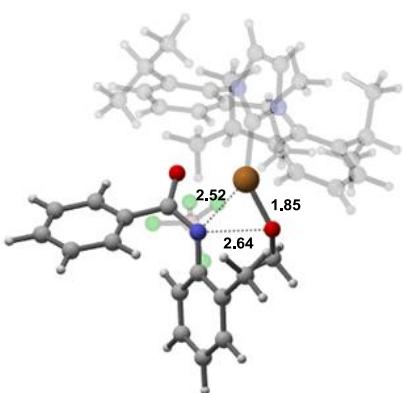
Ps2



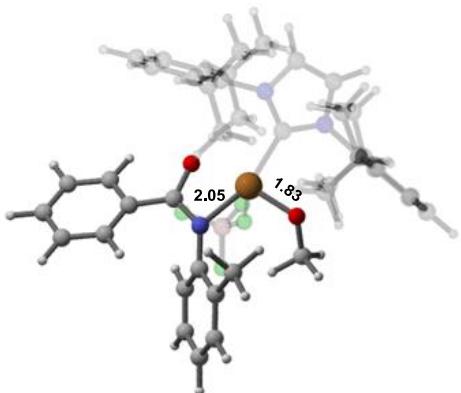
S1a



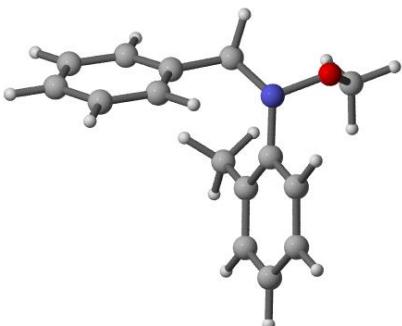
2a



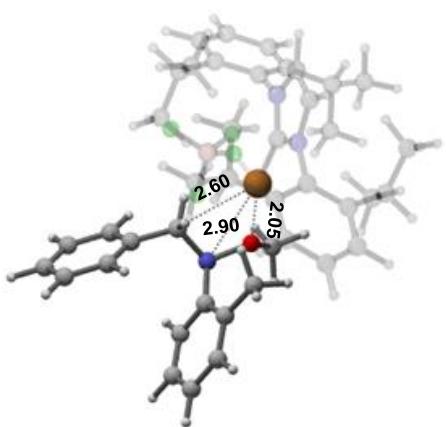
TS<sub>2a-3a</sub>



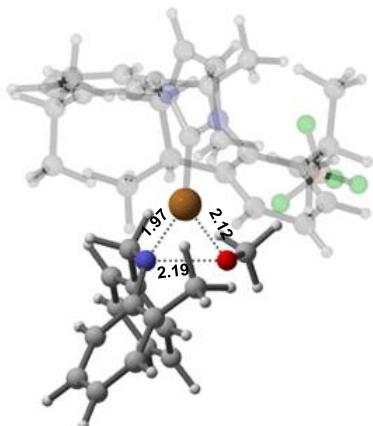
3a



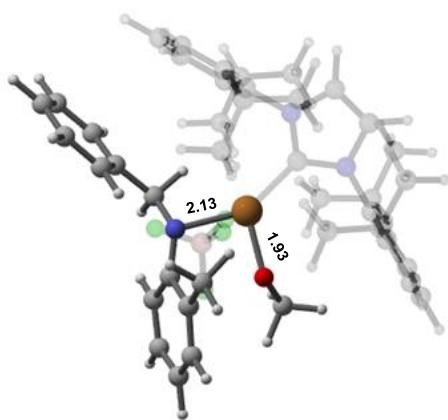
S1b



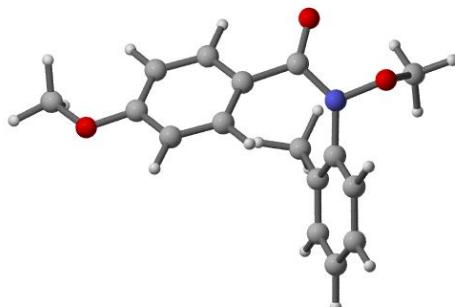
2b



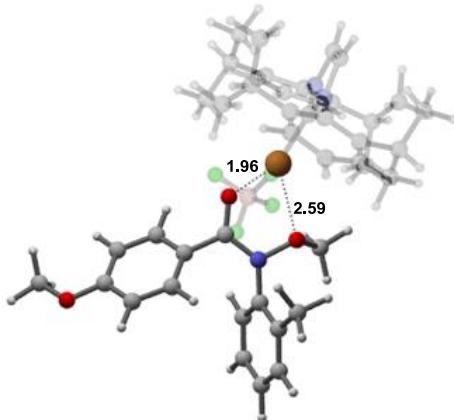
TS<sub>2b-3b</sub>



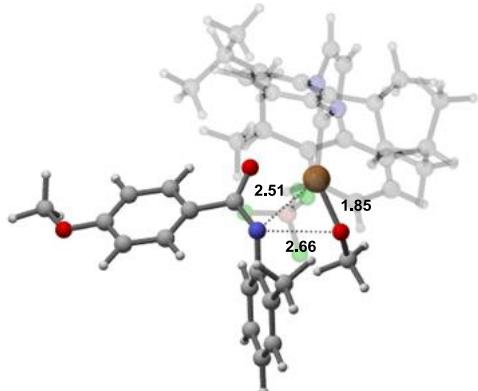
3b



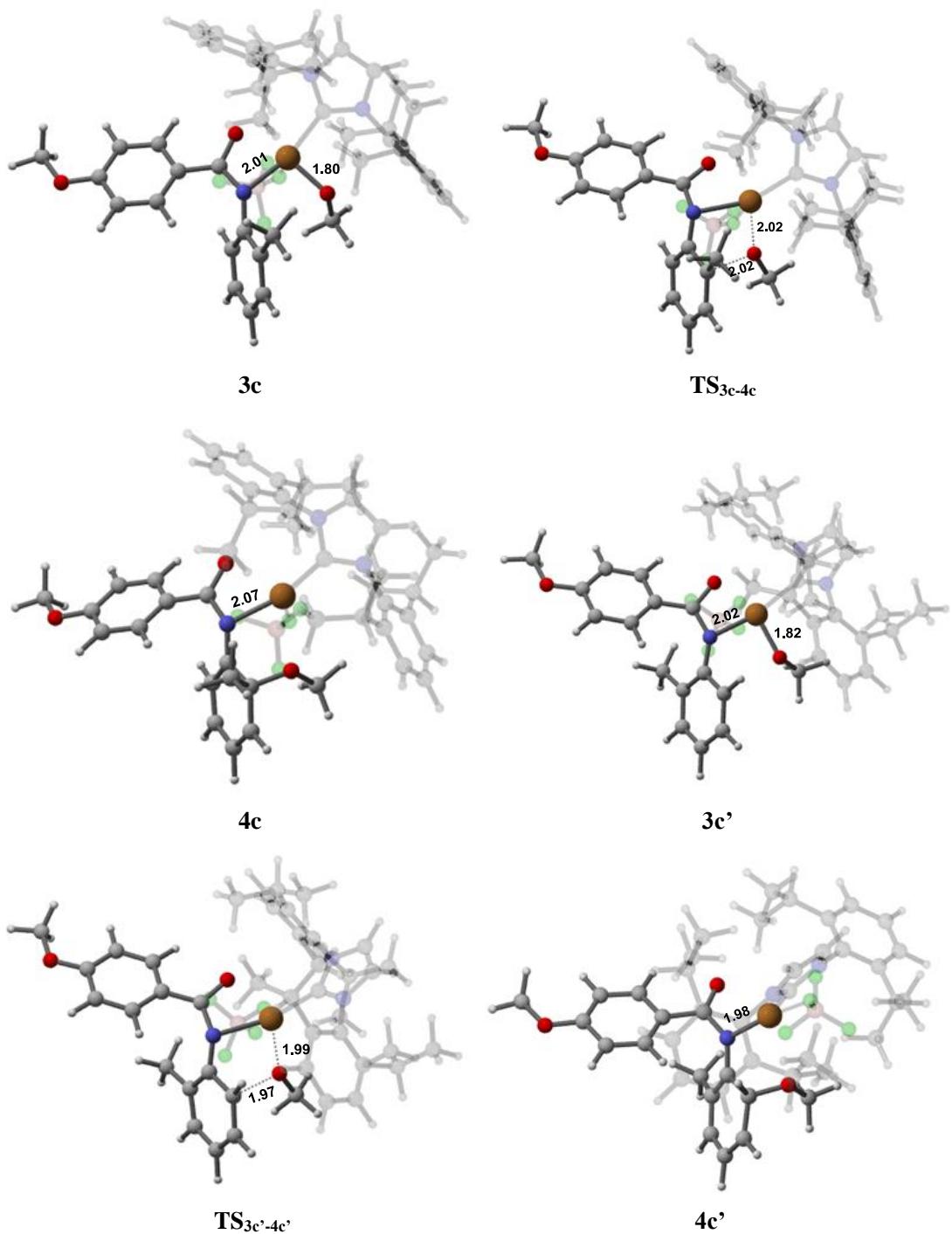
S1c

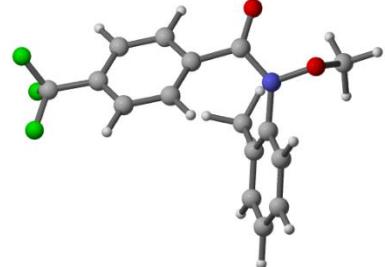


2c

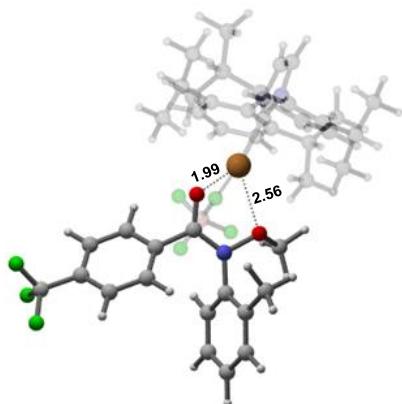


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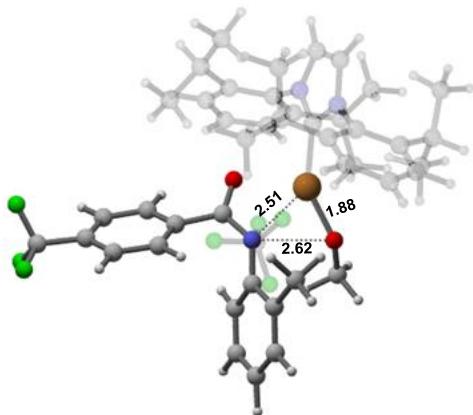




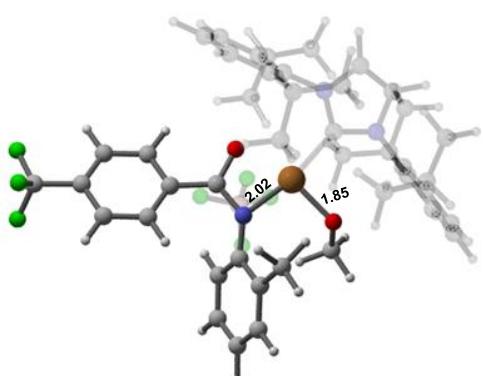
S1d



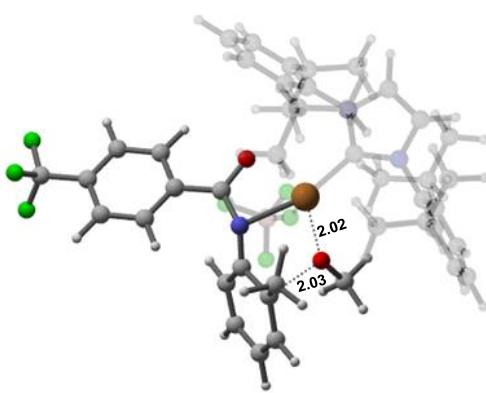
2d



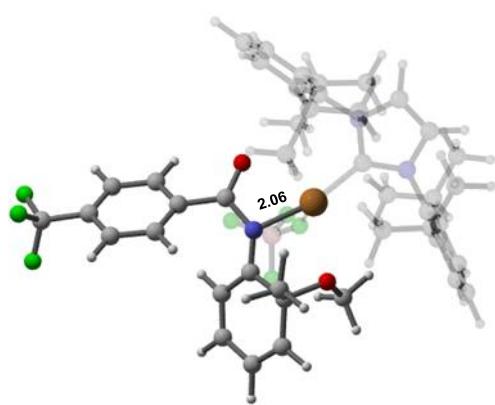
TS<sub>2d-3d</sub>



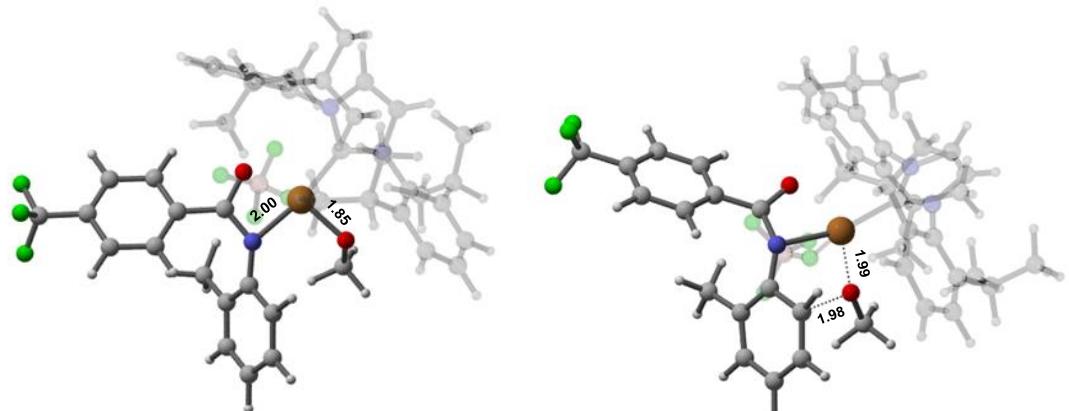
3d



TS<sub>3d-4d</sub>

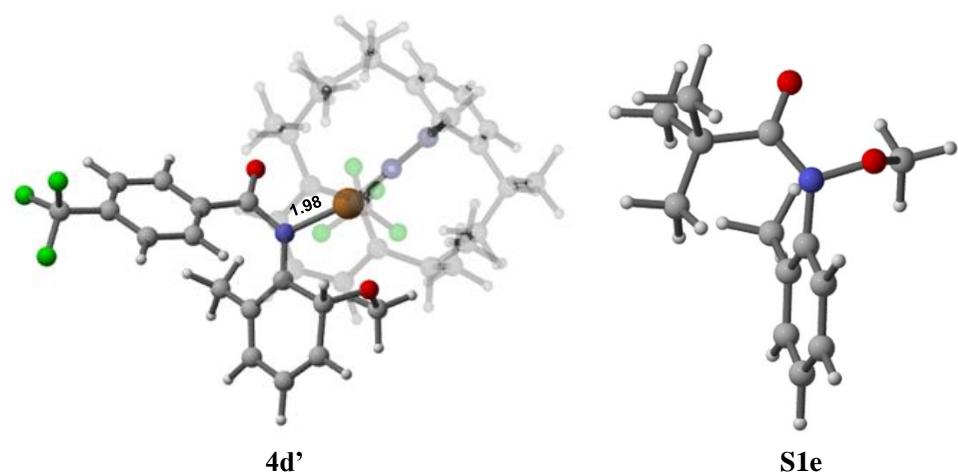


4d



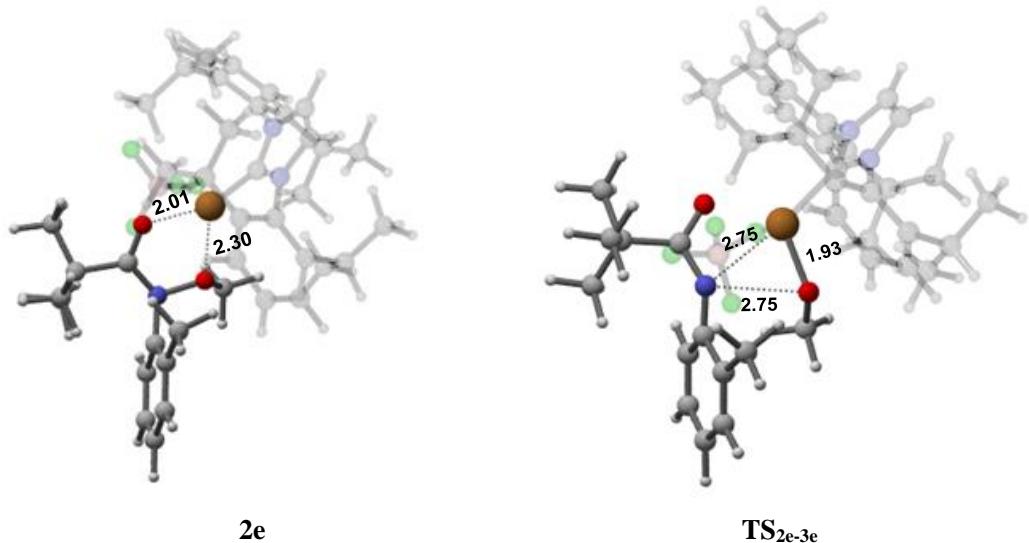
$3d'$

$TS_{3d'-4d'}$



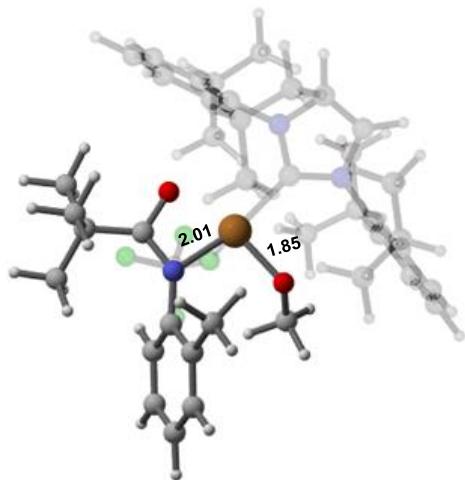
$4d'$

$S1e$

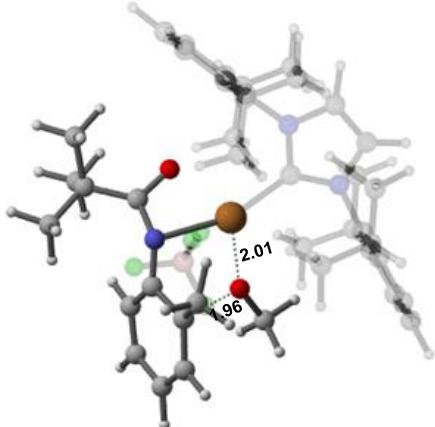


$2e$

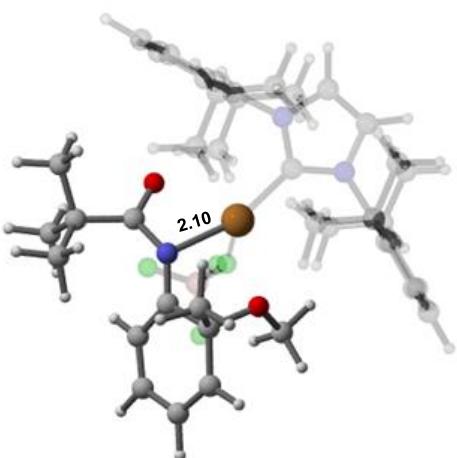
$TS_{2e-3e}$



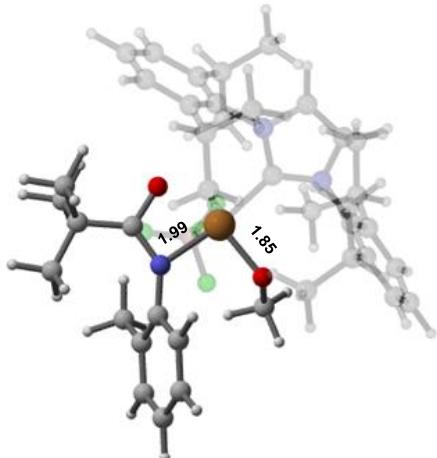
**3e**



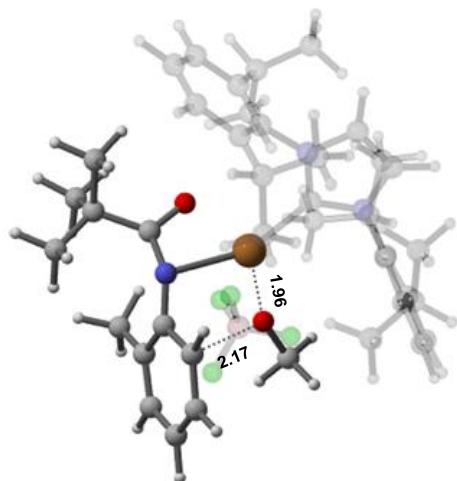
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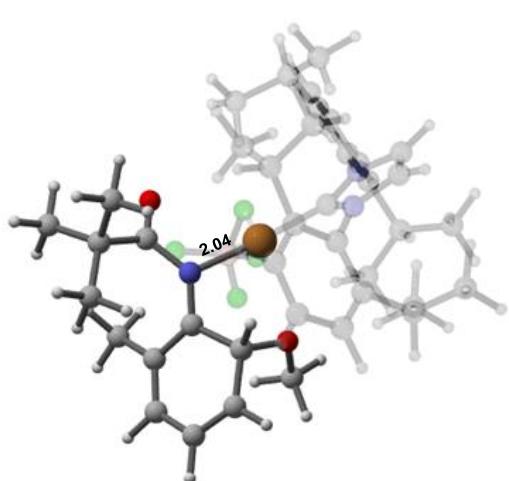
**4e**



**3e'**



**TS<sub>3e'-4e'</sub>**

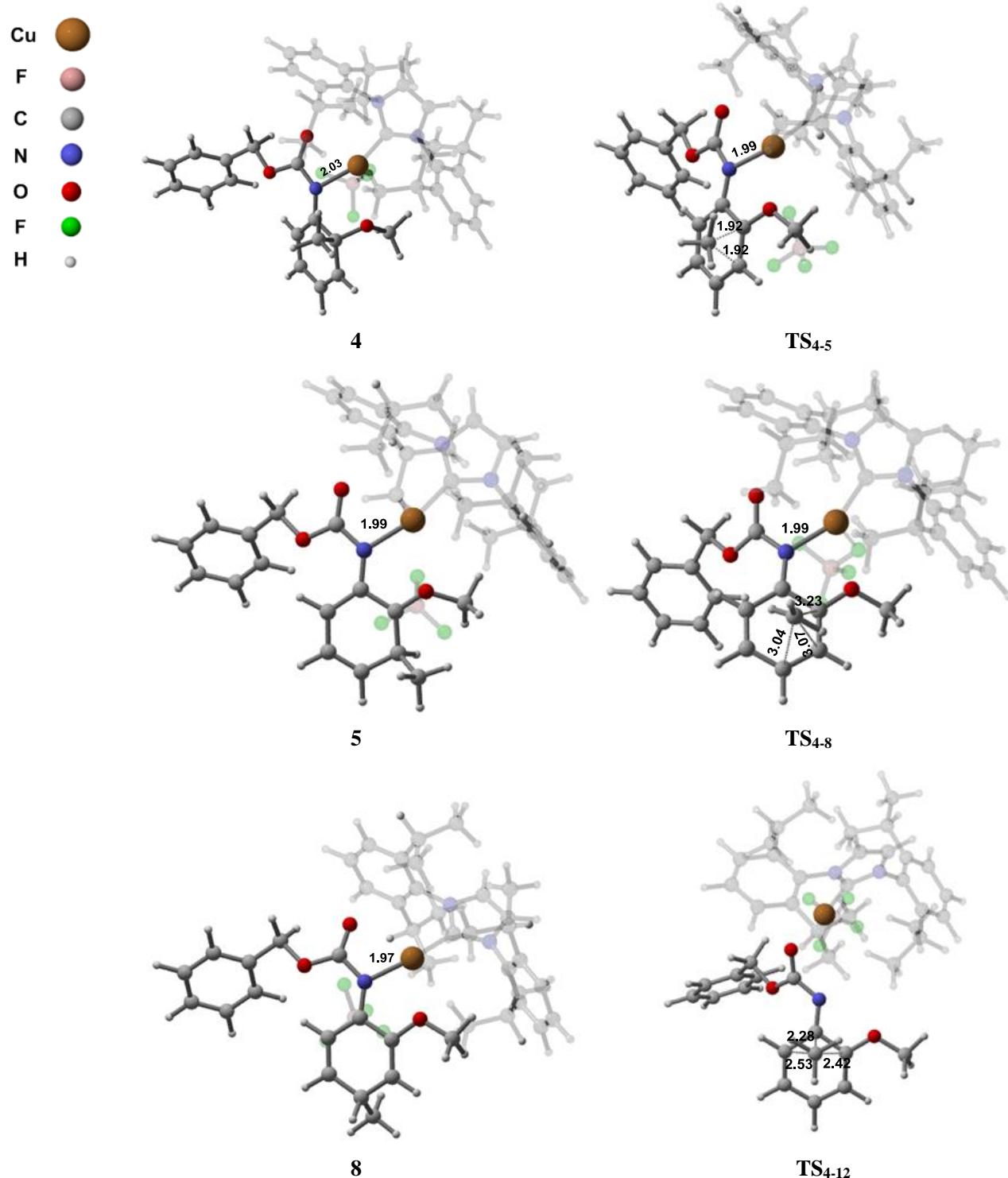


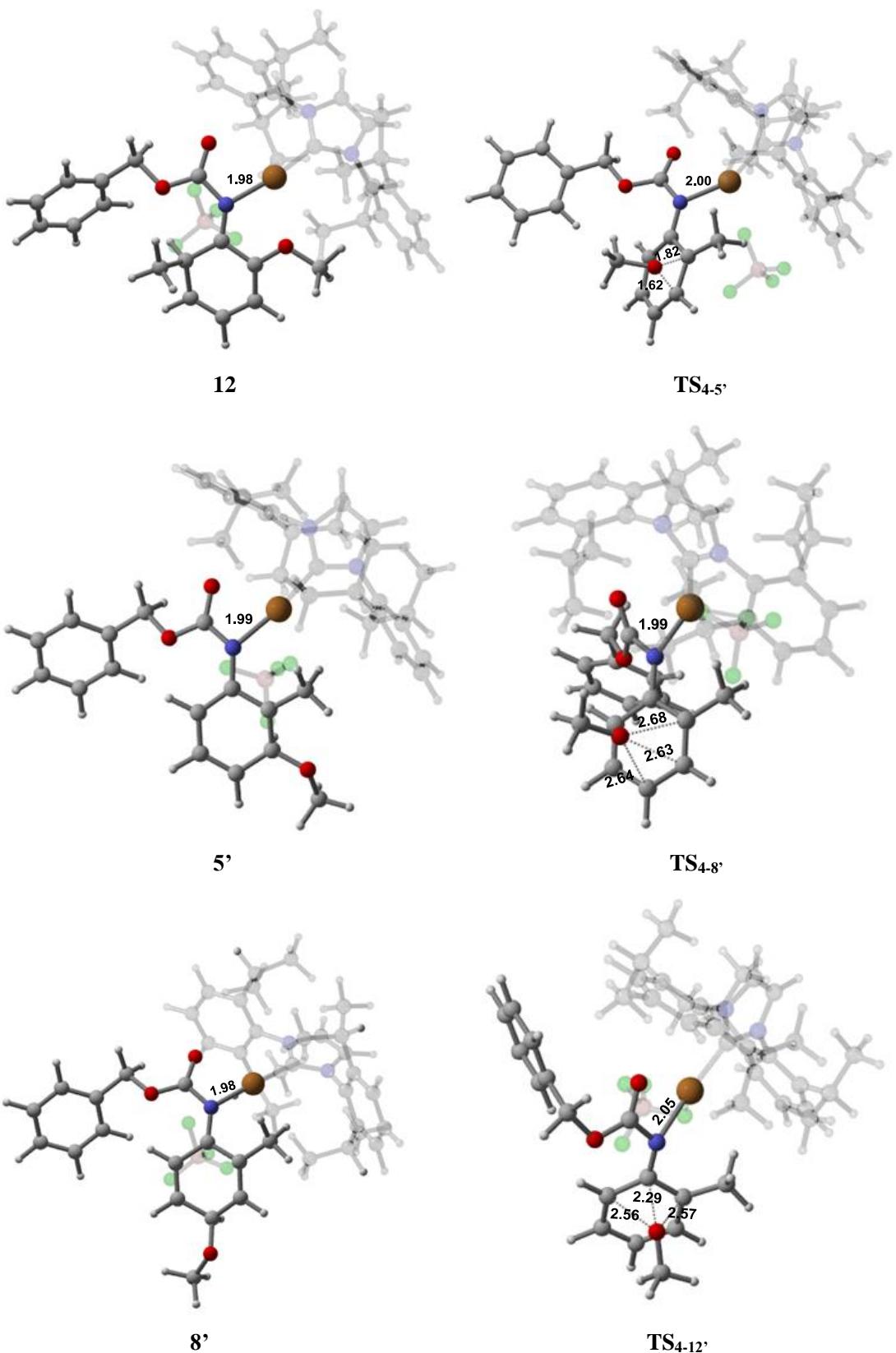
**4e'**

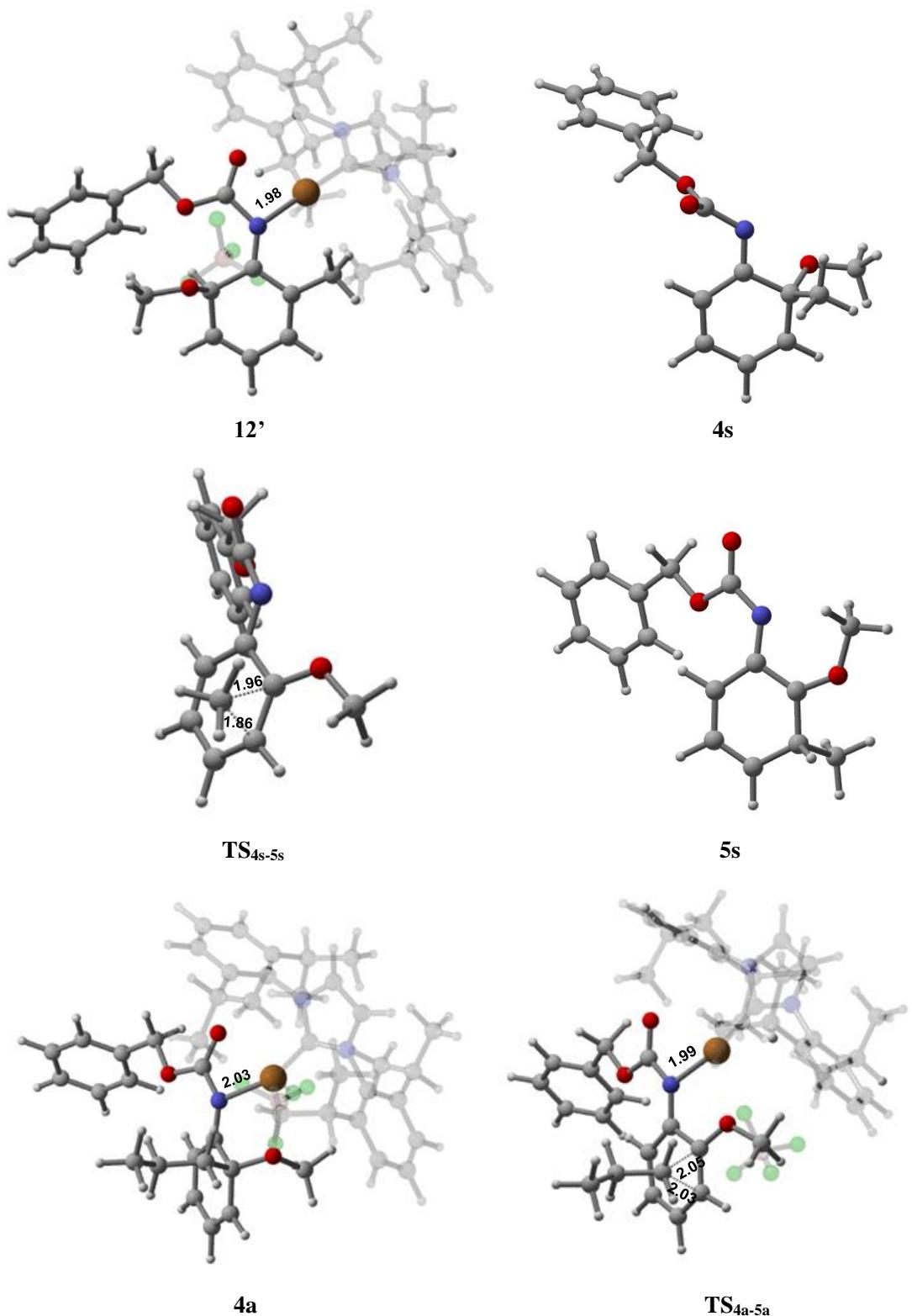
**Table S3.** The gas phase relative electronic energies ( $\Delta E_{\text{gas}}$ ), gas phase relative free energies ( $\Delta G_{\text{gas}}$ ) and solvation corrected relative electronic energies ( $\Delta E_{\text{sol}}$ ) calculated for species involved in the process of domino transfer of the methoxy group or methyl group.

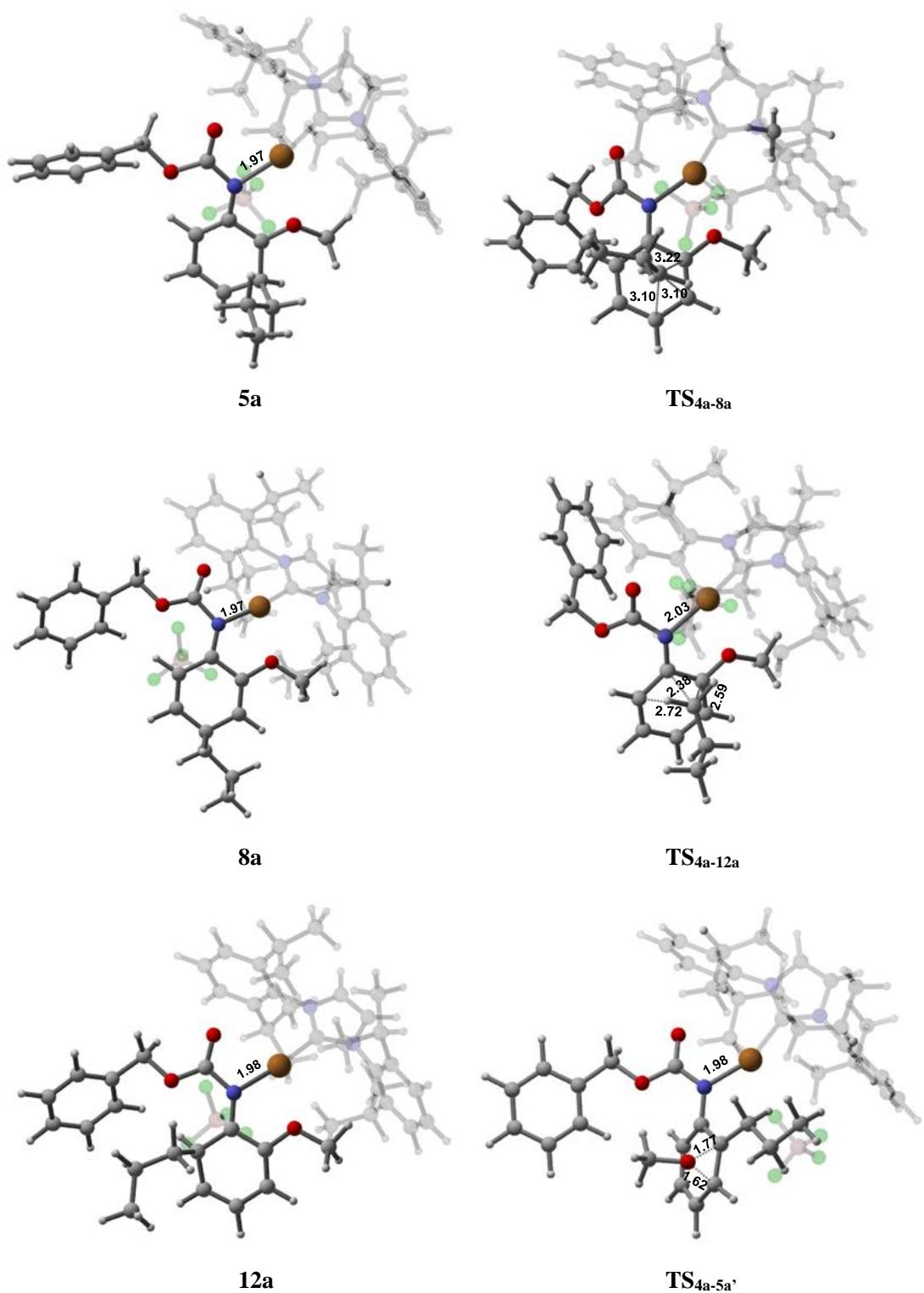
species	$\Delta G_{\text{gas}}$	$\Delta E_{\text{gas}}$	$\Delta E_{\text{sol}}$
<b>4</b>	-11.2	-30.8	-24.4
<b>TS<sub>4-5</sub></b>	24.7	6.6	8.7
<b>5</b>	-0.7	-19.1	-14.2
<b>TS<sub>4-8</sub></b>	36.6	22.3	27.7
<b>8</b>	-14.7	-36.3	-31.2
<b>TS<sub>4-12</sub></b>	36.2	23.1	26.2
<b>12</b>	-14.0	-34.7	-29.4
<b>TS<sub>4-5'</sub></b>	25.0	9.7	14.7
<b>5'</b>	9.0	-7.9	-3.0
<b>TS<sub>4-8'</sub></b>	26.8	12.2	17.0
<b>8'</b>	-10.5	-28.4	-23.5
<b>TS<sub>4-12'</sub></b>	24.0	11.8	16.2
<b>12'</b>	-7.2	-26.4	-21.1
<b>4s</b>	0.7	2.0	1.2
<b>TS<sub>4s-5s</sub></b>	39.3	41.0	37.1
<b>5s</b>	16.4	18.0	16.3
<b>4a</b>	-14.4	-34.3	-27.2
<b>TS<sub>4a-5a</sub></b>	22.2	3.2	5.3
<b>5a</b>	0.0	-20.2	-16.6
<b>TS<sub>4a-8a</sub></b>	25.6	10.8	15.4
<b>8a</b>	-17.8	-38.6	-33.3
<b>TS<sub>4a-12a</sub></b>	27.1	12.2	15.0
<b>12a</b>	-13.3	-36.4	-30.3
<b>TS<sub>4a-5a'</sub></b>	23.4	4.6	10.8
<b>5a'</b>	8.9	-8.5	-2.4
<b>TS<sub>4a-8a'</sub></b>	27.1	10.0	15.6
<b>8a'</b>	-11.6	-31.2	-25.0
<b>TS<sub>4a-12a'</sub></b>	19.5	0.8	6.9
<b>12a'</b>	-8.3	-28.8	-22.1

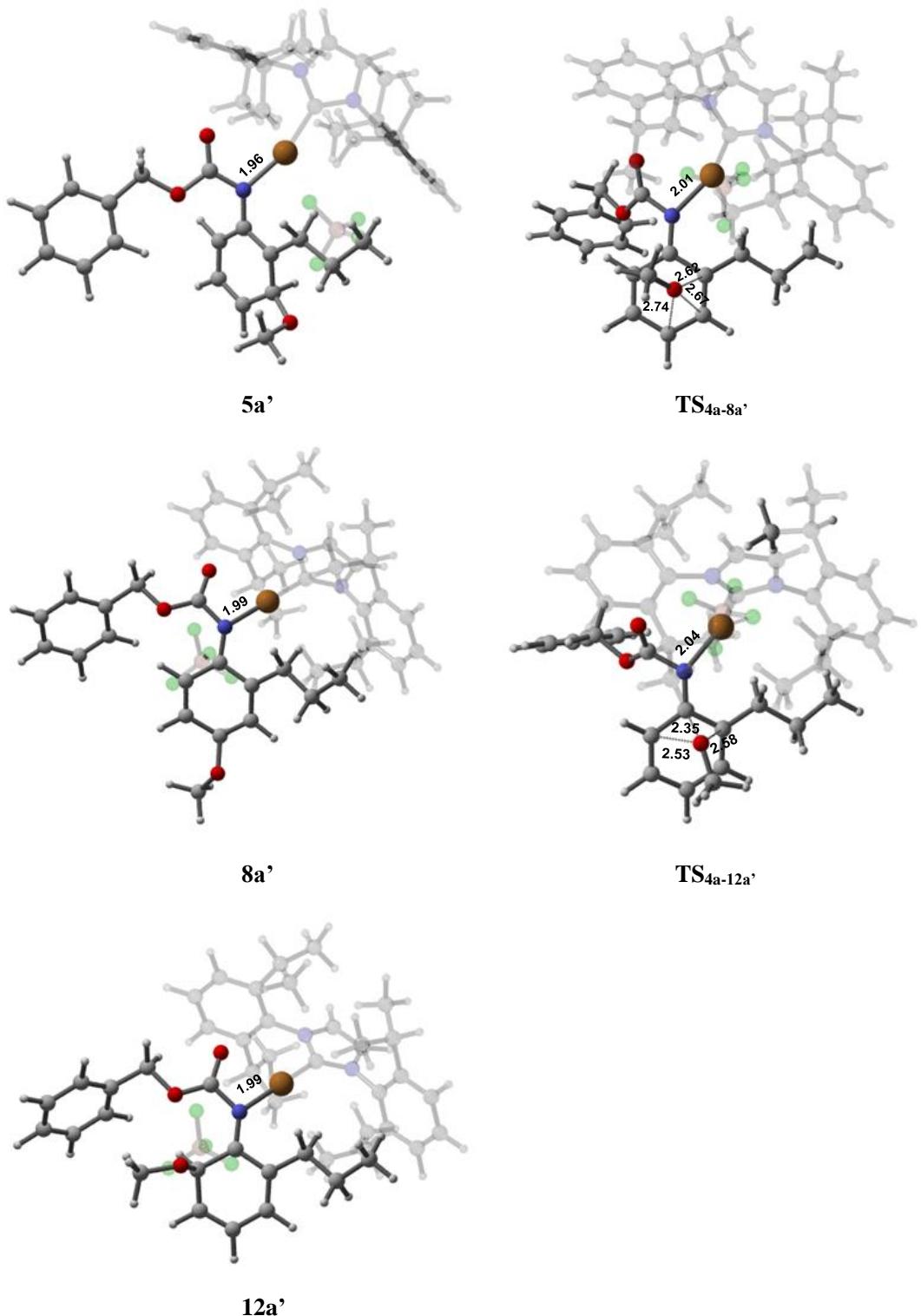
**Figure S10.** Optimized geometries with partial structural parameters (distances in Å) for the species involved in the process of domino transfer of the methoxy group or methyl group. Unimportant hydrogen and carbon atoms are transparent for clarity.







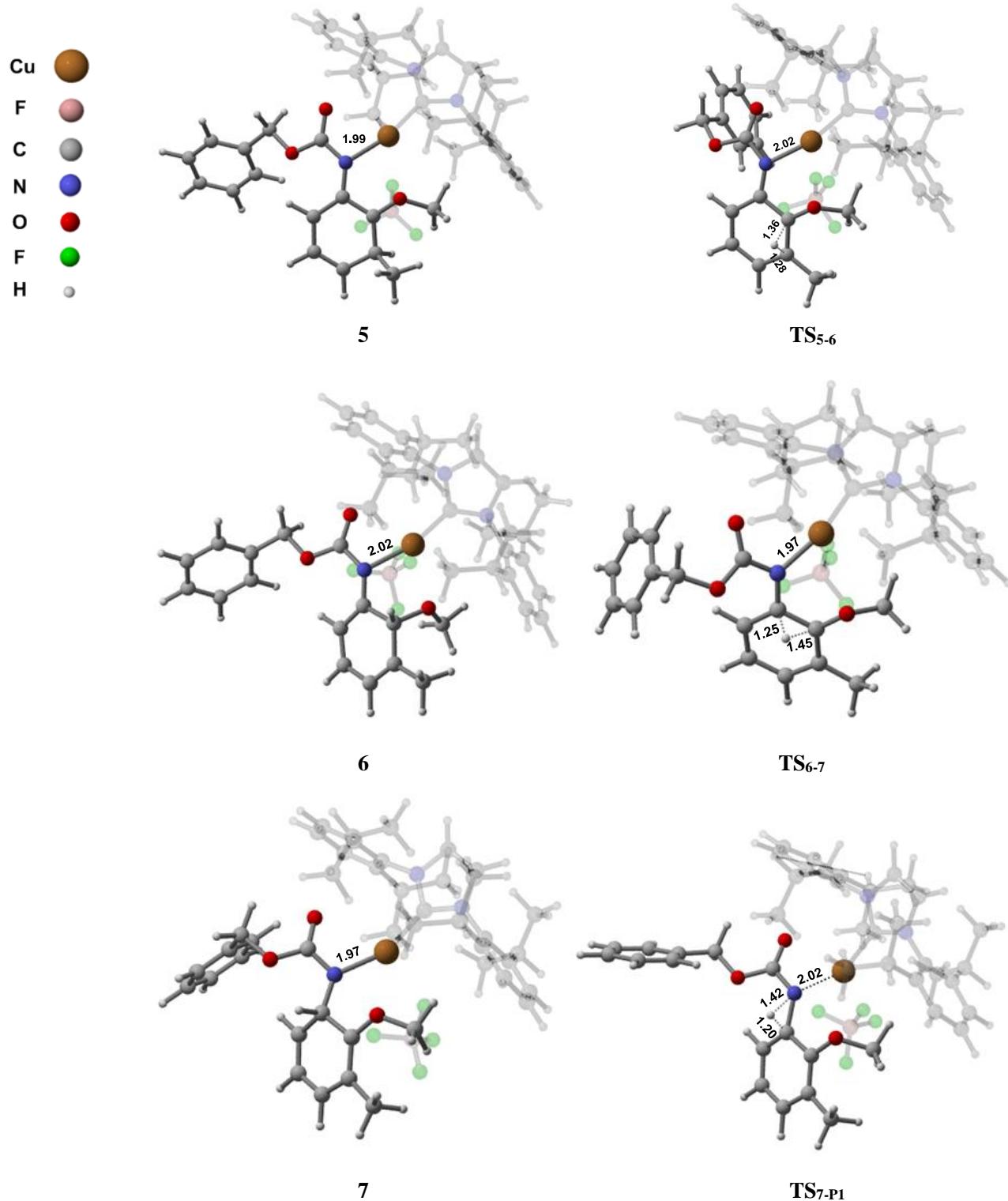


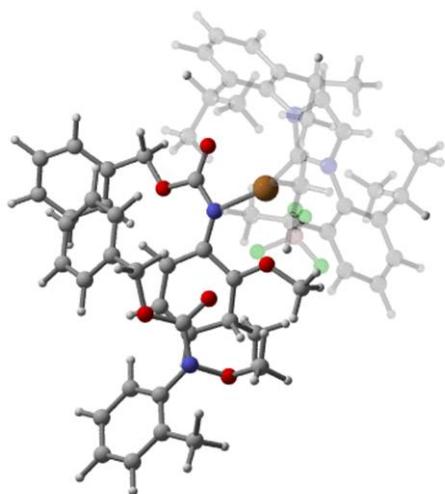
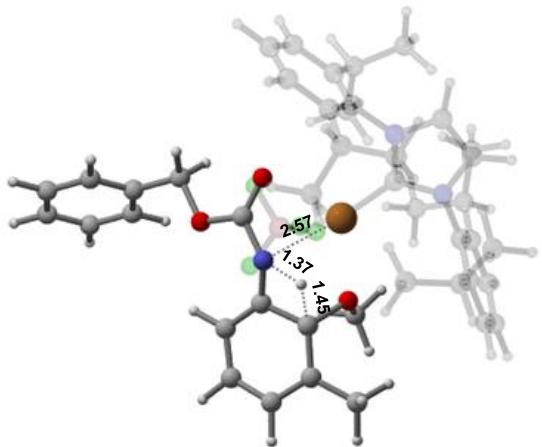


**Table S4.** The gas phase relative electronic energies ( $\Delta E_{\text{gas}}$ ), gas phase relative free energies ( $\Delta G_{\text{gas}}$ ) and solvation corrected relative electronic energies ( $\Delta E_{\text{sol}}$ ) calculated for species involved in the process of proton transfer.

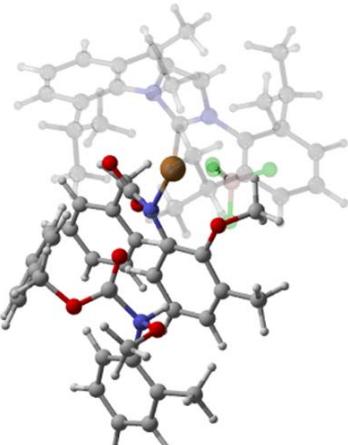
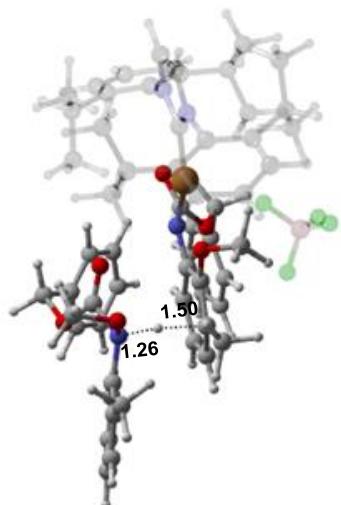
species	$\Delta G_{\text{gas}}$	$\Delta E_{\text{gas}}$	$\Delta E_{\text{sol}}$
<b>5</b>	-0.7	-19.1	-14.2
<b>TS<sub>5-6</sub></b>	10.6	-6.0	-1.1
<b>6</b>	-13.9	-32.6	-27.0
<b>TS<sub>6-7</sub></b>	16.1	-0.5	3.1
<b>7</b>	8.3	-10.5	-4.0
<b>TS<sub>7-P1</sub></b>	26.2	10.2	13.9
<b>P1</b>	-37.4	-37.8	-38.1
<b>TS<sub>6-P1</sub></b>	42.5	27.1	33.2
<b>5n</b>	0.8	-37.1	-25.6
<b>TS<sub>5n-6n</sub></b>	28.7	-5.8	-0.2
<b>6n</b>	24.1	-13.3	-7.5
<b>5s</b>	16.4	18.0	16.3
<b>TS<sub>5s-6s</sub></b>	25.6	27.7	24.8
<b>6s</b>	-4.1	-3.0	-3.4
<b>TS<sub>6s-7s</sub></b>	29.2	31.6	28.7
<b>7s</b>	18.6	19.5	18.3
<b>TS<sub>S7-P1</sub></b>	35.0	39.1	37.8
<b>TS<sub>6s-P1</sub></b>	47.8	52.8	51.5
<b>6s-N</b>	-2.0	-17.8	-12.9
<b>TS<sub>S6s-N-7s-N</sub></b>	23.6	9.2	11.6
<b>7s-N</b>	38.4	-55.9	-51.7

**Figure S11.** Optimized geometries with partial structural parameters (distances in Å) for the species involved in the process of proton transfer. Unimportant hydrogen and carbon atoms are transparent for clarity.

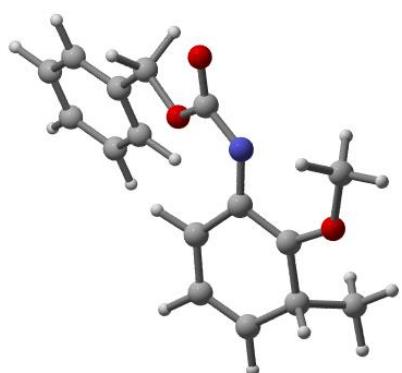




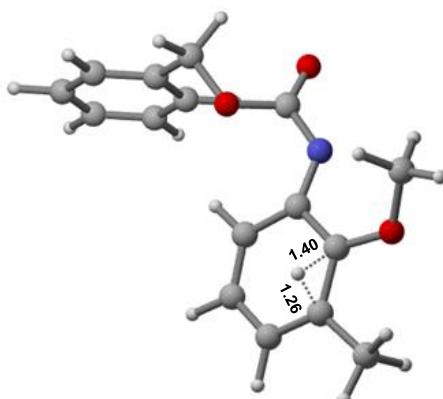
5n

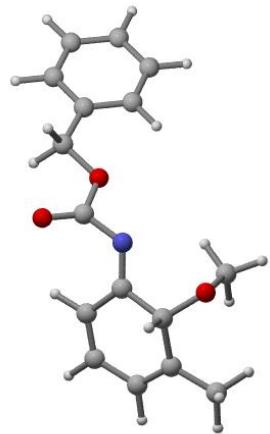


6n

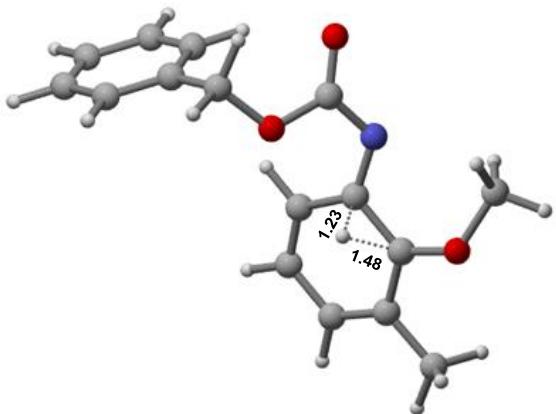


5s

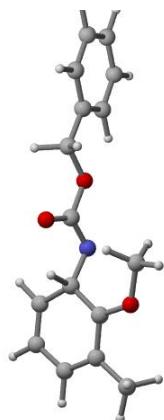




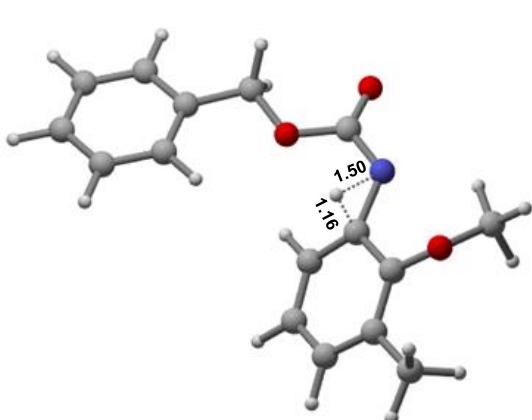
**6s**



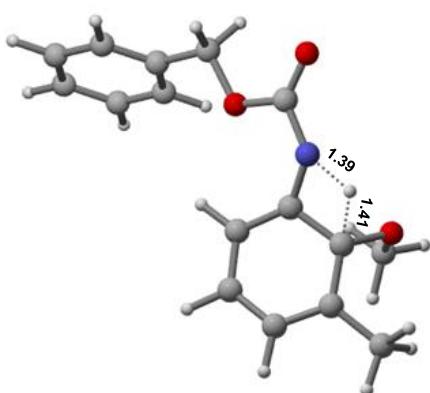
**TS<sub>6s-7s</sub>**



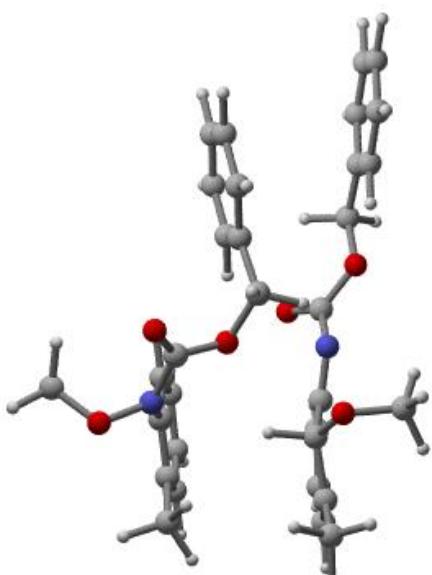
**7s**



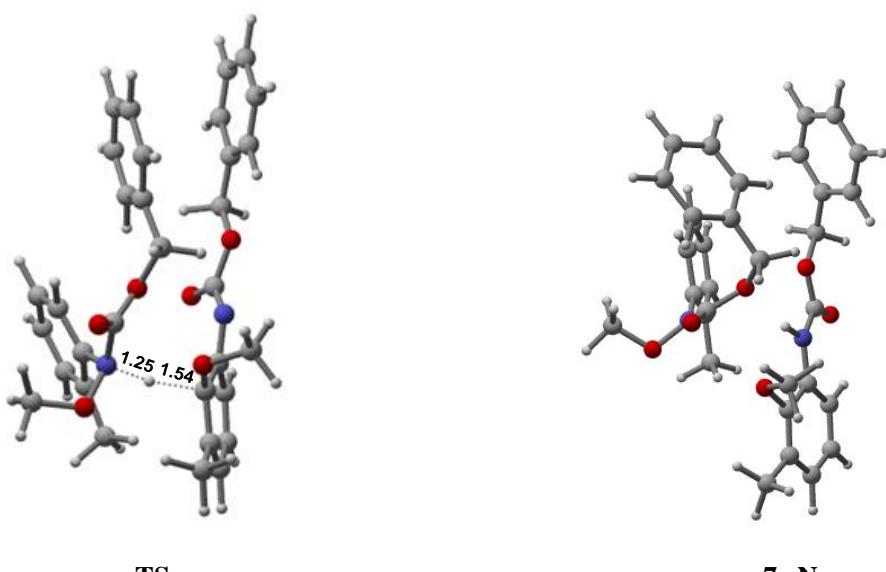
**TS<sub>7s-P1</sub>**



**TS<sub>6s-P1</sub>**



**6s-N**



**Table S5.** Absolute Calculation Energies and imaginary frequencies.

<b>species</b>	<b>E(elec-M06L)<sup>1</sup></b>	<b>G(corr-M06L)<sup>2</sup></b>	<b>H(corr-M06L)<sup>3</sup></b>	<b>E(solv-M06L)<sup>4</sup></b>	<b>IF<sup>5</sup></b>
<b>S1</b>	-900.212193	0.254086	0.319956	-900.452722	-
<b>2</b>	-2680.800954	0.808388	0.953794	-2681.467088	-
<b>TS<sub>2-3</sub></b>	-2680.765499	0.806308	0.949592	-2681.430873	-75.89
<b>3</b>	-2680.798289	0.808634	0.951554	-2681.462959	-
<b>TS<sub>3-4</sub></b>	-2680.794943	0.808803	0.950153	-2681.459892	-182.08
<b>4</b>	-2680.815563	0.811009	0.952976	-2681.480623	-
<b>3'</b>	-2680.789969	0.807161	0.951068	-2681.454765	-
<b>TS<sub>3'-4'</sub></b>	-2680.775043	0.807832	0.950335	-2681.439596	-171.21
<b>4'</b>	-2680.802374	0.810777	0.953624	-2681.466927	-
<b>S1a</b>	-785.687558	0.224796	0.285378	-785.894240	-
<b>2a</b>	-2566.277491	0.778063	0.917937	-2566.911168	-
<b>TS<sub>2a-3a</sub></b>	-2566.238551	0.774988	0.913106	-2566.872794	-82.73
<b>3a</b>	-2566.270937	0.775619	0.914913	-2566.903059	-
<b>S1b</b>	-711.639607	0.243745	0.302872	-711.829650	-
<b>2b</b>	-2492.213787	0.797257	0.935424	-2492.846231	-
<b>TS<sub>2b-3b</sub></b>	-2492.177691	0.791773	0.931648	-2492.811460	-67.40
<b>3b</b>	-2492.220125	0.791845	0.932358	-2492.839369	-
<b>S1c</b>	-900.199856	0.252189	0.320486	-900.437915	-
<b>2c</b>	-2680.790117	0.806343	0.952949	-2681.455167	-
<b>TS<sub>2c-3c</sub></b>	-2680.751830	0.805414	0.948580	-2681.417262	-86.82
<b>3c</b>	-2680.787898	0.808193	0.950936	-2681.451066	-
<b>TS<sub>3c-4c</sub></b>	-2680.780242	0.808523	0.949949	-2681.444589	-191.75
<b>4c</b>	-2680.797603	0.807289	0.952041	-2681.461477	-
<b>3c'</b>	-2680.764876	0.807599	0.951002	-2681.426857	-
<b>TS<sub>3c'-4c'</sub></b>	-2680.760612	0.808613	0.950091	-2681.424066	-193.63
<b>4c'</b>	-2680.792715	0.809422	0.952025	-2681.458289	-
<b>S1d</b>	-1122.708341	0.223348	0.293326	-1122.998514	-
<b>2d</b>	-2903.295462	0.777582	0.924828	-2904.013416	-
<b>TS<sub>2d-3d</sub></b>	-2903.260530	0.775570	0.921459	-2903.977402	-81.29
<b>3d</b>	-2903.295748	0.778581	0.923659	-2904.010277	-
<b>TS<sub>3d-4d</sub></b>	-2903.287937	0.778616	0.922737	-2904.004137	-190.74
<b>4d</b>	-2903.306404	0.778270	0.924987	-2904.021990	-
<b>3d'</b>	-2903.279419	0.777782	0.924180	-2903.992995	-
<b>TS<sub>3d'-4d'</sub></b>	-2903.268659	0.779387	0.922987	-2903.983644	-184.58
<b>4d'</b>	-2903.300400	0.777074	0.925639	-2904.017770	-
<b>S1e</b>	-711.882442	0.257320	0.318031	-712.080882	-
<b>2e</b>	-2492.480156	0.812356	0.950209	-2493.105929	-
<b>TS<sub>2e-3e</sub></b>	-2492.435389	0.804619	0.945346	-2493.060008	-414.44
<b>3e</b>	-2492.473585	0.809474	0.948362	-2493.096670	-
<b>TS<sub>3e-4e</sub></b>	-2492.464902	0.810810	0.947549	-2493.089089	-214.47
<b>4e</b>	-2492.484129	0.813455	0.950431	-2493.107893	-

<b>3e'</b>	-2492.463245	0.811605	0.948998	-2493.087886	-
<b>TS<sub>3e'-4e'</sub></b>	-2492.449383	0.811232	0.947667	-2493.073804	-59.01
<b>4e'</b>	-2492.470114	0.811179	0.948601	-2493.093756	-
<b>TS<sub>s1-ps1</sub></b>	-900.140508	0.248463	0.315967	-900.383388	-270.58
<b>TS<sub>s1-ps2</sub></b>	-900.146512	0.249115	0.316587	-900.388130	-122.90
<b>Ps1</b>	-900.208163	0.252092	0.320819	-900.450500	-
<b>Ps2</b>	-900.220576	0.254412	0.321079	-900.461247	-
<b>TS<sub>4-5</sub></b>	-2680.755870	0.808556	0.951686	-2681.427885	-612.00
<b>5</b>	-2680.796915	0.809120	0.953552	-2681.464417	-
<b>TS<sub>4-8</sub></b>	-2680.730865	0.803512	0.947835	-2681.397724	-130.58
<b>8</b>	-2680.824242	0.814048	0.954760	-2681.491594	-
<b>TS<sub>4-12</sub></b>	-2680.729622	0.800640	0.948626	-2681.399968	-214.76
<b>12</b>	-2680.821708	0.812640	0.954708	-2681.488698	-
<b>TS<sub>4-5'</sub></b>	-2680.750998	0.804132	0.949902	-2681.418417	-358.32
<b>5'</b>	-2680.779058	0.806707	0.950915	-2681.446552	-
<b>TS<sub>4-8'</sub></b>	-2680.746905	0.802734	0.948086	-2681.414653	-69.86
<b>8'</b>	-2680.811667	0.808257	0.953352	-2681.479214	-
<b>TS<sub>4-12'</sub></b>	-2680.747581	0.799036	0.947546	-2681.415911	-153.56
<b>12'</b>	-2680.808443	0.810178	0.953961	-2681.475477	-
<b>4a</b>	-2759.430082	0.862928	1.012403	-2760.119009	-
<b>TS<sub>4a-5a</sub></b>	-2759.370326	0.861482	1.011529	-2760.067162	-542.17
<b>5a</b>	-2759.407611	0.863288	1.013781	-2760.102161	-
<b>TS<sub>4a-8a</sub></b>	-2759.358183	0.854672	1.007469	-2760.051044	-60.21
<b>8a</b>	-2759.436931	0.864346	1.014168	-2760.128706	-
<b>TS<sub>4a-12a</sub></b>	-2759.355960	0.854947	1.008370	-2760.051648	82.47
<b>12a</b>	-2759.433430	0.867897	1.015035	-2760.123927	-
<b>TS<sub>4a-5a'</sub></b>	-2759.367994	0.860941	1.010397	-2760.058397	-343.64
<b>5a'</b>	-2759.388895	0.858829	1.010229	-2760.079430	-
<b>TS<sub>4a-8a'</sub></b>	-2759.359520	0.858440	1.008643	-2760.050841	-51.86
<b>8a'</b>	-2759.425042	0.862312	1.013383	-2760.115504	-
<b>TS<sub>4a-12a'</sub></b>	-2759.374153	0.861015	1.009430	-2760.064646	-119.26
<b>12a'</b>	-2759.421238	0.863729	1.013220	-2760.110794	-
<b>4s</b>	-900.208940	0.251904	0.320555	-900.4508879	-
<b>TS<sub>4s-5s</sub></b>	-900.146770	0.251255	0.318236	-900.3935257	-596.94
<b>5s</b>	-900.183511	0.251461	0.320529	-900.4266887	-
<b>TS<sub>5-6</sub></b>	-2680.775950	0.806197	0.948745	-2681.443536	-1011.50
<b>6</b>	-2680.818407	0.809508	0.952914	-2681.484866	-
<b>TS<sub>6-7</sub></b>	-2680.767293	0.806178	0.949411	-2681.436875	-944.31
<b>7</b>	-2680.783137	0.809677	0.952305	-2681.448258	-
<b>TS<sub>7-P1</sub></b>	-2680.750076	0.805086	0.948562	-2681.419664	-1363.71
<b>P1</b>	-900.272495	0.254715	0.322722	-900.513399	-
<b>TS<sub>6-P1</sub></b>	-2680.723266	0.804229	0.947146	-2681.388818	-1950.51
<b>5n</b>	-3581.037737	1.094152	1.277367	-3581.935333	-

<b>TS<sub>5n-6n</sub></b>	-3580.987925	1.088865	1.271488	-3581.894793	-991.85
<b>6n</b>	-3580.999834	1.093373	1.276227	-3581.906506	-
<b>TS<sub>5s-6s</sub></b>	-900.168097	0.250760	0.317133	-900.413127	-981.56
<b>6s</b>	-900.216958	0.252272	0.320991	-900.458129	-
<b>TS<sub>6s-7s</sub></b>	-900.161805	0.250171	0.316751	-900.406967	-845.39
<b>7s</b>	-900.181146	0.252772	0.319394	-900.423488	-
<b>TS<sub>S7s-P1</sub></b>	-900.149826	0.247558	0.316087	-900.392510	-1034.96
<b>TS<sub>6s-P1</sub></b>	-900.128117	0.246176	0.314400	-900.370623	-2027.38
<b>6s-N</b>	-1800.452747	0.533326	0.644145	-1800.926013	-
<b>TS<sub>S6s-N-7s-N</sub></b>	-1800.409640	0.531122	0.638705	-1800.886878	-1244.36
<b>7s-N</b>	-1800.513463	0.536019	0.645919	-1800.987807	-

<sup>1</sup>The electronic energy calculated by M06L in gas phase. <sup>2</sup>The thermal correction to Gibbs free energy calculated by M06L in gas phase. <sup>3</sup>The thermal correction to enthalpy calculated by M06L in gas phase. <sup>4</sup>The electronic energy calculated by M06L in toluene solvent. <sup>5</sup>The M06L calculated imaginary frequencies for the transition states.

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**Cartesian coordinates for the complexes calculated in this study: [gas phase results optimized at the level of M06L/6-31+G\* (Lanl2dz for Cu)]:**

**IPrCuBF<sub>4</sub>**

C	-3.53303900	5.51466200	0.52598000	H	-2.59860800	-1.71435700	-2.40265300
C	-3.51472700	3.32859900	-0.09708700	C	-0.37359900	0.50559700	1.99737200
C	-3.52904800	5.47849700	-0.82717700	H	0.41841800	1.21686000	1.73255400
N	-3.52375000	4.19866800	0.96821000	H	-1.13681300	1.03758300	2.57569100
N	-3.51859800	4.14025200	-1.19878000	H	0.08221900	-0.24195500	2.66098600
Cu	-3.51075900	1.44840600	0.01420300	N	1.16783900	-0.04456900	-0.40537900
H	-3.53287800	6.27040000	-1.56372200	C	2.18420000	-0.70050500	0.26276700
H	-3.54089600	6.34598100	1.21760600	O	3.36895600	-0.48647600	0.11867200
C	-3.52175100	3.80000900	2.37114200	O	1.58866000	0.56011200	-1.59836600
C	-4.75360900	3.60470500	3.04106500	C	1.77563500	1.95502000	-1.37487900
C	-2.28833300	3.63599900	3.04690200	H	2.07315900	2.35850200	-2.34592400
C	-4.71171200	3.19993900	4.38039500	H	0.83998900	2.42713800	-1.04396900
C	-2.32668400	3.23000300	4.38594900	H	2.57215500	2.12406600	-0.64021400
C	-3.51807000	3.00094700	5.05329000	H	1.64428800	-1.57790900	1.13933900
H	-5.65736900	3.03669200	4.89646900	O	2.57824700	-2.19117600	2.03290900
H	-1.37963000	3.09000300	4.90629300	C	3.27882500	-2.80131700	1.44584600
H	-3.51640500	2.67746000	6.09242000	H	3.17600800	-1.40876900	2.52015200
C	-3.51192700	3.72348200	-2.59085100	H	1.82545400	-3.01533000	3.03396200
C	-4.74043200	3.55872500	-3.26913000	C	0.45837800	-3.27645900	2.91492600
C	-2.27681900	3.56695800	-3.25873200	C	2.52762500	-3.55374600	4.11751600
C	-4.69577600	3.27202200	-4.63851700	C	-0.19126400	-4.06199700	3.86668100
C	-2.30770000	3.27979700	-4.62830900	C	-0.09791700	-2.86309300	2.07567300
C	-3.49838700	3.14317400	-5.32314700	H	1.87883600	-4.33991600	5.06392400
H	-5.64059900	3.13897900	-5.16579300	C	3.59491500	-3.35189400	4.22017300
H	-1.35765700	3.15324000	-5.14768000	H	0.51351300	-4.59638900	4.94161800
H	-3.49313700	2.92509300	-6.38960900	C	-6.45705400	5.19771000	1.97623800
C	-6.14939500	3.78227900	2.46211300	H	-6.51262500	2.70473700	1.44530800
C	-6.45705400	5.19771000	1.97623800	H	-6.23915300	5.93833300	2.75631900
C	-6.51262500	2.70473700	1.44530800	H	-5.89414100	5.47940800	1.08211200
H	-6.23915300	5.93833300	2.75631900	H	-7.52186600	5.28103400	1.72402800
H	-5.89414100	5.47940800	1.08211200	H	-6.39468000	1.70015900	1.86942200
H	-7.52186600	5.28103400	1.72402800	H	-7.55565800	2.81786200	1.12122000
H	-6.39468000	1.70015900	1.86942200	H	-5.88395500	2.75086800	0.55310400
C	-0.89400300	3.84532500	2.47483000	C	-0.89400300	3.84532500	2.47483000
C	-0.50045700	2.77123200	1.46566300	C	-0.50045700	2.77123200	1.46566300
C	-0.61542600	5.26536200	1.98540500	C	-0.61542600	5.26536200	1.98540500
H	-0.58327200	1.76778100	1.90012200	C	-1.13508900	2.78723100	0.57662300
H	-1.13508900	2.78723100	0.57662300	C	0.53667900	2.91581900	1.13516000
H	-0.85603100	6.00397300	2.76077900	H	-0.85603100	6.00397300	2.76077900
H	0.44918100	5.37194900	1.74105400	H	-1.17761900	5.53093400	1.08616200
H	-1.17761900	5.53093400	1.08616200	C	-6.12661300	3.52722100	-2.64664400
C	-6.39450700	2.12228300	-2.09887900	C	-6.39450700	2.12228300	-2.09887900
C	-6.46979500	4.61128300	-1.63438100	H	-6.31772100	1.36705300	-2.88940900
H	-6.31772100	1.36705300	-2.88940900	H	-5.66580400	1.84636500	-1.32511100
H	-7.39575500	2.05488000	-1.65497300	N	-7.39575500	2.05488000	-1.65497300
H	-6.23070000	5.61497100	-2.00838500	C	-6.23070000	5.61497100	-2.00838500
H	-7.54535200	4.58394000	-1.41725300	O	-5.64027800	-2.00100000	-1.41725300
H	-5.95377700	4.47415000	-0.68254900	O	-1.08997100	4.50738900	-0.66804800
C	-0.89583100	3.54776300	-2.62456400	C	-0.50523900	4.62606300	-1.39312300
C	-0.56903700	4.64180300	-1.61752500	H	-0.68751300	1.38818600	-2.85435300
C	-0.62080400	2.14789300	-2.06721800	H	-0.37846100	2.09023500	-1.61759800
H	-0.81489200	5.64027800	-2.00100000	H	-1.35142700	1.87119400	-1.29502600
H	-1.08997100	4.50738900	-0.66804800	Cu	-6.81922800	3.62132400	3.31976500
H	-0.50523900	4.62606300	-1.39312300	H	-0.22535300	3.70367300	3.33678200
H	-0.68751300	1.38818600	-2.85435300	H	-0.19981100	3.69216000	-3.46485900
H	-0.37846100	2.09023500	-1.61759800	N	-3.50268900	-1.22677800	0.17918200
H	-1.35142700	1.87119400	-1.29502600	C	-2.38788300	-0.27643400	0.28433700
H	-6.81922800	3.62132400	3.31976500	C	-4.62883900	-0.29119200	0.03464300
H	-0.22535300	3.70367300	3.33678200	F	-3.36974100	-1.97330200	-0.95308100
H	-6.81689300	3.67196400	-3.49161900	C	-2.382414100	-0.48530500	0.78801200
H	-0.19981100	3.69216000	-3.46485900	C	-0.97076500	-0.12844800	0.78801200
B	-3.50268900	-1.22677800	0.17918200	C	-0.97076500	-0.12844800	0.78801200
F	-3.62946900	-1.93589400	1.33424700	C	-0.97076500	-0.12844800	0.78801200
F	-2.38788300	-0.27643400	0.28433700	C	-0.21375300	-0.39140000	-0.37313300
F	-4.62883900	-0.29119200	0.03464300	C	-2.14713000	-1.27794400	-1.51342300
F	-3.36974100	-1.97330200	-0.95308100	H	-2.91182800	-1.05380700	-0.36916700

**2**

C	-1.96068700	6.13088200	-2.62318200
C	-2.50114900	5.89856700	-1.36072700
C	-2.13423600	4.78212600	-0.60320400
C	-1.20859700	3.89616500	-1.17747900
C	-0.67489000	4.10405900	-2.44966600
C	-1.04158900	5.23554800	-3.16772900
C	-2.25992800	7.01520600	-3.18364400
C	-3.21539600	6.60561100	-0.93806300
C	0.01439800	3.36618300	-2.85414800
C	-0.62259300	5.40652900	-4.15741600
C	-2.70533700	4.54197400	0.75827500
C	-3.11763000	5.46523000	1.17899100
C	-3.51174700	3.79676100	0.73642000
C	-1.94870700	4.15080200	1.44860000
C	-0.80253900	2.73299000	-0.46563900
C	0.44754100	2.43524800	-0.04039800
O	0.75688700	1.39093200	0.55024900
O	-1.78613600	1.80022800	-0.06847000
C	-2.59187000	1.41603500	-1.19785300
C	-1.97004900	1.02703800	-2.00963600
H	-3.24921300	0.64100900	-0.79576800
C	-0.44754100	2.43524800	-0.04039800
O	-0.63552700	-3.94805700	2.33136300
C	-0.45426900	-2.10915400	0.99816000
C	-0.29902500	-4.37513300	1.09176500
N	-0.72713200	-2.56347400	2.27073700
N	-0.19169900	-3.25076000	0.28776200
Cu	-0.23235900	-0.30947900	0.41975400
H	-0.12838000	-5.36824300	0.69910800
H	-0.81980800	-4.48896600	3.24955600
C	-1.05837600	-1.72694000	3.41640700
C	-0.02660000	-1.27026300	4.27158500
C	-2.41389800	-1.41936900	3.68438600
C	-0.38750500	-0.46637200	5.36016400
C	-2.69852300	-0.61095000	4.79153600
C	-1.70360000	-0.12586600	5.62336300
H	0.40494300	-0.10507300	6.01520800
H	-3.74101500	-0.36698400	4.99478000
H	-1.95298000	0.50238100	6.47676300
C	0.17192800	-3.34629900	-1.11851800
C	1.53079900	-3.28981700	-1.49202400
C	-0.84462500	-3.56054100	-2.07288700
C	1.84056400	-3.47732100	-2.84299800
C	-0.46218200	-3.74704200	-3.40489300
C	0.86549800	-3.71187500	-3.79621300
H	2.88518300	-3.40464600	-3.14503100
H	-1.24455700	-3.89631300	-4.14922700
H	1.13713600	-3.84002300	-4.84233000

**Substrate S1**

C	-2.32414100	-0.48530500	0.75628700
C	-0.97076500	-0.12844800	0.78142300
C	-0.21375300	-0.39140000	-0.37313300
C	-0.79762400	-0.94891200	-1.51305100
C	-2.14713000	-1.27794400	-1.51342300
C	-2.91182800	-1.05380700	-0.36916700
H	-2.92925700	-0.28820400	1.64171400

C	1.46423600	-1.55152500	4.14926400	Cu	-0.18005700	0.36895800	-0.53118700
C	1.84336400	-3.02896500	4.23828100	H	1.08167600	-4.48010500	0.76391700
C	2.10672400	-0.82761000	2.97013900	H	0.46655000	-3.16136200	3.13356600
H	1.39775300	-3.49605800	5.12621600	C	0.02093700	-0.39400300	2.71139700
H	1.53616200	-3.60986600	3.36557400	C	1.12418000	0.21398700	3.35480000
H	2.93316600	-3.12706400	4.32116700	C	-1.29703900	0.07285900	2.91709200
H	1.95203500	0.25578400	3.04001800	C	0.88174100	1.39670800	4.06376500
H	3.18733800	-1.02050100	2.94033400	C	-1.46354000	1.25820600	3.64269000
H	1.68669900	-1.14377700	2.01198700	C	-0.38630000	1.94448700	4.17823300
C	-3.62773200	-1.88023500	2.89131800	H	1.72782400	1.88995700	4.54284800
C	-3.71738500	-1.23085400	1.51390300	H	-2.47624700	1.63718100	3.78433500
C	-3.82230100	-3.39500500	2.86176400	H	-0.53730300	2.87900700	4.71679000
H	-3.71107500	-0.13684400	1.60338300	C	0.90221800	-2.86537200	-1.47162300
H	-2.87940400	-1.50828800	0.86922500	C	2.19747300	-2.86882000	-2.04253800
H	-4.64372000	-1.52928100	1.00453500	C	-0.23214100	-3.22781500	-2.22733900
H	-3.81075800	-3.81188900	3.87698600	C	2.30707900	-3.18247800	-3.39986100
H	-4.79262600	-3.63875200	2.41054800	C	-0.04322800	-3.54110000	-3.57956800
H	-3.05796400	-3.91525400	2.27909700	C	1.20456000	-3.50603700	-4.17394500
C	2.71682500	-2.93355600	-0.61017300	H	3.29554500	-3.14336900	-3.85564700
C	2.88285500	-1.41227000	-0.55431800	H	-0.91996200	-3.80974300	-4.16978400
C	2.77446500	-3.56970500	0.77099900	H	1.32112500	-3.73390400	-5.23202300
H	2.94806500	-0.98039100	-1.55963100	C	2.53570000	-0.34233700	3.50404800
H	2.02525500	-0.93200300	-0.06488100	C	2.56251400	-1.43547600	4.57824000
H	3.78536900	-1.13920000	0.00992800	C	3.28041600	-0.78098400	2.25632400
H	2.61692600	-4.65550500	0.73112200	H	2.03220500	-1.12938700	5.48822100
H	3.76007400	-3.39181700	1.22125700	H	2.10815300	-2.36618300	4.21869800
H	2.03602400	-3.14900100	1.45551000	H	3.59900700	-1.67060100	4.85047300
C	-2.34214600	-3.45059900	-1.84088600	H	3.35686700	0.03031500	1.53100300
C	-2.93136100	-4.14314600	-0.61942400	H	4.29453100	-1.10271400	2.52996900
C	-2.73147900	-1.97263100	-1.88736200	H	2.80618000	-1.62822800	1.75334600
H	-2.58108000	-5.17813700	-0.51819100	C	-2.58319400	-0.63330400	2.51065000
H	-2.69757600	-3.61582700	0.30813800	C	-2.95753200	-0.45499500	1.04598600
H	-4.02610200	-4.16721300	-0.70171700	C	-2.64848200	-2.09347300	2.95669400
H	-2.44331100	-1.51204400	-2.83960000	H	-2.98417700	0.60219300	0.75635200
H	-3.81298600	-1.84238000	-1.74028300	H	-2.24225000	-0.94475700	0.38115600
H	-2.20190900	-1.41522800	-1.10423900	H	-3.94448400	-0.89386500	0.84501500
B	0.61173400	0.46678400	-2.94772000	H	-2.41175200	-2.19507800	4.02360800
F	0.01982100	-0.27921400	-1.85598600	H	-3.66063100	-2.48716500	2.79912400
F	-0.43263700	1.06085500	-3.66317000	H	-1.96453100	-2.73924600	2.39790600
F	1.42914400	1.47259100	-2.37873700	C	3.50360600	-2.53237400	-1.34321600
F	1.35972100	-0.38911100	-3.72963400	C	3.85890300	-3.44156800	-0.16776600
O	1.30219100	3.42711000	-0.26713100	H	3.77054800	-4.50189400	-0.44054600
C	2.70667700	3.07527400	-0.12347700	H	4.89866800	-3.26043200	0.13375200
H	2.83944000	2.07366700	-0.54763300	H	3.23999500	-3.26922400	0.71632300
H	2.94721600	3.04366300	0.94649100	C	-1.68899200	-3.25723500	-1.78793500
C	3.50223000	4.11002700	-0.84910100	C	-2.00086000	-3.67949000	-0.35977700
C	3.35417600	4.25918200	-2.23328500	C	-2.35089600	-1.92955600	-2.16024700
C	4.40638000	4.92439500	-0.16653200	H	-1.50882700	-4.62413600	-0.09601900
C	4.10009700	5.21315300	-2.91674700	H	-1.70773200	-2.93265000	0.38083400
H	2.65210200	3.61548800	-2.76249800	H	-3.08359500	-3.82443800	-0.24910600
C	5.16143800	5.87424800	-0.85295700	H	-2.28959400	-1.75168300	-3.24056400
H	4.51935100	4.81332400	0.91262100	H	-3.40855300	-1.91275700	-1.86536900
C	5.00667000	6.02124400	-2.22895100	H	-1.85378600	-1.08184800	-1.67367100
H	3.98023000	5.32312400	-3.99346900	B	1.89626700	1.16324900	-3.25378200
H	5.86580600	6.50348800	-0.31078800	F	1.01033100	0.35752600	-2.43036700
H	5.59186400	6.76552900	-2.76724200	F	1.11816500	1.99728200	-4.05374800
H	-4.48574600	-1.49142600	3.46016500	F	2.68327800	1.95483200	-2.37870300
H	1.89695600	-1.09390300	5.05182500	F	2.69441800	0.31621700	-3.99903100
H	-2.80098300	-3.93339600	-2.71731400	O	2.36134400	3.49857100	0.24381100
H	3.59130900	-3.31952600	-1.15623800	C	3.75961700	3.14333400	0.42610100
				H	3.94401500	2.22667000	-0.14506900
				H	3.91974000	2.93434000	1.49306100
				C	4.57800300	4.29475000	-0.05630300
<b>TS2-3</b>				C	4.72119800	4.50897300	-1.43252200
C	-1.02161900	5.99501100	-2.29842000	C	5.19420300	5.17046000	0.83988500
C	-1.82651500	5.53530900	-1.24153500	C	5.46992700	5.58455100	-1.89871900
C	-1.44579300	4.46504600	-0.45334100	C	4.24408900	3.81878300	-2.12859400
C	-0.17097000	3.84368200	-0.71636700	H	5.94903500	6.24477800	0.37329100
C	0.59835100	4.28150400	-1.84473900	C	5.08235100	5.00611800	1.91247200
C	0.18140600	5.36129800	-2.60397100	H	6.08552300	6.45402600	-0.99730100
H	-1.35822200	6.84042200	-2.89675000	C	5.58073100	5.74183800	-2.97056300
H	-2.77519300	6.03173700	-1.03720100	H	6.42859400	6.92007200	1.08037200
H	1.51221800	3.74732800	-2.09115200	H	6.67520500	7.29311500	-1.36380300
H	0.77848900	5.68518300	-3.45340300	H	3.11283200	0.49860000	3.91882600
C	-2.28795700	3.94732000	0.65714200	H	-3.36378600	-0.11369800	3.08746300
H	-3.23695400	4.48982200	0.72734500	H	-2.15101000	-4.02535600	-2.42779700
H	-2.48580400	2.87849900	0.50110800	H	3.60973700	-1.04539300	-1.02154600
H	-1.76549500	4.01991600	1.61937500	C	3.62342600	-0.45309200	-1.94078400
N	0.19105100	2.82987400	0.08217700	H	2.76664700	-0.68393600	-0.42783700
C	1.51354000	2.45395700	0.21442900	H	4.53210200	-0.83948700	-0.46065300
O	1.85660700	1.29862900	0.42181600	H	4.27467200	-2.73762100	-2.10078800
O	-1.58032600	1.35123400	-1.28385300				
C	-1.57808000	1.87942900	-2.53688300				
H	-1.32311200	1.16453500	-3.33535700				
H	-2.54156500	2.38440300	-2.73540200				
H	-0.81470500	2.69977100	-2.62617200				
C	0.53267800	-2.80323000	2.11618100				
C	0.36582000	-1.29380000	0.42622900				
C	0.82758400	-3.44755700	0.96063000				
N	0.25412000	-1.48696400	1.78066000				
N	0.73518000	-2.51772600	-0.06322100				
			H	-2.67856800	6.12637300	-3.65796000	

H	-2.89711900	5.83885300	-1.20773700	C	6.00371000	4.83158000	-4.27710300
H	0.41966800	3.15349400	-3.75452400	H	5.86639600	3.89661000	-2.33725200
H	-1.02939500	4.76182300	-4.93961100	C	5.42711900	4.95693600	-5.53882900
C	-1.51359600	4.12919500	0.40100000	H	3.82398300	4.32993600	-6.83908400
H	-2.27165500	4.79240900	0.83081500	H	6.90431100	5.39099800	-4.02849600
H	-1.79992200	3.08777700	0.60286200	H	5.87744900	5.61472400	-6.28080900
H	-0.56572000	4.28713500	0.93184100	H	3.37325000	1.18356700	3.17022800
N	0.37945900	2.72676600	-1.07751600	H	3.63823400	-2.76476200	-2.11303500
C	1.57433800	2.24984400	-1.49673700	H	3.37485600	-0.08751300	3.81065800
O	1.87937200	1.09877200	-1.08224300	H	3.14589900	-3.66522300	-1.68797000
O	-1.94281000	0.84475000	-0.34183200				
C	-2.74079700	1.40603300	-1.30993200				
H	-3.20582400	0.63846600	-1.95293600	C	4.43142500	-0.34396000	-1.40972300
H	-3.52269900	2.03084700	-0.83516100	C	3.96570500	-1.11087200	-0.37423700
H	-2.19429800	2.08601200	-1.99916600	C	3.05409600	-0.57655100	0.57847600
C	0.98975500	-2.60766000	1.72660300	C	2.66795600	0.82491800	0.42987700
C	0.07232700	-0.93371200	0.50002600	C	3.18163000	1.59748600	-0.65705900
C	-0.35361700	-2.74597300	1.78882700	C	4.03969900	1.01923000	-1.55023800
N	1.24560200	-1.49590500	0.93806900	H	5.12679600	-0.77214300	-2.13021800
N	-0.90663600	-1.71553500	1.04487100	H	4.29114600	-2.14447900	-0.25774500
Cu	-0.07714300	0.78385300	-0.59547200	H	2.84311400	2.62523700	-0.78610900
H	-0.97865500	-3.47438400	2.28650400	H	4.41518500	1.60256300	-2.38855000
H	1.79419300	-3.18759100	2.15772900	C	2.89217100	-1.26181100	1.89258200
C	2.60759400	-1.04194500	0.66886100	H	2.71269900	-2.33511900	1.75421400
C	3.30746500	-1.57807700	-0.43378500	H	2.07367900	-0.82882100	2.47164900
C	3.20773400	-0.10548500	1.53961200	H	3.81576900	-1.16317200	2.48019800
C	4.61270200	-1.12370000	-0.65618700	N	1.68150100	1.21588100	1.23304600
C	4.51606600	0.30209100	1.25568300	C	1.11182400	2.47007600	1.15060800
C	5.21851500	-0.19001000	0.16772300	O	0.09228300	2.49460100	0.85092800
H	5.15445100	-1.52228100	-1.51379200	O	-1.15100300	-1.01612100	-0.07099100
H	4.98353300	1.02901300	1.91991800	C	-1.08251400	-2.28591700	-0.63216800
H	6.23518600	0.14614700	-0.03224500	H	-0.04128500	-2.53421900	-0.86899400
C	-2.35628100	-1.60049400	0.92131800	H	-1.45466700	-3.06132600	0.06477400
C	-3.00342000	-2.27364700	-0.13583500	H	-1.65989700	-2.34042100	-1.57063300
C	-3.07983900	-0.90594200	1.91434000	C	4.23223000	-0.86643700	-0.13198300
C	-4.39816900	-2.18135900	-0.20472500	C	2.13304900	-0.01462200	0.09939300
C	-4.47259100	-0.85902800	1.78183500	C	4.34433500	0.48024500	-0.07050800
C	-5.13480900	-1.47540000	0.73226500	N	2.87876300	-1.16459400	-0.04074500
H	-4.90437400	-2.68443300	-1.02888600	N	3.06563100	0.98493100	0.07813300
H	-5.04128900	-0.31460200	2.53642200	Cu	0.17250700	0.36535700	0.43073500
H	-6.21938900	-1.42005000	0.65521300	H	5.20511500	1.13280600	-0.11272000
C	2.78483000	-2.58996800	-1.44025800	H	4.97304800	-1.64570900	-0.24453200
C	2.46551700	-3.96218200	-0.84785300	C	2.39997500	-2.53666600	-0.11521300
C	1.67816700	-2.02531500	-2.32392800	C	2.10730700	-3.23540200	1.07863800
H	3.31747800	-4.35523300	-0.27728200	C	2.30271500	-3.17221700	-1.37884100
H	1.59512400	-3.95774800	-0.18675700	C	1.65726400	-4.55723500	0.97126800
H	2.24760500	-4.67179700	-1.65602500	C	1.86622100	-4.50293600	-1.40494400
H	2.00583300	-1.11525600	-2.83587600	C	1.53110700	-5.19396200	-0.25212400
H	1.38478500	-2.74992200	-3.09334200	H	1.41903000	-5.09563300	1.88836900
H	0.77423500	-1.76349100	-1.76627000	H	1.77585800	-4.99312500	-2.37382700
C	2.58412300	0.52623000	2.77466600	H	1.18386900	-6.22430900	-0.30616700
C	1.40745900	1.44553000	2.46268400	C	2.81118500	2.41606000	0.16986900
C	2.29232200	-0.46976200	3.89628900	C	2.95565200	3.05867600	1.41549000
H	1.68773300	2.20917100	1.72634700	C	2.41449600	3.11320200	-0.98992000
H	0.55005800	0.90260100	2.05582600	C	2.71134700	4.43652700	1.45685300
H	1.06488800	1.95612900	3.37286700	C	2.16148500	4.48318500	-0.87083800
H	3.18912100	-1.05030700	4.14656800	C	2.30707000	5.14571100	0.33740900
H	1.97311400	0.06317300	4.80121100	H	2.81132400	4.94662100	2.41675200
H	1.49793600	-1.17761800	3.64336800	H	1.80710700	5.02469200	-1.74596500
C	-2.34947600	-3.01742400	-1.28963700	H	2.08392900	6.20948200	0.40092700
C	-1.97383700	-2.02480500	-2.38727800	C	2.28729600	-2.72438700	2.49941200
C	-1.18119500	-3.93810500	-0.96571600	C	3.75556900	-2.49259900	2.85495700
H	-2.85549400	-1.49885000	-2.77374300	C	1.40426600	-1.54072600	2.87717200
H	-1.29090200	-1.25859900	-2.00835900	H	4.35050700	-3.39896600	2.68818400
H	-1.47682500	-2.51771500	-3.23116000	H	4.20478800	-1.68581200	2.26613000
H	-1.38561500	-4.59771700	-0.11228300	H	3.85245300	-2.21469900	3.91220100
H	-0.96749300	-4.57226200	-1.83537600	H	0.36951000	-1.68354600	2.53527600
H	-0.26478800	-3.38126200	-0.75861200	H	1.39047900	-1.40842200	3.96683400
C	-2.53598400	-0.11511300	3.09812600	H	1.76964600	-0.60733900	2.44475000
C	-1.35652100	-0.69188400	3.86665000	C	2.54151600	-2.54956200	-2.74823500
C	-2.25776600	1.33356800	2.69707600	C	1.47873600	-1.50492300	-3.07984100
H	-1.50017000	-1.74771400	4.12711200	C	3.96296000	-2.06695800	-3.03149000
H	-0.41885200	-0.60249900	3.31369000	H	0.48377600	-1.96156500	-3.14352700
H	-1.22408600	-0.13395300	4.80304200	H	1.42683300	-0.71844500	-2.32192400
H	-3.14218300	1.79773900	2.24292700	H	1.68961800	-1.02116400	-4.04169800
H	-1.96065700	1.92759000	3.57221600	H	4.70543300	-2.82610700	-2.75334000
H	-1.45893500	1.38486900	1.95070800	H	4.07177400	-1.87401700	-4.10586900
B	0.09969500	0.55293500	-4.26754000	H	4.21710900	-1.13823900	-2.51613000
F	-0.36817700	0.61189100	-2.89040200	C	3.18424300	2.41761300	2.77886300
F	-0.73188000	1.35392800	-5.03800200	C	1.83348100	2.05875700	3.40595300
F	1.41626900	1.08272600	-4.25459300	C	4.15109200	1.24829700	2.89867500
F	0.09872900	-0.76360200	-4.68529800	H	1.19054100	2.94209200	3.49738400
O	2.38116000	3.00630100	-2.20764200	H	1.29052900	1.33386700	2.78509300
C	3.63665500	2.37285200	-2.62525900	H	1.96830200	1.61981000	4.40381900
H	3.37489600	1.39110900	-3.03215500	H	5.11615900	1.44988700	2.41853400
H	4.25858200	2.24217700	-1.731518600	H	4.34591800	1.04595200	3.96007800
C	4.26846300	3.26843200	-3.63630200	H	3.74664600	0.32603300	2.47257900
C	3.69656900	3.39342800	-4.90779800	C	2.13894200	2.51923400	-2.36177200
C	5.42151100	3.99255900	-3.32866100	C	3.19557800	1.56548400	-2.90570700
C	4.27332000	4.23693900	-5.85163600	C	0.72450800	1.94009500	-2.43714500
H	2.80158700	2.81813000	-5.14361700				

H	4.20978200	1.97340900	-2.79944100	C	8.23522500	1.56187100	2.34348900
H	3.17405500	0.58902400	-2.41477700	C	8.60076400	2.95297000	2.86005600
H	3.01999500	1.38575000	-3.97449700	C	6.90534900	1.04486500	2.88200200
H	-0.01547100	2.68295900	-2.12671300	H	9.57107800	3.27900500	2.46360500
H	0.48977100	1.63425300	-3.46552700	H	7.86234700	3.71831200	2.60795300
H	0.61158100	1.05259500	-1.79844300	H	8.67820000	2.93126600	3.95467000
B	-1.10634600	5.31744900	-2.10599200	H	6.79474900	-0.02305900	2.66638000
F	-0.25201700	4.92099200	-3.14066400	H	6.84014000	1.19283200	3.96875000
F	-0.42274500	6.18438300	-1.22399000	H	6.04901800	1.54522600	2.41931300
F	-2.26137600	5.92608000	-2.58425700	C	7.44669700	2.72374300	-2.71709700
F	-1.48522700	4.14958000	-1.34954100	C	7.74735900	4.22170600	-2.68508300
O	-1.84391100	3.48684900	1.51333500	H	7.51089100	4.66305600	-3.66144000
C	-1.15023200	4.79820200	1.57085900	H	7.15732000	4.76331800	-1.94149900
H	-0.68294500	4.96318300	0.59703900	H	8.80897500	4.41237000	-2.47922200
H	-0.38024400	4.70163700	2.34669000	C	3.76697500	3.78583000	3.52542000
C	-2.17830900	5.82238500	1.90199500	C	3.54233900	2.27207800	3.56556800
C	-2.89138900	6.45169100	0.87618500	C	5.23659700	4.13877600	3.69982700
C	-2.45062700	6.15276600	3.23298800	H	2.47285700	2.02967600	3.60880400
C	-3.86244100	7.40009600	1.18588000	H	3.93888500	1.79119300	2.66031800
H	-2.66981900	6.20598700	-0.16102300	H	4.03700300	1.82234100	4.43756700
C	-3.42108000	7.10190200	3.54161100	H	5.41487800	5.21807800	3.61475200
H	-1.89288300	5.66152700	4.03212700	H	5.57662400	3.82175900	4.69466100
C	-4.12877800	7.72651700	2.51521700	H	5.87524700	3.63302400	2.97374500
H	-4.40615400	7.89235500	0.38148000	C	2.98458600	5.00128800	-1.51927700
H	-3.62344800	7.35727000	4.58088300	C	4.35905700	5.50718500	-1.93408700
H	-4.88528800	8.47367600	2.75227500	C	2.68644600	3.63335000	-2.13471500
H	3.60931400	3.22402300	3.39631800	H	4.63137900	6.44437300	-1.43102200
H	2.12840500	3.38691700	-3.03648200	H	5.14363300	4.77383100	-1.73626400
H	2.38321500	-3.38139100	-3.45018500	H	4.36849300	5.69310600	-3.01581400
H	1.95324000	-3.56092300	3.13095700	H	1.64461300	3.33177500	-1.97649400
H				H	2.89062800	3.62533000	-3.21306600
H				H	3.30154200	2.85298600	-1.67548700
<b>4</b>				B	2.74047700	-0.06763100	-2.61926600
C	3.77730700	-4.07771700	0.26528700	F	3.08262700	-1.42641900	-2.62087700
C	4.71527000	-3.24772800	0.75278000	F	2.74514000	0.47455600	-3.88729000
C	4.42947600	-1.81566700	1.06496500	F	1.49734100	0.10774100	-1.98160500
C	3.04228400	-1.33042200	0.60552500	F	3.74954000	0.62142300	-1.82601800
C	2.10226600	-2.27728600	0.10121000	H	3.25019100	4.20200400	4.40416300
C	2.46109800	-3.58345000	-0.05536800	H	2.25794900	5.71508800	-1.93804900
H	4.00041000	-5.12656900	0.08137600	H	9.00529100	0.89452500	2.75961300
H	5.722373800	-3.59355500	0.98037900	C	5.98091900	2.41095000	-2.99372900
H	1.13177100	-1.92808200	-0.22986100	H	5.82830700	1.34953200	-3.21702300
H	1.73918200	-4.27592100	-0.48589200	H	5.33638000	2.64133600	-2.14191900
C	4.47543900	-1.63150000	2.58560500	H	5.61598100	2.98913000	-3.85265300
H	5.43655600	-1.97902500	2.97977400	H	8.00899000	2.33989400	-3.58172100
H	4.35160900	-0.56614300	2.81679800	O	5.45454100	-0.95140400	0.54922600
H	3.66914000	-2.19329800	3.07065200	C	5.84017200	-1.23000100	-0.80685400
N	2.88857200	-0.03748700	0.77463900	H	4.96990600	-1.41674900	-1.44569500
C	1.71621700	0.70088300	0.60128300	H	6.35402000	-0.32937900	-1.15818000
O	1.79074000	1.90570000	0.42740300	H	6.53663800	-2.07891300	-0.84354500
C	-0.60803000	0.83848800	0.46474800				
H	-0.44649400	1.30957100	-0.51214300				
H	-0.67700100	1.63203700	1.21937500	C	-2.22355300	5.57886100	-1.88954200
C	-1.79580800	-0.06457000	0.47880000	C	-2.04878100	5.02143300	-0.61783000
C	-1.95860800	-1.02865600	-0.52279600	C	-1.09386600	4.04214000	-0.43981900
C	-2.75786400	0.04251700	1.48406300	C	-0.28518000	3.59317600	-1.51568800
C	-3.06447600	-1.87297300	-0.51016600	C	-0.46737600	4.14889200	-2.81742700
H	-1.21105700	-1.10362000	-1.31414600	C	-1.43671700	5.14773500	-2.95316600
C	-3.87088300	-0.79597800	1.49345400	H	-2.97766300	6.34735000	-2.05206100
H	-2.63232600	0.79272300	2.26553900	H	-2.65864400	5.35128200	0.22130000
C	-4.02341000	-1.75732600	0.49759800	H	-1.58792800	5.58078300	-3.94162000
H	-3.18556300	-2.61887000	-1.29421500	N	0.56429400	2.57174500	-1.16929000
H	-4.61782500	-0.69946100	2.27991600	C	1.71733900	2.10707500	-1.67044700
H	-4.89164100	-2.41453500	0.50166800	O	1.97924800	0.90557500	-1.36026300
C	7.04815400	4.47533200	0.45031400	O	-1.73469300	1.10058200	-0.33623200
C	5.38296900	2.92071700	0.38044100	C	-2.56227600	1.29816300	-1.42551900
C	5.89227800	5.10620500	0.76114200	H	-2.87290600	0.35871200	-1.91354300
N	6.73243200	3.14291000	0.21863700	H	-3.46675800	1.80962200	-1.04243200
N	4.88521400	4.15470300	0.71232100	H	-2.13976000	1.97968200	-2.19078700
Cu	4.33078700	1.30234300	0.26076300	C	0.83954200	-2.61249400	1.73270700
H	5.68406000	6.13878500	1.00551600	C	0.02667600	-1.01691900	0.34418100
H	8.06214300	4.84112900	0.36505300	C	-0.50965400	-2.69578000	1.76002800
C	7.70804700	2.13430200	-0.16648900	N	1.16257300	-1.57899100	0.86591500
C	8.37064800	1.38885400	0.83751600	N	-1.00051600	-1.70570700	0.92289300
C	8.00578300	1.94128400	-1.53723100	Cu	0.04197700	0.66896300	-0.76980200
C	9.26489300	0.39220200	0.42904100	H	-1.17646900	-3.36227600	2.28863700
C	8.91450100	0.92867100	-1.86971200	H	1.60744800	-3.18352300	2.23580100
C	9.52876200	0.14372700	-0.90799700	C	2.54108500	-1.15751700	0.63152600
H	9.76674500	-0.19420400	1.19872400	C	3.28985700	-1.78558300	-0.38636300
H	9.13386900	0.76347900	-2.92433800	C	3.10465200	-0.15938400	1.45772100
H	10.22354500	-0.64308200	-1.19800300	C	4.60809400	-1.35715200	-0.57953800
C	3.49887300	4.48346600	1.00500400	C	4.42882800	0.21766200	1.20673800
C	3.03151200	4.37818300	2.33286700	C	5.17948100	-0.36334500	0.19686700
C	2.66770500	4.95886400	-0.03280200	H	5.18749000	-1.82613600	-1.37443100
C	1.71346500	4.76858000	2.59428900	H	4.87146300	0.99061900	1.83509400
C	1.36097700	5.33170700	0.30167000	H	6.20719500	-0.04792000	0.02152800
C	0.87863200	5.24413000	1.59658100	C	-2.43532700	-1.54184500	0.72007300
H	1.34588000	4.68553000	3.61784200	C	-3.04371000	-2.22637500	-0.35364100
H	0.71031600	5.68795900	-0.49735600	C	-3.19224700	-0.78125800	1.64067800
H	-0.14246300	5.54481000	1.82724400	C	-4.42334100	-2.06369100	-0.53171300

C	-4.56650800	-0.66958000	1.39916700	C	2.15267900	0.30776700	-0.12727600
C	-5.18384700	-1.28185900	0.32017700	C	4.41327000	0.38977300	-0.25512200
H	-4.89633000	-2.57767300	-1.36876300	N	2.68080000	-0.95520700	-0.04990000
H	-5.16009800	-0.07396700	2.09365900	N	3.24153300	1.12719900	-0.23445000
H	-6.25513800	-1.17003700	0.16113200	Cu	0.22301800	0.79159600	0.03640100
C	2.80177500	-2.86790100	-1.33405100	H	5.38157400	0.86394100	-0.33612800
C	2.39590400	-4.17507000	-0.65453400	H	4.67014200	-1.80777300	-0.06347000
C	1.77317700	-2.33857000	-2.32759000	C	1.86498100	-2.15462000	0.02169300
H	3.18383100	-4.53170500	0.02224700	C	1.28028100	-2.50965500	1.25894000
H	1.47041100	-4.09623200	-0.07843000	C	1.63027200	-2.91138000	-1.14741500
H	2.23213200	-4.94933400	-1.41453500	C	0.34600500	-3.55070300	1.26214100
H	2.18522200	-1.51561500	-2.92014200	C	0.69077000	-3.94680900	-1.06750700
H	1.45512300	-3.12395100	-3.02413300	C	0.02153400	-4.24621000	0.10771100
H	0.87128400	-1.95205400	-1.84250900	H	-0.12223900	-3.82113400	2.20916000
C	2.43183600	0.55373000	2.62211600	H	0.48308600	-4.52291200	-1.96950800
C	1.24991700	1.43226500	2.22431900	H	-0.72045700	-5.04316200	0.13290000
C	2.11552800	-0.36789500	3.79980500	C	3.15731500	2.58342100	-0.23229900
H	1.52078700	2.13553600	1.42655900	C	3.26508100	3.29211100	0.98507600
H	0.39636600	0.84892800	1.86698600	C	2.94408700	3.25031900	-1.46343300
H	0.89919700	2.01479600	3.08725000	C	3.05348400	4.67752200	0.93430000
H	3.00369300	-0.93480000	4.10550400	C	2.71831400	4.62708600	-1.42667600
H	1.77930000	0.22207100	4.66215700	C	2.74480400	5.33973400	-0.23862600
H	1.32227900	-1.08642900	3.57316100	H	3.13229900	5.23929700	1.86597100
C	-2.36479100	-3.09562600	-1.40080100	H	2.50452900	5.13892900	-2.36289600
C	-1.89469600	-2.23956400	-2.57185900	H	2.55116000	6.41090200	-0.23465200
C	-1.25123200	-4.02452100	-0.93664800	C	1.63974300	-1.93672300	2.62321700
H	-2.72375100	-1.69475800	-3.03953300	C	3.12978400	-2.05846400	2.93945000
H	-1.16287000	-1.49087800	-2.25213900	C	1.08693300	-0.54433200	2.90559300
H	-1.41230600	-2.84858200	-3.34438200	H	3.47348600	-3.09394200	2.82301100
H	-1.51222300	-4.58168000	-0.02764100	H	3.75134600	-1.42687200	2.29781100
H	-1.03860500	-4.75558700	-1.72683400	H	3.32249700	-1.75313400	3.97575000
H	-0.31723700	-3.48615400	-0.75619200	H	0.00364600	-0.49966800	2.73667900
C	-2.72699600	-0.00447900	2.87088000	H	1.28482900	-0.26216600	3.94875000
C	-1.57578500	-0.56371200	3.69260800	H	1.53964600	0.22184400	2.27049300
C	-2.48251400	1.47192400	2.54895700	C	2.35220600	-2.79487400	-2.48353900
H	-1.72306200	-1.61721100	3.95949700	C	2.44272800	-1.41144400	-3.10144200
H	-0.61455300	-0.47347300	3.18193000	C	3.72050900	-3.48077700	-2.43904300
H	-1.49103700	0.00465900	4.62810500	H	1.45650800	-0.94582100	-3.17341000
H	-3.33566700	1.91570100	2.02057400	H	3.09452400	-0.73340400	-2.54208500
H	-2.31718200	2.03541800	3.47741700	H	2.85285300	-1.48231300	-4.11743500
H	-1.61290600	1.59953700	1.89981600	H	3.65733000	-4.48682800	-2.00742600
B	0.23724500	0.18713200	-4.37742000	H	4.13072000	-3.57169200	-3.45246300
F	-0.29294100	0.43909900	-3.03785900	H	4.44403600	-2.90467800	-1.85128100
F	-0.52388100	0.91696200	-5.27688700	C	3.60388800	2.80059100	2.39545700
F	1.57382500	0.65248100	-4.36420500	C	2.39609800	2.91396900	3.33065500
F	0.18932800	-1.17132900	-4.63059700	C	4.27268500	1.44891700	2.57605100
O	2.54875300	2.88949700	-2.32351500	H	1.95335600	3.91561900	3.29556800
C	3.78316600	2.26380500	-2.81833000	H	1.60709100	2.21012200	3.05303800
H	3.53673100	1.23833700	-3.10715100	H	2.70050800	2.70753700	4.36531600
H	4.49294900	2.25033700	-1.98238000	H	5.21447900	1.36677300	2.02249000
C	4.26358100	3.08697400	-3.96635700	H	4.50475500	1.30200500	3.63903500
C	3.65947500	2.94232600	-5.22125800	H	3.62803100	0.61888400	2.27560700
C	5.29022900	4.01957300	-3.80164900	C	2.99423200	2.62554800	-2.85035600
C	4.08061200	3.72539900	-6.29144400	C	4.29116900	1.87260700	-3.14930900
H	2.85572400	2.21584500	-5.34152200	C	1.75085700	1.81754900	-3.20843000
C	5.71483600	4.79973100	-4.87541400	H	5.17423200	2.44549700	-2.83616600
H	5.75859900	4.13532600	-2.82321800	H	4.33728100	0.89144400	-2.66703500
C	5.10797200	4.65404900	-6.12128700	H	4.37340300	1.69686000	-4.22953500
H	3.60750700	3.60726300	-7.26499500	H	0.87713500	2.46713300	-3.28805400
H	6.51743500	5.52290400	-4.73857300	H	1.89744200	1.29342400	-4.16294600
H	5.43707000	5.26329000	-6.96189700	H	1.52735700	1.06855200	-2.44348000
H	3.20098700	1.24769400	2.99360200	B	-1.15656700	3.68555700	-1.72274800
H	3.68973300	-3.12432100	-1.93184300	F	-0.16367100	4.23372200	-2.52394300
H	3.60347700	-0.02969700	3.53739800	F	-1.27667100	4.41629200	-0.51965100
H	-3.16910100	-3.74861000	-1.77427800	F	-2.37702500	3.62801000	-2.38465800
H	-0.93737700	3.57242200	0.52870000	F	-0.78576100	2.32525300	-1.36313000
C	0.32149300	3.72790200	-4.00737600	O	-2.00456200	3.00717000	2.22667000
H	1.29134900	4.24311200	-4.03743700	C	-1.45024700	4.30805000	2.61646000
H	0.53473100	2.65782200	-4.02053800	H	-0.78880500	4.63612100	1.80953300
H	-0.21674400	3.96742500	-4.92994800	H	-0.86477100	4.14749600	3.53031000
C				C	-2.59777100	5.23642500	2.83377400
C				C	-3.22744000	5.83119000	1.73417400
C				C	-3.06499700	5.50893900	4.12145400
C				C	-4.31256300	6.68050800	1.92704900
C				C	-2.85592300	5.61885300	0.73156800
C				C	-4.14704800	6.36508200	4.31482900
C				C	-2.57428600	5.04571900	4.97866600
C				C	-4.77328300	6.94975300	3.21616200
H				H	-4.79759500	7.14052800	1.06740200
H				H	-4.50167500	6.57459200	5.32300900
H				H	-5.61905300	7.61986800	3.36426000
N				H	-1.84858000	-1.45727800	0.90017900
C				C	-3.99007800	2.67710600	0.11074500
O				H	-4.28538800	2.87249900	1.14925700
O				H	-3.10466500	3.28461600	-0.08810400
C				H	-4.78498100	3.03498000	-0.55097800
H				H	4.33480500	3.54345700	2.75555100
H				H	1.13169200	-2.60511500	3.33521000
H				H	2.99646500	3.49039500	-3.53022900
C				H	1.73869500	-3.39392700	-3.17388100

**4'**

C	-4.48848100	-2.19538800	-0.99984400	C	-4.33952700	4.20776600	2.07948600
C	-3.20626500	-2.60947900	-0.99831700	C	-5.39876100	2.85756500	3.77533000
C	-2.11950400	-1.68536100	-0.58857600	H	-5.54161600	4.87377400	1.86178300
C	-2.58204300	-0.38462200	0.07617900	C	-3.45538000	4.45502000	1.49084900
C	-3.91196900	0.09862600	-0.21200900	H	-6.60274700	3.52505300	3.56018800
C	-4.80720600	-0.82776900	-0.68923800	C	-5.33813800	2.06590600	4.52337700
H	-5.29148900	-2.85871300	-1.31864100	H	-6.67521800	4.53311500	2.60081300
H	-2.90887900	-3.59465500	-1.35611600	H	-5.59577300	5.66162900	1.11204600
H	-5.82347400	-0.48687200	-0.89432900	H	-7.48404200	3.25874300	4.14170800
N	-1.60844600	0.12787300	0.80339500	H	-7.61504800	5.05642600	2.43026100
C	-1.67296800	1.09511200	1.81222400	C	-1.44865000	-2.17686800	0.13785000
O	-0.65321600	1.49895500	2.33545900	H	-4.31814600	1.53928900	-0.13387600
O	-1.22491400	-1.39578300	-1.67670000	H	-4.90199400	1.75694400	0.76699000
C	-1.85715800	-0.88637800	-2.85244400	H	-3.45424400	2.20786800	-0.14234600
H	-1.05189500	-0.47665400	-3.46795300	H	-4.94360900	1.78192300	-1.00160300
H	-2.37545800	-1.68639200	-3.39886700	H	4.56301200	2.11638600	2.44618600
H	-2.55418600	-0.07394900	-2.61779800	H	0.96307800	-3.56793600	3.55926200
C	3.65825800	-2.40835000	-0.29859900	H	3.11438700	1.90611200	-3.98273200
C	2.00876200	-0.84217300	-0.17564500	H	0.52807500	-4.35137300	-2.96888000
C	4.21275000	-1.20644600	-0.58822700				

**S1a**

N	2.31406100	-2.17715600	-0.04290200	C	-3.60077200	0.34002600	-1.86595500
N	3.20271800	-0.25883400	-0.51337400	C	-4.17090200	-0.77845100	-1.26268400
Cu	0.25438900	-0.04087200	0.13444400	C	-3.62225300	-1.29265900	-0.08951800
H	5.23196100	-0.92731500	-0.81857000	C	-2.50840800	-0.70730600	0.51783600
H	4.09203100	-3.39533200	-0.22081300	C	-1.94986400	0.42445900	-0.10333500
C	1.32491800	-3.22192800	0.16747000	C	-2.48100700	0.93121900	-1.29191600
C	0.87552600	-3.51229900	1.47809600	H	-4.01709600	0.74462000	-2.78646700
C	0.82663000	-3.93307000	-0.94836900	H	-5.04487900	-1.25343500	-1.70532100
C	-0.16311500	-4.43954700	1.62407100	H	-4.07583600	-2.16469800	0.38243800
C	-0.20142100	-4.85883500	-0.72433900	H	-2.01424100	1.80075100	-1.75427200
C	-0.71978300	-5.09599000	0.53777500	N	-0.81919900	1.04992000	0.49228900
H	-0.52524700	-4.65172600	2.62991100	C	-0.56047400	2.41582400	0.52822700
H	-0.59900100	-5.39947900	-1.58414600	O	0.57886900	2.86166900	0.49750600
H	-1.53335700	-5.80652600	0.67792700	O	0.31778100	0.22423200	0.56098900
C	3.46704900	1.17250500	-0.64881100	C	0.94742000	0.11933400	-0.71812700
C	3.84186400	1.90630300	0.49522400	H	1.31051900	1.09787300	-1.05063300
C	3.39091100	1.78673600	-1.92014500	H	1.78943300	-0.55745900	-0.55572900
C	4.12246500	3.26897200	0.33431500	H	0.26146700	-0.31673700	-1.45868000
C	3.67206000	3.15271500	-2.00393500	C	-1.93656000	-1.24943700	1.78811100
C	4.03295700	3.89856500	-0.89348300	H	-1.04043100	-1.85264700	1.59905900
H	4.39601700	3.84209200	1.22053700	H	-1.61420300	-0.44067100	2.45557500
H	3.58195300	3.63624800	-2.97596800	H	-2.66408900	-1.87644500	2.31433900
H	4.23841900	4.96358100	-0.98619000	C	-1.75271900	3.30072000	0.67433300
C	1.45736700	-2.97379600	2.77538800	C	-2.90408400	2.93121000	1.37964800
C	2.94986100	-3.26735400	2.92627100	C	-1.66303700	4.58665000	0.13115500
C	1.09413800	-1.52274900	3.06344800	C	-3.95253300	3.83337200	1.52796200
H	3.15276200	-4.33886700	2.80231800	C	-2.72096600	5.47948100	0.26155100
H	3.56820900	-2.72502300	2.20523700	C	-3.86771100	5.10462700	0.96097600
H	3.29164700	-2.97434100	3.92715900	H	-4.83896600	3.54379700	2.08959000
H	0.00747800	-1.37211300	3.04414700	H	-2.64811000	6.47434000	-0.17470100
H	1.46136900	-1.22143600	4.05352900	H	-0.74829700	4.86873600	-0.38733600
H	1.52247800	-0.83506700	2.33194800	H	-2.97459300	1.93928000	1.82421100
C	1.33435500	-3.88379800	-2.38268200	H	-4.69303600	5.80642600	1.07152100
C	1.55038000	-2.50978600	-2.98612300				
C	2.56497100	-4.77589800	-2.56772400				
H	0.67758100	-1.87503500	-2.82608300				
H	2.41772200	-1.99879300	-2.56228300				
H	1.72789300	-2.59779200	-4.06622500				
H	2.41429500	-5.77587700	-2.14305800				
H	2.79008500	-4.89088800	-3.63537800				
H	3.45348400	-4.33722600	-2.09838000				
C	3.85458000	1.44039800	1.94209300				
C	2.47341900	1.70627600	2.53880400				
C	4.33638300	0.03085100	2.24868800				
H	2.20771700	2.76795600	2.48004600				
H	1.69017700	1.17474700	1.98819300				
H	2.42251300	1.39134300	3.58973200				
H	5.29948400	-0.19603500	1.77401800				
H	4.46412700	-0.08219400	3.33335500				
H	3.61893100	-0.73206800	1.93889400				
C	2.98795800	1.12049500	-3.22271400				
C	3.92342700	-0.00155900	-3.67052000				
C	1.49965100	0.77555000	-3.24294300				
H	4.95483300	0.36687400	-3.74844600				
H	3.93353100	-0.86260300	-2.99768400				
H	3.62388200	-0.36890400	-4.66066700				
H	0.89790400	1.68788400	-3.17398000				
H	1.23808900	0.25518500	-4.17523400				
H	1.19886600	0.14033600	-2.40311700				
B	-0.63880200	2.75049600	-0.97917400				
F	-0.14784900	3.71489400	-1.83443300				
F	-1.45846400	3.29547000	0.02143800				
F	-1.35420300	1.75616800	-1.68132600				
F	0.47650100	2.08068300	-0.34019800	Cu	-0.16224400	-0.34919800	0.28142400
O	-2.91124100	1.40590500	2.21888400	H	-0.16036000	-5.38280300	0.79465500
C	-2.97861800	2.44969100	3.23036000	H	-0.93351300	-4.39394100	3.27973500
H	-2.10026300	3.09038600	3.10754600	C	-1.13852900	-1.61851500	3.32612800
H	-2.92229400	1.96231300	4.21193900	C	-0.13548200	-1.11775100	4.19159900
C	-4.26055300	3.19086800	3.03788400	C	-2.50137000	-1.29421300	3.53102000
C	-	-	-	C	-0.52971500	-0.24943100	5.21722400

C	-2.82028300	-0.42362900	4.58013100	C	-2.60023600	1.99683900	-1.47941100
C	-1.85215800	0.10945300	5.41430200	H	-3.11539600	1.19790900	-2.03615700
H	0.24134700	0.14618200	5.87794500	H	-3.31192300	2.73780800	-1.07155100
H	-3.86836900	-0.16713200	4.73421700	H	-2.01331700	2.55239700	-2.25728000
H	-2.12779900	0.78688900	6.22097500	C	0.76804200	-2.59662200	2.23667500
C	0.24327100	-3.41453500	-1.08938700	C	0.35706200	-1.21826400	0.48419200
C	1.61525200	-3.36704000	-1.41451100	C	1.11324800	-3.25517100	1.10366500
C	-0.74059600	-3.61500300	-2.08050100	N	0.30646800	-1.34585100	1.84721900
C	1.96911600	-3.52027500	-2.75936500	N	0.88631000	-2.39316500	0.04430400
C	-0.31484100	-3.77312000	-3.40230300	Cu	-0.43113800	0.27819600	-0.51077400
C	1.02445200	-3.72081100	-3.75076500	H	1.49748800	-4.25348200	0.95140500
H	3.02477100	-3.45293500	-3.02255000	H	0.80014900	-2.89391100	3.27561600
H	-1.07227800	-3.90307000	-4.17529100	C	-0.08694600	-0.26943000	2.74258500
H	1.32868800	-3.81835200	-4.79114400	C	0.88429300	0.68896300	3.11824500
C	1.35531400	-1.41959200	4.14386300	C	-1.41958700	-0.19049200	3.20644700
C	1.70609000	-2.89574100	4.32229700	C	0.46594000	1.75731100	3.91930500
C	2.05534100	-0.77292800	2.95372600	C	-1.76397100	0.90652000	4.00638700
H	1.22372000	-3.31019900	5.21712100	C	-0.84452000	1.88280500	4.35175200
H	1.41563500	-3.51357200	3.46918100	H	1.20456200	2.50602300	4.20607800
H	2.79084500	-3.00734400	4.44474000	H	-2.79292000	0.98242600	4.35752600
H	1.89616200	0.31203500	2.93751600	H	-1.14351100	2.72968400	4.96730900
H	3.13644400	-0.96044200	2.99326500	C	1.09711700	-2.67776600	-1.36507000
H	1.68730100	-1.15846800	2.000027200	C	2.38762900	-2.55387400	-1.92824000
C	-3.69007800	-1.78564400	2.71863200	C	-0.03518800	-2.98583100	-2.15207600
C	-3.72095700	-1.19289200	1.31388300	C	2.47818800	-2.65475100	-3.32196900
C	-3.89720400	-3.29842800	2.74013700	C	0.13264700	-3.03854000	-3.53712400
H	-3.69773600	-0.09625300	1.35849600	C	1.36913800	-2.84043600	-4.12803400
H	-2.86379400	-1.51176000	0.71492300	H	3.46430300	-2.55679900	-3.77806100
H	-4.63246700	-1.49871700	0.78253700	H	-0.74252200	-3.21948600	-1.59843000
H	-3.91698400	-3.67809000	3.76970700	H	1.46756500	-2.86163700	-5.21168000
H	-4.85763900	-3.54934600	2.27192100	C	2.36824600	0.66643200	2.77605500
H	-3.12347900	-3.84620500	2.19670500	C	3.10726800	-0.53998400	3.35309200
C	2.77718400	-3.05438600	-0.48436800	C	2.68520700	0.89488000	1.30136600
C	3.00676500	-1.54124100	-0.44260500	H	2.91264900	-0.65070400	4.42739200
C	2.74682800	-3.66786900	0.90791500	H	2.82790500	-1.47784700	2.86362500
H	3.16000000	-1.13212400	-1.44660800	H	4.18928000	-0.41696100	3.21771800
H	2.13490700	-1.01681300	-0.03065000	H	2.17304000	1.78658800	0.91667000
H	3.87502800	-1.29414200	0.18315000	H	3.76630400	1.03553700	1.16588700
H	2.54103800	-4.74590300	0.88007300	H	2.38449600	0.05659500	0.66679300
H	3.72053800	-3.52647000	1.39552000	C	-2.54963400	-1.16521400	2.91002000
H	2.00130000	-3.20114200	1.55439700	C	-3.07166800	-1.01764500	1.48485600
C	-2.24643900	-3.51545700	-1.90337300	C	-2.27668400	-2.62237400	3.27756300
C	-2.87446500	-4.18802200	-0.69031400	H	3.40331900	0.00708900	1.28081400
C	-2.64419400	-2.04182300	-1.99375500	H	-2.29706600	-1.25123900	0.74926900
H	-2.52833600	-5.22145600	-0.56113600	H	-3.91218300	-1.70102400	1.30547100
H	-2.67129900	-3.64662700	0.23660400	H	-1.86297700	-2.71259900	4.29031500
H	-3.96595200	-4.21405300	-0.80855900	H	-3.21588000	-3.18867800	3.25002200
H	-2.33747600	-1.59909900	-2.94825000	H	-1.58835200	-3.11508100	2.58510400
H	-3.72927800	-1.91590700	-1.86971000	C	3.74460700	-2.31788300	-1.25682400
H	-2.13140600	-1.46709400	-1.21255300	C	4.29604200	-0.92566800	-1.57754500
B	0.58758600	0.31758000	-3.09751800	C	3.91348600	-2.59710700	0.22790300
F	0.10838300	-0.46321800	-1.97407300	H	4.30798000	-0.73151600	-2.65531200
F	-0.21083700	0.01593600	-4.19043300	H	3.68691000	-0.14070700	-1.12038300
F	0.43231200	1.68395300	-2.74267300	H	5.32476100	-0.83254500	-1.20443400
F	1.92719800	0.02749900	-3.30850000	H	3.63354200	-3.62018200	0.50232400
H	-4.56468600	-1.36788000	3.23968400	H	4.97037500	-2.46834300	0.49498400
H	1.75885300	-0.91987600	5.03755200	H	3.34221400	-1.90489500	0.85377300
H	-2.66944400	-4.01983100	-2.78565300	C	-1.45063600	-3.30671400	-1.67859400
H	3.65605000	-3.48883800	-0.98578100	C	-1.61195000	-3.90919600	-0.28928800
C	1.45104600	3.55025800	-0.27258500	C	-2.41045600	-2.13923700	-1.90563600
C	2.61161200	3.23726600	-0.98909000	H	-0.91539700	-4.73951200	-0.11548700
C	1.29887600	4.81930000	0.29526500	H	-1.47005300	-3.17906300	0.51219500
C	3.59870600	4.20200900	-1.15694300	H	-2.63120600	-4.30192800	-0.17872300
H	2.70909330	2.24599200	-1.42858100	H	2.39644700	-1.80215900	-2.94665300
C	2.30122000	5.77197500	0.14253600	H	-3.43456800	-2.42835900	-1.63230000
H	0.40106300	5.05958700	0.86437600	H	-2.13713200	-1.26286200	-1.30299600
C	3.44726800	5.46787300	-0.59108600	B	-0.86408200	0.57450100	-4.32299000
H	4.49038400	3.96355600	-1.73370100	F	-0.94921700	0.21271800	-2.93543000
H	2.18444600	6.75578200	0.59366800	F	-1.80914100	1.58247900	-4.56736100
H	4.22430200	6.21960600	-0.72089200	F	0.43105300	1.08863600	-4.55737800
H				F	-1.10550900	-0.55181400	-5.09911400
				H	-1.77642100	-4.09582500	-2.37540800
				H	-3.36557900	-0.84236900	3.57423500
				H	4.40941000	-3.03306000	-1.76915700
				H	2.77571500	1.54097500	3.30583800
				C	2.62064500	2.40646600	-2.51605400
				C	3.10786800	3.64223300	-2.07299100
				C	3.23399700	1.76224300	-3.59770800
				C	4.20321100	4.22632500	-2.70032500
				H	2.64075600	4.13617100	-1.22082000
				C	4.31192600	2.36361200	-4.23574300
				H	2.81859100	0.81717300	-3.94182100
				C	4.80367400	3.58927700	-3.78512600
				H	4.58863400	5.17933600	-2.34195000
				H	4.77072200	1.87477200	-5.09382500
				H	5.65488600	4.05093400	-4.28355500
				C			
				C	-2.20811700	5.42585900	-3.10501500
				O	-2.26535700	5.29522200	-1.71570600
				O			

C	-1.45731700	4.38523500	-1.04162800	C	2.49910100	3.09295600	-2.20185100
C	-0.53935300	3.61109800	-1.80849300	C	3.53808900	2.42514500	-2.86165500
C	-0.50361200	3.73136600	-3.21531100	C	2.50138600	4.49204100	-2.13118200
C	-1.33042500	4.63686700	-3.85434800	C	4.55950800	3.15318200	-3.45823400
H	-2.86690600	6.13345100	-3.60621300	H	3.50304300	1.33988600	-2.92114200
H	-2.96371300	5.90507700	-1.14238800	C	3.53385400	5.21441100	-2.71804500
H	0.15920400	3.08455000	-3.78529100	H	1.70145000	5.01130500	-1.60517300
H	-1.31030900	4.70744000	-4.93963600	C	4.56050300	4.54642200	-3.38541300
C	-1.52472600	4.20193400	0.43660800	H	5.35488400	2.63405600	-3.98971900
H	-2.28752000	4.84649200	0.88612900	H	3.53664700	6.30117900	-2.65801900
H	-1.75346800	3.15609800	0.68310700	H	5.36287600	5.11452600	-3.85359400
H	-0.56014700	4.42132900	0.91450700				
N	0.25970700	2.72092500	-1.12784600				
C	1.46604300	2.28728300	-1.54052900	C	-2.46692100	-0.17018900	0.19408200
O	1.71454500	1.08825700	-1.18440700	C	-1.08593000	-0.03828600	0.40434400
O	-1.99383200	0.87351400	-0.18119800	C	-0.22222900	-0.52225700	-0.60089900
C	-2.87274900	1.36675300	-1.12060200	C	-0.76243600	-1.04399600	-1.78646200
H	-3.29955300	0.57529600	-1.75932100	C	-2.13197900	-1.12423900	-1.98566700
H	-3.68528200	1.90088500	-0.58928600	C	-2.99532500	-0.70061100	-0.97559000
H	-2.42208500	2.11849600	-1.80162100	H	-3.14092600	0.18988000	0.97246100
C	0.99127400	-2.60111100	1.63011900	H	-2.52443800	-1.53576500	-2.91404000
C	0.01325800	-0.95534300	0.41615600	H	-4.07416200	-0.77338900	-1.10212100
C	-0.34731600	-2.74391900	1.75369700	C	-0.62147800	0.64986400	1.65374800
N	1.20703300	-1.50310100	0.81108100	H	0.07654600	1.46820000	1.43640600
N	-0.93811500	-1.72612800	1.02168900	H	-1.47598400	1.08396300	2.18418300
Cu	-0.18232900	0.77369800	-0.65655000	H	-0.11774900	-0.03001400	2.35280600
H	-0.94697500	-3.46626400	2.28978100	N	1.20100300	-0.54705100	-0.54424000
H	1.81742500	-3.17039000	2.03368100	C	1.96939600	-0.62246100	0.68146800
C	2.55485000	-1.04677000	0.48029500	O	1.79399800	0.36954500	-1.47035300
C	3.22299800	-1.62312400	-0.62067700	C	1.52825100	1.72324200	-1.12823500
C	3.16932100	-0.06328000	1.28674600	H	1.99637000	2.31715200	-1.91772700
C	4.51843600	-1.17226900	-0.90029100	C	0.44695800	1.92783500	-1.11028200
C	4.46100000	0.34687600	0.93972100	H	1.97329700	1.99587600	-0.15889100
C	5.13699400	-0.19249400	-0.14295400	H	-0.06370500	-1.39494900	-2.54411200
H	5.03732100	-1.60472500	-1.75573700	H	3.01500200	-0.68871200	0.34701000
H	4.93803300	1.11540900	1.54781700	H	1.91578000	0.27402000	1.32556700
H	6.14001600	0.14985200	-0.39335600	C	1.61992800	-1.84180700	1.49479900
C	-2.39220700	-1.61248700	0.97149600	C	1.80821800	-1.81834200	2.88018700
C	-3.08679400	-2.27469700	-0.06173300	C	1.14807000	-3.01600800	0.90017500
C	-3.06991300	-0.93662400	2.00986500	C	1.54297800	-2.94275400	3.65730500
C	-4.48330100	-2.18215600	-0.06781600	H	2.16689500	-0.90226100	3.35359500
C	-4.46761500	-0.89231200	1.94072100	C	0.87246100	-4.13868300	1.67758900
C	-5.17692400	-1.49050000	0.91181200	H	0.99449900	-3.04084000	-0.17748800
H	-5.02549400	-2.67759400	-0.87342000	C	1.06986500	-4.10803400	3.05652800
H	-5.00266300	-0.36438000	2.73085300	H	1.69771000	-2.90526200	4.73469300
H	-6.26400300	-1.43570100	0.88566100	H	0.49914900	-5.04420900	1.20121200
C	2.66759200	-2.65802800	-1.58517100	H	0.85071900	-4.98648400	3.66130600
C	2.35261500	-4.01543600	-0.95815100				
C	1.53916300	-2.09898800	-2.44461500				
H	3.21449800	-4.40365100	-0.39914700				
H	1.49710200	-3.99118200	-0.27773300				
H	2.11181600	-4.73939600	-1.74695700				
H	1.84828400	-1.18787500	-2.96757400				
H	1.22664000	-2.82686300	-3.20353600				
H	0.64910600	-1.84173100	-1.86295200				
C	2.57919900	0.60673100	2.51833800				
C	1.35927100	1.47896300	2.23477700				
C	2.37731900	-0.35457700	3.68942200				
H	1.57044200	2.21401800	1.44772200				
H	0.49236500	0.89759400	1.90933900				
H	1.05886700	2.02520000	3.13951400				
H	3.31302000	-0.87441100	3.93063000				
H	2.05769100	0.19592300	4.58367000				
H	1.61738800	-1.11616400	3.49115800				
C	-2.48463300	-3.02890300	-1.23672500				
C	-2.13032600	-2.05707600	-2.35818700				
C	-1.32243500	-3.96944800	-0.94602800				
H	-3.00999100	-1.50424900	-2.70951000				
H	-1.40080800	-1.31177700	-2.02664500				
H	-1.69225200	-2.57578700	-3.21875800				
H	-1.50204600	-4.60634200	-0.07005600				
H	-1.16304600	-4.62630200	-1.81054100				
H	-0.38473900	-3.43027700	-0.79282000				
C	-2.48672100	-0.16942800	3.19342400				
C	-1.23122800	-0.70750300	3.86120900				
C	-2.31554200	1.31309700	2.85443600				
H	-1.31331200	-1.76987000	4.12106200				
H	-0.34205700	-0.57880000	3.24014500				
H	-1.04922000	-0.15284400	4.79122300				
H	-3.24724700	1.74453700	2.46714000				
H	-2.01645600	1.87756700	3.74812900				
H	-1.55632400	1.45512300	2.07999100				
B	-0.15925400	0.54257100	-4.24808400				
F	-0.67489700	0.65996400	-2.88304400				
F	-0.95659300	1.33116800	-5.06716500				
F	1.15983400	1.03925000	-4.21260800				
F	-0.18955700	-0.791118900	-4.61222800				
H	3.36368700	1.30422100	2.84880200				
H	3.49999800	-2.85274200	-2.27840800				
H	-3.27752900	-0.22180100	3.95792300				
H	-3.30539300	-3.66567400	-1.60199400				

C	1.99322500	-3.86821900	-2.51788300	N	1.01430900	-2.14908100	-0.91038700
C	-0.23514000	-4.53112700	-3.05929700	Cu	-0.37732500	0.46006300	-0.64186000
C	1.09728200	-4.42038500	-3.41717900	H	1.81141500	-4.14133300	-0.68341300
H	3.03585700	-3.73293500	-2.80515900	H	1.07403400	-3.70085900	1.96691400
H	-0.95725400	-4.92183000	-3.77595600	C	-0.05833700	-1.17375600	2.36503400
H	1.42971000	-4.73229100	-4.40526900	C	0.83466100	-0.45347400	3.19707300
C	0.99490700	-0.30240100	3.71890000	C	-1.42831200	-1.29997400	2.69463000
C	1.58819000	-1.62891400	4.19157800	C	0.30062100	0.20070300	4.31334400
C	1.55846400	0.19140600	2.38885600	C	-1.89067300	-0.60770300	3.82180900
H	1.20310000	-1.89353200	5.18479600	C	-1.05008700	0.15036000	4.61912100
H	1.38043000	-2.46526100	3.52051000	H	0.97978600	0.76468700	4.95299800
H	2.67910800	-1.54122300	4.26865400	H	-2.94887100	-0.68457600	4.06962600
H	1.29135600	1.24427700	2.22529400	H	-1.44020800	0.67868000	5.48767600
H	2.65357600	0.11735700	2.37378600	C	1.28614500	-2.02207400	-2.33510000
H	1.17664000	-0.37690600	1.53514800	C	2.51939400	-1.47473300	-2.75594900
C	-3.93434100	-1.66232700	2.50346000	C	0.34565600	-2.52609100	-3.26101400
C	-4.03232000	-1.39345800	1.00543600	C	2.78894100	-1.45843400	-4.12933800
C	-3.93552100	-3.14905700	2.85519400	C	0.68632500	-2.48749000	-4.61895700
H	4.16591500	-0.32118100	0.81025700	C	1.89340700	-1.96733900	-5.05791100
H	-3.13731100	-1.71398600	0.46660400	H	3.73735900	-1.03680200	-4.46339400
H	-4.88834100	-1.92716200	0.57179700	H	-0.03899500	-2.86702700	-5.33809200
H	-3.94060200	-3.29282000	3.94315100	H	2.13482600	-1.95525800	-6.11951900
H	-4.83645000	-3.62691700	2.45004800	C	2.33847100	-0.29480500	3.01656200
H	-3.07601300	-3.69036600	2.45141300	C	3.13159500	-1.59990900	2.97464600
C	2.66596600	-2.69687700	-0.45811200	C	2.69176200	0.66221400	1.88028300
C	2.59660500	-1.20033200	-0.77001300	H	2.86043200	-2.25052300	3.81558100
C	2.72430700	-2.95015000	1.04164800	H	2.98984900	-2.16890300	2.05276100
H	2.69127300	-1.00873300	-1.84426400	H	4.20407700	-1.38177800	3.05513300
H	1.62305700	-0.79413900	-0.46245000	H	2.33297600	1.67689100	2.09578500
H	3.37909800	-0.64384800	-0.23559000	H	3.77880500	0.71458000	1.73549400
H	2.67796300	-4.01885300	1.28797600	H	2.24499900	0.35350200	0.93020500
H	3.66438100	-2.55429500	1.44815800	C	-2.47719800	-2.11707100	1.95740400
H	1.91518600	-2.44564200	1.57437600	C	-2.90344100	-1.48383100	0.63871000
C	-2.21500300	-4.17379000	-1.64089900	C	-2.15510600	-3.60461800	1.83522000
C	-2.76101200	-4.59625100	-0.28393700	H	-3.19307700	-0.43505100	0.78485900
C	-2.83738700	-2.85607300	-2.10913900	H	-2.10130800	-1.49409300	-0.10540200
H	-2.28419100	-5.51109700	0.90907200	H	-3.75580700	-2.00782200	0.19314200
H	-2.63904300	-3.81843400	0.47320100	H	-1.89305500	-4.03879900	2.80918100
H	-3.83874100	-4.79079000	-0.36460600	H	-0.03412200	-4.13776100	1.45401700
H	-2.541113500	-2.61364500	-3.13541400	H	-1.33621300	-3.81228600	1.14140600
H	-3.93366000	-2.89779000	-2.04701000	C	3.57025900	-0.80711100	-1.88258200
H	-2.48955400	-2.02124600	-1.48447500	C	3.19777100	0.65990300	-1.64934100
B	0.09537100	-0.77847000	-3.89972000	C	3.94828600	-1.51393400	-0.58871900
F	-0.36776500	-1.04371800	-2.52707200	H	3.11481500	1.19735400	-2.60260800
F	-0.61452300	-1.61250500	-4.74488300	H	2.22969900	0.75077200	-1.13772100
F	-0.17515100	0.57301700	-4.15948900	H	3.95355300	1.16782600	-1.03610800
F	1.46484600	-1.01314000	-3.93378900	H	4.15716000	-2.57867200	-0.75105100
H	-4.86503100	-1.26562500	2.93631200	H	4.85321800	-1.05746300	-0.16679300
H	1.32179200	0.43298700	4.46924100	H	3.17037100	-1.43658700	0.17238900
H	-2.54396200	-4.94450600	-2.35473900	C	-1.08288200	-2.92835800	-2.95284600
H	3.61829900	-3.06424800	-0.86983500	C	-1.35153700	-3.85148200	-1.77315500
H	0.71557700	0.80457200	-1.82647500	C	-1.89588500	-1.64295400	-2.83969600
H	0.78258500	1.47647700	-0.16510300	H	-0.72462400	-4.75293900	-1.71957700
C	1.78501100	2.64883300	-1.65894900	H	-1.20279700	-3.35258000	-0.81242700
C	2.19919400	2.66708300	-2.99434400	H	-2.40304300	-4.16094200	-1.80833400
C	2.39155500	3.50546600	-0.73688900	H	-1.92061900	-1.09549200	-3.79117100
C	3.20575100	3.54038700	-3.39800800	H	-2.92895600	-1.84303900	-2.55213100
H	1.72167100	1.99205400	-3.70461400	H	-1.44870300	-0.98427300	-0.27736000
C	3.39733700	4.37949500	-1.14181000	B	-5.30429300	-1.79892200	-3.04194200
H	2.05709000	3.49683400	0.30302800	F	-5.00182400	-1.66666600	-1.64436500
C	3.80385900	4.39855700	-2.47517700	F	-4.77747100	-0.65911800	-3.69492400
H	3.52675700	3.54874200	-4.43844400	F	-4.64547200	-2.95490600	-3.51647500
H	3.86151700	5.04793400	-0.41795900	F	-6.67439300	-1.88847900	-3.22352900
H	4.59105300	5.08030200	-2.79482500	C	-0.45245900	1.99249700	-3.01801500
				H	0.56430300	2.06440000	-3.44554400
<b>TS2b-3b</b>				H	-0.71510400	0.92917100	-3.15485100
C	0.65284700	5.89973700	0.05476300	C	-1.40706700	2.85215200	-3.81744200
C	0.30345300	4.83022000	0.87868500	C	-1.30737100	2.79760200	-5.21053700
C	-0.06728400	3.59072800	0.36860600	C	-2.39676200	3.64757000	-3.23863400
C	-0.09521800	3.42629100	-1.05562800	C	-2.18646900	3.51779200	-6.01436800
C	0.24557200	4.53191800	-1.88046100	C	-0.54163600	2.16991900	-5.67021400
C	0.63568300	5.73892200	-1.33116000	C	-3.27347400	4.37200700	-4.04257300
H	0.93892500	6.85358800	0.49391200	H	-2.49008400	3.68984300	-2.15425000
H	0.31336800	4.96038400	1.96046100	C	-3.17375200	4.30836000	-5.43069800
H	0.25126300	4.41226100	-2.95917800	H	-2.10329800	3.45499600	-7.09789200
H	0.92301800	6.55913600	-1.98570500	H	-4.04915300	4.97868700	-3.57842400
C	-0.44851100	2.49727200	1.30714800	H	-3.86739700	4.86800300	-6.05532200
H	-0.29725800	2.80541000	2.34749700	H	-3.36132600	-2.06674400	2.61035200
H	-1.49049300	2.18814800	1.18380800	H	-1.44803000	-3.45485100	-3.84613700
H	0.17342700	1.59505800	1.15673800	H	4.48147100	-0.80035300	-2.49992600
N	-0.29646700	2.18281000	-1.58869300	H	2.66812400	0.20407700	3.94000100
O	-2.23275700	1.46347700	-0.85657400				
C	-3.19007400	1.04382600	-1.76371900				
H	-3.64736500	0.08925300	-1.44027200	C	-4.96981300	-2.24903900	0.15317600
H	-3.95941300	1.81560400	-1.91664700	C	-4.23397800	-2.29081300	1.32935900
H	-2.79007600	0.80304100	-2.76689500	C	-3.23573300	-1.35296100	1.57841100
C	0.99665000	-3.07458000	1.08914800	C	-3.00234500	-0.29713500	0.60396000
C	0.43104400	-1.22043900	-0.09311200	C	-3.85258900	-0.22313400	-0.54679600
C	1.35309800	-3.28994000	-0.19947300	C	-4.78424300	-1.20242700	-0.77741900
N	0.44525300	-1.80279300	1.15010000	H	-5.71681000	-3.01678900	-0.04473600

H	-4.40338400	-3.08696600	2.05341900	H	-2.11040100	1.99477700	2.71516900	
H	-3.68635700	0.54409900	-1.29796600	C	-1.64001600	5.32875600	2.19136700	
H	-5.35749400	-1.18851200	-1.70186200	H	-1.22747600	6.22199700	0.26961000	
C	-2.45359000	-1.36916500	2.84350800	H	-2.09419600	4.15838600	3.94368500	
H	-2.70722300	-2.24110900	3.45595800	H	-1.64155400	6.27814600	2.72545600	
H	-1.37959400	-1.39130500	2.63021400	H	-0.56673700	1.49327200	-0.34868500	
H	-2.63399100	-0.46181200	3.43589300	H	-2.21156200	1.71516200	-0.89870900	
N	-1.90056300	0.42957200	0.80245600	<b>S1c</b>				
C	-1.61746700	1.60404400	0.01500900	C	-2.30805300	-0.50035300	0.57318000	
O	-1.31450100	-2.27532200	0.23018000	C	-0.93290800	-0.23696800	0.63077800	
C	-1.60241800	-3.08559900	-0.84262600	C	-0.17918700	-0.48518800	-0.53140900	
H	-1.58723600	-2.55503200	-1.80976700	C	-0.79872600	-0.91806700	-1.71034300	
H	-0.96763600	-3.99098900	-0.88569600	C	-2.16544700	-1.15057600	-1.74276300	
H	-2.65598600	-3.43642800	-0.71862100	C	-2.92340400	-0.95336000	-0.58748500	
C	3.86487300	-1.67678300	0.03285700	C	-2.90721000	-0.31899000	1.46594500	
C	1.75316700	-0.84216900	0.06186000	H	-2.63765400	-1.49229600	-2.66211900	
C	3.95596400	-0.36037500	0.33296600	H	-3.99609200	-1.13911800	-0.59613400	
N	2.51696100	-1.96667800	-0.13135500	H	-0.33068600	0.28692300	1.89743100	
N	2.66313900	0.13815100	0.34743800	C	0.56520800	0.89153300	1.71292800	
Cu	-0.22709100	-0.68539800	0.09568600	H	-1.05348500	0.90753800	2.43886200	
H	4.80922000	0.27087500	0.53832700	H	-0.03024200	-0.52676900	2.57212000	
H	4.62287100	-2.43833800	-0.08600500	C	1.22311000	-0.26184900	-0.57708000	
C	2.03072000	-3.29711700	-0.48723200	N	2.20743200	-0.62388600	0.33103500	
C	1.71253000	-4.21830100	0.53839200	C	3.26098900	-0.00256800	0.41492400	
C	1.95852700	-3.66450600	-1.85167400	O	1.61426500	0.67246700	-1.55052000	
C	1.24869900	-5.48268700	0.15710200	C	1.46129200	2.00124700	-1.05270300	
C	1.49156100	-4.94922800	-2.15568900	C	1.73834900	2.64729700	-1.88926000	
C	1.12460500	-5.85201900	-1.17229700	H	0.41590700	2.19561300	-0.76932900	
H	0.98809800	-6.19179800	0.94265100	H	2.13454600	2.17357000	-0.20524900	
H	1.41763300	-5.23150600	-3.20536500	H	-0.18024200	-1.06796700	-2.59321500	
H	0.75674400	-6.84141400	-1.43941300	C	1.92718600	-1.82425200	1.16178400	
C	2.36008600	1.52616800	0.65406800	C	2.56097300	-1.89902000	2.40490900	
C	2.14016400	1.90372500	1.99859900	C	1.12402700	-2.90131100	0.75487600	
C	2.35591100	2.47903100	-0.39088600	C	2.37962300	-2.98982700	3.24748700	
C	1.87728300	3.25305300	2.26206100	C	3.20821100	-1.07651200	2.70507100	
C	2.08967900	3.81029600	-0.04956100	H	0.94533600	-4.00090000	1.57625700	
C	1.848621900	4.20337100	1.25606600	C	0.64603100	-2.88994500	-0.22283600	
H	1.68193800	3.54821300	3.29352600	C	1.56272100	-4.04812700	2.83320100	
H	2.06422300	4.54883300	-0.85175100	H	2.87896900	-3.01186400	4.21265100	
H	1.62361900	5.24336300	1.48781800	C	0.33488800	-4.84508800	1.26426400	
C	1.85086200	-4.00601900	2.03880400	O	1.31538600	-5.16136000	3.57012200	
C	3.28225100	-3.73793400	2.50133400	C	1.93662700	-5.25789900	4.83719300	
C	0.83681600	-3.02112900	2.60690100	H	1.61834300	-4.44289600	5.50169500	
H	3.97146700	-4.49741700	2.11033600	H	1.61496200	-6.21367700	5.25395600	
H	3.65769200	-2.75773400	2.19420700	H	3.03144200	-5.24679800	4.74717200	
H	3.33305700	-3.77214000	3.59729400	<b>2c</b>				
H	-0.18189700	-3.31222300	2.32890700	C	-2.49241100	6.23415500	-1.85898200	
H	0.91282300	-2.97725900	3.70243600	C	-2.89985700	5.78445700	-0.60496700	
H	0.98699900	-2.00751800	2.22391900	C	-2.36296700	4.62687500	-0.03502700	
C	2.33279000	-2.80842400	-3.05178000	C	-1.39770700	3.93063800	-0.78236300	
C	1.37440300	-1.64448100	-3.26029400	C	-1.00154900	4.35274900	-2.05280200	
C	3.80594600	-2.40658400	-3.11144800	C	-1.54093900	5.51880400	-2.58368100	
H	0.34539700	-1.99287000	-3.39495000	H	-2.92235600	7.14552600	-2.27159800	
H	1.35883700	-0.95488000	-2.41216800	C	-3.64420700	6.34808400	-0.04182200	
H	1.64058900	-1.06357100	-4.15196400	H	-0.27442400	3.75691200	-2.60152500	
H	4.46342800	-3.27584400	-2.97747200	H	-1.22710200	5.85838800	-3.56877200	
H	4.02687600	-1.96873300	-4.09302300	C	-2.79152000	4.15501000	1.31814100	
H	4.08077700	-1.65937000	-2.36221200	H	-3.27836600	4.95965400	1.87926300	
C	2.06543000	0.99283500	3.21513500	H	-3.49824900	3.31729900	1.25077900	
C	0.62631900	0.51141200	3.39347800	H	-1.94110500	3.78335600	1.90327500	
C	3.05382400	-0.16022500	3.31002800	N	-0.82361300	2.74899500	-0.23374500	
H	-0.05888800	1.35540600	3.53676800	C	0.49508800	2.43857200	-0.10473000	
H	0.27676200	-0.02262900	2.49935600	O	0.87874300	1.29496100	0.20398300	
H	0.53320100	-0.16691500	4.25246100	C	-1.72033100	1.68449900	0.01504700	
H	4.08614400	0.15832900	3.11931700	C	-2.44466300	1.33966800	-1.18471000	
H	3.01793600	-0.58792100	4.32039900	H	-1.75973800	1.03535400	-1.98253600	
H	2.81643100	-0.97135000	2.61905100	C	-3.07729500	0.50464300	-0.87534800	
C	2.51585300	2.22262300	-1.88224700	H	-3.07297600	2.17956400	-1.50747100	
C	3.56338700	1.21117800	-2.32599300	C	-0.73616000	-3.90035000	2.34974000	
C	1.15533400	1.89685200	-2.49436400	C	-0.45104800	-2.12352400	0.95196600	
H	4.53630300	1.37021400	-1.84343100	C	-0.35768100	-4.38673400	1.14409200	
H	3.24918100	0.18229200	-2.13532400	N	-0.79243900	-2.51676600	2.22874600	
H	3.71110000	1.29686200	-3.40984700	H	-0.18855200	-3.30015800	0.30119200	
H	0.42084200	2.68995000	-2.30324000	Cu	-0.15517400	-0.36921300	0.27174300	
H	1.221707800	1.75602400	-3.57918800	H	-0.19350600	-5.39928400	0.80142500	
H	0.74413300	0.96836900	-2.08207900	H	-0.97076600	-4.39859800	3.28058700	
B	-1.851326900	0.12798800	-3.24102600	C	-1.15882900	-1.62212500	3.31868300	
F	-0.90453800	0.17520900	-4.24827900	C	-0.15650100	-1.12271500	4.18573400	
F	-1.18348800	-0.27795900	-1.99890200	C	-2.52089000	-1.29127500	3.51823400	
F	-2.40436600	1.40119400	-3.00744900	C	-0.55006000	-0.24810300	5.20625400	
F	-2.85195500	-0.80449000	-3.49379500	C	-2.83928300	-0.41492000	4.56266000	
H	2.28739600	1.65255500	4.06802300	C	-1.87144000	0.11775300	5.39740200	
H	2.83382200	3.19316200	-2.29366800	H	0.22065500	0.14677600	5.86783000	
H	2.18707800	-3.47698400	-3.91349500	H	-3.88669500	-0.15294800	4.71214000	
H	1.58849900	-4.98292400	2.47207500	C	-2.14657600	0.80038900	6.19986400	
C	-1.64404000	2.88376800	0.81811500	C	0.23054900	-3.43768300	-1.08610800	
C	-1.40753200	4.08365900	0.13705000	C	1.60416800	-3.40058100	-1.40573600	
C	-1.90047500	2.92489900	2.18929900	C	-0.75078300	-3.63034600	-2.08125100	
C	-1.40898800	5.29654100	0.81567900	S42				
H	-1.22839700	4.05773600	-0.93928200	C				
C	-1.89131800	4.14038400	2.87309500	C				

C	1.96229000	-3.55602800	-2.74920200	C	0.76140600	-2.60376500	2.24063200
C	-0.32090400	-3.79070000	-3.40139200	C	0.37082700	-1.21792600	0.48866700
C	1.02006800	-3.74813300	-3.74452900	C	1.08984500	-3.26973000	1.10690900
H	3.01950400	-3.49656800	-3.00804100	N	0.32267100	-1.34433100	1.85192700
H	-1.07621600	-3.91410500	-4.17753700	N	0.87528500	-2.40388800	0.04813500
H	1.32761000	-3.84684300	-4.78384000	Cu	-0.40809600	0.27193600	-0.52951700
C	1.33273100	-1.43315000	4.14539800	H	1.45304800	-4.27590600	0.95433000
C	1.67385700	-2.91078500	4.33044300	H	0.79214600	-2.90091500	3.27965700
C	2.04212200	-0.79516700	2.95620600	C	-0.04701800	-0.25967600	2.74693000
H	1.18504200	-3.31928700	5.22451500	C	0.94246800	0.68244000	3.11490200
H	1.38336200	-3.52973000	3.47808400	C	-1.37563200	-0.15649600	3.21724600
H	2.75740600	-3.02849600	4.45799100	C	0.54624700	1.76150300	3.91294400
H	1.88865500	0.29051100	2.93432600	C	-1.69724800	0.94895500	4.01525200
H	3.12204400	-0.98819500	3.00212200	C	-0.75963700	1.91106400	4.35152000
H	1.67689700	-1.18271400	2.00252600	H	1.29902400	2.49848500	4.19316000
C	-3.70909600	-1.77971900	2.70339900	H	-2.72278600	1.04332100	4.37198300
C	-3.73216000	-1.18817800	1.29803500	H	-1.04122800	2.76538400	4.96504600
C	-3.92348200	-3.29145700	2.72627200	C	1.07366700	-2.69102400	-1.36222600
H	3.70944300	-0.09160000	1.34273100	C	2.36231100	-2.58699900	-1.93336800
H	-2.87099500	-1.50696900	0.70464400	C	-0.06754800	-2.98158100	-2.14327200
H	-4.64035500	-1.49431000	0.76124300	C	2.44257000	-2.68454400	-3.32800900
H	-3.94669900	-3.66978000	3.75625300	C	0.09077600	-3.03437900	-3.52916000
H	-4.88464000	-3.53782600	2.25709400	C	1.32572300	-2.85421200	-4.12772800
H	-3.15205600	-3.84397100	2.18441700	H	3.42716700	-2.59926100	-3.78999200
C	2.76488400	-3.09643700	-0.47114800	H	-0.79106700	-3.19866900	-4.14716000
C	3.00672600	-1.58523900	-0.43037000	H	1.41464300	-2.86449600	-5.21217300
C	2.72370500	-3.70667900	0.92231900	C	2.42483800	0.63094100	2.76919500
H	3.16300100	-1.17713600	-1.43434500	C	3.14096800	-0.59043200	3.34385600
H	2.13901800	-1.05402300	-0.01867100	C	2.74276900	0.85522800	1.29410100
H	3.87651400	-1.34485400	0.19601300	H	2.94624400	-0.69777900	4.41852800
H	2.50839300	-4.78288900	0.89625500	H	2.84241000	-1.52259700	2.85487600
H	3.69667100	-3.57251800	1.41348700	H	4.22497200	-0.48850000	3.20670800
H	1.97966100	-3.23177600	1.56464100	H	2.25143200	1.76020800	0.91368000
C	-2.25672300	-3.52029900	-1.91080000	H	3.82651800	0.96948800	1.15522800
C	-2.89421700	-4.18450600	-0.69814800	H	2.41865300	0.02653300	0.65859900
C	-2.64465400	-2.04443400	-2.00809800	C	-2.52351400	-1.11307800	2.93062300
H	-2.55656100	-5.22023200	-0.56461600	C	-3.05154500	-0.96292500	1.50809300
H	-2.69015000	-3.64194500	0.22786500	C	-2.27414600	-2.57363000	3.30203500
H	-3.98547100	-4.20240100	-0.82021100	H	-3.36008600	0.06759600	1.29788900
H	-2.32879600	-1.60658700	-2.96189500	H	-2.28808900	-1.21931600	0.76853800
H	-3.72969200	-1.91150900	-1.89133800	H	-3.90900200	-1.62796800	1.33998000
H	-2.13305500	-1.47052500	-1.22561800	H	-1.85102900	-2.66796100	4.31052100
B	0.60618200	0.28276600	-3.10521200	H	-3.22437200	-3.12181200	3.28713100
F	0.10927600	-0.49346200	-1.98741500	H	-1.60335700	-3.08259800	2.60396700
F	-0.17083400	-0.02692700	-4.21158000	C	3.72554500	-2.37300300	-1.26796600
F	0.44569800	1.65059400	-2.76085400	C	4.29267800	-0.98768200	-1.59151300
F	1.95074600	-0.00806000	-3.29230600	C	3.89485000	-2.65477100	0.21616600
H	-4.58360600	-1.35742500	3.22097100	H	4.33464800	-0.81154800	-2.67175100
H	1.73524100	-0.93272500	5.03917600	H	3.67395900	-0.19351000	-1.16315700
H	-2.67920000	-4.02501500	-2.79317700	H	5.31197300	-0.89311000	-1.19347900
H	3.64204800	-3.53927000	-0.96831900	H	3.59401900	-3.67150000	0.49207200
C	1.48786300	3.51413400	-0.29026800	H	4.95523000	-2.54826200	0.47918000
C	2.65004100	3.19090300	-0.99512200	H	3.34031300	-1.95046500	0.84351500
C	1.34658800	4.80376700	0.24155300	C	-1.48623400	-3.27189700	-1.66119500
C	3.64572400	4.14000800	-1.19590100	C	-1.65229000	-3.87385200	-0.27221900
H	2.75076900	2.19138700	-1.41495300	C	-2.41788800	-2.07982500	-1.87907200
C	2.34395400	5.74756300	0.07010900	H	-0.97290700	-4.71960500	-0.10479900
H	0.45362500	5.06877100	0.80682300	H	-1.48899300	-3.14897900	0.52993400
C	3.49537000	5.42391000	-0.66044900	H	-2.67933900	-4.24415700	-0.15625900
H	4.52668700	3.87012400	-1.77134800	H	-2.41414100	-1.75304500	-2.92314200
H	2.25312300	6.74732000	0.48833300	H	-3.44472600	-2.33659900	-1.58452400
O	4.40878700	6.42086800	-0.79277400	H	-2.10916400	-1.20516500	-1.29029700
C	5.58144200	6.13464500	-1.53053100	B	-0.76726900	0.58053400	-4.40866300
H	6.17065300	7.05324000	-1.52183800	F	0.88076700	0.19786000	-3.03005500
H	6.15840600	5.32445600	-1.06419600	F	-1.71952600	1.58156300	-4.66265000
H	5.34391400	5.86080700	-2.56739100	F	0.52597000	1.11464500	-4.60957000
H				F	-0.97603800	-0.53513300	-5.21104000
H				H	-1.83598900	-4.05066200	-2.35796400
H				H	-3.32975400	-0.77360800	3.59844000
<b>TS<sub>2c-3c</sub></b>				H	4.37819100	-3.09769800	-1.78272400
C	-1.37442800	5.83891500	-2.46093900	H	2.85091800	1.49637300	3.29929300
C	-1.21942500	5.61851000	-1.07980100	H	2.62588300	2.45054300	-2.47335100
C	-0.55749700	4.50653800	-0.59678800	C	3.05981800	3.73202400	-2.09549000
C	-0.006660100	3.57749100	-1.54960000	C	3.29850700	1.78323100	-3.50215300
C	-0.23137400	3.78183400	-2.94944900	C	4.13875000	4.32616200	-2.72413700
C	-0.88875800	4.92036500	-3.38940200	C	2.56065900	4.25866500	-1.28245200
H	-1.90227000	6.72837100	-2.80195600	C	4.36710800	2.38064900	-4.15727900
H	-1.63231400	6.33878900	-0.37342600	H	2.93384800	0.80522600	-3.80658700
H	0.12586600	3.02934500	-3.65372300	C	4.79668300	3.65433300	-3.76382900
H	-1.05228800	5.06794900	-4.45462000	C	4.49443900	5.31087800	-2.42973000
C	-0.40259200	4.21751300	0.85477000	H	4.84912300	1.85587100	-4.97786500
H	-0.85662200	4.99777700	1.47485100	H	5.83665500	4.31832900	-4.32795000
H	-0.86648300	3.25042000	1.09430900	O	6.53313900	3.67152400	-5.37677600
H	0.65598900	4.11812600	1.13224400	C	5.87343100	3.47595300	-6.23261000
N	0.62283400	2.50133000	-1.06448700	H	7.32508100	4.35986900	-5.67653400
C	1.50801100	1.74764600	-1.80177200	H	6.97739700	2.72650000	-5.03625300
O	1.47649800	0.51095600	-1.76728100	C	-5.25762100	-1.96026500	1.03854300
O	-1.79471900	1.49874700	-0.56548100	C	-4.32565100	-2.14561400	2.06409000
C	-2.58398100	1.92086100	-1.58841600				
H	-3.04242700	1.10897000	-2.17494600				
H	-3.33695100	2.64045400	-1.21743900				
H	-1.97533100	2.49906600	-2.33460100				
<b>3c</b>							

C	-3.14484100	-1.41415000	2.10864400	C	-2.24821100	2.62169700	0.75845200
C	-2.91642500	-0.45546100	1.08232000	C	-3.39933500	2.66779200	1.56318100
C	-3.86141400	-0.26377800	0.05222500	C	-1.87307500	3.76740500	0.04803600
C	-5.02718600	-1.01369000	0.03829900	C	-4.15073900	3.82407900	1.65127700
H	-6.16448700	-2.56283400	1.01965700	C	-2.62918800	4.92876100	0.11504700
H	-4.52082200	-2.87964600	2.84619900	C	-3.77526000	4.96001200	0.91964700
H	-3.64681700	0.45382800	-0.73758100	H	-5.03969800	3.87459000	2.27521400
H	-5.74129300	-0.87840400	-0.77139000	H	-2.33043900	5.79607000	-0.46712300
C	-2.15208900	-1.57446300	3.21204300	H	-0.99186900	3.72529700	-0.58795900
H	-2.42463300	-2.40276800	3.87518100	H	-3.69841900	1.79252600	2.13760900
H	-1.15031900	-1.75894100	2.80659900	O	-4.58090600	6.04097200	1.05709100
H	-2.08362400	-0.66046900	3.81883900	C	-4.24623400	7.20570000	0.32496700
N	-1.70957400	0.20449300	1.11698800	H	-5.01388200	7.94121700	0.57036200
C	-1.40303600	1.43654600	0.67177100	H	-3.26097300	7.59164900	0.61954200
O	-0.19278500	1.51366400	0.25941600	H	-4.25490600	7.01251100	-0.75584600
O	-0.41513200	-2.32058600	0.50699700				
C	-1.29388900	-2.84892900	-0.41987700				
H	-0.82024600	-3.06355600	-1.39508500				
H	-1.67203700	-3.79759300	0.00783600				
H	-2.18934500	-2.22171500	-0.59624600				
C	4.02649200	-1.66699100	-0.27978300				
C	1.95067100	-0.79258000	-0.05384800				
C	4.17174200	-0.34468300	-0.03801000				
N	2.66655100	-1.93928100	-0.28437700				
N	2.89717700	0.18115600	0.09565800				
Cu	-0.03484200	-0.49373900	0.24349400				
H	5.04977300	0.28007600	0.04748200				
H	4.75216400	-2.44899800	-0.45391100				
C	2.17040400	-3.29181200	-0.53636700				
C	2.04943100	-4.19409400	0.54560400				
C	1.911178200	-3.69324600	-1.86542100				
C	1.56875400	-5.47695300	0.26585600				
C	1.43368200	-4.99555100	-2.06746600				
C	1.24139900	-5.87889500	-1.02025100				
H	1.45169300	-6.17427200	1.09533900				
H	1.21167200	-5.30565400	-3.08822100				
H	0.857773500	-6.88103000	-1.204083600				
C	2.69024800	1.59216400	0.38725600				
C	2.60067100	2.00602300	1.73281300				
C	2.624245600	2.51143600	-0.68092600				
C	2.43873900	3.37330100	1.98054000				
C	2.48359600	3.86415700	-0.35705100				
C	2.37569300	4.30058100	0.95285700				
H	2.360663300	3.70364200	3.01677500				
H	2.43426900	4.58335100	-1.17528800				
H	2.25140700	5.35992100	1.17317400				
C	2.40105800	-3.93750400	2.00461800				
C	3.88201900	-3.65300300	2.25945700				
C	1.47947400	-2.94072600	2.69753900				
H	4.52084700	-4.39264400	1.75962800				
H	4.19696100	-2.65963800	1.92852100				
H	4.08721100	-3.70856300	3.33631000				
H	0.44245800	-3.29032900	2.67405000				
H	1.78462700	-2.80099200	3.74408400				
H	1.48654300	-1.96241500	2.20983900				
C	2.12908000	-2.87370900	-3.12973900				
C	1.20418600	-1.67210300	-3.25030500				
C	3.59643700	-2.53153500	-3.39090300				
H	0.15100900	-1.96930100	-3.25524300				
H	1.32067800	-0.96576600	-2.42449200				
H	1.39578500	-1.12329500	-4.18120600				
H	4.23247200	-3.42452300	-3.33168700				
H	3.70297300	-2.10857000	-4.39785400				
H	3.99415400	-1.78967000	-2.69232000				
C	2.572720200	1.12170800	2.97087400				
C	1.11645200	0.64874200	3.25585000				
C	3.56926100	-0.02863800	3.03389800				
H	0.45269700	1.49491600	3.33611600				
H	0.76620000	0.00354300	2.45380600				
H	1.10194700	0.07110700	4.18897800				
H	4.58664000	0.29359500	2.77838300				
H	3.59469300	-0.43781000	4.05229000				
H	3.29993900	-0.85461800	2.37221200				
C	2.63076900	2.20099200	-2.16923900				
C	3.58768400	1.13572200	-2.68827400				
C	1.20111300	1.90815200	-2.62156300				
H	4.61034500	1.26103500	-2.30895300				
H	3.25103500	0.12521900	-2.44369000				
H	3.62886100	1.19248800	-3.78334600				
H	0.52192700	2.73907600	-2.39856000				
H	1.15672400	1.71303800	-3.69901100				
H	0.79062600	1.02883900	-2.11531400				
B	-1.95880900	0.29077100	-2.74798900				
F	-1.21353900	0.47809900	-3.89837700				
F	-1.10236600	-0.35150200	-1.74885400				
F	-2.36770900	1.51452100	-2.18968700				
F	-3.04726600	-0.54950600	-2.95620500				
H	2.84299900	1.79857600	3.79598300				
H	2.93738100	3.14418900	-2.64799900				
H	1.84646000	-3.55677500	-3.94501400				
H	2.21460100	-4.90471800	2.49556400				

H	3.71444600	0.19005000	4.14356500	H	3.79090100	-3.85017200	3.35385600
H	3.38229800	-0.17453200	2.45754100	H	0.20228000	-3.24135600	2.57072400
C	2.85864900	3.01212100	-2.01824800	H	1.52351300	-2.81102100	3.68856600
C	3.78264100	1.93177400	-2.56334100	H	1.31740200	-1.95585700	2.14619500
C	1.41590500	2.76362900	-2.45669800	C	2.22987500	-2.81373300	-3.16202000
H	4.81340900	2.02982200	-2.19761900	C	1.36495600	-1.56781100	-3.30272500
H	3.42672600	0.92839500	-2.31924700	C	3.72187200	-2.54347200	-3.35001700
H	3.80830900	1.99605600	-3.65861300	H	0.29932100	-1.81817200	-3.33994400
H	0.76302200	3.61028600	-2.21639200	H	1.48994800	-0.87728400	-2.46490400
H	1.35403800	2.58118400	-3.53548000	H	1.60860800	-1.02047000	-4.22244000
H	0.98555700	1.89196400	-1.95207700	H	4.30916600	-3.46738400	-3.26438200
B	-1.83984100	1.28504400	-2.62874700	H	3.89526900	-2.12799000	-4.35070100
F	-1.01737200	1.38937800	-3.73869700	H	4.12285100	-1.82257900	-2.63306500
F	-1.10148700	0.59437700	-1.57219800	C	2.72230600	1.00342700	3.06339200
F	-2.18524300	2.54956800	-2.12288700	C	1.24830700	0.66085300	3.29421000
F	-2.97817600	0.52754100	-2.89567900	C	3.59768900	-0.24016100	3.11909600
H	3.10898800	2.47274200	3.93548200	H	0.64169700	1.56762200	3.41341000
H	3.18287800	3.95535000	-2.48546100	H	0.83334900	0.11306900	2.43567000
H	1.97969200	-2.62792000	-3.96534000	H	1.12389400	0.03665000	4.18979700
H	2.06649600	-4.14043600	2.44496200	H	4.64596500	-0.01998600	2.88161700
C	-2.05432400	3.70463700	0.84416400	H	3.56618000	-0.66764700	4.12996500
C	-3.23539300	3.75757200	1.60245100	H	3.25321500	-1.01994400	2.43720200
C	-1.66942900	4.83345400	0.11171500	C	2.90696700	2.16770100	-2.04838800
C	-4.00680500	4.90398000	1.62878600	C	3.82018700	1.07082800	-2.57903700
C	-2.44226800	5.98530400	0.11751700	C	1.46445800	1.94979200	-2.50553900
C	-3.61824200	6.02334100	0.87841000	H	4.84834300	1.15735600	-2.20318900
H	-4.92108600	4.95964300	2.21472600	H	3.44987700	0.07314200	-2.33340600
H	-2.13506800	6.83930900	-0.47963800	H	3.85790400	1.12966600	-3.67440300
H	-0.76555700	4.78010400	-0.49153600	H	0.83054900	2.81475000	-2.27956900
H	-3.54383900	2.89036600	2.18433200	H	1.41948900	1.75918800	-3.58426100
O	-4.44391300	7.09564200	0.95065300	H	1.00527400	1.09356500	-1.99798400
C	-4.10474800	8.23706200	0.18426700	B	-1.86648300	0.44782700	-2.71435500
H	-4.89374100	8.96673600	0.37275500	F	-1.15367700	0.63333400	-3.88355100
H	-3.13777800	8.65363100	0.49683800	F	-0.99014800	-0.21885900	-1.74746000
H	-4.07159500	8.00054500	-0.88732400	F	-2.25846400	1.66812600	-2.14370400
H				F	-2.96800800	-0.38972900	-2.89770200
<b>4c</b>				H	3.03462400	1.63400800	3.91031300
C	-4.84521800	-2.11057800	0.52243500	H	3.25556400	3.10368600	-2.51270600
C	-3.73843700	-2.57237200	1.13600200	H	1.95268000	-3.47286100	-3.99869600
C	-2.51063500	-1.73798800	1.31017200	H	1.87907400	-4.93647600	2.41748500
C	-2.63852500	-0.31295200	0.75082100	C	-2.41006700	2.75551500	0.89936200
C	-3.82123700	0.07570400	0.05565200	C	-3.37585700	2.59203800	1.90519400
C	-4.87154300	-0.78832700	-0.04718200	C	-2.41961200	3.92814700	0.13853700
H	-5.72215200	-2.74676700	0.41267300	C	-4.32356100	3.57196800	2.14070600
H	-3.68191600	-3.59061000	1.52206600	C	-3.38198300	4.90744000	0.34579900
H	-3.83768100	1.03262000	-0.45873000	C	-4.33977000	4.73111900	1.35199000
H	-5.74676400	-0.48625700	-0.62009600	H	5.06984300	3.46281100	2.92420900
C	-2.15312800	-1.65715300	2.79137100	H	-3.38698100	5.79397400	-0.28233300
H	-2.04718900	-2.66356100	3.21090800	H	-1.67887800	4.03896600	-0.65063000
H	-1.20877300	-1.11372000	2.91232900	H	-3.37313500	1.69060100	2.51787200
H	-2.93497300	-1.12170500	3.34806800	O	-5.32108700	5.62386300	1.63748300
N	-1.55007700	0.40039000	0.93322300	C	-5.38445600	6.79967500	0.85230900
C	-1.37676000	1.75018300	0.60518600	H	-6.23231500	7.36856100	1.23758800
O	-0.27109900	2.05031800	0.15120100	H	-4.46744800	7.39611900	0.95107000
O	-1.37335400	-2.36765600	0.67389400	H	-5.55229000	6.56302800	-0.20699500
C	-1.63692100	-2.86789700	-0.64646900				
H	-0.65698000	-2.99136700	-1.11726800				
H	-2.14291200	-3.84123200	-0.59742800	C	-5.23639200	-2.24406500	-0.73695400
H	-2.22454100	-2.16064100	-1.24342900	C	-4.18707800	-2.94572100	-0.14281400
C	4.13294400	-1.80009000	-0.22909400	C	-3.09950000	-2.24403300	0.34234800
C	2.09014700	-0.81253800	-0.01205700	C	-3.03987200	-0.82500200	0.26586600
C	4.43491600	-0.49501400	0.05840500	C	-4.10691200	-0.10474900	-0.35245100
N	2.75756400	-1.98961400	-0.27152700	C	-5.18390100	-0.85249700	-0.82800600
N	3.09661800	0.09703000	0.18121600	H	-6.09783900	-2.77769700	-1.13615400
Cu	0.20050200	-0.36584100	0.14162400	H	-4.21484800	-4.03135000	-0.06980000
H	5.25569300	0.07396200	0.17822000	H	-6.00540000	-0.31796300	-1.30483500
H	4.82207700	-2.61354800	-0.40960900	N	-1.87075800	-0.29464100	0.73741600
C	2.13429400	-3.27084800	-0.57321300	C	-1.46331700	0.90711600	1.16716000
C	1.82573600	-4.16056100	0.48382700	O	-0.21918900	1.10759900	0.92468500
C	1.88533400	-3.62496400	-1.92171900	O	-0.75563100	-2.06163700	-1.07557700
C	1.17598300	-5.35816700	0.16253000	C	-0.70846000	-2.12993200	-2.45417600
C	1.24420000	-4.84591400	-2.16711400	H	-0.88588900	-1.16012500	-2.94808000
C	0.86854900	-5.70071300	-1.14416000	H	0.23074600	-2.57390900	-2.83551500
H	0.91933700	-6.03692800	0.97605800	H	-1.53023400	-2.80294700	-2.76327700
H	1.03412100	-5.11460800	-3.20195800	C	3.87657800	-1.95534000	-0.18477800
H	0.35812300	-6.63700600	-1.36515000	C	1.87995800	-0.89898200	-0.33756200
C	2.93621100	1.50754900	0.49412900	C	4.12121900	-0.62604500	-0.26371300
C	2.84842900	1.90566500	1.84544900	N	2.49914400	-2.11569600	-0.23197800
C	2.93310900	2.45145900	-0.55540000	N	2.89447900	0.00943400	-0.33476500
C	2.76956400	3.27552100	2.11881400	Cu	-0.10001800	-0.51141300	-0.24979400
C	2.84792500	3.80489800	-0.20834500	H	5.04524600	-0.06542100	-0.25824500
C	2.76970800	4.22391100	1.10903200	H	4.54237000	-2.79989600	-0.08199600
H	2.70008800	3.58992400	3.16074400	C	1.81239400	-3.39216700	-0.20692600
H	2.83340000	4.53911900	-1.01423600	C	1.11941600	-3.76233400	0.96810300
H	2.71048400	5.28459700	1.34837500	C	1.83456600	-4.22291400	-1.34814400
C	2.14584400	-3.97178200	1.95971200	C	0.29895900	-4.89081900	0.90735100
C	3.63042300	-3.78795900	2.26982900	C	0.99166200	-5.34322400	-1.33353800
C	1.25144900	-2.93479300	2.63116500	C	0.19500400	-5.65599500	-0.24484600
H	4.23262800	-4.57466200	1.79713800	H	-0.25716800	-5.17535600	1.80099300
H	4.02519100	-2.82320100	1.94254000	H	0.97302900	-5.98273700	-2.21620100

H	-0.46681000	-6.51994600	-0.27685300	C	-1.07261600	-0.71953300	-2.36751500
C	2.71319400	1.45338600	-0.37125200	H	-0.38725500	-0.00200700	-2.83925100
C	2.73118500	2.19691800	0.82947400	H	-0.90843600	-1.72650400	-2.79057300
C	2.51950000	2.05955500	-1.63378200	H	-2.08718800	-0.37756500	-2.63268200
C	2.47088200	3.56983200	0.71943400	C	4.05033500	-0.89712900	-0.09514300
C	2.24598900	3.42820900	-1.65545900	C	2.11591700	0.28744500	-0.21488600
C	2.19981700	4.17950900	-0.49174700	C	4.37807800	0.40639700	-0.26970500
H	2.47930300	4.16568000	1.63336400	N	2.66335000	-0.95959900	-0.05581200
H	2.04939700	3.89886600	-2.61584400	N	3.19363900	1.12089600	-0.32618600
H	1.97093200	5.24302400	-0.53456600	Cu	0.17174000	0.75520400	-0.12297400
C	1.28963800	-3.13513900	2.34681500	H	5.33993000	0.89460900	-0.34382300
C	2.74565800	-3.16918100	2.81366100	H	4.66761800	-1.77384200	0.03980900
C	0.64566800	-1.77081300	2.56390900	C	1.86558800	-2.16677200	0.06489500
H	3.15802100	-4.18385900	2.74949800	C	1.25473400	-2.45936400	1.30587100
H	3.39135600	-2.50973200	2.22406500	C	1.66916700	-2.99262400	-1.06397700
H	2.81797000	-2.84004200	3.85825700	C	0.33451400	-3.51202700	1.34619100
H	-0.41015200	-1.76858100	2.26666400	C	0.74298500	-4.03642400	-0.94734200
H	0.69814200	-1.49671800	3.62649000	C	0.04857900	-4.27832400	0.22666600
H	1.14247200	-0.97161100	2.00579400	H	-0.15299600	-3.73460200	2.29597200
C	2.77458000	-4.16140200	-2.55161100	H	0.56698800	-4.66653000	-1.81951700
C	3.01620400	-2.83928100	-3.26366300	H	-0.68281400	-5.08362900	0.28013700
C	4.10192600	-4.84906400	-2.21015700	C	3.08685800	2.57291800	-0.40591500
H	2.08344500	-2.39188600	-3.61624800	C	3.13758000	3.34978200	0.77299600
H	3.53590600	-2.09741900	-2.64952400	C	2.91584600	3.16628600	-1.67998200
H	3.64583200	-3.01895800	-4.14468500	C	2.91152100	4.72707700	0.63516200
H	3.94246500	-5.82986600	-1.74701300	C	2.67752900	4.54006200	-1.73195600
H	4.69856800	-4.99359700	-3.11947700	C	2.64702100	5.31840500	-0.58559300
H	4.70891700	-4.25008800	-1.52078400	H	2.94336900	5.34106100	1.53610000
C	3.01515600	1.75852100	2.27071100	H	2.49443800	4.99518000	-2.70327600
C	1.76225000	1.82623600	3.15131300	H	2.44163300	6.38548100	-0.65028100
C	3.74433200	0.45025100	2.52934600	C	1.57657300	-1.80898900	2.64465600
H	1.22613300	2.77368900	3.02823800	C	3.06221100	-1.88522400	2.99476500
H	1.05678000	1.02627800	2.90941400	C	0.98611800	-0.41761300	2.84775200
H	2.04595600	1.72848100	4.20760900	H	3.42507900	-2.91946200	2.94212600
H	4.72284000	0.40497800	2.03882500	H	3.68699700	-1.27883600	2.33273800
H	3.91590400	0.34507200	3.60850200	H	3.22786400	-1.52082700	4.01667500
H	3.16567100	-0.42341100	2.21586200	H	-0.10185900	-0.42114900	2.70580000
C	2.69442000	1.39113300	-2.99256200	H	1.19843400	-0.05998500	3.86461500
C	4.12638000	0.89870300	-3.21557900	H	1.39249600	0.32025400	2.15013500
C	1.67346000	0.32401600	-3.36664400	C	2.42447000	-2.94138600	-2.38544800
H	4.86851000	1.65798100	-2.93625200	C	2.50479700	-1.59610600	-3.08403800
H	4.34544600	-0.01323900	-2.64733900	C	3.80507600	-3.59219100	-2.26226100
H	4.27687500	0.65461800	-4.27515500	H	1.51290000	-1.15302800	-3.20629200
H	0.66297100	0.73401400	-3.36712200	H	3.13270600	-0.87506100	-2.55203600
H	1.89738100	-0.05906800	-4.37205800	H	2.93921000	-1.71995200	-4.08475400
H	1.69580200	-0.52923100	-2.68390800	H	3.74998600	-4.57503300	-1.77891700
B	-1.29480500	2.30522500	-2.25930700	H	4.24915800	-3.72752700	-3.25629900
F	-0.25193300	2.73922600	-3.07449000	H	4.49663200	-2.96901000	-1.68395300
F	-1.39250800	3.09658700	-1.10700200	C	3.43551700	2.94287500	2.21985100
F	-2.49495400	2.26951900	-2.95532800	C	2.20397400	3.09947700	3.11773900
F	-1.00338100	0.93912100	-1.81778700	C	4.10645200	1.60864700	2.49711300
H	-2.26113400	-2.75520700	0.80808900	H	1.73246500	4.08076700	2.99545200
C	-4.12681000	1.37814000	-0.49407000	H	1.43993700	2.35333600	2.88503400
H	-4.59220800	1.85400600	0.38163500	H	2.49230900	2.98549300	4.17128200
H	-3.13234900	1.81408100	-0.60283500	H	5.07018100	1.50438500	1.98619300
H	-4.70281200	1.67107800	-1.37679900	H	4.29704400	1.52083500	3.57483400
H	3.68626100	2.54896300	2.64542000	H	3.47939100	0.75825500	2.21729400
H	0.74762800	-3.82106800	3.01563000	C	3.01376300	2.46140600	-3.02535600
H	2.53617000	2.20868500	-3.71028700	C	4.32130800	1.69869200	-3.24093000
H	2.29086900	-4.80953100	-3.29812000	C	1.78449900	1.62580700	-3.36613100
C	-2.22857800	1.85408600	1.96949500	H	5.19442700	2.30281300	-2.96008200
C	-1.81471100	3.18853500	2.02201300	H	4.36651800	0.76081500	-2.67873200
C	-3.35649100	1.45499500	2.70404700	H	4.42373000	1.43738900	-4.30207600
C	-2.51655800	4.11802900	2.77840000	H	0.90372300	2.26132200	-3.47789300
C	-4.04704900	2.36684200	3.47966200	H	1.94766900	1.06857300	-4.29914900
C	-3.63452300	3.70740600	3.51532200	H	1.56458700	0.90275200	-2.57542700
H	-2.19549700	5.15592800	2.77937000	B	-1.20047200	3.54251300	-2.02752400
H	-4.91599000	2.07298200	4.06360600	F	-0.20316500	4.04978000	-2.85436800
H	-0.95951500	3.49347500	1.42284100	F	-1.33257400	4.32658200	-0.87140400
H	-3.68535300	0.41640800	2.66876600	F	-2.41359300	3.43107700	-2.70109700
O	-4.38317700	4.53022500	4.29067700	F	-0.82016000	2.19679600	-1.60544800
C	-4.01982600	5.89790300	4.33618800	H	-1.88798400	-1.51919600	0.80052900
H	-4.07996300	6.35876200	3.34127000	C	-3.97071400	2.59845400	-0.21013800
H	-4.74043100	6.37376500	5.00313300	H	-4.46522900	2.81627200	0.74681100
H	-3.00597700	6.02772200	4.73849000	H	-3.04734700	3.18365600	-0.23796800
H				H	-4.60883600	2.97127800	-1.01631300
H				H	4.15237900	3.71050600	2.55585700
C	-4.40882900	-1.01482900	-1.37583900	H	1.07031000	-2.45171200	3.38138800
C	-3.43745200	-1.71385100	-0.70408600	H	3.03128400	3.28363800	-3.75613700
C	-2.51404700	-0.99405400	0.08445600	H	1.84284800	-3.59483200	-3.05371300
C	-2.68632700	0.43672700	0.32196300	C	-2.05321500	3.06838000	2.27766200
C	-3.73091100	1.13791200	-0.37601800	C	-1.67356700	4.41119100	2.36918500
C	-4.54196600	0.38910000	-1.20490000	C	-3.16243500	2.61706900	3.00972500
H	-5.10794400	-1.53306600	-2.03100500	C	-2.39221000	5.29835700	3.15914700
H	-3.32908100	-2.79146000	-0.81034500	C	-3.86975000	3.48540700	3.81952400
H	-5.32992200	0.90701700	-1.75117600	C	-3.49290900	4.83502800	3.89178900
N	-1.67782100	0.93003600	1.03735600	H	-2.09897200	6.34399100	3.19004100
C	-1.27353400	2.17707200	1.42287700	H	-4.72443800	3.15166900	4.40324700
O	-0.07774400	2.43105600	1.12515900	H	-0.83146700	4.75424100	1.77108200
O	-0.88378700	-0.69754300	-0.98058800	O	-3.46142600	1.57085200	2.94434600
				O	-4.25681000	5.61334300	4.69734600

C	-3.92626200	6.98727400	4.78639400	H	-1.57055900	-1.71183200	-0.69190100	
H	-4.00371900	7.47870300	3.80743300	C	-4.23966700	2.07870600	-0.35218000	
H	-4.65353300	7.42334400	5.47295800	H	-4.45610800	2.13165900	0.72231400	
H	-2.91303600	7.12777700	5.18653600	H	-3.42717000	2.78428100	-0.56286300	
<b>4c'</b>								
C	-4.47685200	-1.37066700	-2.04122700	H	-5.13325000	2.42588900	-0.88124100	
C	-3.21347100	-1.83960200	-2.04896800	H	4.13607900	3.10393800	1.42912700	
C	-2.11190200	-0.107170700	-1.41489000	H	0.50802300	-1.98310600	4.10137100	
C	-2.54555400	0.16752900	-0.63821100	C	3.92174100	0.41408200	-4.57853000	
C	-3.88253100	0.69579600	-0.80122700	C	0.39656100	-4.83880600	-1.81557800	
C	-4.78711300	-0.08497300	-1.46862400	C	-2.57519800	1.21200900	2.26827500	
H	-5.27919000	-1.93103100	-2.51930000	C	-2.79252600	2.15777900	3.27551700	
H	-2.94186200	-2.76671100	-2.55354300	C	-3.12215900	-0.07215000	2.42719300	
H	-5.79557500	0.30517300	-1.61135300	C	-3.54584400	1.85468000	4.40195800	
N	-1.57876500	0.67085100	0.08365100	C	-3.86673300	-0.39246500	3.54931800	
C	-1.72413600	1.62435600	1.12050300	C	-4.08802100	0.57060500	4.54332300	
O	-1.06567000	2.64930500	1.13532900	H	-3.70392700	2.61533900	5.16171000	
O	-1.07325800	-0.73368700	-2.34929200	H	-4.28476400	-1.38782800	3.68451700	
C	-1.51182500	0.11543500	-3.42194200	H	-2.35250900	3.14575500	3.15294300	
H	-0.62239300	0.32818800	-4.01664600	C	-2.94249200	-0.84339300	1.67963100	
H	-2.26499700	-0.39530400	-4.03641600	O	-4.82853600	0.16548200	5.60436300	
H	-1.90043600	1.06541200	-3.03665600	H	-5.06139000	1.10561500	6.63745700	
C	3.49688300	-2.20730900	0.38848800	H	-5.61284800	1.97902500	6.26451700	
C	1.96598100	-0.65310800	-0.26422300	H	-5.66400500	0.58481600	7.38312300	
C	4.16953800	-1.19367600	-0.20929400	H	-4.11895000	1.43705900	7.09373300	
N	2.15149800	-1.86634200	0.35894400	<b>S1d</b>				
N	3.23020000	-0.25731100	-0.61171800	C	-2.34978600	-0.42350500	0.45780400	
Cu	0.27304900	0.29456100	-0.50763300	C	-0.97589400	-0.17229700	0.57383600	
H	5.22659800	-1.04174600	-0.38085400	C	-0.16377900	-0.52137200	-0.52053700	
H	3.84646700	-3.11643900	0.85759400	C	-0.72041500	-1.03964200	-1.69598200	
C	1.05445000	-2.71228000	0.80167300	C	-2.08677400	-1.25712800	-1.78857200	
C	0.50165900	-2.52994100	2.09083900	C	-2.90504500	-0.95927300	-0.69764300	
C	0.54033400	-3.69385000	-0.07870600	H	-2.99548700	-0.16590900	1.29752100	
C	-0.65666500	-3.24803000	2.41414100	H	-2.51198400	-1.66341000	-2.70430100	
C	-0.61238300	-4.38480300	0.31596600	H	-3.97844100	-1.13129000	-0.75391700	
C	-1.23396600	-4.14749000	1.53218700	C	-0.43720300	0.44445800	1.82719800	
H	-1.09980900	-3.09060300	3.39799500	H	0.47942500	1.01914000	1.64874300	
H	-1.02378300	-5.12961700	-0.36555600	H	-1.17650900	1.11841700	2.27350600	
H	-2.13998900	-4.68696900	1.80472400	H	-0.19532900	-0.31459100	2.58375400	
C	3.59828000	1.01947600	-1.21818200	N	1.24324900	-0.31668900	-0.50267400	
C	3.76908200	2.14729400	-0.38994100	C	2.17404800	-0.63307500	0.46786400	
C	3.78765200	1.10110600	-2.61570300	O	3.25648200	-0.06509100	0.54083900	
C	4.10806000	3.36047900	-1.00030400	O	1.71085700	0.51341700	-1.53220200	
C	4.12596500	2.34466000	-3.15625700	C	1.56418600	1.88597700	-1.16674800	
C	4.27900600	3.47293800	-2.36736900	H	1.91029900	2.44583800	-2.03853600	
H	4.20942500	4.24121700	-0.36602600	H	0.50941600	2.12788300	-0.96929400	
H	4.23990100	2.42050900	-4.23725300	H	2.18845600	2.12186800	-0.29747100	
H	4.51653900	4.43473900	-2.81805400	H	-0.05598900	-1.26543500	-2.52774400	
C	1.06719800	-1.66555700	3.20788100	C	1.81383200	-1.74123500	1.40422500	
C	2.53427000	-1.94268300	3.53166700	C	2.36846400	-1.68280000	2.68872100	
C	0.76360600	-0.18323900	3.02698400	C	1.02845300	-2.84131900	1.04692300	
H	2.71358300	-3.01674000	3.67087100	C	2.11057800	-2.68338700	3.61310200	
H	3.22113900	-1.58360500	2.76110600	H	3.00396300	-0.83683900	2.94272600	
H	2.80781200	-1.43443200	4.46487100	C	0.78082800	-3.85579200	1.96632400	
H	-0.31885800	-0.00628700	3.01537000	H	0.61433600	-2.91798500	0.04362400	
H	1.19388500	0.40808800	3.84594800	C	1.30866200	-3.76946600	3.25291300	
H	1.16869000	0.20420500	2.08919700	H	2.52859400	-2.62763600	4.61637400	
C	1.14702100	-4.15052900	-1.39756300	H	0.17362100	-4.71189100	1.68401500	
C	1.36395200	-3.06350400	-2.43352400	C	1.07230900	-4.86044800	4.25163600	
C	2.41540700	-4.98325700	-1.19535900	F	2.16910200	-5.64218900	4.40649800	
H	0.47551300	-2.43688700	-2.56984600	F	0.05725700	-5.67581700	3.89782700	
H	2.18947800	-2.40467000	-2.15770400	F	0.78064800	-4.36749000	5.47757100	
H	1.62421000	-3.51134700	-3.40203900	<b>2d</b>				
H	2.28613700	-5.74853700	-0.42001900	C	-2.53015700	6.17933500	-2.11144000	
H	2.68180600	-5.49164600	-2.13047000	C	-2.88616900	5.80002600	-0.81814500	
H	3.27005600	-4.35476700	-0.91957900	C	-2.36568400	4.64586500	-0.22798400	
C	3.51765600	2.25217900	1.10509500	C	-1.47209600	3.88203300	-0.99915500	
C	2.06290700	2.65742200	1.34018400	C	-1.12710900	4.23073000	-2.30410400	
C	3.94218900	1.08049900	1.97899900	C	-1.65005000	5.39632000	-2.85520600	
H	1.80533400	3.57758100	0.80461700	H	-2.94542100	7.09070100	-2.53875900	
H	1.36979900	1.89572600	0.96284200	H	-3.57307700	6.41908200	-0.24062900	
H	1.85490200	2.80006500	2.40928300	H	-0.44719600	3.58342800	-2.85621200	
H	4.97675100	0.77113900	1.78020900	H	-1.37616400	5.68317400	-3.86834900	
H	3.87740200	1.36745900	3.03697900	C	-2.72966000	4.25257600	1.16884000	
C	3.30068400	0.20560000	1.85254500	H	-3.20233000	5.08533500	1.70152800	
C	3.54274900	-0.00003400	-3.63199800	H	-3.42695200	3.40484900	1.18400100	
C	4.32956200	-1.29479400	-3.44161300	H	-1.85078000	3.92771100	1.74067200	
C	2.03860800	-0.18681600	-3.83426000	N	-0.89964700	2.70648100	-0.42946500	
H	5.40485700	-1.08881200	-3.35527500	C	0.38356600	2.48451000	-0.06173900	
H	4.03456900	-1.87471600	-2.56391600	O	0.73986700	1.44239500	0.52053600	
H	4.18593000	-1.94386400	-4.31535900	O	-1.80396600	1.68662000	-0.05373100	
H	1.59765400	0.74685700	-4.20161700	C	-2.63895400	1.32501400	-1.17293400	
H	1.83136100	-0.98924100	-4.55634700	H	-2.03505600	0.97591500	-2.01696700	
H	1.51918800	-0.42599200	-2.90031700	H	-3.25790000	0.51529000	-0.77977400	
B	0.04168300	3.05044500	-2.32079400	H	-3.27623600	2.16951200	-1.46379800	
F	0.20116400	2.90602600	-3.69780800	C	-0.64473600	-3.91407100	2.32978100	
F	0.56280400	4.23383800	-1.84630700	C	-0.43266400	-2.08750800	0.98554700	
F	-1.30487700	2.88021200	-1.96028300	C	-0.27948400	-4.35160800	1.10182700	
F	0.79430100	1.94834000	-1.69704100	N	-0.73493300	-2.52985400	2.25538000	

N	-0.15384000	-3.23461600	0.29035600	H	-1.46795800	6.42327800	-0.33847300
Cu	-0.23605100	-0.28833200	0.40727400	H	0.05312400	3.08481400	-3.70787200
H	-0.10059900	-5.34840200	0.72237400	H	-1.05379600	5.18740100	-4.44933400
H	-0.84894900	-4.44761200	3.24808000	C	-0.29935000	4.23384800	0.82640800
C	-1.08777700	-1.67813700	3.38403700	H	-0.70740900	5.02159200	1.46841200
C	-0.07234000	-1.20610600	4.25087400	H	-0.79163400	3.28058000	1.06379700
C	-2.44793000	-1.36498900	3.62097700	H	0.76188900	4.09305600	1.07534900
C	-0.45343300	-0.38241600	5.31755100	N	0.57946000	2.49174500	-1.14004400
C	-2.75329300	-0.53899400	4.70951300	C	1.45737700	1.71907800	-1.84650300
C	-1.77405900	-0.03842400	5.55078000	O	1.44570100	0.48555200	-1.77976700
H	0.32675700	-0.00897900	5.98036000	O	-1.78542700	1.55769000	-0.48643000
H	-3.79956400	-0.29259300	4.88964200	C	-2.62514300	2.00247600	-1.46065100
H	-2.03919100	0.60397900	6.38884700	H	-3.13950300	1.20300400	-2.01695000
C	0.23588400	-3.33343100	-1.10924300	H	-3.33778400	2.73587300	-1.04133500
C	1.60295300	-3.28550800	-1.45633400	H	-2.04892600	2.56789900	-2.23901600
C	-0.76297000	-3.53764100	-2.08508300	C	0.78678500	-2.58764800	2.22550900
C	1.93759000	-3.45680800	-2.80341200	C	0.35447100	-1.21323900	0.47584400
C	-0.35648700	-3.69971000	-3.41307700	C	1.13170700	-3.24298500	1.09058000
C	0.97824700	-3.66282100	-3.77925400	N	0.31236500	-1.34098900	1.83892200
H	2.98883700	-3.39083500	-3.08346300	N	0.89223100	-2.38286000	0.03250800
H	-1.12549600	-3.83107300	-4.17417700	Cu	-0.44916800	0.28048400	-0.51017100
H	1.26775800	-3.77028800	-4.82274900	H	1.52403000	-4.23774500	0.93599500
C	1.41986700	-1.49103900	4.16244200	H	0.82627300	-2.88511600	3.26614400
C	1.79204800	-2.96769800	4.28422700	C	-0.08525400	-0.26791800	2.73669400
C	2.08578700	-0.79158000	2.98197800	C	0.88022600	0.69834500	3.10727300
H	1.33014600	-3.41807600	5.17245400	C	-1.41592200	-0.20024000	3.20781200
H	1.49610500	-3.56151500	3.41630800	C	0.45709900	1.76363400	3.90985300
H	2.87991400	-3.06850600	4.38621900	C	-1.76521000	0.89421700	4.00908400
H	1.92751200	0.29266100	3.02190000	C	-0.85220500	1.87849300	4.34886900
H	3.16724800	-0.98113100	2.98073800	H	1.19106000	2.51820200	4.19320900
H	1.68831500	-1.13270100	2.02296900	H	-2.79270700	0.96151700	4.36608800
C	-3.64680600	-1.83112400	2.80883400	H	-1.51488200	2.72297900	4.96586000
C	-3.70064700	-1.19767200	1.42233300	C	1.10048800	-2.66610100	-1.37757900
C	-3.84823300	-3.34480900	2.79100900	C	2.38895300	-2.53683100	-1.94428200
H	-3.66291800	-0.10256300	1.49730800	C	-0.03261700	-2.97981900	-2.16123200
H	-2.86260500	-1.50870100	0.79298800	C	2.47585100	-2.63832100	-3.33830800
H	-4.62803000	-1.47685500	0.90369900	C	0.13127000	-3.03174300	-3.54677200
H	-3.86343900	-3.75031000	3.81068000	C	1.36532100	-2.83243500	-4.14124800
H	-4.80826800	-3.58953000	2.31879600	H	3.46041900	-2.53821800	-3.79726600
H	-3.07215300	-3.87445700	2.23291800	H	-0.74480000	-3.21750700	-4.16681300
C	2.77217200	-2.94658400	-0.54579500	H	1.46096900	-2.85112000	-5.22511100
C	2.94807200	-1.42649400	-0.49241100	C	2.36309100	0.68653200	2.75974600
C	2.79018900	-3.57822500	0.83852600	C	3.11363100	-0.51285800	3.33648200
H	3.05603200	-1.00875600	-1.49969300	C	2.67347400	0.91307400	1.28341900
H	2.07170200	-0.93731300	-0.04637200	H	2.92337600	-0.62340600	4.41148400
H	3.82752900	-1.15313600	0.10640700	H	2.84020000	-1.45362000	2.84916000
H	2.62013500	-4.66204000	0.79876600	H	4.19415700	-0.38139600	3.19753100
H	3.76794100	-3.411138800	1.30961200	H	2.15108900	1.79854600	0.89771700
H	2.04257100	-3.14585600	1.50572600	H	3.75278200	1.06403600	1.14450200
C	-2.26545300	-3.45102700	-1.87722900	H	2.37944600	0.06951400	0.65270800
C	-2.86479400	-4.15274500	-0.66602400	C	-2.53884900	-1.18513700	2.91813800
C	-2.67094100	-1.97873200	-1.93195300	C	-3.07159700	-1.04002900	1.49670600
H	-2.50590700	-5.18450600	-0.56123100	C	-2.24986800	-2.64017200	3.28143900
H	-2.65221300	-3.62583800	0.26707900	H	-3.41584200	-0.01839600	1.29777900
H	-3.95771200	-4.18846500	-0.76641100	H	-2.29916700	-1.26406400	0.75580500
H	-2.39723900	-1.52134400	-2.88870500	H	-3.90603200	-1.73167600	1.32088000
H	-3.75175000	-1.85744600	-1.77091100	H	-1.82754100	-2.72793400	4.29078700
H	-2.13827100	-1.41273500	-1.15613400	H	-3.18392700	-3.21506700	3.26059300
B	0.38272000	0.44121400	-3.18303800	H	-1.56250500	-3.12561400	2.58295900
F	0.14036800	0.15525600	-1.77603000	C	3.74764800	-2.29481300	-1.27784800
F	-0.78933500	0.14143000	-3.87737100	C	4.29376900	-0.90123500	-1.60208400
F	0.66495400	1.81977400	-3.25478100	C	3.92462000	-2.57193000	0.20625600
F	1.46272600	-0.30903400	-3.60996300	H	4.29095300	-0.70499900	-2.67960600
H	4.51489300	-1.43070000	3.35375800	H	3.69100000	-0.11818500	-1.13074000
H	1.83665700	-1.01777400	5.06434300	H	5.32742900	-0.80860300	-1.24327000
H	-2.70260000	-3.94037300	-2.76089100	H	3.65335900	-3.59684400	0.48217000
H	3.65522600	-3.34328700	-1.06999400	H	4.98168500	-2.43582900	0.46864700
C	1.40186700	3.51645100	-0.38157700	H	3.35126700	-1.88362400	0.83456800
C	2.59068500	3.04860600	-0.95476000	C	-1.44436100	-3.30864900	-1.68250900
C	1.25732800	4.87534700	-0.09299800	C	-1.59552000	-3.91735600	-0.29467300
C	3.60959900	3.93660800	-1.26115300	C	-2.41011100	-2.14440900	-1.90002400
H	2.68572600	1.98898800	-1.18247100	H	-0.89180700	-4.74277200	-0.12676200
C	2.28788300	5.76370000	-0.38174100	H	-1.45618100	-3.18910100	0.50902700
H	0.34026500	5.24931000	0.35935500	H	-2.61105900	-4.31863400	-0.18133400
C	3.45788000	5.29541500	-0.97511800	H	-2.40294100	-1.80251400	-2.93959900
H	4.52348600	3.57914100	-1.73139500	H	-3.43167900	-2.43818500	-1.62243300
H	2.17715500	6.82081100	-0.15466700	H	-2.13662300	-1.27005000	-1.29442500
C	4.58440800	6.22716300	-1.29924300	B	-0.88684800	0.58732400	-4.30852100
F	5.65686800	6.01879200	-0.49455900	F	-0.96573800	0.22855500	-2.91886600
F	5.02405000	6.05936200	-2.56711300	F	-1.83232700	1.59394400	-4.55006700
F	4.24339700	7.52572900	-1.16446100	F	0.40865900	1.10369800	-4.54657300
				F	-1.12684500	-0.53984800	-5.08108100
				H	-1.77018100	-4.09630900	-2.38082000
				H	-3.35321200	-0.87077800	3.58826600
				H	4.41302100	-3.00757100	-1.79253700
				H	2.76570500	1.56555400	3.28570300
				C	2.59377600	2.40735000	-2.52896700
				C	3.09950800	3.62565100	-2.06618300
				C	3.19778900	1.76917600	-3.61918600
				C	4.21143200	4.19997400	-2.67237700
				H	2.63628500	4.11768900	-1.21140600

C	4.29134200	2.35487300	-4.23918700	H	3.25199100	0.13173800	-2.43912300
H	2.77200700	0.83532000	-3.97841900	H	3.63314800	1.20098600	-3.77621000
C	4.80447300	3.56373400	-3.76042300	H	0.51518100	2.73987700	-2.41279800
H	4.61695500	5.13772800	-2.30128600	H	1.15972900	1.71567900	-3.70900200
H	4.75320200	1.87485600	-5.10032400	H	0.78502600	1.02826100	-2.12831000
C	6.02462300	4.13391300	-4.41430000	B	-1.96398300	0.28260600	-2.73562600
F	7.11845400	3.36744500	-4.17436900	F	-1.23512500	0.48451100	-3.89119800
F	6.31614900	5.37901800	-3.98205200	F	-1.09405800	-0.37322900	-1.75572400
F	5.89621100	4.19773500	-5.75910300	F	-2.36205100	1.50073000	-2.15117900
				F	-3.05743900	-0.55100900	-2.93516400
<b>3d</b>				H	2.78279300	1.80315100	3.79889800
C	-5.29901400	-1.95286200	1.06659100	H	2.92929900	3.14997600	-2.64307800
C	-4.35610700	-2.13733500	2.08245400	H	1.87499200	-3.55562200	-3.94827600
C	-3.16738500	-1.41751800	2.10466300	H	2.24107800	-4.90858100	2.49150500
C	-2.94456100	-0.47238800	1.06522300	C	-2.26384100	2.60210600	0.72651700
C	-3.89931200	-0.28097500	0.04509500	C	-3.36482000	2.66690500	1.59004900
C	-5.07255100	-1.01886100	0.05367100	C	-1.90359600	3.72338800	-0.02704400
H	-6.21168300	-2.54675500	1.06517400	C	-4.09130700	3.84299500	1.70054800
H	-4.54885200	-2.86152100	2.87413400	C	-2.63765100	4.89788400	0.07456500
H	-3.68546700	0.42406700	-0.75594800	C	-3.72660200	4.95832300	0.94291500
H	-5.79593300	-0.88394300	-0.74762500	H	-4.94210800	3.90109200	2.37676800
C	-2.15837800	-1.57818600	3.19357400	H	-2.36734700	5.76636800	-0.52011800
H	-2.43603800	-2.38700500	3.87797600	H	-1.05902000	3.64921800	-0.70750500
H	-1.16785900	-1.79217000	2.77408500	H	-3.64240900	1.80120600	2.18883400
H	-2.05700600	-0.65444600	3.78085000	C	-4.53156000	6.21323400	1.09299400
N	-1.73080800	0.17709200	1.07199000	F	-4.04090300	7.23988200	0.37121700
C	-1.41636200	1.40354300	0.64174500	F	-4.57461300	6.61998800	2.38613000
O	-0.20302600	1.49859400	0.25111200	F	-5.81774700	6.03471300	0.71005800
O	-0.40005900	-2.34136200	0.48889800				
C	-1.28729600	-2.86855700	-0.43055200				
H	-0.82583900	-3.07769700	-1.41143600				
H	-1.65516300	-3.81997400	0.00001900				
H	-2.18828700	-2.24504700	-0.59168100				
C	4.03421700	-1.65208400	-0.27224100				
C	1.95164100	-0.79670400	-0.05531200				
C	4.16633100	-0.32865800	-0.02815900				
N	2.67687600	-1.93688600	-0.28387200				
N	2.88698500	0.18619600	0.09972400				
Cu	-0.03365500	-0.51425700	0.22823300				
H	5.03834800	0.30374500	0.06254100				
H	4.76760000	-2.42747900	-0.44332700				
C	2.19101000	-3.29289500	-0.53867600				
C	2.07337500	-4.19647600	0.54246600				
C	1.93524500	-3.69337600	-1.86855100				
C	1.59915000	-5.48135400	0.26068500				
C	1.46231000	-4.99727000	-2.07221600				
C	1.27368500	-5.88279300	-1.02603800	O	-0.06598300	2.52475900	0.31857700
H	1.48536500	-6.18054100	1.08900300	O	-0.99846000	-1.25247300	0.63685000
H	1.24264200	-5.30749200	-3.09341700	C	-1.30931600	-2.10266100	-0.43004900
H	0.89497900	-6.88648600	-1.21215700	H	-0.43420500	-2.16444700	-1.09313100
C	2.66473000	1.59564700	0.38963100	H	-1.54185700	-3.12181100	-0.07967100
C	2.55388000	2.00790000	1.73418600	H	-2.13750600	-1.70923900	-0.10294900
C	2.61835000	2.51429600	-0.67908100	C	4.17953700	-0.92580400	-0.22310700
C	2.37067100	3.37280000	1.97983700	C	2.11797100	0.00831300	0.02724300
C	2.43936400	3.86495900	-0.35690900	C	4.36182700	0.38322300	0.06335600
C	2.30909900	4.29969100	0.95153200	N	2.80999800	-1.14933800	-0.24395700
H	2.27603300	3.70218800	3.01501400	N	3.10228400	0.94337500	0.20675600
H	2.39147100	4.58396600	-1.17532200	Cu	0.16052300	0.36923100	0.29620000
H	2.16795600	5.35714700	1.17016200	H	5.25930800	0.97667300	0.17053400
C	2.41966800	-3.93893300	2.00261800	H	4.88430700	-1.72260500	-0.41670500
C	3.89673700	-3.63967300	2.26279500	C	2.23310400	-2.45343000	-0.54515800
C	1.48626700	-2.95208100	2.69426200	C	1.98088800	-3.36333700	0.50885200
H	4.54502100	-4.36908500	1.76028500	C	1.98375600	-2.80693400	-1.89331700
H	4.20146900	-2.64078000	1.93901900	C	1.38850500	-4.58950500	0.18432500
H	4.09989700	-3.69956500	3.33970700	C	1.40124600	-4.05640900	-2.14147100
H	0.45191100	-3.30930400	2.66344900	C	1.08273500	-4.93699800	-1.12130900
H	1.78375200	-2.81453200	3.74322100	H	1.17522700	-5.28688700	0.99446600
H	1.49022200	-1.97133500	2.21124400	H	1.19010000	-4.32656500	-3.17559400
C	2.15166800	-2.87174500	-3.13174300	H	0.61704200	-5.89589200	-1.34332700
C	1.22011800	-1.67535700	-3.25429600	C	2.93028100	2.35207100	0.52639600
C	3.61783100	-2.52135900	-3.38817600	C	2.85979500	2.74368200	1.87969700
H	0.16882100	-1.97899900	-3.26334100	C	2.89605800	3.29712100	-0.52097800
H	1.32987300	-0.96901100	-2.42749900	C	2.74752500	4.11049900	2.15775600
H	1.41132200	-1.12428300	-4.18394900	C	2.78121300	4.64725800	-0.16913300
H	4.25804200	-3.41128300	-3.32954900	C	2.70608600	5.06108200	1.15051700
H	3.72494300	-2.09552500	-4.393377800	H	2.68860900	4.42123000	3.20133400
H	4.01017900	-1.77923200	-2.68681400	H	2.74344200	5.38356900	-0.97261000
C	2.52648100	1.12313600	2.97209600	H	2.62210100	6.11928100	1.39363300
C	1.10368400	0.63440200	3.24916300	C	2.30808800	-3.17150500	1.98269000
C	3.53717400	-0.01444600	3.04267500	C	3.79005200	-2.95226800	2.28064000
H	0.40167700	1.47396000	3.32958000	C	1.39695600	-2.15884000	2.66509900
H	0.73281900	-0.01319800	2.44428400	H	4.40798800	-3.72500200	1.80553700
H	1.06051500	0.05410000	4.18064700	H	4.15725900	-1.97870100	1.94683600
H	4.55216700	0.32261100	2.79720200	H	3.96114500	-3.00635200	3.36339300
H	3.55927000	-0.42458300	4.06068200	H	0.34910900	-2.46044700	2.56754900
H	3.28625300	-0.84329300	2.37735900	H	1.64421900	-2.06884200	3.73215600
C	2.62225400	2.20529600	-2.16791900	H	1.47338600	-1.16432200	2.21507600
C	3.58585900	1.14371500	-2.68146900	C	2.26315800	-1.96482800	-3.12917900
C	1.19660600	1.90926900	-2.63100900	C	1.35085200	-0.74873100	-3.22963600
H	4.60583900	1.27319800	-2.29673500	C	3.74071100	-1.64610600	-3.35398800

H	0.29435600	-1.03722400	-3.25090800	C	2.94051000	2.44831500	-0.54545600
H	1.46823300	-0.06338400	-2.38653500	C	2.79878800	3.26637900	2.13210900
H	1.55382500	-0.18033600	-4.14594800	C	2.87131300	3.80160200	-0.19414400
H	4.35381500	-2.55598300	-3.31256200	C	2.80483800	4.21757900	1.12493700
H	3.87270900	-1.19802200	-4.34675600	H	2.73786400	3.57879000	3.17510900
H	4.14577000	-0.93585500	-2.62877500	H	2.86056000	4.53847400	-0.99758000
C	2.78401200	1.83515400	3.09697100	H	2.75836900	5.27804800	1.36749600
C	1.32825800	1.44174500	3.35228000	C	2.14297200	-3.98509100	1.95081700
C	3.70347300	0.62233300	3.13774600	C	3.62751600	-3.80362000	2.26229700
H	0.68798000	2.32424700	3.47342100	C	1.24965400	-2.95095800	2.62792800
H	0.91930600	0.87383600	2.50491200	H	4.22925300	-4.58855900	1.78630600
H	1.23815400	0.81750200	4.25170500	H	4.02297400	-2.83758600	1.93942200
H	4.73980900	0.87946200	2.88576400	H	3.78779500	-3.87081400	3.34598300
H	3.70171900	0.19419000	4.14871500	H	0.19930300	-3.25155700	2.55623400
H	3.37795600	-0.17055300	2.46102600	H	1.51413200	-2.84200800	3.68883000
C	2.86109300	3.01682600	-2.01435800	H	1.32611100	-1.96609100	2.15647900
C	3.78932800	1.93912100	-2.55745900	C	2.25160200	-2.81217700	-3.16716500
C	1.42023000	2.76624100	-2.45739700	C	1.38916500	-1.56497200	-3.31500600
H	4.81866500	2.04017300	-2.18879900	C	3.74521200	-2.54383500	-3.34484300
H	3.43598700	0.93431200	-2.31535600	H	0.32502400	-1.81718900	-3.37073700
H	3.81821900	2.00454500	-3.65252300	H	1.49953500	-0.87814000	-2.47199600
H	0.76617000	3.61284900	-2.21987200	H	1.64841500	-1.01355300	-4.22816300
H	1.36162700	2.58403800	-3.53629700	H	4.33165400	-3.46707500	-3.24744900
H	0.98941200	1.89388000	-1.95410000	H	3.92644500	-2.13676400	-4.34753900
B	-1.84216200	1.28983300	-2.61062700	H	4.14097900	-1.81692400	-2.63118000
F	-1.02711600	1.42447200	-3.71966500	C	2.73180700	0.99084900	3.06933100
F	-1.09521000	0.58130400	-1.57094200	C	1.25644500	0.65061700	3.29509700
F	-2.18981200	2.54130200	-2.06798400	C	3.60495400	-0.25448200	3.12390900
F	-2.97837300	0.53470500	-2.88548400	H	0.65268200	1.55882700	3.41783000
H	3.08755400	2.47457000	3.94021900	H	0.84327700	0.10825300	2.43179100
H	3.18455300	3.96097300	-2.47983900	H	1.12779400	0.02184400	4.18684900
H	1.98481800	-2.62021500	-3.96816300	H	4.65438600	-0.03458800	2.89170300
H	2.06699300	-4.14324800	2.43959200	H	3.56897000	-0.68559200	4.13304000
C	-2.08504300	3.69659400	0.79698700	H	3.26263800	-1.03145700	2.43764200
C	-3.24879400	3.744480900	1.57430400	C	2.90452900	2.16766300	-2.03917900
C	-1.69482100	4.82032700	0.06153200	C	3.81805700	1.07423500	-2.57662300
C	-4.00759900	4.90460700	1.62235600	C	1.45951800	1.94835400	-2.48789200
C	-2.45887900	5.97943300	0.09950200	H	4.84800200	1.16489200	-2.20675800
C	-3.61091200	6.02204400	0.88432000	H	3.45369000	0.07483600	-2.32912600
H	-4.90783900	4.94801700	2.23233700	H	3.84934900	1.13385300	-3.67210500
H	-2.16546600	6.85005100	-0.48111600	H	0.82571200	2.81076900	-2.25186800
H	-0.79871100	4.76086700	-0.55169800	H	1.40523400	1.76471900	-3.56776400
H	-3.55147300	2.87454300	2.15369700	H	1.00643500	1.08637700	-1.98515900
C	-4.44571700	7.26384800	0.97093900	B	-1.88471200	0.44357000	-2.65586200
F	-3.95365000	8.27961000	0.23566600	F	-1.25144100	0.65852400	-3.86217700
F	-4.53601400	7.70579400	2.25036000	F	-0.94086100	-0.21972400	-1.75714800
F	-5.71593200	7.04755700	0.55493900	F	-2.26202500	1.65240400	-2.04331800
				F	-2.98596600	-0.40672400	-2.77622800
				H	3.04259400	1.61800900	3.91918800
				H	3.24805400	3.10521200	-2.50370400
				H	1.97988000	-3.47054600	-4.00613300
				H	1.87485200	-4.95163700	2.40373500
				C	-2.43222800	2.76598800	0.89273800
				C	-3.35859200	2.60918500	1.93080900
				C	-2.46849500	3.91583900	0.09994000
				C	-4.31702400	3.58582000	2.16250000
				C	-3.44166600	4.88381500	0.31379000
				C	-4.36563000	4.71742100	1.34485700
				H	-5.03535500	3.47129100	2.97230700
				H	-3.48691800	5.76554700	-0.32017100
				H	-1.74223300	4.01459600	-0.70318600
				H	-3.32435000	1.72148700	2.56177600
				C	-5.44951600	5.72252800	1.58396000
				F	-5.31678700	6.82748100	0.82466000
				F	-5.48557100	6.12836700	2.87674900
				F	-6.67336200	5.20313600	1.31702500

#### 4d

C	-4.85670100	-2.09896700	0.57102500	<b>3d'</b>			
C	-3.72498500	-2.56454800	1.13469800	C	-5.57019800	-2.10483600	0.12605200
C	-2.50134500	-1.72151200	1.28764300	C	-4.52350400	-2.76040100	0.78335400
C	-2.64732800	-0.29560600	0.73568100	C	-3.31218500	-2.11418400	0.93704300
C	-3.85672100	0.09781300	0.09520500	C	-3.12303800	-0.79736600	0.46023800
C	-4.90978800	-0.76802700	0.02685400	C	-4.16790700	-0.13682800	-0.24484700
H	-5.73432600	-2.73725400	0.48414300	C	-5.38105200	-0.82102900	-0.37476800
H	-3.64930400	-3.58755900	1.50418800	C	-6.52866100	-2.60307600	-0.01029200
H	-3.89696600	1.05812400	-0.40996500	H	-4.65676100	-3.77120600	1.16429200
H	-5.81022200	-0.45807600	-0.50119300	H	-6.19246200	-0.32759300	-0.90939400
C	-2.12673800	-1.63721600	2.76580500	N	-1.86089000	-0.27463800	0.66575000
H	-2.01248200	-2.64242000	3.18545100	C	-1.42214300	0.94471600	0.95701700
H	-1.18185000	-1.09164900	2.87410200	O	-0.16992600	1.09310000	0.71814800
H	-2.90355900	-1.10893000	3.33117200	O	-0.52927800	-2.36280500	-0.87401200
N	-1.54741700	0.41157400	0.88331300	C	-1.48801700	-2.35327000	-1.87169900
C	-1.37401700	1.76734700	0.60074200	C	-2.39031900	-1.76192900	-1.62338800
O	-0.26460200	2.11322500	0.20367300	H	-1.10724300	-2.01748100	-2.84756300
O	-1.36614700	-2.33931100	0.63771400	C	-1.83750200	-3.39961200	-1.96487900
C	-1.64157800	-2.85353500	-0.67615300	C	3.92488900	-1.96960900	-0.23335800
H	-0.66405400	-2.99813200	-1.14650600	C	1.88983500	-0.99157400	-0.28568300
H	-2.15714800	-3.82229800	-0.61008300	C	4.11402300	-0.63333600	-0.13234100
H	-2.22229400	-2.14888700	-1.28103700	N	2.55785100	-2.18495000	-0.33193300
C	4.13643400	-1.80328500	-0.23001100	N	2.86119000	-0.04470200	-0.13865800
C	2.09269400	-0.82037600	-0.00698500				
C	4.34490500	-0.49826200	0.05936300				
N	2.76164300	-1.99518600	-0.27101800				
N	3.09664200	0.09127200	1.8537200				
Cu	0.19590700	-0.40486000	0.15581600				
H	5.25541800	0.07283300	0.17851800				
H	4.82693800	-2.61490000	-0.41326400				
C	2.13823300	-3.27460700	-0.57925200				
C	1.82344400	-4.16653400	0.47385000				
C	1.89505300	-3.62386000	-1.93014700				
C	1.17001800	-5.36051700	0.14644100				
C	1.24979900	-4.84146800	-2.18162000				
C	0.86593900	-5.69744300	-1.16257300				
H	0.90917700	-6.04179000	0.95653300				
H	1.04407700	-5.10713200	-3.21811000				
H	0.35306400	-6.63116300	-1.38855300				
C	2.94006800	1.50175200	0.50174000				
C	2.86273900	1.89660100	1.85453200				

Cu	-0.10534500	-0.65871400	-0.22927600	C	-2.69797200	0.43383100	0.31964900
H	5.01252600	-0.04230900	-0.02755000	C	-3.74392400	1.12793200	-0.37901500
H	4.62227400	-2.79540900	-0.24783500	C	-4.54984200	0.37325900	-1.20856600
C	1.99158600	-3.53128100	-0.37071700	H	-5.10333100	-1.55373500	-2.03073200
C	1.51235200	-4.10237300	0.82889600	H	-3.32654000	-2.80074300	-0.79579700
C	1.97444900	-4.25060500	-1.58569100	H	-5.34006000	0.88563600	-1.75659600
C	0.93096100	-5.37294500	0.75927600	N	-1.68645400	0.94020600	1.02394700
C	1.38703100	-5.52137600	-1.57661300	C	-1.27593100	2.17414000	1.41789200
C	0.84654900	-6.07805600	-0.42974500	O	-0.07245500	2.42286100	1.15865600
H	0.54720900	-5.81411900	1.67904000	O	-0.88243300	-0.69708900	-0.97043000
H	1.35199500	-6.07487100	-2.51503100	C	-1.06882300	-0.71897600	-2.35764500
H	0.38571200	-7.06413000	-0.45779900	H	-0.37873900	-0.00501100	-2.82791800
C	2.64095500	1.39409700	-0.06035000	H	-0.90916100	-1.72663900	-2.77965200
C	2.52445400	2.03376300	1.19177900	H	-2.08082500	-0.36990000	-2.62375300
C	2.54589100	2.10681500	-1.27573400	C	4.05066100	-0.89746700	-0.09988300
C	2.18552300	3.39296800	1.17709600	C	2.11582900	0.28453900	-0.21055700
C	2.16501200	3.44939500	-1.21129000	C	4.37620600	0.40726300	-0.27003600
C	1.96182500	4.08835600	0.00138900	N	2.66396900	-0.96243700	-0.05828000
H	2.07811200	3.90154900	2.13673500	N	3.19093300	1.12049500	-0.32118300
H	2.02681900	3.98909800	-2.14689700	Cu	0.17363100	0.74943800	-0.11118500
H	1.65795900	5.13400400	0.02785700	H	5.33711400	0.89727200	-0.34414900
C	1.60626300	-3.51189700	2.22819300	H	4.66928500	-1.77390500	0.03029400
C	3.04873900	-3.37180500	2.71248500	C	1.86855100	-2.17187800	0.05781200
C	0.77866600	-2.25316800	2.46291600	C	1.25773400	-2.46980900	1.29757100
H	3.57455900	-4.33286200	2.65626400	C	1.67569500	-2.99476500	-1.07386300
H	3.62102300	-2.64636900	2.12550300	C	0.34112000	-3.52575300	1.33431300
H	3.07140800	-3.03385300	3.75650500	C	0.75290700	-4.04206100	-0.96052600
H	-0.23948900	-2.36595200	2.06853600	C	0.05880300	-4.28991900	0.21240500
H	0.71075200	-2.03707700	3.53760300	H	-0.14539700	-3.75365800	2.28333600
H	1.21636200	-1.37078900	1.98911900	H	0.58014700	-4.67086500	-1.83424100
C	2.44894000	-3.77600200	-2.95081600	H	-0.66878300	-5.09878700	0.26333900
C	1.43267700	-2.81226200	-3.55956400	C	3.08199800	2.57302900	-0.39642100
C	3.88576800	-3.27152900	-3.05730900	C	3.13583400	3.34632100	0.78476100
H	0.49168000	-3.33349900	-3.76951300	C	2.90723900	3.16970000	-1.66853200
H	1.19988100	-1.98987400	-2.87690400	C	2.90752900	4.72373500	0.65152500
H	1.80451500	-2.38344800	-4.49839700	C	2.66783200	4.54348400	-1.71555000
H	4.58995300	-3.94526000	-2.55145200	C	2.63920200	5.31839300	-0.56679800
H	4.17294600	-3.22987500	-4.11510700	H	2.94223800	5.33553400	1.55378900
H	4.02648800	-2.26570300	-2.65471000	H	2.48350300	5.00179200	-2.68511400
C	2.71847800	1.47547700	2.60066900	H	2.43366400	6.38560300	-0.62783600
C	1.38790000	1.28063400	3.33447700	C	1.57629400	-1.82206400	2.63839300
C	3.61488600	0.26179900	2.78167700	C	3.06150600	-1.89543400	2.99050900
H	0.78230500	2.19473300	3.31477500	C	0.98341000	-0.43204900	2.84349500
H	0.78636400	0.48652000	2.88294900	H	3.42661700	-2.92873400	2.93711900
H	1.57389200	1.01673200	4.38404500	H	3.68559600	-1.28696200	2.32968500
H	4.60318500	0.40349400	2.32836500	H	3.22546500	-1.53194900	4.01294100
H	3.76908600	0.07967800	3.85309400	H	-0.10323700	-0.43496600	2.68945100
H	3.18106900	-0.64976200	2.36483100	H	1.18358800	-0.08065700	3.86488200
C	2.97847300	1.61054500	-2.64581600	H	1.39923100	0.31018300	2.15618600
C	4.50359700	1.69358100	-2.76691900	C	2.43098300	-2.93757900	-2.39522000
C	2.47915800	0.25254000	-3.10479400	C	2.50839500	-1.58990900	-3.08946200
H	4.88487600	2.68345400	-2.48737900	C	3.81275900	-3.58640400	-2.27475200
H	4.99864600	0.94942500	-2.12711000	H	1.5152600	-1.14873800	-3.21081500
H	4.81478500	1.48840700	-3.79935100	H	3.13461900	-0.86892600	-2.55539000
H	1.40854100	0.13499400	-2.91930400	H	2.94313700	-1.70964800	-4.09045500
H	2.64068600	0.14786300	-4.18565700	H	3.75987000	-4.57009800	-1.79303100
H	3.01930500	-0.57068100	-2.62488000	H	4.25551600	-3.71954800	-3.26959000
B	-0.97326900	1.80908900	-2.64798700	H	4.50443100	-2.96322000	-1.69664800
F	0.12258300	2.22094400	-3.39467400	C	3.44095800	2.93624600	2.22930400
F	-1.17509600	2.65868000	-1.54774200	C	2.21401900	3.08687100	3.13451500
F	-2.12035200	1.70035100	-3.41530300	C	4.11662100	1.60316700	2.50063700
F	-0.68503700	0.47371700	-2.10583200	H	1.73049500	4.06184500	3.00882000
H	-2.46682100	-2.60320500	1.41769400	H	1.45735000	2.32980000	2.91322200
C	4.01650400	1.22064100	-0.84250800	H	2.51079100	2.98350000	4.18662300
H	-4.40374600	1.99936800	-0.16865600	H	5.07843000	1.50261300	1.98549200
H	-2.98066000	1.47899600	-1.06997900	H	4.31222500	1.51355900	3.57721700
H	-4.57838500	1.29502900	-1.77922600	H	3.49059900	0.75152400	2.22166900
H	3.22837400	2.29725100	3.12919700	C	3.00386800	2.46947800	-3.01652600
H	1.15328000	-4.27988900	2.87278100	C	4.31321900	1.71145400	-3.23746300
H	2.55845200	2.34184200	-3.34677000	C	1.77656600	1.63128900	-3.35833200
H	2.42641500	-4.68464600	-3.57098900	H	5.1849600	2.31741700	-2.95678600
C	-2.17786200	2.03001100	1.59789100	H	4.36256300	0.77119560	-2.67833300
C	-1.76187000	3.34682100	1.37877500	H	4.41408900	1.45377500	-4.29957800
C	-3.27114100	1.76685400	2.43266700	H	0.89377300	2.26435300	-3.46811400
C	-2.45222860	4.39732500	1.97231600	H	1.94043500	1.07694100	-4.29285700
C	-3.94807200	2.81550100	3.03740000	H	1.55974600	0.90521500	-2.56944500
C	-3.54327200	4.13157400	2.79860200	B	-1.20433700	3.53527900	-1.99892400
H	-2.14963500	5.42453300	1.78637200	F	-0.20961800	4.05055500	-2.82013800
H	-4.79556300	2.61800800	3.69110800	F	-1.34149200	4.3100600	-0.83588200
H	-0.92170600	3.52739400	0.71228200	F	-2.41595200	3.41780700	-2.67163200
H	-3.58631900	0.73995100	2.61257100	F	-0.81708400	2.18860800	-1.57947400
C	-4.29819600	5.24130900	3.46508200	H	-1.8920600	-1.51672500	0.81152500
F	-3.87870000	6.46195700	3.08025400	C	-3.99152900	2.58641700	-0.20915100
F	-5.62431200	5.17226400	3.20321900	H	-4.49779900	2.79644500	0.74352500
F	-4.17616100	5.18607300	4.81546300	H	-3.07016300	3.17576100	-0.22603900
				H	-4.62282000	2.96251100	-1.01888600
				H	4.15702800	3.70505300	2.56373400
				H	1.06977600	-2.46704900	3.37283300
				H	3.01723900	3.29417400	-3.74450300
				H	1.85044000	-3.58984200	-3.06549400
				C	-2.06704100	3.08151500	2.26579500

C	-1.68902200	4.42517300	2.33773500	H	4.19162700	-1.94163900	-4.32590000		
C	-3.15986800	2.61858600	3.00848500	H	1.61047700	0.75569900	-4.20609900		
C	-2.41316600	5.30655100	3.13128800	H	1.83877500	-0.98000000	-4.56289600		
C	-3.86887000	3.49303400	3.81772400	H	1.53057600	-0.41856300	-2.90554900		
C	-3.49854200	4.83952800	3.87175300	B	-0.00416500	3.06954200	-2.26699300		
H	-2.14087000	6.35774900	3.17270900	F	0.08654200	2.94443300	-3.65022300		
H	-4.71461800	3.13919500	4.40458000	F	0.52735000	4.24953600	-1.79916200		
H	-0.85065300	4.76474300	1.73372500	F	-1.33096600	2.87621800	-1.84307200		
H	-3.44613000	1.56890800	2.95135900	F	0.78884700	1.96525000	-1.69444600		
C	-4.30022100	5.76117100	4.73934000	H	-1.54506200	-1.72155400	-0.69551300		
F	-3.84260800	7.02811500	4.72213100	C	-4.25570900	2.03588100	-0.31763700		
F	-4.29945600	5.35477700	6.03297200	H	-4.51585600	2.06502100	0.74811000		
F	-5.59916600	5.80028900	4.35746100	H	-3.43951300	2.74874200	-0.48434700		
<b>4d'</b>									
C	-4.45234700	-1.39701500	-2.04629400	H	4.15840400	3.09200600	1.43016500		
C	-3.18359500	-1.85210700	-2.05735800	H	0.50613100	-1.97827400	4.09030500		
C	-2.09321400	-1.07909600	-1.41192900	H	3.93394300	0.41757400	-4.58418800		
C	-2.53983700	0.14786100	-0.62630000	C	0.37914700	-4.82440400	-1.83154600		
C	-3.87964000	0.66318700	-0.78341300	C	-2.59225600	1.19539000	2.27003600		
C	-4.77585800	-0.12167700	-1.45993400	C	-2.87875100	2.17371700	3.22762800		
H	-5.24828200	-1.96006000	-2.53144300	C	-3.07821300	-0.10562200	2.45173000		
H	-2.90073600	-2.77021200	-2.57192400	C	-3.65228400	1.86810100	4.33935800		
H	-5.78888800	0.25833000	-1.59726000	C	-3.84180300	-0.41878300	3.56974500		
N	-1.57066900	0.66215800	0.08842400	C	-4.13547900	0.57006400	4.50984700		
C	-1.71216800	1.60148600	1.12705200	H	-3.88215000	2.63397100	5.07613200		
O	-1.03583200	2.61178700	1.17963200	H	-4.21073500	-1.43312400	3.71331400		
O	-1.05746400	-0.71631200	-2.33950900	H	-2.47833700	3.17428500	3.07823900		
C	-1.50075100	0.13254900	-3.41110900	C	-2.83539700	-0.89027500	1.73638600		
H	-0.61370800	0.34529000	-4.00889300	F	-4.91992900	0.20616100	5.73371200		
H	-2.25473100	-0.38038900	-4.02225400	F	-5.42969300	1.28640000	6.35786800		
H	-1.88976700	1.08258800	-3.02629000	F	-5.95061800	-0.62188600	5.45007000		
C	3.49416000	-2.21352700	0.37832000	<b>S1e</b>					
C	1.97220400	-0.65141300	-0.27420900	C	-2.49851600	-0.28524600	0.05195400		
C	4.17243400	-1.20226800	-0.21730400	C	-1.14909600	-0.04806700	0.34564000		
N	2.15049000	-1.86589200	0.34792800	C	-0.19323900	-0.53604300	-0.56197500		
N	3.23819400	-0.26057600	-0.61916600	C	-0.58375100	-1.18711400	-1.73622000		
Cu	0.28146300	0.30121000	-0.52558700	C	-1.92716100	-1.40025500	-2.00881700		
H	5.23050700	-1.05526000	-0.38682900	C	-2.88976000	-0.95296700	-1.10279900		
H	3.83917100	-1.32466400	0.84689200	H	-3.25477700	0.08074100	0.74691800		
C	1.04775800	-2.70543600	0.78899200	H	-2.22417900	-1.91691600	-2.91957400		
C	0.49552000	-2.52106300	0.207829200	H	-3.94769200	-1.11576400	-1.30208500		
C	0.52825800	-3.68299500	-0.09263300	C	-0.77157000	0.67386600	1.60250800		
C	-0.66798400	-3.23181500	2.39983500	H	0.16749600	1.22968500	1.50386100		
C	-0.62895600	-4.36738300	0.30075600	H	-1.55566500	1.37933000	1.89830700		
C	-1.25014300	-4.12731200	1.51669500	H	-0.63840200	-0.02209800	2.44329900		
H	-1.10780400	-3.07659800	3.38571100	H	1.20008800	-0.31272800	-0.37154600		
H	-1.04297300	-5.11103600	-0.38040100	N	2.00598700	-0.51769600	0.74010300		
H	-2.15802200	-4.66373500	1.78915700	C	2.96195400	0.21440900	0.95794200		
C	3.61138600	1.01652000	-1.22243800	O	1.71179600	0.62022800	-1.30347900		
C	3.78598400	2.14173600	-0.39128700	O	1.38737100	1.95738100	-0.93208900		
C	3.80238300	1.10076800	-2.61960400	C	1.77139500	2.57321900	-1.74907400		
C	4.12822100	3.35552100	-0.99870200	H	0.29790400	2.09331500	-0.85643100		
C	4.14570100	2.34436500	-3.15692800	H	1.88350200	2.22714600	0.00726000		
C	4.30090800	3.47053300	-2.36540400	H	0.19176800	-1.52235500	-2.42249900		
H	4.23346800	4.23410200	-0.36213200	C	1.83395600	-1.80650700	1.57388200		
H	4.26271100	2.42198500	-4.23745400	C	3.03899300	-2.66970600	1.15509400		
H	4.54311700	4.43237400	-2.81341600	C	3.97880800	-2.13123500	1.31219100		
C	1.06793900	-1.66411600	3.19738800	H	3.05702600	-3.59082200	1.75136800		
C	2.53269800	-1.95295600	3.52091100	H	2.97770500	-2.95415800	0.09684000		
C	0.77639600	-0.17943100	3.01781500	C	0.56990800	-2.63855300	1.36977400		
H	2.70404400	-3.02874800	3.65573600	H	-0.34041400	-2.13512900	1.71424800		
H	3.22261300	-1.59518000	2.75249500	H	0.42097100	-2.92826000	0.32343700		
H	2.80868600	-1.45103100	4.45663800	H	0.66607900	-3.56279400	1.95462600		
H	-0.30489000	0.00433000	3.01045900	H	1.98068000	-1.43979900	3.05196400		
H	1.21239800	0.40901700	3.83553100	C	2.89634700	-0.86562600	3.22241100		
H	1.18072100	0.20498800	2.07857600	H	1.13366700	-0.84016000	3.40966600		
C	1.13455100	-4.14348600	-1.41037800	H	2.02071300	-2.35206900	3.66024700		
C	1.36501100	-3.05795200	-2.44501000	H	<b>2e</b>				
C	2.39454900	-4.98782000	-1.20398600	C	-3.03070300	5.92598000	0.14489600		
H	0.48246900	-2.42379000	-2.58449700	C	-2.58871800	5.06135800	1.14504100		
H	2.19515800	-2.40590900	-2.16656100	C	-1.80745700	3.94071700	0.85008000		
H	1.62465000	-3.50788400	-3.41265200	C	-1.46286900	3.73433700	-0.49917700		
H	2.25493200	-5.75363200	-0.43109700	C	-1.92729200	4.57520800	-1.50887100		
H	2.66089100	-5.49640700	-2.13891200	C	-2.70744000	5.68219800	-1.18775700		
H	3.25335400	-4.36751100	-0.92265400	C	-3.63679200	6.79075700	0.40965700		
C	3.53735100	2.24296600	1.10441800	H	-2.85631800	5.25483200	2.18404300		
C	2.08404400	2.65117100	1.34220600	H	-1.64717400	4.35594500	-2.53807100		
C	3.95934000	1.06749300	1.97438400	H	-3.06119700	6.34678300	-1.97332500		
H	1.82875100	3.57449500	0.81110700	C	-1.37165500	2.98936000	1.91976700		
H	1.38969500	1.89236900	0.96125600	H	-1.59289200	3.38706600	2.91564400		
H	1.87669200	2.78941300	2.41191300	H	-1.87448100	2.01598700	1.82660400		
H	4.99221200	0.75491500	1.77270400	H	-0.29519000	2.77691600	1.87491200		
H	3.89820600	1.35213200	3.03310800	H	-0.70563700	2.57569700	-0.86322300		
H	3.31412200	0.19539600	1.84717500	N	0.61532200	2.33681600	-0.55872800		
C	3.55423600	0.00268700	-3.63836000	C	0.98682300	1.21341900	-0.20143800		
C	4.33677100	-1.29500000	-3.45069800	O	-1.51938700	1.40066800	-0.72160500		
C	2.04938400	-0.17941200	-3.83989100	O	-2.28669000	1.22996000	-1.92667600		
H	5.41256300	-1.09256500	-3.36342900	C					
H	4.03947600	-1.87581100	-2.57437500	C					

H	-1.62420900	1.06947800	-2.78149500	C	-1.77123700	5.41435100	-1.32733700
H	-2.89944600	0.34501100	-1.73506300	C	-0.77661000	4.60365000	-0.82158200
H	-2.93720100	2.10125700	-2.07986300	C	-0.05403800	3.75756000	-1.74450200
C	-0.92720900	-3.55812000	2.46606900	C	-0.45525900	3.71199900	-3.12414100
C	-0.52808700	-2.00336900	0.84839000	C	-1.45406100	4.55506900	-3.58640900
C	-0.45254200	-4.21267900	1.37973300	H	-2.89697000	6.06147800	-3.05437300
N	-0.97017400	-2.20623000	2.13865400	H	-2.31993800	6.06806700	-0.64943400
N	-0.21443500	-3.25984100	0.40234800	H	0.05411700	3.01343400	-3.78599900
Cu	-0.22573900	-0.39430500	-0.10384200	H	-1.74478900	4.52034600	-4.63384800
H	-0.26217800	-5.26303500	1.20598400	C	-0.45067400	4.52989900	0.62755600
H	-1.23684400	-3.91722800	3.43820400	H	-1.06201500	5.22422200	1.21328400
C	-1.42049000	-1.16441900	3.05120300	H	-0.62159700	3.50575700	0.98470800
C	-0.49293800	-0.55062500	3.92842300	H	0.60891700	4.74337800	0.81954300
C	-2.79069000	-0.80848900	3.08414500	N	0.86744800	2.96271500	-1.22830000
C	-0.96515800	0.44594200	4.79218400	C	1.96100900	2.33413800	-1.71691500
C	-3.191114300	0.19395800	3.97647700	O	2.14606500	1.13440600	-1.47878900
C	-2.29607600	0.82727200	4.82194500	O	-1.23183500	1.38780200	-0.39780700
H	-0.25037800	0.92395600	5.46200000	C	-2.09716100	1.62634000	-1.41652300
H	-4.24460300	0.47233500	3.99625800	H	-2.59570600	0.72100200	-1.81085200
H	-2.63478900	1.60469800	5.50553300	H	-2.84647500	2.38904700	-1.12878800
C	0.31388300	-3.57395100	-0.916774400	H	-1.58817600	2.06982000	-2.31603900
C	1.70965100	-3.55859100	-1.12589900	C	0.48024200	-2.68870000	2.28656200
C	-0.582324300	-3.89884100	-1.95768500	C	0.42893800	-1.36269300	0.43413000
C	2.17736200	-3.87655400	-2.40557000	C	0.68771400	-3.48446600	1.21053500
C	-0.04370200	-4.21014200	-3.20982500	N	0.31391900	-1.39747700	1.80521700
C	1.32068300	-4.19657000	-3.44385200	N	0.65669700	-2.66804800	0.09155400
H	3.25244500	-3.84055200	-2.58218000	Cu	0.34120500	0.31034300	-0.72632500
H	-0.73211900	-4.43729200	-4.02413700	H	0.85514800	-4.54989700	1.13158200
H	1.71335800	-4.41939300	-4.43410300	H	0.43314200	-2.91330100	3.34326900
C	0.99451900	-0.84929700	4.04730400	C	0.04833200	-0.23527300	2.64118300
C	1.32289100	-2.28275000	4.46073900	C	1.12968000	0.57086100	3.06847600
C	1.78870000	-0.36793400	2.83654400	C	-1.28123200	0.06164100	3.02600700
H	0.76822000	-2.56716700	5.36428500	C	0.83523900	1.72455800	3.80507800
H	1.09934100	-3.01928300	3.68543900	C	-1.49828900	1.22988500	3.76658200
H	2.39382500	-2.36749800	4.68499000	C	-0.46319700	2.07078900	4.14043600
H	1.64555900	0.70880500	2.67438600	H	1.66454000	2.35518200	4.12563600
H	2.85986300	-0.55512200	2.97450000	H	-2.52156400	1.47278300	4.05226400
H	1.47730600	-0.86677500	1.91530200	H	-0.66544400	2.97753500	4.70873900
C	-3.90712100	-1.39858400	2.23606300	C	0.83807800	-3.17035800	-1.26205700
C	-3.79791900	-0.99558800	0.76881500	C	2.14106100	-3.33019600	-1.77880800
C	-4.13979500	-2.89362400	2.44434800	C	-0.30289900	-3.51396600	-2.02009300
H	-3.78501600	0.09816400	0.66843300	C	2.26212800	-3.80282900	-3.09197700
H	-2.881159400	-1.37115200	0.30522400	C	-0.10516000	-3.96919100	-3.32638400
H	-4.64948300	-1.38372700	0.19390100	C	1.16034700	-4.10440400	-3.87170200
H	-4.26859600	-3.12471800	3.50954600	H	3.26507500	-3.90963100	-3.50642700
H	-5.05298700	-3.20497700	1.92149400	H	-0.98307100	-4.20478900	-3.92767500
H	-3.32525500	-3.51460600	2.06405500	H	1.28535000	-4.44088600	-4.89914700
C	2.79223200	-3.12730400	-0.14869000	C	2.61219300	0.30319300	2.84687100
C	3.04066400	-1.62316800	-0.28774700	C	3.09955400	-1.02565400	3.42032900
C	2.63550800	-3.54092400	1.30712900	C	3.05643500	0.53405400	1.40824500
H	3.29179400	-1.34671900	-1.31678200	H	2.81645500	-1.12836400	4.47575900
H	2.14374500	-1.04688300	-0.02887800	H	2.70743000	-1.89337400	2.88265200
H	3.85240100	-1.30011800	0.37884400	H	4.19406900	-1.07884000	3.35934900
H	2.39744800	-4.60729600	1.41532300	H	2.74386300	1.52556900	1.05746200
H	3.57343700	-3.35215800	1.84639000	H	4.14981500	0.46651700	1.31836500
H	1.85916800	-2.96918300	1.81906900	H	2.62625500	-0.19382100	0.71584500
C	-2.09964600	-3.80941900	-1.92476300	C	-2.53270700	-0.75375100	2.72964600
C	-2.82032500	-4.28122300	-0.67036300	C	-2.96868800	-0.64510100	1.27323000
C	-2.51274200	-2.38367700	-2.29237300	C	-2.50645500	-2.19835100	3.22675800
H	-2.47315400	-5.26549500	-0.33119400	H	-3.21840900	0.38929000	1.01378300
H	-2.70359800	-3.57885200	0.15823200	H	-2.17346000	-0.95245900	0.58962200
H	-3.89722900	-4.35784800	-0.87132600	H	-3.84676100	-1.27694600	1.08368700
H	-2.12860300	-2.09028300	-3.27597200	H	-2.14180500	-2.26251400	4.26033800
H	-3.60670600	-2.27616400	-2.28655400	H	3.52409000	-2.60878800	3.20685100
H	-2.08518500	-1.67485400	-1.57245500	H	-1.88868200	-2.85413500	2.60822200
B	0.87623100	-0.00308500	-3.36608800	C	3.47078900	-2.95508900	-1.13674100
F	0.15410500	-0.66868600	-2.29063400	C	3.87214200	-1.55698900	-1.60642600
F	0.27829000	-0.37593300	-4.56129000	C	3.62145500	-3.07680800	0.37136700
F	0.73533900	1.39035600	-3.16290000	H	3.88643400	-1.48633300	-2.70073900
F	2.21094600	-0.37145700	-3.29371500	H	3.16262400	-2.60878800	-3.20685100
H	-4.81954900	-0.91205700	2.61294700	H	4.86804100	-1.28899100	-1.22663700
H	1.32695400	-0.22670500	4.89184100	H	3.32352300	-4.06292000	0.74850200
H	-2.43931600	-4.46554800	-2.74096200	H	4.67413400	-2.92285000	0.64332400
H	3.70334400	-3.63012500	-0.50862000	H	3.04395700	-2.31938800	0.90759700
C	1.64495200	3.45996900	-0.70581600	C	-1.75866700	-3.37128200	-1.60648500
C	3.00095100	2.77999800	-0.93344300	C	-2.12841400	-3.79632500	-0.19081800
H	2.98341200	2.16566800	-1.84004200	C	-2.25908400	-1.96436100	-1.93234300
H	3.77112200	3.55292800	-1.04510900	H	-1.70725700	-4.77661900	0.06755300
H	3.27643000	2.13194400	-0.09482400	H	-1.80088200	-3.07805000	0.56388600
C	1.35363600	4.38686200	-1.88887600	H	-3.22030800	-3.86877100	-0.10250100
H	1.13165500	3.81181600	-2.79395500	H	-2.12262200	-1.72719600	-2.99359200
H	0.52505000	5.07290600	-1.68929800	H	-3.32260400	-1.85845000	-1.67685000
H	2.24127600	5.00106200	-2.08418600	H	-1.69402600	-1.21014500	-1.37190300
C	1.69729800	4.26860200	0.59830500	B	0.16902100	0.32660000	-4.22364700
H	0.75651200	4.79753700	0.79811100	F	0.10382600	-0.19110600	-2.87155500
H	1.92987300	3.62832300	1.45921900	F	-1.05886500	0.94208100	-4.50048000
H	2.49051000	5.02278700	0.52214500	F	1.19324000	1.30658500	-4.26163000
H				F	0.43774500	-0.71534500	-5.08275800
H				H	-2.30029500	-4.05844000	-2.27467000
C	-2.10435900	5.40593100	-2.69621500	H	-3.31739300	-0.26262200	3.32467900
H				H	4.19428900	-3.66240000	-1.57232100

H	3.11546600	1.07899700	3.44402800	H	-0.21959800	-3.41153100	-0.69152400	
C	3.11837100	3.18879800	-2.27899600	C	-2.74355300	-0.04633900	2.95883400	
C	4.18664300	2.23381200	-2.81040100	C	-1.51268200	-0.50442500	3.72294100	
H	3.78327300	1.59531600	-3.60330400	C	-2.64583200	1.45133600	2.66069700	
H	5.02273400	2.81772000	-3.21616800	H	-1.55041600	-1.56621700	3.99342500	
H	4.56847600	1.58328600	-2.01598000	H	-0.59154700	-0.32773200	3.16385700	
C	2.67419700	4.13331400	-3.39261600	H	-1.43191700	0.07057500	4.65461000	
H	2.24242500	3.58456700	-4.23654000	H	-3.55132900	1.82566600	2.16717000	
H	1.94984800	4.88149000	-3.04809000	H	-2.50267100	2.01296200	3.59379600	
H	3.54998200	4.68267600	-3.76120100	H	-1.81100100	1.66281100	1.98771500	
C	3.68296400	4.00585800	-1.10796300	B	-0.02734000	0.37044200	-4.31651400	
H	2.94831300	4.72522000	-0.72464600	F	-0.40895300	0.38041400	-2.90881700	
H	3.99335100	3.35770000	-0.27830300	F	-1.07180700	0.93484300	-5.03834400	
H	4.56492700	4.56709800	-1.44231100	F	1.12849600	1.17796600	-4.40824300	
<b>3e</b>								
C	-2.53479800	5.16663800	-2.75007900	H	0.23138200	-0.93153400	-4.69644100	
C	-2.20009600	5.14259000	-1.39319700	H	3.11269300	1.50520300	3.02758100	
C	-1.18962600	4.31814700	-0.91012600	H	3.74523800	-2.79430600	-1.94507000	
C	-0.48363500	3.51289100	-1.84562800	H	-3.58803100	-0.16606000	3.65608300	
C	-0.83511800	3.52688000	-3.21147000	C	-3.07380300	-3.84935900	-1.64753000	
C	-1.84832900	4.36003200	-3.65868700	C	2.77496100	3.01014100	-2.33694700	
H	-3.34177500	5.81187900	-3.09441700	C	3.80919400	2.04853600	-2.92574100	
H	-2.74257400	5.77692700	-0.69173900	H	3.37526900	1.46737900	-3.74505400	
H	-0.31475500	2.86110400	-3.89374400	H	4.65699300	2.62792600	-3.31296900	
H	-2.11797000	4.35652100	-4.71264400	H	4.18471300	1.35022100	-2.16959900	
C	-0.82011500	4.28721600	0.53566800	C	3.40011900	3.77688900	-1.15403100	
H	-1.52072400	4.87453600	1.13929700	H	2.68429600	4.47724900	-0.70383100	
H	-0.81471400	3.25569200	0.90641800	H	3.75297700	3.08954000	-0.37406800	
H	0.18981900	4.68776300	0.70257500	C	4.26082200	4.35632400	-1.51110200	
N	0.45328800	2.64553100	-1.33534800	C	2.31943800	4.00918200	-3.39779400	
C	1.64939300	2.20502900	-1.72278600	H	1.85728600	3.50226000	-4.25033400	
O	1.89115600	1.02728500	-1.27682200	H	1.61040100	4.74431100	-2.99929400	
O	-1.76289000	1.19989100	-0.19817500	H	3.19481100	4.56107200	-3.76339000	
C	-2.67771900	1.19713800	-1.23632900	<b>TS3e-4e</b>				
H	-3.03032900	0.18416000	-1.49799600	C	-2.61680100	4.40611600	-2.91183800	
H	-3.54453100	1.79640000	-0.89764300	C	-2.53191100	4.36128200	-1.54878800	
H	-2.30888900	1.69230300	-2.15521800	C	-1.36964500	3.83539300	-0.90232900	
C	0.93114800	-2.47850700	1.77538800	C	-0.20628100	3.51586600	-1.74424600	
C	0.03216300	-0.90435500	0.41502500	C	-0.35402700	3.55986200	-3.16307500	
C	-0.41196700	-2.63031100	1.80671700	C	-1.52410500	3.98058900	-3.72555600	
N	1.19630600	-1.41758100	0.92270000	H	-3.52505200	4.77060400	-3.38963900	
N	-0.95616600	-1.65583600	0.98469900	H	-3.36493900	4.68565500	-0.92602600	
Cu	-0.00293500	0.79231900	-0.69733000	H	0.44876300	3.18138600	-3.78880900	
H	-1.04203300	-3.33883500	2.32584200	H	-1.63072900	3.96051500	-4.80825000	
H	1.72984200	-3.01708300	2.26622200	C	-1.16577500	4.12572000	0.54718500	
C	2.55387800	-0.93822500	0.68127000	H	-2.11169100	4.04372500	1.09259100	
C	3.31961700	-1.52479700	-0.34875700	H	-0.43632900	3.44523900	0.99526500	
C	3.07615000	0.08273400	1.50514700	H	-0.78901300	5.15060700	0.67449900	
C	4.62294800	-1.05076800	-0.53519400	N	0.80623900	2.97957800	-1.08992400	
C	4.38646200	0.50762500	1.25849400	C	1.95004500	2.38197300	-1.52589200	
C	5.16005600	-0.04468400	0.25055900	O	2.09138800	1.19926400	-1.14981200	
H	5.21656900	-1.48659000	-1.33846100	O	-1.66025700	1.90617600	-0.71613100	
H	4.79814000	1.29848200	1.88611100	C	-2.80508700	1.42011800	-1.36322100	
H	6.17528600	0.30942100	0.07682700	H	-2.74497900	1.54837900	-2.45509300	
C	-2.39990300	-1.56515700	0.79842900	N	0.80623900	2.97957800	-1.08992400	
C	-2.99201100	-2.29932200	-0.25389800	C	1.95004500	2.38197300	-1.52589200	
C	-3.18109500	-0.83936300	1.72793300	H	-3.72058300	1.89087100	-0.96718900	
C	-4.38250400	-2.21524100	-0.40288000	C	0.88886300	-2.57892900	1.68477700	
C	-4.56336500	-0.80119800	1.50975000	C	0.03482100	-0.86909000	0.44219100	
C	-5.16737600	-1.46125000	0.45189800	C	-0.45747900	-2.69789800	1.70830400	
H	-4.84403400	-2.76585100	-1.22266900	N	1.18497300	-1.46521300	0.91228600	
H	-5.17492500	-0.23187500	2.21077100	Cu	-0.96659800	-1.65096600	0.95508200	
H	-6.24590100	-1.40936900	0.31236500	H	0.03877300	0.83538700	-0.63181800	
C	2.86041400	-2.59940200	-1.32015700	H	-1.10660700	-3.42170700	2.18130500	
C	2.53384300	-3.94277300	-0.66849400	C	1.67062400	-3.17633600	2.13365000	
C	1.78103800	-2.10010500	-2.27540800	C	2.56555600	-1.05102600	0.67291700	
H	3.35973700	-4.28579300	-0.03126100	C	3.28403500	-1.62446200	-0.40003300	
H	1.62796900	-3.91792000	-0.05712100	C	3.17697600	-0.13461000	1.55833600	
H	2.37240300	-4.70119200	-1.44480300	C	4.61931900	-1.23819000	-0.56869200	
H	2.11058800	-1.21299600	-2.82578600	C	4.51542100	0.20275700	1.32936100	
H	1.52257400	-2.87130900	-3.01150500	C	5.23988900	-0.33713400	0.27948900	
H	0.85537700	-1.82011500	-1.76362900	H	5.17468300	-1.66940100	-1.40137900	
C	2.36770600	0.78642100	2.65365900	C	4.98915100	0.91490500	2.00553100	
C	1.17626700	1.63980100	2.22397600	C	6.28016400	-0.05500800	0.12212500	
C	2.06572000	-0.12963900	3.83896600	C	-2.39794700	-1.48921700	0.77215400	
H	1.45510800	2.32728800	1.41387800	C	3.02847100	-2.14340800	-0.31060700	
H	0.32610300	1.04705000	1.87001600	C	-3.14030500	-0.76178000	1.72892600	
H	0.81218900	2.24372600	3.06696100	C	-4.41840500	-2.01587600	-0.42607600	
H	2.97754600	-0.63533500	4.18039100	C	-4.52605900	-0.67562500	1.54834600	
H	1.67053400	0.45462700	4.68005100	C	-5.16774300	-1.28842400	0.48402400	
H	1.32565200	-0.90058600	3.60615300	H	-4.90918900	-2.50516000	-1.26746900	
C	-2.29572700	-3.14726100	-1.30951500	H	-5.10428700	-0.10601000	2.27661600	
C	-1.91051900	-2.28420600	-2.50661700	C	6.24750400	-1.20729500	0.37032100	
C	-1.11894100	-4.00629400	-0.86912100	C	2.75834600	-2.61507200	-1.42648300	
H	-2.77650800	-1.76350200	-2.93406000	C	2.37888800	-3.97823700	-0.84765700	
H	-1.18629100	-1.51507800	-2.22528900	C	1.69915100	-2.00858300	-2.33995100	
H	-1.44965800	-2.88510700	-3.29963600	H	3.20417000	-4.40020000	-0.25864400	
H	-1.33268600	-4.58991200	0.03569200	H	1.49417200	-3.94730700	-0.20709000	
H	-0.86978800	-4.71357700	-1.67026900	H	2.15792100	-4.67789100	-1.66383300	
H				H	2.08547400	-1.13317300	-2.87115600	
H				H	1.36542100	-2.73401000	-3.09201500	

H	0.81234400	-1.66693600	-1.79967300	C	1.30683100	5.21163800	0.15274300
C	2.53713400	0.53732300	2.76350500	C	0.79288300	5.12741900	1.43549000
C	1.41671700	1.50663600	2.39906700	H	1.20838200	4.57275400	3.46952300
C	2.16426800	-0.43385300	3.88296500	H	0.67346400	5.55687100	-0.66469700
H	1.76503200	2.25198600	1.67145500	H	-0.23655400	5.41948100	1.63864400
H	0.55541400	1.00032900	1.95343600	C	8.21586100	1.62022400	2.39931000
H	1.06053100	2.03846500	3.29233300	C	8.52615300	3.03196800	2.89485400
H	3.03299800	-1.03444200	4.18054300	C	6.89048100	1.07288800	2.91857900
H	1.82036800	0.12030200	4.76601200	H	9.49160200	3.38353700	2.50846700
H	1.36418200	-1.12552100	3.60400600	H	7.76681800	3.76623300	2.61478100
C	-2.35655500	-2.88943700	-1.45135300	H	8.58527100	3.03404800	3.99080900
C	-1.95596400	-1.89675000	-2.54216600	H	6.82122000	-0.00357600	2.73025500
C	-1.20720400	-3.82453500	-1.10708900	H	6.79230200	1.24833000	3.99872700
H	-2.81777200	-1.33304800	-2.91755900	H	6.03093500	1.53070500	2.41977300
H	-1.22796400	-1.16140700	-2.17504600	C	7.48781100	2.65035400	-2.69876200
H	-1.49085900	-2.40370100	-3.39452200	C	7.73766700	4.15765000	-2.69816800
H	-1.44269800	-4.49356800	-0.26909100	H	7.47550000	4.57258200	-3.67955200
H	-0.97487200	-4.44865600	-1.97905900	H	7.14008300	4.69425400	-1.95734500
H	-0.29345500	-3.27877200	-0.86525800	H	8.79502200	4.38566500	-2.50884100
C	-2.60460900	0.03644500	2.90906300	C	3.65118700	3.70705800	3.44134200
C	-1.45176400	-0.54745200	3.71076700	C	3.48841500	2.18564200	3.46601000
C	-2.27852100	1.45662300	2.44977100	C	5.10036200	4.11899800	3.65944200
H	-1.61784300	-1.59589800	3.98647400	H	2.42835200	1.89929000	3.47958200
H	-0.50337500	-0.48277100	3.17327900	H	3.92742600	1.72671800	2.56908500
H	-1.32818700	0.02526100	4.63923000	H	3.97629900	1.74870300	4.34819700
H	-3.160688200	1.94862300	2.02060900	H	5.23582900	5.20453300	3.57549100
H	-1.91026200	2.06768900	3.28541300	H	5.42326400	3.81882700	4.66510600
H	-1.51632000	1.44624100	1.66251200	H	5.78041900	3.63894300	2.95367900
H	3.33980700	1.16324000	3.18216400	C	2.97824400	4.88850000	-1.62560300
H	3.62550600	-2.81860400	-2.07310700	C	4.36315500	5.38505600	-2.01364500
H	-3.45581000	0.10827300	3.60363100	C	2.69068700	3.52417700	-2.25354700
H	-3.15262300	-3.52381700	-1.87138900	H	4.63388100	6.32322800	-1.51169700
B	-0.32953500	0.52057000	-4.35140200	H	5.13659800	4.64528500	-1.79702000
F	-1.70848100	0.72442100	-4.42855700	H	4.39528400	5.56316700	-3.09623000
F	0.07852800	0.75488400	-2.96405900	H	1.64959100	3.21688600	-2.10393800
F	0.01897900	-0.77728400	-4.68990600	H	2.90130100	3.53486100	-3.32964600
F	0.35587100	1.45187600	-5.14736800	H	3.30678500	2.73833800	-1.80194800
C	3.07832800	3.09416200	-2.25128300	B	2.97484200	-0.07310900	-2.82912700
C	4.33175700	2.95234800	-1.37651800	F	3.37618900	-1.38382700	-3.09418000
H	4.55376600	1.98969000	-1.17868900	F	3.12227300	0.74997400	-3.92582600
H	5.19108500	3.40356600	-1.88847700	F	1.67143500	-0.04636400	-2.31808400
H	4.20883100	3.46074300	-0.40986000	F	3.86432000	0.42658000	-1.76784500
C	3.29735800	2.35159600	-3.57724300	H	3.09272500	4.09583700	4.30680400
H	3.55345300	1.30221700	-3.39074000	H	2.26313100	5.60393100	-2.06120400
H	2.40616600	2.35820900	-4.21589700	H	8.99713900	0.98599200	2.84499400
H	4.12265700	2.82128900	-4.12734000	C	6.04073600	2.27085500	-2.99209900
C	2.79446000	4.57442000	-2.49086200	H	5.93887000	1.19821900	-3.19071200
H	1.96276700	4.73763800	-3.18474000	H	5.36742000	2.49205800	-2.15973600
H	2.56183000	5.09941800	-1.55557200	H	5.66474100	2.80674400	-3.87310900
H	3.68134800	5.04985200	-2.92758700	H	8.07754400	2.26687800	-3.54521800
O				O	5.52222700	-0.93591000	0.57525700
C				C	6.01832600	-1.22032600	-0.74321400
H				H	5.21252800	-1.49288900	-1.43407700
C	4.06411600	-4.04052800	-0.05389500	H	6.47733000	-0.28946800	-1.09017100
C	4.85802100	-3.26164500	0.70674400	H	6.77986200	-2.01032200	-0.70720600
C	4.50513200	-1.85179000	1.05472100	C	0.32183400	0.12013000	1.11330600
C	3.15255600	-1.38947800	0.49170100	C	-0.27765800	1.29956400	1.89311200
C	2.40618700	-2.25554600	-0.35861900	H	-0.34208600	2.19314400	1.26503300
C	2.84276200	-3.52111600	-0.61267300	H	-1.28482100	1.03636800	2.24053300
H	4.35406000	-5.06375700	-0.28705400	H	0.32706900	1.55349100	2.77421400
H	5.80936000	-3.62600700	1.09528000	C	-0.58175200	-0.15816400	-0.09491700
H	1.53618300	-1.85508900	-0.87101200	H	-0.26108200	-1.03101100	-0.67220800
H	2.27341400	-4.14832000	-1.29674100	H	-1.60492600	-0.34412200	0.25723200
C	4.49199000	-1.68177000	2.57033000	H	-0.59435700	0.69714200	-0.77859200
H	5.44890000	-2.00243700	2.99646400	C	0.39352800	-1.09684100	2.03404300
H	4.32151800	-0.62724000	2.81755700	H	0.72072300	-2.00353200	1.51288900
H	3.68916900	-2.27904300	3.01858400	H	1.07627200	-0.92493000	2.87755500
N	2.85720000	-0.15647300	0.81803900	H	-0.60131900	-1.30095800	2.44942400
C	1.69521000	0.58325800	0.61008900				
O	1.85152500	1.72434400	0.18113500				
C	6.99266200	4.45377700	0.43554300				
C	5.36113600	2.86459500	0.35384900				
C	5.81937100	5.06451100	0.72022400				
N	6.70885600	3.11226200	0.21427600				
N	4.83401400	4.09099200	0.66391200				
Cu	4.29798300	1.24002600	0.19174700				
H	5.58590100	6.09522400	0.94896500				
H	8.00065300	4.83848500	0.36351300				
C	7.72169000	2.12544500	-0.13171600				
C	8.38845300	1.42250400	0.90002300				
C	8.05459800	1.91651800	-1.49217600				
C	9.32399900	0.44923800	0.52964900				
C	9.00458500	0.92987100	-1.78595600	O	1.68484900	2.42242600	-1.38952800
C	9.62490300	0.18516900	-0.79671800	O	1.99393600	1.21350600	-1.05810100
H	9.82963700	-0.10441600	1.32074800	C	-1.74967600	1.01700300	-0.43400800
H	9.25057100	0.75157500	-2.83249400	H	-2.51251900	1.11271000	-1.58493900
H	10.35286900	-0.58198100	-1.05644200	H	-2.75872100	0.13463500	-2.02773200
C	3.43433400	4.39151700	0.917811300	H	-3.45245200	1.61854000	-1.28936300
C	2.93169300	4.28177300	2.23066000	C	-2.06285100	1.74925800	-2.36978300
C	2.62552400	4.84906900	-0.14737400	C	0.97035300	-2.48193800	1.76825300
C	1.60411400	4.65917100	2.45664500	C	0.12312200	-0.91500000	0.37069400
				C	-0.37515200	-2.61401000	1.77487700

N	1.27068900	-1.43547100	0.90906500	C	-0.57950400	3.97012500	-0.31651800
N	-0.88771900	-1.64500100	0.92727200	C	0.17736500	3.56877500	-1.48548300
Cu	0.07393400	0.77358600	-0.73469700	C	-0.28856300	3.96028600	-2.79061400
H	-1.02644600	-3.30578400	2.29017400	C	-1.40892300	4.76002200	-2.84370900
H	1.75128100	-3.02566000	2.28140800	H	-2.97876800	5.83066800	-1.80862300
C	2.64651200	-0.98577800	0.70637500	H	-2.20802500	5.15136400	0.46377400
C	3.42360600	-1.57708200	-0.31174200	H	-1.79922900	5.03385900	-3.82254600
C	3.18298600	-0.01079900	1.57720000	N	1.14855200	2.70443900	-1.22736500
C	4.74918000	-1.14689200	-0.44733700	C	2.07249100	2.00027700	-1.90814900
C	4.51898500	0.35876500	1.39080900	O	1.92961100	0.75072600	-1.88716700
C	5.30189200	-0.19188200	0.38882400	O	-1.31665500	1.93281000	-0.26540800
H	5.35165100	-1.58766400	-1.24102700	C	-2.60120600	1.83033200	-0.79945700
H	4.94112300	1.11416000	2.05399600	H	-2.78023800	0.80731000	-1.16530300
H	6.33658900	0.12309400	0.26084200	H	-3.37255600	2.08169000	-0.05343600
C	-2.32552800	-1.53895800	0.70265400	H	-2.71628400	2.47213900	-1.69005300
C	-2.89777100	-2.27653100	-0.35573100	C	0.87910800	-2.54411200	1.78506400
C	-3.11643200	-0.77862400	1.59379400	C	0.12960300	-0.95425600	0.33587400
C	-4.28089500	-2.16425900	-0.54975700	C	-0.45489000	-2.71440300	1.65327100
C	4.49098800	-0.72109500	1.33912600	N	1.23141500	-1.46965500	0.97618000
C	-5.07598900	-1.384757500	0.27204800	N	-0.90064900	-1.73064600	0.78680900
H	-4.72846700	-2.71597000	-1.37658600	Cu	0.09348400	0.69979000	-0.83603500
H	-5.11108900	-0.12636000	2.01077900	H	-1.13035700	-3.44015700	2.08242700
H	-6.14868800	-1.31419300	0.09935300	H	1.61842600	-3.07915600	2.36485200
C	2.96826400	-2.63586400	-1.30173600	C	2.59936200	-0.97662300	0.93375500
C	2.62531200	-3.97898800	-0.65781500	C	3.54682800	-1.62134300	0.10399900
C	1.90335800	-2.12914500	-2.26624500	C	2.97917900	0.05823200	1.81934700
H	3.44638300	-4.33606200	-0.02211500	C	4.87659000	-1.19024200	0.18189200
H	1.71998300	-3.94299600	-0.04545800	C	4.32655900	0.44076000	1.83594900
H	2.45224600	-4.73144400	-1.43738000	C	5.27435100	-0.17387100	1.03499700
H	2.22835800	-1.21881800	-2.78151700	H	5.61229900	-1.67785100	-0.45782900
H	1.67795000	-2.88286300	-3.03017200	H	4.62660400	1.23886500	2.51553300
H	0.96021900	-1.88563900	-1.76965300	H	6.31603400	0.14192800	1.06962900
C	2.46909900	0.69405900	2.72237300	C	-2.28176900	-1.58547600	0.37229400
C	1.29573700	1.56843600	2.29009100	C	-2.65978000	-2.14361600	-0.87090000
C	2.12339900	-0.23009200	3.88998500	C	-3.20559700	-0.91493000	1.20779900
H	1.59757500	2.29108000	1.52129500	C	-3.96263300	-1.90311900	-1.31634900
H	0.46578200	0.98517000	1.88136100	C	-4.50256400	-0.74655300	0.70571900
H	0.90001000	2.12929000	3.14794700	C	-4.87544500	-1.19585700	-0.55049300
H	3.00739500	-0.78888200	4.22156100	H	-4.25081600	-2.28125300	-2.29648900
H	1.75731500	0.35702200	4.74213200	H	-5.22964900	-0.22582900	1.33087200
H	1.34374900	-0.95590400	3.64078500	H	-5.88224100	-1.01648300	-0.92352500
C	-2.18272700	-3.15626300	-1.37037800	C	3.28430800	-2.76016800	-0.87062700
C	-1.72953600	-2.33175000	-2.57116800	C	2.87305600	-4.07668700	-0.20925000
C	-1.04545800	-4.03664100	-0.86997900	C	2.35754900	-2.37221600	-0.01568600
H	-2.57003700	-1.85122100	-3.08626200	H	3.52919300	-4.32739000	0.63470200
H	-1.03682400	-1.53618800	-2.27567500	H	1.84169700	-4.06603200	0.15512400
H	-1.20344600	-2.95325500	-3.30372400	H	2.94386000	-4.89124700	-0.94092200
H	-1.30390300	-4.58962700	0.04246800	H	2.77616100	-1.55462200	-2.61174000
H	-0.79396300	-4.77143600	-1.64504700	H	2.18328200	-3.23249000	-2.67510400
H	-0.13348300	-3.46474000	-0.68045500	H	1.38475300	-2.02867600	-1.65626100
C	-2.68115000	0.05334200	2.79747800	C	2.09140500	0.76131300	2.83792600
C	-1.53451400	-0.46040800	3.65549700	C	0.88845300	1.50783900	2.27190200
C	-2.45037300	1.51950900	2.42274900	C	1.71792500	-0.15232900	4.00589900
H	-1.66826700	-1.50780900	3.95254800	H	1.17192500	2.12006500	1.40512100
H	-0.56692100	-0.36911900	3.15722400	H	0.07990100	0.84816300	1.94609200
H	-1.47371300	0.13808600	4.57386300	H	0.46812000	2.17460400	3.03768800
H	-3.30126400	1.93181000	1.86611600	H	2.61351300	-0.57437500	4.47902200
H	-2.30412300	2.11979900	3.33142500	H	1.16438500	0.41040800	4.76867500
H	-1.57338100	1.63676900	1.78065200	H	1.08167900	-0.98677300	3.69305300
B	-0.03941900	0.15392400	-4.42358700	C	-1.80298500	-3.00570600	-1.79266500
F	0.08054800	0.38886500	-2.97565500	C	-1.08751100	-2.17720400	-2.85719600
F	-1.30370400	0.61320600	-4.79673000	C	-0.85082700	-3.99548400	-1.13144800
F	0.98115500	0.88444600	-5.03312900	H	-1.79587700	-1.63182000	-3.48274100
F	0.10064900	-1.20428000	-4.65720800	H	-0.42144900	-1.42776600	-2.41261400
H	3.22199500	1.39244200	3.11855700	H	-0.47852800	-2.82618900	-3.50005500
H	3.85990900	-2.83246700	-1.916133900	H	-1.32063400	-4.55203000	-0.30967200
H	-3.56655900	0.04350800	3.45227400	H	-0.51721000	-4.72642600	-1.87936800
H	-2.96307400	-3.84670000	-1.72686100	H	0.05181100	-3.51334400	-0.74587600
C	2.79557300	3.35033200	-1.83033000	C	-3.00597400	-0.30353900	2.59701300
C	3.84205100	3.34283600	-0.70490400	C	-1.92997600	-0.86438600	3.51271700
H	4.18582000	2.32558300	-0.49067700	C	-2.87654800	1.22079100	2.51597400
H	4.70617700	3.94864100	-1.00501200	H	-2.00832700	-1.94943700	3.64340200
H	3.43893000	3.77101000	0.22368100	H	-0.91971700	-0.63551000	3.16383400
C	2.32553600	4.78201100	-2.06897600	H	-2.03525100	-0.40743600	4.50505600
H	1.65157800	4.86272000	-2.92713400	H	-3.77030000	1.67169600	2.06859700
H	1.81277300	5.19629600	-1.19145900	H	-2.75424300	1.64348300	3.52226800
H	3.19591800	5.41684500	-2.27566900	H	-2.01893700	1.52192000	1.90275200
C	3.41793300	2.75577900	-3.10221400	H	2.74309000	1.53815400	3.26559700
H	3.77767000	1.73673500	-2.91917800	H	4.26806400	-2.96017500	-1.32144500
H	2.70306900	2.70868400	-3.93144600	H	-3.96158400	-0.50496400	3.10758000
H	4.26860900	3.37519000	-3.41377800	H	-2.54182900	-3.62140600	-2.32904600
H	-0.98706300	3.73399300	0.64284500	B	-1.91206300	0.97028600	-3.95869400
C	-0.24103000	3.50686400	-3.98837500	F	-2.99039500	0.21647600	-3.48328500
H	0.17727600	4.31447600	-4.60409300	F	-0.89458900	1.02499300	-2.90082200
H	0.55332300	2.79431100	-3.76282500	F	-1.32372800	0.38791100	-5.06979700
H	-0.95439900	2.96056300	-4.61699200	F	-2.32336600	2.28039100	-4.21786900
C				C	3.37616400	2.61556900	-2.40200600
C				C	4.47233700	2.04870900	-1.48737100
C				H	4.50130400	0.95547500	-1.53968400
C				H	5.45041300	2.44140100	-1.79408600
C				H	4.30575300	2.33115200	-0.43970700

C	3.64762800	2.15362500	-3.83733500	H	4.20471700	1.26472300	-3.98269500	
H	3.59031000	1.06215500	-3.91384700	H	0.93458800	2.50544400	-2.66989100	
H	2.93695300	2.58021700	-4.55280400	H	1.69355900	1.35382800	-3.80267500	
H	4.65571800	2.46654500	-4.13746900	H	1.48422800	0.94272700	-2.08785600	
C	3.38009200	4.13733000	-2.29224500	B	-0.90140500	2.93664800	-0.43197500	
H	2.60389400	4.60813000	-2.90406900	F	-0.42918700	3.90108200	-1.30248400	
H	3.23136600	4.46340300	-1.25563800	F	-1.96924700	3.38080200	0.32688700	
H	4.34787300	4.52835700	-2.62969000	F	-1.29235400	1.76004400	-1.16124300	
H	-0.14483800	3.74367900	0.65213500	F	0.16540100	2.48598900	0.41873500	
C	0.37790900	3.49994900	-4.04184800	H	-1.05624800	-2.36684900	-0.49113600	
H	1.26461000	4.10078800	-4.28505600	C	-4.23821400	0.96100800	0.16190900	
H	0.68443000	2.44995100	-3.97583700	H	-4.42227900	0.83938500	1.23771900	
H	-0.31381400	3.56896600	-4.88514400	H	-3.51931500	1.78491200	0.06114800	
<b>4e'</b>								
C	-3.91215300	-2.16655700	-2.07135200	H	3.52070400	2.95098900	3.43645800	
C	-2.61597400	-2.51722100	-1.95650500	H	1.08780800	-3.38690200	3.27443800	
C	-1.68287200	-1.71470500	-1.11917200	H	3.14656900	3.26751600	-3.13911000	
C	-2.38606300	-0.75692900	-0.16363800	C	1.77782900	-3.46719000	-3.28995400	
C	-3.71670600	-0.28402000	-0.47607000	C	-2.95836000	-0.71469200	3.01526100	
C	-4.43123400	-1.00164800	-1.39451500	H	-1.98609300	-1.47240700	3.93656800	
H	-4.58158900	-2.72812400	-2.72184400	H	-1.29941800	-0.78321000	4.44115500	
H	-2.18675900	-3.33384700	-2.53647300	H	-2.55535100	-2.01708200	4.70104100	
H	-5.44283000	-0.67472500	-1.63883800	C	-1.39139300	-2.20591700	3.37558700	
N	-1.65505400	-0.40089200	0.86270700	C	-3.85095300	-1.74718400	2.33183000	
C	-2.05330000	0.14427800	0.29295700	H	-4.63894200	-1.29605600	1.71967000	
O	-1.48598200	1.12781000	2.53524200	H	-3.28203600	-2.44410600	1.70171800	
O	-0.70524200	-1.02413500	-1.92074500	C	-4.35003400	-2.34736400	3.10381400	
C	-1.23599200	-0.31603300	-3.04542700	C	-3.80230300	0.23138500	3.87171300	
H	-0.44411600	0.36406900	-3.36679900	H	-4.54225100	0.77768900	3.27346800	
H	-1.48694800	-1.00757700	-3.86094800	H	-4.34770200	-0.34273000	4.63146200	
H	-2.10927400	0.28719800	-2.77405400	H	-3.17144100	0.97026100	4.37420600	
C	4.05859000	-1.32192800	0.04450400	<b>TS<sub>S1-Ps1</sub></b>				
C	2.11665000	-0.12512900	0.09468100	C	-0.68072300	0.17169500	1.07066800	
C	4.38647800	-0.00748700	0.02017200	C	-0.16817200	0.57008400	-0.16286700	
N	2.67259000	-1.38520100	0.09206300	C	-0.33534800	1.86284200	-0.64899800	
N	3.20232100	0.71417600	0.05494000	C	-1.09028900	2.80028100	0.17597100	
Cu	0.18067200	0.24977100	0.24374900	C	-1.56996000	2.36324400	1.45766500	
H	5.34790100	0.48830400	0.00646300	C	-1.39184900	1.06992500	1.88454400	
H	4.67393100	-2.21017200	0.05584200	H	-0.52128300	-0.85115100	1.40927900	
C	1.89103000	-2.60750100	0.02809200	H	0.40209100	-0.14107100	-0.75936100	
C	1.34199300	-3.14399800	1.21683700	H	-2.10720500	3.10003800	2.05052600	
C	1.68820200	-3.24137600	-1.21872000	H	-1.78364500	0.74432600	2.84570200	
C	0.47890200	-4.24038900	1.10555700	N	-1.27845000	4.08091100	-0.07903800	
C	0.82889600	-4.34830400	-1.25325700	C	0.22772100	2.24113700	-1.97325800	
C	0.20029100	-4.83171400	-0.11753600	H	-0.55020700	2.23451800	-2.74831900	
H	0.03846000	-4.64431300	2.01741000	H	0.67447700	3.24044900	-1.95032800	
H	0.65428000	-4.83063700	-2.21552300	H	1.00401200	1.52968900	-2.27249400	
H	-0.48123700	-5.67904300	-0.17992200	O	1.12668600	3.69994900	0.41626700	
C	3.19560500	2.17642700	0.11419200	C	1.33909100	3.76295600	1.74168000	
C	3.26057400	2.81296400	1.37255200	H	1.95306400	4.62963100	2.05814900	
C	3.17703800	2.92604000	-1.08335200	H	0.39178100	3.72722000	2.34011200	
C	3.28846000	4.21232800	1.39488300	H	1.89812400	2.85511000	2.06862800	
C	3.19709500	4.32012600	-0.98365100	C	-1.18385600	4.69500900	-1.31419300	
C	3.24903800	4.96927500	0.23780800	O	-0.50508700	5.66357300	-1.57463900	
H	3.32021800	4.70739900	2.36569200	O	-2.09391100	4.14533000	-2.16556000	
H	3.15132300	4.90085300	-1.90421900	C	-2.16591900	4.80479600	-3.45296800	
H	3.25222700	6.05663500	0.28703900	H	-2.50059300	5.83683100	-3.28743600	
C	1.69805100	-2.73084200	2.63478100	H	-1.15637500	4.85017300	-3.88007700	
C	3.16012700	-3.04330900	2.96047500	C	-3.10490900	4.02578900	-4.31502800	
C	1.36701600	-1.29992700	3.01860300	C	-4.47503400	4.00022300	-4.03277000	
H	3.41605300	-4.08627800	2.73722100	C	-2.62720300	3.30992700	-5.41493300	
H	3.84201700	-2.39525500	2.39535000	C	-5.34821400	3.27340500	-4.83499700	
H	3.35718100	-2.86428200	4.02519500	H	-4.85217100	4.55309000	-3.17232400	
H	0.39073700	-0.97279200	2.64316100	C	-3.50018400	2.58561400	-6.22466900	
H	1.36696900	-1.18572900	4.11095700	H	-1.55992700	3.32494600	-5.63996800	
H	2.10877400	-0.61061600	2.62352400	C	-4.86207300	2.56530900	-5.93466100	
C	2.37341100	-2.92364900	-2.54043100	H	-6.41254700	3.26136800	-4.60565700	
C	2.38259300	-1.47216000	-2.98020500	H	-3.11541000	2.03547700	-7.08195100	
C	3.77841500	-3.53048400	-2.59690600	H	-5.54586900	1.99905900	-6.56498500	
H	1.37818600	-1.04568300	-2.94539800	<b>Ps1</b>				
H	3.03178500	-0.85071900	-2.35881000	C	-2.59926800	0.07208300	0.94540300	
H	2.75803700	-1.39560600	-4.00936500	C	-1.18586100	-0.39440500	1.14793400	
H	3.78427900	-4.58069200	-2.28065200	C	-0.42435300	-0.62729500	-0.16279500	
H	4.16833800	-3.48193700	-3.62129700	C	-1.05570600	-0.28378700	-1.41923800	
H	4.48075000	-2.97872500	-1.96104900	C	-2.32423300	0.18850500	-1.46162700	
C	3.17940200	2.16496200	2.74513500	C	-3.11593100	0.35526800	-0.26266400	
C	1.71037300	1.91202900	3.09388400	H	-3.20277500	0.18445600	1.84645400	
C	4.11108700	0.98873900	3.02423600	H	-2.77573400	0.43230600	-2.42287900	
H	1.14835000	2.85198600	3.10869800	H	-4.14472600	0.69897600	-0.35866700	
H	1.20560500	1.28715200	2.34993200	C	-0.41293700	0.64944500	1.95472300	
H	1.60973100	1.42833100	4.07496100	H	-0.31172100	1.57322700	1.37403700	
H	5.15589400	1.25786600	2.81918400	H	-0.92596100	0.89794100	2.89079100	
H	4.04213300	0.71129900	4.08462300	H	0.59173500	0.26807000	2.16996900	
H	3.89019600	0.08861500	2.44715300	N	0.77102200	-1.08708700	-0.04174700	
C	3.09138700	2.37650200	-2.49593900	C	1.59585100	-1.26709100	-1.14014900	
C	4.28506100	1.52126000	-2.91819400	O	2.37303200	-0.43554600	-1.56737600	
C	1.72577800	1.75577300	-2.77985400	O	1.49016200	-2.52893800	-1.60904900	
H	5.22498100	2.07102500	-2.77698700	C	2.43143100	-2.85733400	-2.66038500	

H	2.30283900	-2.13038100	-3.47234200	H	-1.95847100	-0.21682900	3.48553700
H	3.44811300	-2.73847400	-2.26757700	O	-1.31473300	-0.32349500	-2.19615200
C	2.15662300	-4.25817200	-3.09984400	C	-0.61830000	0.03364700	-3.37099600
C	1.02028300	-4.54918000	-3.86180400	H	-0.80303600	1.08096000	-3.65907900
C	3.02022100	-5.29797300	-2.75020900	H	0.46401800	-0.12480700	-3.24221900
C	0.75195600	-5.85334600	-4.26357000	H	-0.99500500	-0.61655300	-4.16548800
H	0.33940200	-3.74158500	-4.13339300	H	0.15768000	0.68334300	-1.16794900
C	2.75794800	-6.60521300	-3.15518800				
H	3.90559200	-5.07848200	-2.15298800				
C	1.62243900	-6.88504100	-3.91152300	<b>TS4-5</b>			
H	-0.13662100	-6.06808000	-4.85512800	C	-4.62040400	0.74908200	-0.11598700
H	3.44022700	-7.40688900	-2.87665700	C	-4.74501500	-0.58867600	-0.41410500
H	1.41466100	-7.90602900	-4.22777900	C	-3.61464600	-1.41056600	-0.22742600
H	-0.48092200	-0.42817800	-2.33342700	C	-2.36060200	-0.85126900	0.17663300
O	-1.20680100	-1.68372100	1.78525000	C	-2.24513700	0.57844900	0.48689100
C	-1.50968500	-1.69357800	3.16028500	C	-3.42703600	1.31661000	0.35315800
H	-2.46598600	-1.19672400	3.39223900	H	-5.47194600	1.41151100	-0.26305800
H	-1.59354800	-2.74706200	3.43834300	H	-5.66087600	-1.01879900	-0.80584400
H	-0.71441400	-1.23154700	3.76337700	H	-3.61403700	-2.42859800	-0.60153300
			H	-3.40707500	2.37867200	0.55111600	
			N	-0.99686500	0.96255500	0.85640200	
			O	-1.20256100	-1.51796600	0.11309000	
C	-0.68675200	0.36628900	0.02688100	C	-1.20964800	-2.86888900	-0.35931500
C	0.12207600	0.93632800	1.03056900	H	-1.57638000	-2.89957200	-1.38959700
C	0.71909200	2.16636700	0.85981400	H	-0.16877700	-3.18834400	-0.30901400
C	0.52755300	2.86021000	-0.39933200	H	-1.81372100	-3.50301500	0.30571800
C	-0.31813800	2.25592400	-1.40957600	C	-3.34001700	-1.58491600	1.66166500
C	-0.905559700	1.02001500	-1.17980300	H	-3.86276800	-2.54354000	1.67205200
H	-1.14210200	-0.60748400	0.20346800	H	-2.38398300	-1.69601300	2.18577400
H	0.26598500	0.39981900	1.96787800	H	-3.94556000	-0.78224600	2.07804200
H	-0.39853400	2.73360300	-2.37640200	C	-0.60686800	2.24639200	1.14554100
H	-1.53001300	0.56513600	-1.94562500	O	0.54216400	2.51548500	1.47811100
N	1.03282200	4.07739600	-0.46771800	C	4.47844900	-1.53866900	-0.41070100
C	1.53705600	2.80191000	1.92782800	C	2.50149900	-0.54517700	0.13716300
H	2.56383500	2.98793300	1.59174800	C	4.74462500	-0.24633400	-0.11031700
H	1.12951000	3.78485000	2.19204000	N	3.10904400	-1.71801300	-0.25955300
H	1.56996000	2.17630800	2.82531500	N	3.53829100	0.34580400	0.22392100
O	-1.34503700	4.34319400	-0.87072800	Cu	0.68101100	-0.03792400	0.47384800
C	-2.18316400	5.23817800	-1.43991500	H	5.67052800	0.31217900	-0.10090100
H	-3.14044900	5.39017000	-0.90436200	H	5.12128500	-2.34926200	-0.72535100
H	-1.64899000	6.21607300	-1.44693000	C	2.46214600	-2.99699500	-0.52309900
H	-2.38478600	5.03013000	-2.51362300	C	2.30460700	-3.92927000	0.53288500
C	1.04539700	4.85703000	-1.61892500	C	2.06645200	-3.31971600	-1.84488300
O	0.90761600	6.06288500	-1.62426000	C	1.70288800	-5.15936100	0.23934200
O	1.39574500	4.13997800	-2.72196200	C	1.47631400	-4.57228500	-2.06218800
C	1.55581800	4.92069200	-3.91605400	C	1.28504600	-5.48738300	-1.04058600
H	0.60480800	5.41934700	-4.14743100	H	1.57456000	-5.87542600	1.05104500
H	2.28516200	5.711775900	-3.71263400	H	1.15533100	-4.81611600	-3.07440500
C	1.99558200	4.02243100	-5.03051000	H	0.82104200	-6.45192600	-1.24096100
C	1.67888400	4.36227100	-6.34884500	C	3.44894700	1.74515900	0.60746600
C	2.74818300	2.86943400	-4.79057800	C	3.64816500	2.09682300	1.95901100
C	2.11192500	3.57127700	-7.40983200	C	3.22095300	2.72188500	-0.38449600
H	1.08363400	5.25492400	-6.54525100	C	3.65064600	3.45675500	2.28412400
C	3.17478400	2.07374700	-5.85125100	C	3.23592500	4.06385200	0.01213600
H	2.98892000	2.59338400	-3.76581700	C	3.45508700	4.43902400	1.32700100
C	2.86103400	2.42234200	-7.16348400	H	3.79526800	3.73590000	3.32841900
H	1.85513600	3.84848900	-8.43097700	H	3.05867600	4.82494600	-0.74850000
H	3.75630700	1.17525300	-5.64980800	H	3.46530300	5.49152500	1.60643700
H	3.19463700	1.79874000	-7.99125600	C	2.73232100	-3.74845100	1.98132900
			C	2.42364700	-3.61601200	2.16225100	
			C	1.93371600	-2.67813600	2.71832500	
			C	4.76737100	-4.45645500	1.68953300	
C	-2.09632700	1.36057100	1.38317600	H	4.64664200	-2.69277800	1.73854000
C	-1.54754700	0.11624300	1.40583000	H	4.49753000	-3.62055800	3.22989400
C	-1.00359100	-0.43573600	0.17315700	H	0.85768100	-2.89644100	2.67666900
C	-0.92395200	0.44782200	-1.06658300	H	2.22888600	-2.63525900	3.77499800
C	-1.67676200	1.73197400	-0.98042300	H	2.07554400	-1.68234100	2.29192800
C	-2.19228700	2.16277800	0.18394900	C	2.16715000	-2.43162400	-3.07423500
H	-2.52020300	1.76154100	2.30458700	C	1.19244200	-1.26019400	-3.00135000
H	-1.77218400	2.31331600	-1.89671600	C	3.59199700	-2.05554100	-3.47811100
H	-2.71474600	3.11671700	0.23835800	H	0.15659300	-1.61011000	-2.94456700
N	-0.56261600	-1.64704000	0.17920700	H	1.35806700	-0.62440100	-2.12681200
C	0.09279900	-2.16844400	-0.92601900	H	1.25809700	-0.62538600	-3.89325800
O	1.14802900	-1.74648100	-1.37197200	H	4.22591600	-2.94845900	-3.56313200
O	-0.52302800	-3.28353600	-1.35425600	H	3.57538100	-1.56444700	-4.45907300
C	0.10840800	-3.92335200	-2.48470600	H	4.07923300	-3.36650000	-2.78486700
H	0.35073900	-3.16396600	-3.23742800	C	3.71711900	1.15225100	3.14842900
H	1.05595700	-4.35845600	-2.13998400	C	2.29453100	0.83432900	3.61743900
C	-0.83263000	-4.95263800	-3.02176200	C	4.55001500	-0.11433100	3.01245800
C	-1.39141900	-4.80139900	-4.29225900	H	1.74835400	1.74821000	3.87438300
C	-1.17182300	-6.07725000	-2.26204700	H	1.71728400	0.34604400	2.81953800
C	-2.27112500	-5.75491100	-4.80116700	H	2.31148600	0.16966500	4.49195400
H	-1.13470300	-3.92373500	-4.88676800	H	5.55054500	0.08531700	2.60846000
C	-2.05448100	-7.02797400	-2.76392900	H	4.67454700	-0.57989700	3.99910800
H	-0.74600300	-6.19636300	-1.26580300	H	4.07164600	-0.85782500	2.37137100
C	-2.60542100	-6.86936100	-4.03615100	C	2.84585000	2.48270500	-1.83772100
H	-2.69920900	-5.62424000	-5.79375000	C	3.60131600	1.39423000	-2.58575200
H	-2.31425100	-7.89760800	-2.16240700	C	1.33336400	2.28122700	-1.95237900
H	-3.29511300	-7.61473800	-4.42894300	C	4.68748100	1.46183800	-2.44052600
C	-1.52336500	-0.73835900	2.62681800	H	3.27716700	0.39568100	-2.28634000
H	-2.07615900	-1.67149000	2.46379500	H	3.39996800	1.47812300	-3.66121800

H	0.77987200	3.13233600	-1.53497600	H	1.02392700	-1.12338000	-2.19833500
H	1.02041400	2.14364300	-2.99467500	H	1.09990300	-1.17027600	-3.96653300
H	1.00599600	1.38763900	-1.40376800	H	4.00503500	-3.47553500	-3.30732900
B	-2.18184500	-0.13439000	-3.12947300	H	3.39436800	-2.19935000	-4.37421900
F	-1.58565000	-0.14429300	-4.38521900	H	3.77457800	-1.82834500	-2.69847000
F	-1.27886300	0.40140000	-2.16959700	C	3.38191500	0.85617500	3.14666800
F	-3.36756600	0.59709600	-3.11181800	C	1.97345600	0.58776900	3.68438900
F	-2.46573600	-1.48769500	-2.72917900	C	4.17536200	-0.43710000	3.03322700
O	-1.55412900	3.20793700	1.01975600	H	1.46041400	1.52166000	3.93725400
C	-1.09193600	4.55662600	1.20967500	H	1.35049800	0.09313100	2.92627000
H	-0.13615400	4.67053500	0.68017900	H	2.01345600	-0.05196300	4.57649900
H	-0.88865600	4.72313500	2.27583500	H	5.16986200	-0.28422300	2.59564700
C	-2.14498900	5.48529700	0.69148200	H	4.31368500	-0.86920500	4.03318400
C	-2.75354500	5.25431700	-0.54700100	H	3.65488500	-1.18835500	2.43509100
C	-2.50625600	6.61650300	1.42564300	C	2.39939000	2.02070400	-1.86438200
C	-3.70998900	6.14121000	-1.03566400	C	3.19661000	0.94360700	-2.58770600
H	-2.48544200	4.36900700	-1.12339600	C	0.89538900	1.75880300	-1.96148800
C	-3.45463100	7.51082700	0.93211700	H	4.27917100	1.05878100	-2.44435400
H	-2.04195700	6.79578700	2.39634100	H	2.91424300	-0.05991400	-2.26271400
C	-4.06047800	7.27326400	-0.29906600	H	2.99233900	0.99237800	-3.66488200
H	-4.18078100	5.94837300	-1.99838500	H	0.31343000	2.59910600	-1.56122100
H	-3.72722600	8.38859700	1.51612800	H	0.57880800	1.58564500	-2.99768400
H	-4.80645200	7.96657500	-0.68439100	H	0.60635500	0.86778700	-1.38880400
H	4.18978600	1.74278700	3.94860700	B	-2.39386800	-0.40809000	-2.78948200
H	3.08267700	3.42971900	-2.34726300	F	-1.80178400	0.07815400	-3.93781800
H	2.46727000	-4.70145400	2.46371100	F	-1.43984800	-0.43726500	-1.72389600
H	1.80441700	-3.06721900	-3.89579500	F	-3.48770600	0.36062000	-2.37234600
H				F	-2.83427200	-1.75760500	-2.98009000
<b>5</b>				O	-1.94029900	2.78440600	1.29597300
C	-5.11865100	0.46056600	0.51220200	C	-1.46507200	4.13920000	1.30192400
C	-5.26167200	-0.74903700	-0.07297300	H	-0.58598300	4.19970400	0.64601000
C	-4.12900200	-1.69492900	-0.13468700	H	-1.12763700	4.40459200	2.31272900
C	-2.84475800	-0.117499300	0.39796400	C	-2.58455500	5.01825500	0.83794400
C	-2.67124800	0.16143400	0.87122700	C	-3.34030600	4.67294500	-0.28932900
C	-3.85698400	0.90028900	0.98940000	C	-2.87108600	6.20894300	1.50782500
H	-5.96042500	1.14621700	0.58834200	C	-4.36116100	5.50797600	-0.73282900
H	-6.20547900	-1.07974400	-0.50135300	H	-3.12962300	3.73923700	-0.81238400
H	-3.93403300	-1.87408800	-1.21571200	C	-3.88857500	7.04963100	1.05984100
H	-3.80245400	1.89376900	1.41602100	H	-2.29259100	6.47801200	2.39259100
N	-1.38219000	0.53853800	1.16208700	C	-4.63738400	6.69945100	-0.06093600
O	-1.78071800	-1.94280000	0.47713600	H	-4.94246300	5.22801800	-1.60998000
C	-1.58256300	-3.08827400	-0.37586200	H	-4.10211600	7.97471400	1.59363300
H	-2.23038800	-3.04332400	-1.25500100	H	-5.43666300	7.35146500	-0.41030600
H	-0.53980000	-3.01843200	-0.69464200	H	3.89837300	1.46591600	3.90347700
H	-1.72914300	-3.99919400	0.21103600	H	2.59640800	2.96159900	-2.40147300
C	-4.55757100	-3.03005900	0.51034200	H	1.86239500	-4.97052600	2.62782300
H	-5.48734900	-3.37332800	0.04672200	H	1.59802300	-3.64012200	-3.82290300
H	-3.81489700	-3.81953500	0.38442000				
H	-4.74210600	-2.89427400	1.58132600				
C	-0.97552500	1.82356400	1.36068400				
O	0.20115700	2.12248300	1.55002700				
C	4.05928900	-1.94956800	-0.32416700				
C	2.08005800	-0.93185500	0.17801000				
C	4.32784900	-0.65016000	-0.06118900				
N	2.68748000	-2.11723400	-0.18384800				
N	3.12201000	-0.04372200	0.24722000				
Cu	0.27552500	-0.40967000	0.59650400				
H	5.25585200	-0.09514300	-0.05911400				
H	4.70082800	-2.77186600	-0.60916000				
C	2.02983100	-3.39369400	-0.42140500				
C	1.77106200	-4.25951000	0.67001600				
C	1.70305800	-3.77362700	-1.74724600				
C	1.11254500	-5.46685100	0.40770800				
C	1.05646000	-5.00328700	-1.93233200				
C	0.74436100	-5.84102600	-0.87461700				
H	0.90263000	-6.13004500	1.24699600				
H	0.78519900	-5.29019500	-2.94781800				
H	0.23419500	-6.78705900	-1.05040100				
C	3.04260500	1.36633800	0.59199300				
C	3.28184300	1.75794600	1.92557600				
C	2.78768500	2.31117000	-0.42376400				
C	3.29181200	3.12795800	2.20722200				
C	2.80316000	3.66455700	-0.06813800				
C	3.05987800	4.07975200	1.22817700				
H	3.46794600	3.43971600	3.23735500				
H	2.60215400	4.40186600	-0.84613400				
H	3.07261700	5.14025500	1.47582100				
C	2.17337100	-0.40442250	2.12134100				
C	3.68652200	-3.96566300	2.31987100				
C	1.41213900	-2.92135200	2.81678300				
H	4.18250700	-4.84740800	1.89455800				
H	4.13194000	-3.07934900	1.85962700				
H	3.92572700	-3.92975600	3.39033200				
H	0.32700300	-3.06769900	2.73136600				
H	1.66774000	-2.88902500	3.88412800				
H	1.63569700	-1.94004800	2.39328200				
C	1.90626900	-2.95836300	-3.01621400				
C	0.93767100	-1.78076300	-3.06951100				
C	3.35124500	-2.59417500	-3.35142600				
H	-0.10217000	-2.12410600	-3.09505200				

F	0.89659600	-3.71049400	-2.64688500	Cu	0.36450000	0.23073300	1.78831700
H	-5.34140800	-3.77103000	-5.15436700	H	4.27991500	-2.99766300	1.18164100
H	-3.15058800	-4.49299800	-6.70592300	H	5.29848200	-0.41124000	1.02910800
C	-4.64587200	-3.16820400	-2.52819000	C	3.34916900	1.54712800	1.33748400
C	-5.06526600	-1.83213400	-2.32454500	C	3.18645100	2.15406500	0.07287500
C	-5.06651500	-4.20230000	-1.66453300	C	3.63119900	2.31492000	2.48944900
C	-5.90699300	-1.56686800	-1.24051100	C	3.25531800	3.55066900	0.00777300
C	-5.90746300	-3.86269700	-0.59720300	C	3.70035800	3.70388000	2.34731100
C	-6.33013500	-2.56485900	-0.37755200	C	3.50120600	4.32750900	1.12609500
H	-6.22823600	-0.53806800	-1.07901100	H	3.10267500	4.02353100	-0.96219000
H	-6.22831600	-4.65954700	0.07399000	H	3.90652800	4.30165100	3.23522000
H	-6.98663300	-2.33053100	0.45857500	H	3.54149000	5.41301900	1.04700200
C	-0.74001600	-4.31303800	-5.33004800	C	1.61165700	-3.09113300	1.77986100
C	0.01345100	-3.20309100	-5.76186300	C	1.08911000	-3.81508900	0.68030200
C	-0.20080100	-5.61954100	-5.35792000	C	1.42262300	-3.54243800	3.10604600
C	1.32291400	-3.43093600	-6.19826100	C	0.39792100	-5.00246100	0.95101800
C	1.11463000	-5.77208400	-5.80287500	C	0.71868900	-4.73783500	3.30163200
C	1.88168700	-4.69484500	-6.21386200	C	0.21502900	-5.47375800	2.24177800
H	1.91164000	-2.57139800	-6.51997500	H	-0.00840000	-5.56179600	0.10816100
H	1.54272700	-6.77374900	-5.80446900	H	0.57283000	-5.08665600	4.32439800
H	2.90728400	-4.84306500	-6.54697900	H	-0.31785300	-6.40667600	2.41969900
C	-4.65261800	-5.66571200	-1.69666000	C	3.01384700	1.45706200	-1.26575100
H	-5.46865600	-6.18956900	-1.17420900	C	4.35720700	0.97326600	-1.81726100
C	-4.64554800	-0.62003900	-3.14046000	C	1.97857400	0.35407200	-1.31842400
H	-5.21398500	0.21484400	-2.70213500	H	5.11124600	1.77023100	-1.82384100
C	-0.88723000	-6.89279000	-4.89276600	H	4.75406800	0.13649200	-1.22579300
H	-0.17386600	-7.69330500	-5.14117900	H	4.23441200	0.61172400	-2.84605800
C	-0.39311100	-1.73812600	-5.73812800	H	1.04046400	0.65564500	-0.83243000
H	0.22931100	-1.27100900	-6.51887700	H	1.73357100	0.11988700	-2.36028700
C	-3.39590900	-5.86818000	-0.84619800	H	2.34035800	-0.56269900	-0.84849500
H	-2.53379100	-5.32237800	-1.24819300	C	3.85769100	1.78899300	3.89641200
H	-3.55373900	-5.51195500	0.17899400	C	2.56848300	1.27833200	4.53452000
H	-3.12069600	-6.92937500	-0.80158900	C	5.04025000	0.83114800	4.03170900
C	-4.53576800	-6.33522200	-3.05742400	H	1.81578500	2.07500300	4.56994600
H	-5.41602300	-6.14972700	-3.68587700	H	2.12791000	0.45388600	3.96797600
H	-3.65063500	-6.01238600	-3.60729300	H	2.75140700	0.92535600	5.55878500
H	-4.44319100	-7.42054200	-2.92434900	H	5.95247300	1.28218300	3.62063100
C	-1.03580700	-6.91475900	-3.37474500	H	5.22627700	0.60862800	5.09062400
H	-0.05858600	-6.85982700	-2.88553000	H	4.88788400	-0.12531900	3.52515100
H	-1.60812800	-6.05817000	-3.00810200	C	1.11131300	-3.38756000	-0.77834600
H	-1.54548500	-7.83050000	-3.04515900	C	0.14718700	-2.21800900	-1.00098500
C	-2.16448100	-7.25843400	-5.64711700	C	2.49170300	-3.20835600	-1.40916700
H	-3.00690800	-6.59828700	-5.42578200	H	-0.89261800	-2.55113900	-0.88742100
H	-2.00168100	-7.24234600	-6.73299600	H	0.29554200	-1.39945800	-0.28631800
H	-2.47634100	-8.27455600	-5.37332300	H	0.24178100	-1.79100800	-2.00527700
C	0.02494900	-1.10484500	-4.41129800	H	3.10481900	-4.10763600	-1.26273800
H	-0.50161700	-1.55547000	-3.56079600	H	2.37832800	-3.05447400	-2.48923000
H	1.09056800	-1.25099500	-4.20663100	H	3.05461700	-2.35556000	-1.02504300
H	-0.19047600	-0.02692600	-4.40196700	C	1.81721800	-2.81731000	4.38193600
C	-1.83119100	-1.39588800	-6.09844800	C	3.21349700	-2.21505500	4.43685600
H	-1.92648300	-0.31105000	-6.24331000	C	0.72803700	-1.80485400	4.74990600
H	-2.15356700	-1.88679100	-7.02483000	H	3.98103100	-2.93560600	4.12764400
H	-2.53330400	-1.66988600	-5.30857300	H	3.31326400	-1.32722100	3.81162700
C	-3.17111200	-0.28289500	-2.92948300	H	3.44078800	-1.90487200	5.46472100
H	-2.96216000	-0.09007500	-1.86948200	H	-0.23666400	-2.30535300	4.90392900
H	-2.51212100	-1.10237900	-3.22868600	H	0.98369700	-1.26652500	5.67141700
H	-2.88745900	0.60860600	-3.50571600	H	0.58482500	-1.06088300	3.95230000
C	-5.06123200	-0.65233600	-4.61006900	B	-1.06330900	1.80477300	-2.13542800
H	-4.52784400	-1.40485300	-5.19576200	F	-0.20300800	1.61162100	-3.20718900
H	-6.13605700	-0.85219300	-4.70748500	F	-0.44369200	2.64141400	-1.15569400
H	-4.86022000	0.32086500	-5.07597700	F	-2.26178300	2.41583500	-2.54620000
H	0.26908700	0.57201600	1.50633700	F	-1.35827700	0.56515000	-1.50599600
O	1.82136800	0.86489300	-2.71294800	O	-1.56561000	3.65338700	1.30355400
C	2.53764900	1.60466900	-3.68832700	C	-0.97088400	4.95289900	1.03119900
H	3.61824200	1.55585200	-3.50607100	H	-0.07739300	4.77171200	0.42156800
H	2.30658200	1.12682100	-4.64164000	H	-0.66726000	5.40255300	1.98463800
H	2.21337700	2.65368700	-3.70879900	C	-2.02195300	5.74309200	0.32291100
C				C	-2.68890400	6.79372000	0.95485200
C				C	-2.38714800	5.37617300	-0.97772100
C				C	-3.71123000	5.74637300	0.29647900
C				C	-2.40909100	7.07526300	1.97111800
C				C	-3.41602300	6.04887700	-1.62923900
C				H	-1.87231400	4.54781600	-1.46511600
H				C	-0.47880500	7.10058200	-0.99386300
H				H	-4.22565100	8.29680300	0.79487200
H				H	-3.69742300	5.74908900	-2.63776000
N				H	-4.88214700	7.62857600	-1.50595800
C				H	4.14486800	2.67825700	4.47779600
O				H	2.65102900	2.24266800	-1.94408600
C				H	1.79305400	-3.59367200	5.16192100
O				H	0.67617900	-4.24259600	-1.31772700
C				C	-3.36465200	1.84485400	0.30213400
H				H	-2.82951000	2.62489400	-0.25181500
H				C	-4.26309900	2.54023900	1.36103800
H				H	-3.66269900	3.06322600	2.10802800
C				H	-4.90447000	3.27594300	0.86351200
C				H	-4.90451500	1.80623700	1.86324800
N				C	3.38971900	-3.78700800	1.80851500
N							

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C

3.38971900 -3.78700800 1.80851500

S60

C	4.27974000	-3.06535200	1.02184300	F	2.63210800	-0.03492100	-3.79875700
C	4.05260200	-1.71366900	0.78892500	F	1.62957900	0.77634700	-1.88614100
C	2.83520900	-1.06762200	1.23727000	F	3.92319600	0.60505100	-2.00749000
C	1.93406100	-1.85791300	2.00745400	H	3.61905300	3.95694200	4.4612500
C	2.21208900	-3.17593600	2.29002800	H	2.18497300	5.93881100	-1.48977500
H	3.57916900	-4.83892800	2.01132600	H	8.77447500	0.22855900	2.16396700
H	5.17459100	-3.54215100	0.62871500	C	5.67996000	2.75614300	-3.20837200
H	1.01446100	-1.40520900	2.36192600	H	5.40877900	1.75335400	-3.55157400
H	1.51417500	-3.75652600	2.88987000	H	5.09503400	2.93960500	-2.30389800
C	4.85414400	-2.13592600	3.89219600	H	5.35799500	3.48074800	-3.96784800
H	3.83417600	-1.91946000	3.61101800	H	7.67164100	2.56839600	-3.88801800
H	5.22556000	-1.80923000	4.86008500	O	4.86177800	-0.92529700	0.07021000
H	5.54183400	-2.57553800	3.18403900	C	5.83638000	-1.52782300	-0.77423400
N	2.68490300	0.21394100	0.88040600	H	5.35687000	-2.27225400	-1.41925300
C	1.47382300	0.89548800	0.88457600	H	6.23866300	-0.71340400	-1.38032100
O	1.41455600	2.11155600	0.94873400	H	6.63993700	-1.98348000	-0.17912800
O	0.40614500	0.09544700	0.71501500				
C	-0.80141200	0.76195900	0.29763400				
H	-0.51585400	1.52810100	-0.43451900				
H	-1.25270000	1.72726600	1.15896200	C	-4.37571000	1.21902300	-0.37896900
C	-1.71176500	-0.27026900	-0.28662800	C	-4.60857000	-0.23670400	-0.48672800
C	-1.21385900	-1.22067400	-1.18607000	C	-3.72209700	-1.03682400	0.39407700
C	-3.07013300	-0.27643700	0.03474000	C	-2.44701500	0.95553700	1.06987500
C	-2.07138600	-2.16062100	-1.74917100	C	-3.38747500	1.77405500	0.34849100
H	-0.15340900	-1.21575400	-1.43581600	H	-5.00346100	1.86768300	-0.99027900
C	-3.92936000	-1.21321300	-0.53716300	H	-3.23540100	2.84366900	0.32184300
H	-3.45824000	0.45787900	0.74227000	N	-1.33958000	1.34259700	1.68093900
C	-3.42973200	-2.15923500	-1.42901700	C	-0.84586700	2.65181200	1.75848300
H	-1.67634100	-2.89614800	-2.44821700	O	0.32434700	2.82609300	2.05681000
H	-4.98720800	-1.20860400	-0.27818800	C	-2.71481500	-0.48585500	1.10376700
H	-4.09737000	-2.89601000	-1.87364800	O	-1.84823700	-1.17712900	1.89537700
C	7.07370200	4.23283900	0.41273500	C	-2.05238600	-2.57303900	2.00828500
C	5.26445900	2.85307000	0.29042200	H	-1.96439000	-3.06811700	1.03127100
C	6.00914600	4.91616000	0.89215600	H	-1.26235400	-2.93982900	2.66811600
N	6.61514400	2.97366400	0.04605200	H	-3.03851600	-2.78768900	2.44396700
N	4.91657500	4.06593300	0.81990300	C	4.19602600	-0.76669800	1.11527700
Cu	4.06195600	1.35254200	0.00000800	C	1.98302100	-0.61066400	1.59850700
H	5.91808400	5.92252800	1.27714100	C	3.71556600	-2.02942600	1.21316200
H	8.11016300	4.51572900	0.29061300	N	3.13866100	0.09242100	1.36574400
C	7.47409000	1.94148200	-0.51659200	N	2.35923800	-1.92704700	1.49845500
C	8.12121600	1.02861100	0.35221200	Cu	0.27603800	0.21920700	1.78944700
C	7.69807800	1.90428600	-1.91464400	H	4.20109600	-2.99030400	1.11038500
C	8.92641100	0.03733900	-0.22137500	H	5.19170700	-0.39724700	0.91139800
C	8.50918200	0.87685400	-2.41577300	C	3.22029900	1.54689400	1.24336000
C	9.11057200	-0.05945700	-1.59105300	C	3.01585200	2.13610500	-0.02332000
H	9.42089800	-0.67145000	0.44346100	C	3.51199100	2.33205300	2.38088400
H	8.67011400	0.83115500	-3.49244500	C	3.03621500	3.53375300	-0.10095300
H	9.73622500	-0.84541300	-2.01157200	C	3.53726500	3.72074200	2.22515800
C	3.59371000	4.47458800	1.26375000	C	3.28432000	4.32704600	1.00537600
C	3.24108000	4.31584400	2.62067600	H	2.84724600	3.99308300	-1.07098700
C	2.71760500	5.07798100	0.33755300	H	3.74874200	4.33218200	3.10242500
C	1.99323100	4.80067300	3.02689000	H	3.28665500	5.41264900	0.91712000
C	1.48393100	5.53456900	0.81245100	C	1.54776800	-3.10337700	1.77500800
C	1.11777600	5.40715800	2.14183300	C	1.01042600	-3.85685000	0.70252400
H	1.70983900	4.67767100	4.07283800	C	1.39183900	-3.53060700	3.11372000
H	0.79609800	5.98972200	0.09968100	C	0.33796700	-5.04550500	1.01228300
H	0.15204100	5.77394700	2.48604900	C	0.70427700	-4.72868600	3.34877900
C	8.07010440	1.02376100	1.87351200	C	0.18612600	-5.49175300	2.31583000
C	8.62528000	2.29337900	2.51882200	H	-0.07893300	-5.62655800	0.18958400
C	6.71559700	0.60344600	2.43331300	H	0.58407500	-5.05713200	4.38155500
H	9.62257700	2.52904400	2.12565700	H	-0.33380600	-6.42567800	2.52415600
H	7.98980700	3.16905600	2.36548200	C	2.86533800	1.42184500	-1.35538600
H	8.71811900	2.14873900	3.60269900	C	4.23221400	1.01211700	-1.91015700
H	6.46020500	-0.41926000	2.12676900	C	1.89364400	0.26212500	-1.39921800
H	6.72124800	0.63527000	3.53127900	H	4.93738000	1.85248100	-1.92847400
H	5.90110300	1.24482900	2.08533500	H	4.68178400	0.20689800	-1.31239800
C	7.17665500	2.88388700	-2.95731300	H	4.12636400	0.63400000	-2.93488100
C	7.61787700	4.33198500	-2.74382000	H	0.94055400	0.51530200	-0.92401800
H	7.41955700	4.91045000	-3.65481300	H	1.66707200	0.00461500	-2.44046600
H	7.08074700	4.82832200	-1.93111600	H	2.30202200	-0.63061000	-0.91806600
H	8.69331300	4.40083800	-2.53270500	C	3.79209000	1.82534900	3.78505100
C	4.01496100	3.56706700	3.69543800	C	2.53125100	1.30224200	4.46806300
C	3.65485700	2.08032100	3.64274300	C	4.99310900	0.88712600	3.89243000
C	5.52294800	3.76477400	3.75529700	H	1.77383800	2.09217800	4.53197000
H	2.57376900	1.92997200	3.75179900	H	2.07764300	0.47567700	3.91439400
H	3.93932000	1.64276300	2.67803100	H	2.75354700	0.94847400	5.48431300
H	4.16904100	1.52366100	4.43851900	H	5.88290400	1.34443900	3.44090800
H	5.80605000	4.82429300	3.72261600	H	5.22062600	0.68509100	4.94728500
H	5.91254700	3.34397900	4.69181300	H	4.83697000	-0.07988300	3.40773000
H	6.03875900	3.25216500	2.94081800	C	1.00330800	-3.46633100	-0.76656900
C	2.91899800	5.18509500	-1.16472800	C	0.05022100	-2.29175400	-1.00326400
C	4.27233500	5.68620600	-1.65442700	C	2.37350000	-3.31642600	-1.42602400
C	2.51568900	3.86604200	-1.82541900	H	-0.99292000	-2.60531100	-0.86232700
H	4.59105200	6.59455100	-1.12634100	H	0.22480000	-1.45703900	-0.31494100
H	5.06157900	4.93890200	-1.54816800	H	0.13427000	-1.89382200	-2.02038600
H	4.21016200	5.92524300	-2.72396100	H	2.98733900	-4.21056200	-1.25389300
H	1.48834300	3.58481400	-1.57130600	H	2.24440600	-3.20400300	-2.50937300
H	2.60295700	3.92066000	-2.91841100	H	2.94175800	-2.44977300	-1.08318700
H	3.15048300	3.03702300	-1.48808300	C	1.80949900	-2.78047700	4.36751600
B	2.65465000	-0.01521900	-2.42155700	C	3.20195500	-2.16773700	4.37770300
F	2.61869900	-1.29983700	-1.86942400	C	0.71883400	-1.77400300	4.74686700

H	3.96615500	-2.88991600	4.06390600	H	2.19381700	-0.95867600	-2.79584500	
H	3.28181700	-1.29176700	3.73349900	H	2.67808700	-1.38475400	-4.44589800	
H	3.45194400	-1.83651900	5.39364500	H	4.90006000	-3.77633000	-2.64899000	
H	-0.23672500	-2.28243100	4.92958000	H	4.74692300	-2.76409500	-4.09595100	
H	0.98971500	-1.22045500	5.65479500	H	4.77101300	-2.01313300	-2.50597200	
H	0.54909700	-1.04211600	3.94335800	C	3.17968800	1.70190500	2.60348800	
B	-1.14341200	1.81794700	-2.03347700	C	1.68189100	1.44037200	2.78604200	
F	-0.23215100	1.79173700	-3.08327100	C	4.00741300	0.45844000	2.89975500	
F	-0.60248400	2.56750800	-0.94502900	H	1.11340300	2.37816900	2.76347500	
F	-2.35833900	2.40160100	-2.43028300	H	1.28639400	0.81178400	1.97617800	
F	-1.39044200	0.49386000	-1.56864400	H	1.48557000	0.93641200	3.74201100	
O	-1.72008800	3.63591900	1.54944900	H	5.07619100	0.62024700	2.71116400	
C	-1.13596400	4.95163800	1.35687400	H	3.89294800	0.18459800	3.95693300	
H	-0.18303700	4.80769200	0.83352300	H	3.68983900	-0.40613700	2.31350900	
H	-0.92881700	5.38906300	2.34152400	C	3.54665600	2.07513400	-2.59815900	
C	-2.10748300	5.76473300	0.56403600	C	4.47087100	0.91267900	-2.94165300	
C	-2.59214300	6.97955400	1.05077000	C	2.09673400	1.80518900	-3.00893800	
C	-2.52604600	5.31017400	-0.69293300	H	5.49492400	1.08569500	-2.58570400	
C	-3.48110800	7.74046400	0.29211100	H	4.12605100	-0.03822800	-2.52980500	
H	-2.27090400	7.33308400	2.03174000	H	4.51199500	0.78621200	-4.03105300	
C	-3.42445100	6.06286000	-1.44185900	H	1.48099600	2.70496200	-2.89873900	
H	-2.14344000	4.36611100	-1.08187900	H	2.03730100	1.46086800	-4.04921500	
C	-3.90173400	7.28062800	-0.95352900	H	1.63582600	1.03250600	-2.37936000	
H	-3.85094000	8.68883200	0.67937300	B	-1.33694400	-1.59769900	-2.91771300	
H	-3.74328300	5.69702700	-2.41704600	F	-1.34505600	-1.40454900	-4.28050700	
H	-4.59967600	7.87151400	-1.54536100	F	-0.52823700	-0.57272900	-2.29182600	
H	4.08398900	2.72502900	4.34763100	F	-2.63409800	-1.50371700	-2.36438000	
H	2.45751600	2.18275400	-2.03486300	F	-0.78529300	-2.84240700	-2.56927500	
H	1.81212500	-3.54439600	5.16000700	O	-1.58221900	2.98301300	0.84280200	
H	0.54997300	-4.33131000	-1.27432000	C	-1.21308300	4.34601500	1.05619600	
C	-4.47783800	-0.68420400	-1.95994800	H	-0.88583300	4.77894500	0.09979600	
H	-5.18341500	-0.13240300	-2.59089100	H	-0.33819800	4.38665900	1.72199500	
H	-3.46317800	-0.48741600	-2.31873800	C	-2.37837000	5.09143900	1.63296300	
H	-4.69508500	-1.75452300	-2.05428800	C	-2.15853700	6.35505500	2.19108600	
H	-5.65704700	-0.43411300	-0.19300600	C	-3.67929900	4.58277800	1.60826600	
H	-3.88326500	-2.11318400	0.40669100	C	-3.21434800	7.09838200	2.70896400	
<b>TS4-5*</b>								
C	-4.56886500	0.65927400	-0.78730400	H	4.73684500	5.32573400	2.13136600	
C	-4.88881500	-0.62823500	-0.46545300	C	-3.85922500	3.59698500	1.18266400	
C	-3.85618400	-1.44118200	0.11511300	C	-4.51024700	6.58445200	2.68185400	
C	-2.47028700	-0.95050600	0.19365700	H	-3.02460800	8.08011900	3.14021700	
C	-2.21900100	0.46805500	-0.06717200	H	-5.74581100	4.91586200	2.10613600	
C	-3.28311400	1.21318200	-0.55931100	C	-5.33797000	7.16233300	3.08970400	
H	-5.31835100	1.29916500	-1.25290300	C	-1.38264400	-1.91484300	0.45133200	
H	-5.86178600	-1.06128000	-0.67390400	H	-0.60645500	-1.47254800	1.08564300	
H	-3.97572800	-2.52232900	0.08469800	H	-1.76993600	-2.82525900	0.92042600	
H	-3.11139500	2.25046800	-0.82971700	O	-3.50615300	-1.15666600	1.67305900	
N	-0.94038200	0.89216100	0.13761800	C	-4.08417500	-0.00935500	2.28712600	
C	-0.61465900	2.21357000	0.26241800	H	-5.11040700	0.14546400	1.93593600	
O	0.48609700	2.66784700	-0.02545700	H	-4.07295800	-0.24288700	3.35532900	
C	4.59458900	-1.60620500	-0.14300000	H	-3.49135500	0.89347600	2.09483600	
C	2.59736000	-0.51914100	-0.26367000	H	3.46420400	2.44117200	3.36838300	
C	4.84842200	-0.28180500	-0.02977900	H	3.89228300	2.92361300	-3.20905300	
N	3.22084500	-1.74571300	-0.28076300	H	1.99688400	-4.21268100	2.74188900	
N	3.62646300	0.37054800	-0.09746100	H	2.65302800	-3.80729900	-3.76218400	
Cu	0.73759000	-0.04791200	-0.42840300	<b>5'</b>				
H	5.77523900	0.26223900	0.09142900	C	3.45558200	-4.03416500	-0.70943600	
H	5.25316800	-2.46304100	-0.14274400	C	4.52791600	-3.05841500	-0.82571300	
C	2.52159900	-3.01400800	-0.43075900	C	4.49277900	-1.84730300	-0.02133500	
C	2.05975600	-3.69254300	0.72383200	C	3.22530900	-1.39510000	0.45166100	
C	2.31596700	-3.54445600	-1.72515500	C	2.20099900	-2.37084800	0.50801500	
C	1.28093400	-4.83911400	0.53450100	C	2.31340500	-3.64417100	-0.06497800	
C	1.53101400	-4.69786700	-1.83481400	H	3.52796400	-4.97336200	-1.25095000	
C	0.98686200	-5.32670900	-0.72937200	H	1.26870300	-2.11256200	0.99356300	
H	0.90843900	-5.35941900	1.41783800	H	1.46042500	-4.31796000	-0.00744100	
H	1.32935100	-5.08565800	-2.83220500	H	3.13695800	-0.09027600	0.85437700	
H	0.35868800	-6.20769700	-0.85008600	N	1.96765600	0.60253800	0.99726100	
C	3.51874400	1.81470800	0.00469500	C	1.97125100	1.83483300	1.05682200	
C	3.41232500	2.41049700	1.27881100	O	0.81422500	-0.09807600	1.06637200	
C	3.58063600	2.59230700	-1.16975100	O	-0.37564600	0.70617700	0.92100900	
C	3.40098300	3.80774500	1.34467600	C	-0.28390300	1.26585200	-0.01974900	
C	3.56339600	3.98397000	-1.03185200	H	-0.42114800	1.43612000	1.73843500	
C	3.48153100	4.59616300	0.20841200	H	-1.55218500	-0.21553700	0.92654200	
H	3.31219700	4.27585400	2.32594800	C	-1.68442100	-1.20996400	-0.05076100	
H	3.60418200	4.59092200	-1.93656300	C	-2.53888200	-0.08977700	1.90546500	
H	3.47498400	5.68232100	0.28855500	C	-2.78557000	-2.06095600	-0.03915100	
C	2.36102700	-3.34224800	2.17564900	C	-0.91629600	-1.30685700	-0.81938200	
C	3.84828200	-3.24586400	2.51251900	H	-3.64637200	-0.93591500	1.91344100	
C	1.56662200	-2.14531400	2.68955500	C	-2.43504600	0.68034200	2.67065900	
H	4.40141900	-4.10814700	2.11862300	H	-3.76985500	-1.92523000	0.94158700	
H	4.31836500	-2.33878500	2.12389900	C	-2.88305800	-2.82940100	-0.80482600	
H	3.98004400	-3.23299700	3.60206300	H	-4.41010300	-0.82454700	2.68169900	
H	0.49370000	-2.37088500	2.71599900	H	-4.63282600	-2.58951700	0.94433400	
H	1.87631100	-1.87669100	3.70851400	H	7.06255200	4.59556400	0.49773000	
H	1.70096900	-1.26310100	2.05530800	C	5.39992200	3.04200300	0.52878300	
C	2.88508300	-3.01545700	-3.03453600	C	5.89198900	5.25596100	0.66415700	
C	2.18298800	-1.75980600	-3.53993500	C	6.75703700	3.24319400	0.41505800	
C	4.40797700	-2.88400000	-3.05913600	N	4.88839600	4.30113600	0.68875400	

Cu	4.34747700	1.45547400	0.53793300	O	2.04289400	1.74986100	1.16289900
H	5.67402200	6.30995900	0.76921600	O	1.67149500	0.32195500	2.87134300
H	8.08055800	4.95267600	0.42338500	C	0.64554600	1.23610200	3.30883700
C	7.74576000	2.18896400	0.23154900	H	1.08040100	2.23912800	3.40563800
C	8.31362600	1.55965300	1.36608800	H	0.39534800	0.86648900	4.30969400
C	8.14226400	1.82441800	-1.07768700	C	-0.55325000	1.25954400	2.40353300
C	9.22205800	0.51624900	1.15122100	C	-1.36804400	2.39473500	2.38240800
C	9.06027400	0.77519900	-1.21432200	C	-0.88239100	0.17298000	1.59064000
C	9.58914100	0.11006700	-0.12128100	C	-2.50319900	2.43674000	1.57669300
H	9.65318400	0.02298600	2.02244600	H	-1.10104400	3.25936800	2.99244900
H	9.35659900	0.48321000	-2.22161100	C	-2.00970900	0.21896600	0.77479200
H	10.29643000	-0.70635300	-0.25888500	H	-0.23477400	-0.70227300	1.55656600
C	3.48347700	4.63617700	0.85691800	C	-2.82838300	1.34628600	0.77104100
C	2.95620700	4.75916800	2.15982300	H	-3.12732200	3.32980100	1.56785600
C	2.68789200	4.85946100	-0.28595500	H	-2.23420100	-0.62608700	0.12616400
C	1.61739300	5.14601300	2.28564800	H	-3.70774200	1.38205200	0.12979500
C	1.35540100	5.23748400	-0.08596200	C	4.26784500	3.46588700	-3.71507600
C	0.81739600	5.38810700	1.18122100	C	3.73749800	2.29775000	-1.83767500
H	1.20112200	5.23876600	3.28941200	C	3.62248400	4.31400000	-2.87857600
H	0.73247500	5.40482200	-0.96502300	N	4.35069800	2.24428000	-3.06425200
H	-0.220203400	5.68804700	1.30737700	N	3.29606200	3.59502200	-1.73728100
C	8.06514600	1.90898000	2.82646000	Cu	3.38416400	0.83338800	-0.59232100
C	8.44393700	3.34156900	3.19936600	H	3.36768600	5.36039700	-2.97807500
C	6.67743900	1.50720300	3.31384400	H	4.69696000	3.61906500	-4.69535100
H	9.47350400	3.56684800	2.89336400	C	4.89173400	1.02477300	-3.64926900
H	7.79065700	4.09277600	2.74828600	C	6.24576800	0.68030500	-3.42972100
H	8.38168600	3.47191400	4.28726600	C	4.04347700	0.20248500	-4.42163100
H	6.51765300	0.42725600	3.19848200	C	6.68259400	-0.56561400	-3.89228100
H	6.55338600	1.75291100	4.37687900	C	4.54820500	-1.02774700	-4.85742500
H	5.88219100	2.01134300	2.75952400	C	5.84164200	-1.43131400	-4.57478200
C	7.65901600	2.43528500	-2.38432600	H	7.72022900	-0.84663500	-3.70921200
C	7.89902500	3.93648400	-2.53228100	H	3.88382600	-1.68317800	-5.41953200
H	7.70208800	4.23625000	-3.56930200	H	6.20081200	-2.40463400	-4.90515500
H	7.25329500	4.54760300	-1.89838400	C	2.69113900	4.23642300	-0.57282500
H	8.94085400	4.19634400	-2.30234800	C	3.52675700	4.68319500	0.47374500
C	3.63714600	4.38991100	3.46928300	C	1.29399700	4.45302200	-0.53224500
C	3.39710800	2.90523700	3.75887500	C	2.93141900	5.34325800	1.55595000
C	5.10206100	4.76070100	3.65014400	C	0.76860500	5.12308700	0.57763900
H	2.32576800	2.68054000	3.80848800	C	1.56755100	5.56867100	1.61798900
H	3.80734900	2.27347900	2.95950600	H	3.57665900	5.68281100	2.36695600
H	3.86463500	2.61266800	4.70868300	H	-0.30957100	5.27852200	0.61697600
H	5.29966400	5.81123000	3.40238800	H	1.12943700	6.08849200	2.46929000
H	5.39099200	4.60508900	4.69811600	C	7.31101900	1.54504500	-2.77259400
H	5.76692300	4.14125800	3.04506400	C	7.47109200	2.93644700	-3.38339200
C	3.07871200	4.62309600	-1.73543500	C	7.19482500	1.55960500	-1.25106000
C	4.46597600	5.07136500	-2.17271200	H	7.55568600	2.87743700	-4.47614000
C	2.81685700	3.16034700	-2.10176700	H	6.64854100	3.61588800	-3.14773700
H	4.69511000	6.09637200	-1.85203900	H	8.38897900	3.40240500	-3.00263000
H	5.25058300	4.41347100	-1.79410100	H	7.43037700	0.57267400	-0.83688300
H	4.53219200	5.04002200	-3.26783300	H	7.88700100	2.28622800	-0.80539400
H	1.76802400	2.88546100	-1.94027700	H	6.18182300	1.81285500	-0.92324400
H	3.06513600	2.95891500	-3.15102200	C	2.65304200	0.54732900	-4.92839700
H	3.41574700	2.47378400	-1.48833300	C	2.74297300	1.43474400	-6.17306400
B	2.78346200	-0.40883900	-2.72608200	H	1.75115100	1.55396700	-6.62735800
F	3.09225600	-1.81255000	-2.95766600	H	3.10487000	2.44021000	-5.91870700
F	2.57369900	0.21732100	-3.93446800	H	3.41682200	1.01493200	-6.92999100
F	1.66764700	-0.33439600	-1.88886600	C	5.02439800	4.46545600	0.61464400
F	3.91509500	0.13149400	-2.06223200	C	5.29424100	3.11492800	1.28178200
H	3.08621600	4.95312500	4.23881100	C	5.87247400	4.68782500	-0.63005800
H	2.36674200	5.22851600	-2.31797300	H	4.80756300	3.05707500	2.26317000
H	8.77229400	1.27334100	3.38059600	H	4.89259400	2.28740800	0.68229600
C	6.23434200	1.99916700	-2.71283900	H	6.37101800	2.94843900	1.41901000
H	6.17409600	0.91370800	-2.84550900	H	5.63219200	5.64034900	-1.11978100
H	5.52323700	2.24917700	-1.91965500	H	6.93492000	4.71244400	-0.35514400
H	5.87656400	2.46663100	-3.63937000	H	5.75776100	3.89257400	-1.36826400
H	8.30085900	1.97296500	-3.14954000	C	0.26509400	3.92622300	-1.51665500
C	5.72367500	-1.04300300	0.11889100	C	0.39708400	4.41067600	-2.95840500
H	6.62137300	-1.63905100	-0.05593200	C	0.14897200	2.41244300	-1.36637600
H	5.72220000	-0.20212300	-0.59613100	H	0.45818200	5.50639400	-3.00398000
H	5.76670300	-0.58928700	1.11833200	H	1.26752700	4.00633500	-3.48024900
O	5.81168400	-3.48903200	-1.16146300	H	-0.48759500	4.10282400	-3.53015800
C	5.88247500	-4.24897700	-2.35519000	H	-0.18801300	2.15344900	-0.35684200
H	5.36141800	-3.74450400	-3.18152100	H	-0.55895700	1.98587400	-2.08913600
H	6.94437700	-4.33788600	-2.59418500	H	1.11071600	1.91252000	-1.50337900
H	5.46752800	-5.25909800	-2.22578400	B	1.97986000	-1.64056100	-1.49657500
H	4.05002800	-2.49347900	-1.73850700	F	1.92000300	-2.73366200	-0.64570900
				F	1.52537800	-1.92521400	-2.76788800
				F	1.27064300	-0.54450700	-0.92848200
				F	3.36170300	-1.18749100	-1.57766100
				F	5.34777600	5.23363200	1.33400700
				H	-0.69107800	4.34430300	-1.16448600
				H	8.25577600	1.02808300	-3.00011100
				C	1.67457000	1.12050200	-3.92313500
				H	1.66590300	0.54121900	-2.99742800
				H	1.89118300	2.16510100	-3.68325700
				H	0.65725600	1.09250200	-4.33525300
				H	2.23049300	-0.41549700	-5.24886700
				C	5.73765900	-1.13616300	0.38579900
				H	5.46649300	-0.80137100	-0.62398800
				H	5.87713800	-0.24085500	1.00397200
				H	6.68982500	-1.67376700	0.31021200

O	4.67023500	-1.43541100	3.46355400	C	-2.86876900	6.63454500	1.30119400
C	5.35701900	-2.49883500	3.91844400	C	-2.34790800	5.38832800	-0.70210400
H	4.81882500	-3.46440400	3.71786300	C	-3.78693300	7.40295800	0.58676200
H	6.37195500	-2.61618800	3.47790300	H	-2.71695000	6.81310300	2.36671800
H	5.43265800	-2.47164600	5.02594700	C	-3.27223300	6.14803500	-1.41217000
<b>12'</b>							
C	-4.43150300	0.97104200	-0.62805400	H	-4.34651300	8.18955400	1.09097900
C	-4.52974000	-0.36621400	-0.71051500	H	-3.43190700	5.94528400	-2.47017800
C	-3.74342800	-1.19254900	0.16287600	H	-4.71434200	7.75191000	-1.32709300
C	-2.52011400	0.70128800	1.01988400	H	4.15226100	2.81041800	4.24131000
C	-3.52233700	1.62755500	0.35667100	H	2.41436000	2.12285200	-2.10211400
H	-5.03900300	1.62857800	-1.24704000	H	1.80036900	-3.41046900	5.20367900
H	-2.97040200	2.43091200	-0.15441400	H	0.61464200	-4.41193300	-1.19889600
N	-1.45808200	1.12502300	1.67635500	H	-5.21616300	-0.84129800	-1.40851100
C	-1.00200400	2.44869600	1.80617700	C	-2.01582400	-1.64606800	1.89904200
O	0.16447700	2.61001100	2.20793900	H	-0.98890400	-1.83104200	1.54518600
C	-2.77600500	-0.71898100	1.00474100	H	-1.92980300	-1.24491000	2.91695700
C	4.22859200	-0.75140000	1.08875600	H	-2.51192000	-2.62223500	1.95323400
C	2.02123500	-0.58845600	1.58084300	H	-3.92690800	-2.26888600	0.15156300
C	3.74911200	-2.01272900	1.21733600	O	-4.28684000	2.17750500	1.44176700
N	3.17227500	0.11252300	1.32803400	C	-4.99848400	3.34273300	1.07574500
N	2.39518000	-1.90511900	1.50730300	H	-5.33562900	3.80318800	2.00886200
Cu	0.31084600	0.23485400	1.78102000	H	-4.35281200	4.04936100	0.53449300
H	4.23564800	-2.97473200	1.13154600	H	-5.87901500	3.11074600	0.45686000
H	5.22333900	-0.38682600	0.87176900				
C	3.23610000	1.56509500	1.17818900				
C	2.99778800	2.12857500	-0.09457200				
C	3.53225000	2.37517700	2.29754100				
C	2.98086900	3.52492700	-0.19404600				
C	3.52141200	3.76162600	2.11924500				
C	3.22907800	4.34176400	0.89509200				
H	2.75943300	3.96318800	-1.16685700				
H	3.73682100	4.39193200	2.98205000				
H	3.20269700	5.42549800	0.78984300				
C	1.55932400	-0.305715700	1.81405800				
C	1.01470000	-3.83591600	0.76317200				
C	1.34712200	-3.41122900	3.16612600				
C	0.26228400	-4.96455600	1.10990500				
C	0.572229600	-4.54653400	3.43680700				
C	0.030404900	-5.32570600	2.42814300				
H	-0.16404500	-5.56143200	0.30380600				
H	0.40284000	-4.81431900	4.48009100				
H	-0.55652700	-6.20881400	2.66632400				
C	2.84975200	1.38731900	-1.41204500				
C	4.22224100	1.00044000	-1.96903300				
C	1.90618300	0.20377700	-1.42417400				
H	4.90525900	1.85797300	-2.01095900				
H	4.69686600	0.22072600	-1.35683200				
H	4.11896100	0.59738500	-2.98437000				
H	0.95330700	0.44635500	-0.94284900				
H	1.67373200	-0.07873800	-2.45753500				
H	2.33924400	-0.67071900	-0.93128800				
C	3.85020700	1.89861000	3.70424100				
C	2.60615700	1.38351600	4.42194500				
C	5.05327700	0.96262300	3.80574800				
H	1.84559000	2.16968900	4.49014000				
H	2.14681200	0.54846200	3.88650500				
H	2.84992000	1.04258100	5.43752900				
H	5.93116700	1.40256700	3.31526600				
H	5.30939500	0.79422200	4.85985200	Cu	4.12873600	1.39321500	-0.05781700
H	4.88117200	-0.01954700	3.35819900	H	5.90358400	5.97526100	1.40652300
C	1.04797500	-3.51890500	-0.72345100	H	8.11431500	4.55473900	0.48161300
C	0.07989300	-2.37158600	-1.02129900	C	7.43908400	1.97468100	-0.38800900
C	2.42425700	-3.37712100	-1.36884200	C	8.02430600	1.02612700	0.48456500
H	-0.95393900	-2.68178000	-0.82151400	C	7.64107200	1.91330400	-1.78730000
H	0.27266700	-1.49291500	-0.39648000	C	8.71248200	-0.04784000	-0.09201000
H	0.13549700	-2.04461100	-2.06599400	C	8.32554700	0.80051500	-2.29090800
H	3.05166440	-4.24991400	-1.14430800	C	8.83721300	-0.18718400	-1.46506100
H	2.30860400	-3.32259900	-2.45824800	H	9.15387200	-0.79119600	0.57218000
H	2.97255000	-2.48397200	-1.06436100	H	8.46194400	0.72803600	-3.36948300
C	1.80791500	-2.65564600	4.40246000	H	9.35847800	-1.04413700	-1.88885200
C	3.22006200	-2.08963400	4.38625400	C	3.56971100	4.56463300	1.30489700
C	0.75457900	-1.61534200	4.79327700	C	3.18252000	4.40517500	2.65178800
H	3.95529500	-2.84310700	4.07662200	C	2.73413400	5.20388100	0.36480900
H	3.32479800	-1.22758200	3.72675800	C	1.93599300	4.91547900	3.03201500
H	3.49279300	-1.75099000	5.39394100	C	1.50041100	5.68656900	0.81387600
H	-0.21022000	-2.09615500	4.98852600	C	1.09787400	5.55334500	2.13275900
H	1.05474500	-1.06590600	5.69449700	H	1.62610400	4.79269900	4.07031400
H	0.59636500	-0.88212800	3.98854300	H	0.84501800	6.17276300	0.09101600
B	-1.06813500	1.88317500	-1.96677000	H	0.13458800	5.94293700	2.45820700
F	-0.15036200	1.81093300	-3.00643900	C	8.01684100	1.05797200	2.00698300
F	-0.48348700	2.56885800	-0.85496500	C	8.59983700	2.33329300	2.61552000
F	-2.22816100	2.57382700	-2.36094300	C	6.67251800	0.67139800	2.62038700
F	-1.42657500	0.58442200	-1.52049700	H	9.55400800	2.60011200	2.14274800
O	-1.83440700	3.43548600	1.51355300	H	7.93159600	3.19487500	2.53650400
C	-1.20567400	4.75090500	1.42082400	H	8.78939100	2.17490200	3.68470800
H	-0.24654400	4.61405800	0.91004400	H	6.42368200	-0.38326100	2.44688800
H	-1.01674300	5.10955300	2.43968400	H	6.69210000	0.82415600	3.70819000
C	-2.14629900	5.62563700	0.66270900	H	5.84722300	1.27078900	2.22125700

C	7.24635700	2.95851100	-2.82374500	H	1.59017500	-0.18596700	-2.49990800
C	7.77277500	4.36602800	-2.54196000	H	2.28676500	-0.75731700	-0.97894300
H	7.69765700	4.97074100	-3.45421500	C	3.93936400	1.92051500	3.55542200
H	7.20121100	4.88913000	-1.76981800	C	2.70954500	1.44188500	4.32060400
H	8.82725600	4.35425700	-2.23616800	C	5.13529200	0.97524800	3.65304400
C	3.92091100	3.64361000	3.74116000	H	1.95565000	2.23551200	4.37404600
C	3.54648500	2.16154200	3.68574800	H	2.23250300	0.59070500	3.82798300
C	5.42925000	3.82354800	3.84195900	H	2.97481900	1.13737400	5.34232900
H	2.46226900	2.02222900	3.77478300	H	6.00778000	1.39727300	3.13787400
H	3.85130900	1.70741700	2.73415700	H	5.40939400	0.82522900	4.70543000
H	4.03719700	1.61107600	4.49835400	H	4.94639700	-0.01391200	3.22808400
H	5.72592600	4.87953000	3.82064700	C	0.86133700	-3.53779300	-0.60686400
H	5.78593100	3.39577200	4.78812000	C	-0.06656100	-2.35412800	-0.88755600
H	5.96205700	3.30426100	3.04255700	C	2.21505500	-3.47173000	-1.30973700
C	2.98507500	5.33128800	-1.12805200	H	-1.10251900	-2.61127200	-0.62985600
C	4.35409400	5.84300500	-1.56167500	H	0.19429000	-1.46817200	-0.29811500
C	2.59787900	4.02455500	-1.82070900	H	-0.04716300	-2.05520800	-1.94175500
H	4.64889100	6.74253000	-1.00574200	H	2.80921900	-4.37003700	-1.09549800
H	5.14366000	5.09805000	-1.44198300	H	2.05942200	-3.42737300	-2.39469600
H	4.32802900	6.10237700	-2.62768200	H	2.81726400	-2.60187500	-1.04166900
H	1.55507300	3.75947500	-1.61611500	C	1.86882300	-2.57716200	4.45450200
H	2.73294500	4.08878900	-2.90809600	C	3.28758400	-2.03525100	4.36772800
H	3.20248100	3.18061000	-1.46570000	C	0.84672300	-1.50912100	4.85397200
B	2.80764500	0.17958900	-2.53710800	H	3.99824000	-2.80917800	4.05121800
F	2.70961700	-1.13684000	-2.09195700	H	3.37991200	-1.19392100	3.68026500
F	2.78351700	0.29092300	-3.90467300	H	3.60496400	-1.67286100	5.35382800
F	1.83028000	0.97723200	-1.91874000	H	-0.11865700	-1.96849000	5.10041500
F	4.10539400	0.70047900	-2.06043900	H	1.18913600	-0.93761300	5.72592200
H	3.50623800	4.03664700	4.68247000	H	0.66747100	-0.79884700	4.03340300
H	2.26328200	6.09088800	-1.46621200	B	-1.16279600	1.84846200	-1.86982500
H	8.71811600	0.26007400	2.29350000	F	-0.19775500	1.89288600	-2.86950600
C	5.76163100	2.95904500	-3.13633200	F	-0.67661900	2.50827500	-0.70202800
H	5.43785000	1.99983600	-3.57619600	F	-2.35216200	2.46624300	-2.28881000
H	5.14426000	3.14284200	-2.28050600	F	-1.43761100	0.49556200	-1.51565400
H	5.54090500	3.74680100	-3.89615400	O	-1.83850600	3.47979500	1.86709700
H	7.76969500	2.63338000	-3.73538000	C	-1.27420700	4.81253900	1.70619200
C	5.27251000	-1.35490500	-0.03510800	H	-0.31459300	4.69424000	1.18943000
H	4.86935000	-1.23930600	-1.04932900	H	-1.08628900	5.22819900	2.70360800
H	5.58355600	-0.34769800	0.28713200	C	-2.25750900	5.62275400	0.92534600
H	6.16961100	-1.98057600	-0.08065400	C	-2.77069300	6.81639800	1.43461000
O	4.63633600	-1.88242000	3.51884000	C	-2.66115200	5.18398500	-0.34197100
C	4.48388600	-1.24564900	4.69739500	C	-3.67513400	7.57097200	0.68798700
H	4.86823500	-1.87565200	5.53197500	H	-2.46114300	7.15776400	2.42360600
H	5.10419400	-0.32229900	4.76494800	C	-3.57531900	5.92946200	-1.07848000
H	3.43267600	-0.96714800	4.94264600	H	-2.25524100	4.25820700	-0.74978200
				C	-4.08230400	7.12570500	-0.56742500
<b>8'</b>				H	-4.06772800	8.50286000	1.09231300
C	-4.30782700	1.17479800	-0.38821600	H	-3.88119800	5.57548500	-2.06226000
C	-4.28828900	-0.25768400	-0.77442700	H	-4.79328300	7.71126000	-1.14888800
C	-3.64978800	-1.11844900	0.24643300	H	4.26510200	2.84447500	4.05688400
C	-2.51899600	0.79854800	1.20267600	H	2.41493200	1.99773800	-2.23192300
C	-3.45592000	1.67023700	0.52639700	H	1.88029600	-3.30978300	5.27600400
H	-4.94786600	1.85033000	-0.95345400	H	0.36859700	-4.41953700	-1.04384800
N	-1.43831200	1.18008500	1.86680000	H	-3.60478500	-0.28792600	-1.65711400
C	-0.95882800	2.49304800	1.98604700	C	-2.08569000	-1.55919800	2.12209000
O	0.22977900	2.65478300	2.23642500	H	-1.03341200	-1.73657600	1.84502800
C	-2.77816700	-0.64509900	1.16129100	H	-2.07483800	-1.14734000	3.13858200
C	4.20194700	-0.82212300	1.01157300	H	-2.57773300	-2.53821700	2.14317500
C	2.01311300	-0.58928300	1.55433000	H	-3.86425600	-2.18546400	0.18138800
C	3.69590100	-2.06673400	1.19340400	H	-3.41525100	2.73556100	0.70671200
N	3.17318200	0.07517200	1.24907600	O	-5.54756900	-0.80042600	-1.13991500
N	2.35365800	-1.91624300	1.51634700	C	-6.00405100	-0.32958700	-2.38894000
Cu	0.32591000	0.26765100	1.79958500	H	-5.26057100	-0.51522500	-3.18061600
H	4.15713100	-3.04268600	1.12729800	H	-6.92120600	-0.87932500	-2.61376500
H	5.19897600	-0.49005100	0.75652900	H	-6.23365700	0.74691900	-2.37327700
C	3.26335600	1.52160700	1.05431800				
C	3.01052900	2.05231500	-0.23035300				
C	3.58942800	2.35934100	2.14415000	C	3.76182000	-4.09686500	0.24929600
C	2.99806200	3.44534500	-0.36745400	C	4.69498800	-3.26772300	0.75461400
C	3.57915400	3.74075000	1.92914300	C	4.41516500	-1.82943100	1.03432000
C	3.26328200	4.28964300	0.69682600	C	3.04029200	-1.34533900	0.54648100
H	2.76583700	3.85927800	-1.34826100	C	2.11047700	-2.28578600	0.01401000
H	3.81353400	4.39266000	2.77076500	C	2.46377900	-3.59580000	-0.11995000
H	3.23646700	5.37030100	0.56412600	H	3.98605100	-5.14939800	0.08315100
C	1.50090400	-3.03668800	1.89002500	H	5.69594400	-3.61728300	1.00953200
C	0.88377600	-3.82249800	0.88539600	H	1.15498000	-1.92995800	-0.35170500
C	1.34447300	-3.35532700	3.25840400	H	1.75165400	-4.28685300	-0.56882000
C	0.11899000	-4.92182400	1.29236900	C	4.47315900	-1.58154200	2.55648400
C	0.55804100	-4.46607200	3.59094800	H	5.43292200	-1.97639400	2.92274300
C	-0.05024500	-5.25112900	2.62752800	H	4.50747200	-0.48895000	2.68178400
H	-0.36287300	-5.52214700	0.52090800	N	2.88371300	-0.05400700	0.72328600
H	0.43358800	-4.70794800	4.64685800	C	1.70983800	0.68027700	0.55443500
H	-0.65020900	-6.11347300	2.91327500	O	1.77497100	1.88546300	0.38412500
C	2.83687800	1.27360600	-1.52242400	O	0.56588600	0.00342200	0.71262200
C	4.19251100	0.83408000	-2.08101900	C	-0.61622200	0.80141900	0.43697400
C	1.86182000	0.11599400	-1.48140300	H	-0.46340100	1.27485400	-0.54029400
H	4.89748000	1.67151000	-2.15355600	H	-0.68629200	1.59372800	1.19291200
H	4.65273100	0.05844600	-1.45347000	C	-1.79803200	-0.10922600	0.45623400
H	4.06750400	0.40670000	-3.08387300	C	-1.95950100	-1.07368300	-0.54518900
H	0.93164800	0.39476400	-0.97755800	C	-2.75590300	-0.00888800	1.46610800

				<b>TS<sub>4a-5a</sub></b>			
C	-3.05996700	-1.92491100	-0.52803700	C	-4.65268700	0.75892800	-0.09751300
H	-1.21543700	-1.14283200	-1.34048100	C	-4.79930200	-0.59889600	-0.28384600
C	-3.86360300	-0.85429800	1.48016100	C	-3.66480800	-1.40700600	-0.10718700
H	-2.63133900	0.74167700	2.24740300	C	-2.39337300	-0.82767500	0.19218000
C	-4.01485400	-1.81585500	0.48432500	C	-2.26615700	0.60290900	0.45904500
H	-3.18020800	-2.67093200	-1.31209100	C	-3.44089300	1.34477700	0.29285400
H	-4.60753400	-0.76288900	2.27009600	C	-5.50250000	1.41883000	-0.26708800
H	-4.87908900	-2.47830600	0.49184500	H	-5.73769800	-1.04622500	-0.59663000
C	7.05193900	4.44928300	0.48315700	H	-3.68244300	-2.44037900	-0.43728600
C	5.39211400	2.89094500	0.38643500	H	-3.40696200	2.41748800	0.41824500
C	5.89492700	5.06979700	0.81031500	N	-1.01427600	0.99455200	0.81763000
N	6.74043200	3.12058600	0.22589200	N	-1.23979000	-1.49134800	0.07533100
N	4.89097400	4.11602000	0.74489400	O	-1.26442800	-2.84422100	-0.38976400
Cu	4.34017800	1.27467900	0.23506500	C	-1.67264200	-2.87890700	-1.40465900
H	5.68388100	6.09683200	1.07496600	H	-0.22209000	-3.16257900	-0.38035400
H	8.06445700	4.82009000	0.40260000	C	-1.84017600	-3.47820300	0.29951200
C	7.71834100	2.12244700	-0.18107400	C	-3.26802500	-1.61390800	1.87323200
C	8.39193800	1.36639100	0.80752900	C	-3.82249700	-2.55510200	1.80929400
C	8.00664600	1.94968400	-1.55641400	H	-2.22929700	-1.83630800	2.13975600
C	9.28434300	0.37670200	0.37865600	H	-0.62007900	2.28216600	1.07342700
C	8.91416400	0.94303100	-1.190971300	C	0.53511200	2.55892900	1.38004700
C	9.53688900	0.14577800	-0.96364800	O	4.45521500	-1.54971000	-0.37958700
H	9.79372500	-0.21872500	1.13642100	C	2.48111300	-0.53003700	0.13149300
H	9.12630500	0.79319000	-2.96810900	C	4.73256000	-0.26113000	-0.07377200
H	10.23032900	-0.63600300	-1.26991000	C	3.08090400	-7.11105000	-0.25295200
C	3.50403200	4.43370900	1.04780100	N	3.52824100	0.34748900	0.23747500
C	3.03666600	4.29052500	2.37226200	Cu	0.65867100	-0.00681900	0.43150300
C	2.67127400	4.93363800	0.02291900	H	5.66537600	0.28537200	-0.04855400
C	1.71854900	4.67342800	2.64460200	H	5.09317300	-2.36889700	-0.68164400
C	1.36479600	5.29779600	0.36820300	C	2.42224800	-2.98242200	-0.52275800
C	0.88353700	5.17664100	1.66066400	C	2.24341400	-3.91188700	0.53256700
H	1.35107800	4.56205500	3.66551900	C	2.03681400	-3.30261500	-1.84824700
H	0.71289400	5.67353000	-0.42084400	C	1.63422500	-5.13697800	0.23363000
H	-0.13739400	5.47119400	1.89983000	C	1.43993300	-4.55105000	-2.07113900
C	8.26638700	1.51599200	2.31688400	C	1.22959100	-5.46355800	-1.05091500
C	8.61299600	2.90292100	2.85665600	C	1.48991200	-5.85067400	1.04478100
C	6.94817300	0.96570700	2.85130600	H	1.12880000	-4.79369200	-3.08669600
H	9.57282400	3.25420100	2.45625300	H	0.76041600	-6.42471400	-1.25565200
H	7.85852100	3.65999000	2.62943400	C	3.45287100	1.74957100	0.61533300
H	8.70395000	2.85999100	3.94960300	C	3.61395300	2.10327000	1.97109600
H	6.86144700	-0.10182800	2.62377000	C	3.27623200	2.72642400	-0.38688900
H	6.87779400	1.09884800	3.93995400	C	3.62756000	3.46431600	2.29149100
H	6.08076200	1.45212900	2.39297800	C	3.30063400	4.06962500	0.00492600
C	7.44125000	2.75035400	-2.72081500	C	3.48053900	4.44609300	1.32525200
C	7.73935800	4.24812000	-2.66458600	H	3.74147600	3.74527900	3.33910800
H	7.49697700	4.70579500	-3.63196400	H	3.15922000	4.83018400	-0.76365700
H	7.15218300	4.77596600	-1.90895700	H	3.49747900	5.49929900	1.60173600
H	8.80166800	4.43732700	-2.46101200	C	2.65410400	-3.73269900	1.98634700
C	3.773755300	3.66757700	3.54792300	C	4.16334700	-3.60892000	2.18910200
C	3.56694800	2.15064200	3.54364000	C	1.85218200	-2.65684900	2.71155700
C	5.24028200	4.02773000	3.73286300	H	4.68959900	-4.45077600	1.72168300
H	2.50128300	1.88795000	3.58037100	C	2.15958600	-2.41700300	-0.07751200
H	3.96940200	1.70359700	2.62399300	C	1.20734400	-1.22643700	-0.01678200
H	4.07214300	1.68415100	4.40071300	H	4.40143100	-3.61798500	3.26040400
H	5.41087500	5.10983400	3.67064200	H	0.77581600	-2.87077200	2.65800400
H	5.58209800	3.69162700	4.72077500	H	2.13554100	-2.61252400	3.77147300
H	5.88259700	3.54188100	2.99640000	H	2.00332700	-1.66267400	2.28463100
C	2.98432000	5.00576900	-1.46337800	C	2.15958600	-2.41700300	-0.07751200
C	4.35731700	5.51948300	-1.87334100	C	3.59526200	-2.06926700	-3.46866500
C	2.68379900	3.64888400	-2.10210500	H	0.16407300	-1.55421300	-2.95755800
H	4.62987300	6.44915300	-1.35667600	H	1.38369400	-0.58356000	-2.14981900
H	5.14325400	4.78408600	-1.68874700	H	1.28825200	-0.60284700	-3.91536700
H	4.36399300	5.72217200	-2.95206500	H	4.21009900	-2.97533700	-3.55435400
H	1.64365400	3.34374900	-1.94061600	H	3.59783200	-1.57086800	-4.44610000
H	2.88127700	3.65950100	-3.18117800	H	4.09127100	-1.39620500	-2.76588400
H	3.30186100	2.86106500	-1.65973600	C	3.63654300	1.16288800	3.16519100
B	2.74804300	-0.05670200	-2.66526700	C	2.19857700	0.86000700	3.59521200
F	3.08392900	-1.41644600	-2.69306300	C	4.46375600	-0.11019300	3.05661300
F	2.75327600	0.50956900	-3.92281400	C	1.65353000	1.78045500	3.83081600
F	1.50439300	0.10964400	-2.02465400	H	1.63948100	0.37128500	2.78489700
F	3.76035600	0.61323700	-1.86007900	H	2.18484800	0.20172100	4.47475300
H	3.25225600	4.05300100	4.43786500	H	5.47717600	0.08296300	2.68253900
H	2.25600800	5.72685900	-1.86654200	H	4.55619300	-0.57502600	4.04714600
H	9.04977800	0.85424100	2.71681300	H	4.00075500	-0.85170600	2.40232500
C	5.97545700	2.43920900	-2.99823300	H	2.93231700	2.48613300	-1.84710600
H	5.82357200	1.37975100	-3.23120600	C	3.68446800	1.38149400	-2.57458800
H	5.33187000	2.66134600	-2.14349600	C	1.41944500	2.30601500	-1.98639800
H	5.60901800	3.02531300	-3.85117200	C	1.06924600	1.42958500	-1.42467300
H	8.00129000	2.38220300	-3.59368700	H	-2.13996300	0.04836500	-3.06010400
O	5.45136800	-0.98424100	0.49964500	H	-1.58874100	-0.0070900	-4.33592000
C	5.83516400	-1.28713200	-0.85140300	H	0.87205800	3.17250500	-1.59384200
H	4.96333400	-1.46541300	-1.49081600	H	1.12121400	2.15235600	-3.03066200
H	6.36705700	-0.40032000	-1.21114700	H	1.06924600	1.42958500	-1.42467300
H	6.51556800	-2.14931900	-0.87638800	B	-1.58874100	-0.0070900	-4.33592000
C	3.31858200	-2.15564800	3.36272000	F	-1.18023900	0.55664300	-2.14311200
H	2.38053700	-1.66660700	3.05881600	F	-3.28940400	0.83650000	-3.01554000
H	3.19213400	-3.22523700	3.13492400	F	-2.47150900	-1.28322000	-2.62902100
C	3.53085200	-1.96587600	4.85475900	O	-1.57149700	3.24233400	0.95669600
H	2.68615300	-2.35120000	5.43666400				
H	4.43514000	-2.48472600	5.19854000				
H	3.64900500	-0.90335000	5.10536500				

C	-1.10417700	4.59293500	1.11648900	H	3.30181500	-1.98439800	-4.44666400
H	-0.15032100	4.69344100	0.58123200	H	3.83890300	-1.88414900	-2.77275100
H	-0.89579100	4.78043100	2.17835100	C	3.38251900	0.78867300	3.15238000
C	-2.15618100	5.51558300	0.58592800	C	1.92561900	0.52910000	3.54386700
C	-2.75977100	5.27588100	-0.65433800	C	4.18071200	-0.50497300	3.07570800
C	-2.52294300	6.65066300	1.31121600	H	1.39629500	1.46726700	3.74327200
C	-3.71379000	6.15822800	-1.15260900	H	1.37840300	0.03629900	2.72797500
H	-2.48466100	4.38813200	-1.22496500	H	1.86842100	-0.11004200	4.43561700
C	-3.47032800	7.54055100	0.80795100	H	5.21020600	-0.33804600	2.73371200
H	-2.06295200	6.83668500	2.28273300	H	4.22984500	-0.96792700	4.07018600
C	-4.06992400	7.29415300	-0.42448300	H	3.72104700	-1.23742900	2.40953400
H	-4.17948200	5.95860300	-2.11643200	C	2.88454000	2.09385900	-1.88836100
H	-3.74684100	8.42170400	1.38506700	C	3.60851000	0.95519500	-2.59243900
H	-4.81521700	7.98377100	-0.81777900	C	1.36841600	1.97593800	-2.05522700
H	4.09135400	1.75184100	3.97676800	H	4.69237400	0.97610200	-2.41807200
H	3.19455600	3.42642500	-2.35665900	H	3.23337100	-0.02326300	-2.28525100
H	2.37675200	-4.68366800	2.46580500	H	3.44130000	1.02865600	-3.67464600
H	1.79192700	-0.34750400	-3.90088900	H	0.85332500	2.87345300	-1.69080500
C	3.92197100	-0.61670200	2.77804300	H	1.08492000	1.81148900	-3.10189600
H	-3.24832600	0.22856200	2.96204800	H	0.96873300	1.13200400	-1.47805400
H	-4.82179500	-0.20462500	2.30306100	B	-2.37535200	-0.13865700	-2.91317800
C	-4.30396800	-1.28149500	4.09870500	F	-2.00363700	-0.40741600	-4.22257600
H	-4.75952900	-0.55175900	4.77683100	F	-1.29661200	0.41431500	-2.19171900
H	-5.02803700	-2.09163600	3.94745000	F	-3.47999200	0.71415100	-2.84261800
H	-3.43063200	-1.70595600	4.60890300	F	-2.71954600	-1.38891600	-2.26380400
O				O	-1.81270100	2.88985900	0.92330500
C				C	-1.36549500	4.24903900	1.04726100
<b>5a</b>				C	-0.43135700	4.35662800	0.47981500
C	-4.89126900	0.40415400	-0.14168000	H	-1.12773300	4.45904900	2.09881900
C	-5.09180300	-0.92967500	-0.09640100	C	-2.44546800	5.14929100	0.53488800
C	-3.97078300	-1.83262600	0.23944000	C	-3.05504200	4.90514200	-0.70180400
C	-2.64593500	-1.17232000	0.31528200	C	-2.83222000	6.27056700	1.27102500
C	-2.47599100	0.23327100	0.46737800	C	-4.03426400	5.76793600	-1.18508600
C	-3.61945600	0.97413000	0.14530800	H	-2.76021300	4.03172000	-1.28512300
H	-5.679796100	1.08044800	-0.41650600	C	-3.80465200	7.14178900	0.78296800
H	-6.06541100	-1.38088800	-0.27770700	H	-2.36686100	6.46063500	2.23916700
H	-3.92206400	-2.61800500	-0.52749300	C	-4.41008000	6.89017600	-0.44545800
H	-3.52550500	0.204960700	0.06806300	H	-4.50302800	5.56528500	-2.14688500
N	-1.20729400	0.65832200	0.77892600	H	-4.09520300	8.01291800	1.36838300
O	-1.55125300	-1.89945900	0.37500700	H	-5.17436700	7.56539200	-0.82736200
C	-1.52536500	-3.22505900	-0.18816100	H	3.82936100	1.37184700	3.97256800
H	-1.88043800	-3.16974100	-1.22209000	H	3.19652200	3.01828600	-2.39884600
H	-0.47529900	-3.51539200	-0.15508300	H	2.07916400	-5.04258900	2.48039200
H	-2.12245900	-3.92054500	0.40961500	H	1.42450200	-3.38944600	-3.87573600
C	-4.25188300	-2.53819900	1.61017700	C	-4.24418200	-1.61005400	2.81719800
H	-5.22967200	-3.01381800	1.51878700	H	-3.23217900	-1.20603500	2.96776500
H	-3.51668100	-3.34029900	1.76255700	H	-4.88859300	-0.74200700	2.61686900
C	-0.82816300	1.94817100	0.98320900	H	-4.70468400	-2.32035400	4.07769800
O	0.33838800	2.26091900	1.21763900	C	-4.68388600	-1.65198900	4.94523400
C	4.21257600	-1.97800200	-0.36949800	H	-5.73136900	-2.69458500	3.97380800
C	2.26646900	-0.89476100	0.11539600	H	-4.06470800	-3.18150800	4.31066000
N	2.83207300	-2.09669100	-0.25425400				
N	3.33871100	-0.04813200	0.22536200				
Cu	0.46939500	-0.30754100	0.41126300				
H	5.47584700	-0.17975600	-0.03683800				
H	4.82860400	-2.81844400	-0.65828700				
C	2.13777500	-3.355114800	-0.51379500				
C	1.96341300	-4.28172400	0.54192300				
C	1.71386000	-3.65748000	-1.83058800				
C	1.33694700	-5.49980000	0.24946100				
C	1.08896500	-4.89372100	-2.04478800				
C	0.89644000	-5.81263400	-1.02658200				
H	1.19947400	-6.21477300	1.06063500				
H	0.74947200	-5.12559600	-3.05384200				
H	0.41203800	-6.76728600	-1.22647900				
C	3.30080200	1.35894500	0.59324200				
C	3.42380000	1.71844100	1.95122200				
C	3.19758200	2.33338900	-0.42147700				
C	3.47112400	3.08101000	2.26227500				
C	3.25452500	3.67802500	-0.03893700				
C	3.39562300	4.05919900	1.28464000				
H	3.55455400	3.36638700	3.31146100				
H	3.16580000	4.43635700	-0.81748400				
C	3.43653900	5.11346900	1.55436500				
C	2.36840300	-4.09749400	1.99637400				
C	3.87562700	-3.98318900	2.21654900				
C	1.56004600	-3.01054600	2.69906500				
H	4.40043600	-4.83504300	1.76564800				
H	4.30328500	-3.06949700	1.79688600				
H	4.09939300	-3.98276900	3.29092900				
H	0.48320500	-3.21633800	2.62640200				
H	1.82485200	-2.95785100	3.76326900				
H	1.72364500	-2.02078000	2.26620100				
C	1.84432600	-2.77742300	-3.06339600				
C	0.96418700	-1.53453000	-2.99389400				
C	3.28906600	-2.50753500	-3.48230100				
H	-0.08987800	-1.79624500	-2.84877600				
H	1.23643000	-0.86055200	-2.17796200				
H	1.01931900	-0.96075700	-3.92716700				
H	3.84531400	-3.44676300	-3.60286900				
				Cu			

H	5.95217900	5.89352700	1.31597500	O	-1.86953300	-1.14971900	1.97977700
H	8.13360000	4.52039300	0.26211700	C	-2.08099800	-2.54274900	2.11224100
C	7.49978400	1.94790700	-0.56354700	H	-2.01858400	-3.04861600	1.13851500
C	8.17282600	1.02654300	0.27618800	H	-1.27929200	-2.90864500	2.75855600
C	7.68751700	1.92804000	-1.96708900	H	-3.05872400	-2.74627700	2.57154400
C	8.96557900	0.04485100	-0.32951300	C	4.16399200	-0.79379600	1.05985100
C	8.48774300	0.90880200	-2.50171100	C	1.96339900	-0.62040600	1.59131700
C	9.11297400	-0.03567500	-1.70480200	C	3.67747900	-2.05278600	1.17488200
H	9.47927300	-0.67058700	0.31341400	N	3.11804400	0.07368200	1.32863400
H	8.61893800	0.87595000	-3.58284500	N	2.32848800	-1.93967100	1.48982200
H	9.72774600	-0.81569600	-2.15145200	Cu	0.26714900	0.22444600	1.80747500
C	3.64157400	4.41942000	1.33792900	H	4.15413000	-3.01747100	1.06667600
C	3.31893700	4.22925300	2.69814600	H	5.15720500	-0.43214800	0.83120600
C	2.73920600	5.03217100	0.44379100	C	3.20687500	1.52693400	1.19626300
C	2.07659700	4.69393100	3.14235100	C	2.97778600	2.11043000	-0.06908900
C	1.51359700	5.46987000	0.95561900	C	3.52924700	2.31616700	2.32233500
C	1.17758100	5.31238400	2.28960000	C	3.00770400	3.50734400	-0.15557500
H	1.81702900	4.54587700	4.19137400	C	3.56179400	3.70376300	2.15768700
H	0.80594400	5.93225500	0.26733400	C	3.28689000	4.30499200	0.94026700
H	0.21674300	5.66414200	2.66198500	H	2.80013300	3.96265900	-1.12373400
C	8.16090800	1.00213100	1.79809600	H	3.79660000	4.31860600	3.02656200
C	8.71676600	2.26921500	2.44717500	H	3.29565700	5.39001900	0.84565400
C	6.82465000	0.55592400	2.38511700	C	1.51470100	-3.10880400	1.78940000
H	9.70260400	2.51796700	2.03386600	C	0.94406300	-3.86089600	0.73341600
H	8.07164600	3.14196400	2.31946200	C	1.38874400	-3.53072600	3.13299700
H	8.83659400	2.11201100	3.52683000	C	0.26873900	-5.04237800	1.06374300
H	6.58502200	-0.47305800	2.08613600	C	0.69642100	-4.72181600	3.38912400
H	6.85555200	0.59554600	3.48321700	C	0.14542500	-5.48320800	2.37211200
H	5.99009600	1.17797400	2.04956100	H	-0.17417700	-5.62167500	0.25354900
C	7.13511500	2.91819000	-2.98351500	H	0.59939800	-5.04603000	4.42565000
C	7.57103900	4.36637300	-2.76000600	H	-0.37809000	-6.41137700	2.59657000
H	7.34244200	4.95683100	-3.65609000	C	2.78713400	1.38857600	-1.39190100
H	7.05290000	4.84583400	-1.92507200	C	4.13310000	0.95073000	-1.97528900
H	8.65149300	4.44140800	-2.57823900	C	1.79491200	0.24531600	-1.40233700
C	4.12333000	3.46509300	3.73908900	H	4.85268100	1.77800400	-2.01473500
C	3.76903800	1.97727000	3.67148500	H	4.58184900	0.14039400	-1.38396100
C	5.63171100	3.66782300	3.76417400	H	3.99628800	0.56925900	-2.99508700
H	2.69385000	1.81680700	3.82254200	H	0.85763300	0.51775300	-0.90614800
H	4.01581400	1.55458400	2.68940100	H	1.53874600	-0.01744800	-2.43539700
H	4.31861200	1.41380000	4.43956600	H	2.20014500	-0.64970800	-0.92305700
H	5.90979300	4.72891600	3.74553200	C	3.83445400	1.81572100	3.72352100
H	6.04673500	3.23046100	4.68253400	C	2.58536600	1.30078300	4.43347900
H	6.12886700	3.17447700	2.92652800	C	5.03342700	0.87297800	3.81273100
C	2.90318500	5.16494800	-1.06100200	H	1.83081200	2.09280900	4.50479700
C	4.24101300	5.68078000	-1.57652000	H	2.12006800	0.47043700	3.89529700
C	2.48974300	3.85309500	-1.73124200	H	2.82540100	0.95487200	5.44842600
H	4.56790900	6.58343700	-1.04353500	H	5.91710200	1.32498200	3.34418700
H	5.03662900	4.93662100	-1.50112100	H	5.27850600	0.67313500	4.86405200
H	4.15042100	5.93477100	-2.64059600	H	4.86445200	-0.09479600	3.33383800
H	1.46942500	3.56525100	-1.45696000	C	0.90284900	-3.47591200	-0.73663100
H	2.55241100	3.92414200	-2.82497800	C	-0.05249800	-2.29928200	-0.95345000
H	3.13296600	3.02038100	-1.41934300	C	2.25690300	-3.33241900	-1.42971800
B	2.67126400	-0.03533900	-2.41715100	H	-1.09192600	-2.60884100	-0.77879100
F	2.63514100	-1.31954800	-1.86323700	H	0.14514600	-1.46128600	-0.27526800
F	2.66640800	-0.06127900	-3.79634600	H	0.00293900	-1.90873500	-1.97547600
F	1.63260200	0.75078300	-1.90090300	H	2.86971700	-4.23010900	-1.27321700
F	3.92930000	0.59219400	-1.99135100	H	2.10206000	-3.21832500	-2.50955200
H	3.75062700	3.83624600	4.70657600	H	2.83869700	-2.46952900	-1.10040300
H	2.15729600	5.91913700	-1.35562700	C	1.84384600	-2.78021500	4.37353500
H	8.88117200	0.21227400	2.06069000	C	3.24028600	-2.17688500	4.34698600
C	5.63329000	2.78292800	-3.19838800	C	0.77017500	-1.76486000	4.77682200
H	5.36147000	1.78549600	-3.55619200	H	3.99105100	-2.90383400	4.01263300
H	5.07200000	2.94016800	-2.27417000	H	3.30891700	-1.30113800	3.70111600
H	5.28513900	3.52125400	-3.93262600	H	3.51914600	-1.84764200	5.35602100
H	7.609044600	2.61923500	-3.93034900	H	-0.18390700	-2.26599700	4.98550200
O	4.90359100	-0.92985000	0.08451200	H	1.06750600	-1.21026300	5.67577300
C	5.86632300	-1.52832200	-0.77447200	H	0.58559800	-1.03458000	3.97527500
H	5.38176500	-2.28018800	-1.40723500	B	-1.22233200	1.82784100	-2.01251200
H	6.25121300	-0.71391100	-1.39216700	F	-0.33468400	1.79613900	-3.08207600
H	6.68689400	-1.97545200	-0.19541800	F	-0.65683700	2.57829800	-0.93809100
C	4.99409700	-1.46538200	5.27198500	F	-2.44492800	2.41192400	-2.38493100
H	5.67410400	-2.10235700	5.86425600	F	-1.46152900	0.50517800	-1.53868600
H	5.56721300	-0.51667900	5.18071200	O	-1.71563000	3.65328500	1.58418500
C	3.69180100	-1.20412000	6.01273300	C	-1.13728300	4.96870600	1.37326300
H	3.86592000	-0.71858700	6.97881700	H	-0.19402700	4.82301600	0.83321800
H	3.03209400	-0.55571400	5.42311400	H	-0.91261500	5.41173300	2.35156400
H	3.15297100	-2.14062400	6.19757500	C	-2.12588600	5.77538000	0.59490000
C	-	-	-	C	-2.60972300	6.98851800	1.08663100
C	-	-	-	C	-2.56394000	5.31449600	-0.65317200
C	-	-	-	C	-3.51723500	7.74117000	0.34181400
C	-	-	-	H	-2.27366800	7.34711700	2.06075300
C	-	-	-	C	-3.48029200	6.05902100	-1.38823700
C	-	-	-	H	-2.18350300	4.37118100	-1.04586600
C	-	-	-	C	-3.95698600	7.27497100	-0.89492000
H	-	-	-	H	-3.88664300	8.68808600	0.73303700
H	-	-	-	H	-3.81416000	5.68792600	-2.35636400
H	-	-	-	H	-4.66990200	7.85920000	-1.47545900
N	-	-	-	H	4.14045100	2.71710100	4.27578400
C	-	-	-	H	2.37663200	2.15063800	-2.06835000
O	-	-	-	H	1.86121300	-3.54196600	5.16790500
C	-	-	-	H	0.43436700	-4.34106300	-1.23016900

**8a**

C	-4.52528900	-0.64349600	-1.87172100	H	-0.10227600	-6.90308300	-2.91327200
H	-5.20280900	-0.00377900	-2.45686300	H	-1.63537800	-6.07140500	-3.04719700
H	-3.50724900	-0.40606500	-2.20508900	H	-1.60274000	-7.84332000	-3.11402800
H	-5.70138400	-0.43000100	-0.09700000	C	-2.16514400	-7.24600000	-5.70971800
H	-3.94189500	-2.08734700	0.55308100	H	-3.01619200	-6.60193500	-5.47383400
C	-4.85417700	-2.10530500	-2.13284500	H	-1.99616400	-7.19712500	-6.79384900
H	-4.12996400	-2.74943400	-1.61140700	H	-2.46721900	-8.27280800	-5.46570500
H	-5.84115500	-2.34960500	-1.70703400	C	0.00778700	-1.10664500	-4.40358800
C	-4.83528400	-2.43105100	-3.61645300	H	-0.54812500	-1.54613900	-3.56518700
H	-5.05391700	-3.48882500	-3.80360400	H	1.06419100	-1.27938400	-4.17537300
H	-5.57775400	-1.83664500	-4.16377000	H	-0.18171700	-0.02331100	-4.39654900
H	-3.85461800	-2.20888700	-4.05470400	C	-1.82988400	-1.38089000	-6.11724100
H				H	-1.92363600	-0.29460700	-6.25028900
H				H	-2.13989300	-1.86114400	-7.05430300
<b>TS<sub>4a-12a</sub></b>				H	-2.54520200	-1.66404700	-5.34240800
N	0.61081600	-0.63153400	-1.00211000	C	-3.22570000	-0.28676400	-2.95202300
C	0.05054400	-1.53279200	-0.16710000	H	-3.01960100	-0.12333100	-1.88665200
O	-0.87008000	-2.29802800	-0.49226600	H	-2.55942400	-1.09057200	-3.27581500
C	1.16681200	0.49297700	-0.59705500	H	-2.94987100	0.62288400	-3.50388100
C	1.00123100	1.14995500	0.68115900	C	-5.09825800	-0.66305900	-4.64560600
C	2.01119200	1.21635300	-1.54461500	H	-4.54589700	-1.40383100	-5.22894700
C	1.75900700	2.23639800	1.05640200	H	-6.16876900	-0.87968500	-4.75561000
C	2.77158900	2.31539100	-1.14500400	H	-4.90713000	0.31580600	-5.10422900
C	2.65699800	2.81927600	0.14801100	H	0.31171400	0.69699800	1.38867400
H	3.45414300	2.78709600	-1.84692100	O	2.07563700	0.66542100	-2.76221200
H	3.27162500	3.66552700	0.44964900	C	2.85848300	1.31047600	-3.74991500
C	-0.41762700	2.33418100	-1.38616600	H	3.92265900	1.30226700	-3.48156600
O	0.59890400	-1.62670600	1.06241400	H	2.70813400	0.73402300	-4.66476600
C	0.18523300	-2.77323200	1.85352300	H	2.52573600	2.34684300	-3.90596200
H	-0.83223400	-2.59151100	2.22359800	H	-1.08713600	1.63337900	-0.89308000
H	0.16401400	-3.64375500	1.18948400	H	-0.15527800	2.07307700	-2.40968500
C	1.16904300	-2.92333600	2.96754100	C	-0.28788600	3.70121500	-0.89585300
C	2.48236700	-3.31630900	2.68370300	H	0.77294900	3.85911600	-0.57892300
C	0.80280800	-2.67705300	4.29202200	H	-0.40113000	4.41625200	-1.72818100
C	3.40898300	-3.45500300	3.71163000	C	-1.19523100	4.04034600	0.27568400
H	2.75983000	-3.51577900	1.64964400	H	-0.98865100	5.04265400	0.66590700
C	1.72962400	-2.82180800	5.32393900	H	-2.25266600	4.00118700	-0.00947500
H	-0.22103500	-2.37378700	4.51688900	H	-1.04402700	3.32557200	1.09456700
C	3.03567300	-3.20844600	5.03379500				
H	4.42770300	-3.76450300	3.48214200				
H	1.43116900	-2.63075200	6.35402000				
H	3.76248000	-3.32344300	5.83692800				
H	1.63851500	2.66131100	-2.05141400	C	-4.29292300	1.10789700	-0.63861000
C	-3.21950200	-4.18081000	-5.69082900	C	-4.41897300	-0.23323900	-0.63596100
C	-2.44452100	-3.66305200	-3.61305400	C	-3.62236600	-1.02611200	0.25335700
C	-4.29006400	-3.82178900	-4.94315300	C	-2.37089300	0.94819300	0.97718100
N	-2.10266600	-4.09412000	-4.87212600	H	-4.87287600	1.73268800	-1.31458000
N	-3.80900100	-3.49798100	-3.68089300	N	-5.10389700	-0.73903800	-1.31316600
Cu	-1.29635900	-3.29082800	-2.13738900	C	-1.27527400	1.35783800	1.59029700
B	1.17989300	-4.62278800	-1.56131000	O	-0.77450000	2.66703300	1.63752800
F	1.90064100	-3.95842700	-0.57062400	C	0.37107300	2.85618300	2.01098700
F	1.82895200	-5.753373700	-2.01595000	O	-2.63297500	-0.47483900	1.01771300
F	-0.11591100	4.97273800	-1.03825700	C	-1.79025900	-1.18184100	1.82241600
F	0.91952600	-3.72544300	-2.64452000	C	-2.00121200	-2.57826900	1.91414500
H	-5.34454700	-3.77826000	-5.17969300	H	-1.89062400	-3.06366300	0.93453400
H	-3.14266500	-4.48809600	-6.72486600	H	-1.22866500	-2.95513100	2.58863000
C	-4.67223800	-3.18019600	-2.55665100	H	-2.99799200	-2.79589500	2.32354900
C	-5.11332000	-1.84968100	-2.36217100	C	-3.77884300	-2.10256700	0.27068600
C	-5.09243100	-4.22052800	-1.69899500	C	4.27536000	-0.77104300	1.19122400
C	-5.97713200	-1.59507600	-1.29171100	C	2.04961900	-0.60246600	1.60890300
C	-5.95560700	-3.89183600	-0.64519000	C	3.78456200	-2.03099300	1.27148400
C	-6.40047500	-2.59890100	-0.43416400	N	3.21625300	0.09386400	1.41174800
H	-6.31539100	-0.57052500	-1.13595700	N	2.42102800	-1.92118700	1.51717400
H	-6.27586300	-4.69220400	0.02243400	Cu	0.33959800	0.23187700	1.75524000
H	-7.07319900	-2.37302500	0.39177900	H	4.26709400	-2.99469400	1.18143600
C	-0.74158500	-4.30383600	-5.34436900	H	5.27878600	-0.40701500	1.01843200
C	0.01020900	-3.19140100	-5.77474500	C	3.30725400	1.54744200	1.28767300
C	-0.20503800	-5.61131600	-5.38068200	C	3.15658400	2.13287800	0.01191200
C	1.31884700	-3.41839100	-6.21683000	C	3.55336200	2.33576600	2.43399400
C	1.11116000	-5.76227800	-5.82667500	C	3.17275500	3.53033200	-0.06758000
C	1.87796900	-4.68310600	-6.23600700	C	3.57873900	3.72397400	2.27678100
H	1.90793400	-2.55784800	-6.53651800	C	3.36990400	4.32671400	1.04654100
H	1.54077600	-6.76357200	-5.82905100	H	3.01569700	3.98640500	-1.04477600
H	2.90474600	-4.83008400	-6.56704100	H	3.75326200	4.33813600	3.16034700
C	-4.65476600	-5.67676900	-1.72726200	C	3.36793700	5.41223600	0.95675200
H	-5.45486900	-6.21097600	-1.19122200	C	1.59877300	-3.09555200	1.76943600
C	-4.69631700	-0.63246800	-3.17219900	C	1.08679100	-3.84367000	0.68066800
H	-5.23771100	0.19636000	-2.73423600	C	1.41117500	-3.52901100	3.10204400
C	-0.89735900	-6.88852200	-4.93461900	C	0.40962200	-5.03505500	0.96824700
H	-0.18016100	-7.68565500	-5.18210800	C	0.72083000	-4.72970400	3.31454000
C	-0.39649900	-1.72660000	-5.74075500	H	0.22936200	-5.48885900	2.26560900
H	0.23636300	-1.25290300	-6.50897000	H	0.01274800	-5.61238400	0.13310800
C	-3.38233000	-5.85130100	-0.89435600	H	0.57603900	-5.06346200	4.34244200
H	-2.54358700	-5.27484800	-1.30384000	C	-0.29282300	-6.42516100	2.45693800
H	-3.53648000	-5.50863600	0.13619700	C	3.06502500	1.41276200	-1.32233600
H	-3.07273800	-6.90361400	-0.86486200	C	4.45684700	1.01826900	-1.82402500
C	-4.54859000	-6.34925600	-3.08802000	H	2.10931100	0.24139000	-1.39569300
H	-5.43988200	-6.17503900	-3.70449900	H	5.15166600	1.86742100	-1.81982500
H	-3.67505500	-6.02038500	-3.65269500	H	4.89421000	0.22104200	-1.20703000
H	-4.44254300	-7.43320700	-2.95275700	H	4.39401100	0.63522000	-2.85046900
C	-1.07186100	-6.93118100	-3.41993300	H	1.14097100	0.48584800	-0.94841200
				H	1.91812300	-0.01907000	-2.44312100

H	2.51219500	-0.64663900	-0.90107300	C	1.79727200	-5.14009000	0.01564300
C	3.78932000	1.83099500	3.84677900	C	1.84760800	-4.69779200	-2.32820700
C	2.50929900	1.30891500	4.49351700	C	1.53010000	-5.54425700	-1.28087100
C	4.98579200	0.89143900	3.98976700	H	1.55540300	-5.79892300	0.85024200
H	1.74619600	2.09541100	4.52428400	H	1.63024900	-4.99931300	-3.35205000
H	2.07849100	0.47476500	3.93362900	H	1.06645100	-6.51005700	-1.47338500
H	2.70049200	0.96567800	5.51965300	C	3.59248700	1.74689500	0.20767700
H	5.88919900	1.34817400	3.56554600	C	3.65556600	2.19351800	1.54440100
H	5.18136600	0.68800400	5.05080400	C	3.50891800	2.65507600	-0.86781600
H	4.84325300	-0.07495700	3.49927500	C	3.66438800	3.57383300	1.77089300
C	1.11456800	-3.44181400	-0.78501600	C	3.51883100	4.02216900	-0.56907600
C	0.19251200	-2.24409500	-1.02784500	C	3.60498200	4.48794900	0.73201800
C	2.50185900	-3.32187600	-1.41453800	H	3.70562700	3.92537700	2.80232500
H	-0.85876900	-2.53835000	-0.91331600	H	3.44939700	4.72931000	-1.39633000
H	0.36925600	-1.42297600	-0.32436900	H	3.61767100	5.55778300	0.93601800
H	0.30379400	-1.83218700	-2.03696300	C	2.63387900	-3.62223200	1.77448900
H	3.08295900	-4.23897600	-1.24910800	C	4.12190100	-3.65064800	2.12609900
H	2.39886800	-3.18302200	-2.49757300	C	1.95704000	-2.38330200	2.34375900
H	3.09052400	-2.48160100	-1.04144600	H	4.59930700	-4.57327600	1.77343400
C	1.79403000	-2.78220100	4.36899700	H	4.66323600	-2.80292500	1.68968200
C	3.18532300	-2.16886900	4.42078200	H	4.25690300	-3.59288700	3.21430000
C	0.69404500	-1.77538500	4.71922100	H	0.91517000	-2.29889800	2.01235500
H	3.95930000	-2.88975100	4.12871200	H	1.96449300	-2.41563100	3.44433900
H	3.28292900	-1.29154200	3.78078700	H	2.46548600	-1.46840700	2.04437900
H	3.40489800	-1.83888300	5.44417500	C	2.75341700	-2.65654100	-3.38385000
H	-0.26758800	-2.28246800	4.87117600	C	1.89988200	-1.40542300	-3.56211800
H	0.93898000	-1.22584400	5.63697200	C	4.24767300	-2.40428500	-3.59073500
H	0.55001500	-1.04016000	3.91383300	H	0.84507200	-1.66973300	-3.67323100
B	-0.90768400	1.83306900	-2.02894300	H	1.96545600	-0.73154500	-2.70333100
F	-0.04960900	1.66454020	-3.10473800	H	2.22008500	-0.84900300	-4.45386700
F	-0.26815000	2.62117700	-1.02763800	H	4.82640500	-3.33133000	-3.48236700
F	-2.08859000	2.48650900	-2.42950200	H	4.42049200	-2.01895400	-4.60404600
F	-1.24513500	0.58212900	-1.44257400	H	4.66182000	-1.66887200	-2.89556100
O	-1.62425700	3.63987800	1.30394500	C	3.57795800	1.33308500	2.79510800
C	-1.03049500	4.95213700	1.11937400	C	2.11244200	0.97681400	3.06799300
H	-0.09120700	4.80813400	0.57334200	C	4.51912800	0.13691100	2.89065900
H	-0.80082400	5.37432200	2.10567800	H	1.52254000	1.88556900	3.23782400
C	-2.02977000	5.76602700	0.36371000	H	1.65091000	0.46552000	2.21203200
C	-2.63613400	6.88263300	0.94035500	H	2.02110700	0.32832200	3.94967900
C	-2.38874700	5.37889300	-0.93340000	H	5.56049900	0.43274600	2.70840700
C	-3.59260300	7.61072300	0.23313200	H	4.46654800	-0.28989700	3.90103100
H	-2.36122600	7.18107800	1.95324200	H	4.27997100	-0.66851200	2.19409100
C	-3.34909000	6.10084200	-1.63473900	C	3.29905400	2.30986200	-2.33237400
H	-1.92718300	4.49870200	-1.38327700	C	4.17594100	1.21327000	-2.92260200
C	-3.95292200	7.21744400	-1.05376100	C	1.81007700	2.07234300	-2.60018400
H	-4.06100000	8.48098300	0.69121300	H	5.23552900	1.36008900	-2.67597500
H	-3.62476000	5.78727100	-2.64079400	H	3.88520500	0.21643200	-2.58826900
H	-4.70424500	7.78145500	-1.60522200	H	4.08343600	1.21608800	-4.01634400
H	4.06543200	2.73125000	4.41656700	H	1.22048500	2.95202000	-2.31601400
H	2.67462100	2.16453000	-2.02241200	H	1.63210100	1.85359300	-3.66104200
H	1.77359900	-3.54789800	5.15952900	H	1.42299600	1.22659100	-2.01392800
H	0.65128500	-4.29204400	-1.30842200	B	-1.30831800	-2.57896600	-1.82072500
C	-3.40891700	1.81068100	0.32417600	F	-1.17340700	-2.96683400	-3.13943600
H	-2.90915000	2.64007800	-0.18777400	F	-0.59203500	-1.34358600	-1.60542900
C	-4.29695200	2.44080900	1.45416200	F	-2.66539800	-2.32961900	-1.49570600
H	-3.61900800	2.83911700	2.21503600	F	-0.79846300	-3.53812800	-0.93720600
H	-4.87478600	1.63377800	1.93025400	O	-1.61053000	2.95156400	0.91647200
C	-5.23427500	3.54326800	0.95225100	C	-1.30053900	4.32507600	1.13696100
H	-5.27063800	4.34064200	1.70750800	H	-0.67812300	4.68895800	0.30616000
H	-4.80052800	4.01688200	0.05869400	H	-0.68687800	4.42396800	2.04404400
C	-6.65321700	3.07658300	0.66780400	C	-2.57944500	5.09895800	1.25234300
H	-7.27691100	3.89775400	0.29518400	C	-2.55882700	6.36390500	1.84771200
H	-6.68313600	2.27361800	-0.07903000	C	-3.78922500	4.61029500	0.75022200
H	-7.12832900	2.68610800	1.57738000	C	-3.71809500	7.12929300	1.93392100
<b>TS4a-5a'</b>							
C	-4.28436500	0.71229500	-1.09416100	H	-4.92144800	6.63501000	1.43234600
C	-4.84428300	-0.38629700	-0.51517500	H	-3.68316700	8.11297700	2.39986800
C	-4.05734000	-1.11621200	0.44437600	H	-5.88804500	4.97862100	0.44909600
C	-2.64353300	-0.77849900	0.67440500	H	-5.83018100	7.23060700	1.50141400
C	-2.14133900	0.47274700	0.09549000	C	-1.71592000	-1.72617600	1.34896200
C	-2.97256100	1.15513600	-0.76981400	H	-0.91154100	-1.92801800	0.62340800
H	-4.83968100	1.26844800	-1.84936100	H	-1.22633000	-1.19114500	2.17869700
H	-5.82526700	-0.75841400	-0.79359800	O	-3.87592900	-0.43999300	1.90122500
H	-4.36012900	-2.13234400	0.68090000	C	-4.31173400	0.90783100	2.10007400
H	-2.58786700	2.04874100	-1.25602900	H	-5.16849400	1.13989100	1.45767800
N	-0.85934500	0.84228900	0.42222100	H	-4.60626700	0.93770100	3.15249400
C	-0.53719200	2.15402300	0.59832600	H	-3.50166100	1.62101500	1.91077800
O	0.60209200	2.60055900	0.56695800	H	3.88532600	2.00444800	3.61198200
C	4.67506600	-1.59869500	-0.49204500	H	3.56589700	3.23047500	-2.87472300
C	2.66023600	-0.56482500	-0.25921800	H	2.18314800	-4.48220100	2.29384900
C	4.92198600	-0.29649600	-0.22089500	H	2.46406000	-3.33337000	-4.20148900
N	3.29624600	-1.75437400	-0.52191900	C	-2.31094700	-3.05175400	1.79852500
N	3.69031700	0.32377000	-0.07305600	H	-2.75100600	-3.55081400	0.92509500
Cu	0.78116000	-0.15208100	-0.08799300	H	-3.12003100	-2.87471500	2.52298700
H	5.84763700	0.25226800	-0.11349100	C	-1.26003300	-3.96593500	2.40196400
H	5.33970100	-2.43100200	-0.67973900	H	-1.69889500	-4.91752400	2.72289400
C	2.65862800	-3.03915400	-0.78533600	H	-0.48211400	-4.18902300	1.66054200
C	2.36156200	-3.89253300	0.30169400	H	-0.77597100	-3.51040600	3.27673400

**5a'**

C	-4.63934900	1.00361400	-1.04865300	C	-5.31484400	5.43364500	1.13241100
C	-5.19130100	-0.13240500	-0.52653300	H	-4.25807800	3.55291600	1.03695000
C	-4.35112700	-1.06110100	0.21746300	C	-5.20750000	6.81644800	1.25212700
C	-3.01451000	-0.63337200	0.66742000	H	-3.84777900	8.47953800	1.45753900
C	-2.49753200	0.57029400	0.12792400	H	-6.29635500	4.96931000	1.04429300
C	-3.31368200	1.33033600	-0.73163900	H	-6.10070300	7.43872400	1.25620600
H	-5.21102400	1.65531600	-1.70638400	C	-2.11387400	-1.49970000	1.47340500
H	-6.20960200	-0.45037200	-0.73974200	H	-1.23090300	-1.67600900	0.82347900
H	-3.94604100	-1.63607700	-0.70871500	O	-1.69729600	-0.87052700	2.28119000
H	-2.87577800	2.22054600	-1.17829200	C	-5.06089400	-1.97903700	0.99592700
N	-1.19857200	0.93817600	0.42157300	C	-5.59354800	-1.37850200	2.16143400
C	-0.87461300	2.22865100	0.69017200	H	-6.30214500	-0.57262700	1.91215300
O	0.27235200	2.65656900	0.75854600	H	-6.11897500	-2.16651900	2.70560200
C	4.22090100	-1.69845700	-0.49375900	H	-4.79714700	-0.96488000	2.80151500
C	2.26153300	-0.57083700	-0.25192400	H	3.59890900	1.98952900	3.65237300
C	4.53035400	-0.41705300	-0.18430700	H	3.28561100	3.16415800	-2.83646800
N	2.83655900	-1.78225100	-0.54323500	H	1.61490600	-4.42679200	2.29014700
N	3.33080200	0.26161900	-0.02798900	H	1.83572900	-3.28906300	-4.21158200
Cu	0.42752300	-0.05120500	-0.04450500	C	2.58884700	-2.84480600	2.00825200
H	5.48244800	0.08013900	-0.05835000	H	-3.07947700	-3.40623200	1.20826300
H	4.84554300	-2.55506400	-0.70557900	C	-3.33950500	-2.70473500	2.79784900
C	2.11897300	-3.02404700	-0.80122900	H	-1.42201600	-3.65571100	2.54073500
C	1.79956200	-3.86464500	0.28966200	H	-1.75686900	-4.62548000	2.92712400
C	1.80919700	-3.39287100	-2.13043000	H	-0.69935200	-3.84832800	1.73653500
C	1.11293700	-5.05278800	0.01724500	H	-0.89289900	-3.13824100	3.35319600
C	1.11812300	-4.59329000	-2.32447400				
C	0.75731600	-5.41466300	-1.27093900				
H	0.84847100	-5.69790200	0.85583400				
H	0.83833700	-4.86439600	-3.34076300				
H	0.19653000	-6.32950200	-1.45350600				
C	3.28734700	1.69064200	0.24872900				
C	3.39490100	2.14625300	1.58149900				
C	3.20432000	2.59612000	-0.82959400				
C	3.43876300	3.52692700	1.79789800				
C	3.24747100	3.96468100	-0.53892100				
C	3.37121900	4.43674500	0.75582400				
H	3.51049800	3.88372900	2.82558500				
H	3.17696300	4.66780700	-1.36949800				
H	3.40077100	5.05722200	0.95316200				
C	2.18571400	-3.65787700	1.74691300				
C	3.66351800	-3.95735200	2.00797300				
C	1.80404400	-2.32071000	2.36099700				
H	3.95743700	-4.93408300	1.60498100				
H	4.31222300	-3.19420000	1.55952700				
H	3.86731100	-3.95856100	3.08691400				
H	0.79861500	-1.99203200	2.06723100				
H	1.83397000	-2.38390400	3.45756400				
H	2.49966900	-1.53473600	2.06846100				
C	2.17906300	-2.63477300	-3.39648200				
C	1.42065900	-1.32226400	-3.56865000				
C	3.68688700	-2.48802400	-3.60889500				
H	0.35225000	-1.50615300	-3.70300700				
H	1.52061700	-0.67350500	-2.69514900				
H	1.79939400	-0.77443400	-4.44241400				
H	4.20158300	-3.45134000	-3.49395300				
H	3.88377500	-2.12384700	-4.62556900				
H	4.15151900	-1.77576300	-2.92104300				
C	3.33664000	1.29510500	2.83936600				
C	1.88631200	0.87741100	3.10342900				
C	4.35453500	0.16308000	2.96112500				
H	1.26550200	1.76461100	3.27313200				
H	1.44314300	0.35314500	2.24671600				
H	1.81684400	0.22396200	3.98330600				
H	5.37663300	0.54541600	2.84088200				
H	4.28393600	-0.28815400	3.95952400				
H	4.22019800	-0.64189600	2.23580400				
C	2.97715800	2.25729900	-2.29313600				
C	3.80773600	1.12472600	-2.88223600				
C	1.47857400	2.09206900	-2.56201800				
H	4.87279500	1.23305600	-2.63941000				
H	3.48196800	0.13998800	-2.54497900				
H	3.71230400	1.12748600	-3.97567500				
H	0.93154500	2.99801200	-2.27397800				
H	1.28963800	1.88639400	-3.62533000				
H	1.05120200	1.26344400	-1.97972600				
B	-1.85699700	-2.47292800	-1.99989300				
F	-1.39682200	-3.03862600	-3.17169800				
F	-1.16284200	-1.26567400	-1.70777100				
F	-3.25161900	-2.13088000	-2.15917800				
F	-1.74390000	-3.33221700	-0.90523300				
O	-1.95825600	3.03744800	0.94589300				
C	-1.64450700	4.39744000	1.22858500				
H	-0.92870400	4.77072500	0.48285600				
H	-1.12892900	4.45319300	2.19929100				
C	-2.90472200	5.21101900	1.23279900				
C	-2.80536800	6.60151600	1.35418200				
C	-4.17205700	4.63398300	1.12464300				
C	-3.94503100	7.39889000	1.36533200				
H	-1.82020800	7.06308700	1.43731100				

C	7.31719600	3.29548500	-2.55482900	C	4.11015500	0.88001100	-2.06601000
C	7.58848300	4.78016700	-2.30970600	C	1.79808200	0.10845500	-1.45078800
H	7.37275600	5.34628800	-3.22464900	H	4.79808800	1.73213900	-2.13140600
H	6.96625700	5.20708800	-1.51870500	H	4.59085100	0.10335700	-1.45567000
H	8.63969900	4.95866100	-2.04747100	H	3.98504400	0.46653100	-3.07468600
C	3.58868400	3.71884800	3.84924200	H	0.86793500	0.36989000	-0.93831200
C	3.29536800	2.21874900	3.85632900	H	1.52130000	-0.18904000	-2.46914300
C	5.08242400	3.97466600	3.98759400	H	2.24123100	-0.76165700	-0.95827100
H	2.21720500	2.01923800	3.888763100	C	3.81662400	1.92593500	3.59384300
H	3.68529500	1.73622400	2.95060200	C	2.61794800	1.37158700	4.35776100
H	3.76362400	1.74225200	4.72685300	C	5.06301800	1.04437700	3.66805700
H	5.33249600	5.04162800	3.93884000	H	1.82369300	2.12387700	4.42303900
H	5.42817000	3.59648600	4.95872300	H	2.18327000	0.49796900	3.86477700
H	5.66475500	3.45337100	3.22426300	H	2.90592200	1.07629700	5.37612900
C	2.73431000	5.22129700	-1.10290800	H	5.91154300	1.53185900	3.17124300
C	4.08566000	5.82051500	-1.47395400	H	5.34259500	0.87313700	4.71578500
C	2.48529000	3.89223200	-1.81238300	H	4.93037600	0.06172700	3.20732900
H	4.31174100	6.72631700	-0.89614600	C	0.78351000	-3.53794700	-0.56962700
H	4.90728400	5.11427500	-1.33429000	C	-0.15845900	-2.34487800	-0.72778300
H	4.08583300	6.09359700	-2.53692400	C	2.08314500	-3.44354700	-1.36858300
H	1.46170600	3.53656200	-1.65560100	H	-1.16692300	-2.60443000	-0.37764100
H	2.66377200	3.97292900	-2.89231800	H	0.16325400	-1.47189900	-0.15058800
H	3.14710300	3.10499800	-1.43093500	H	-0.24099200	-2.02342200	-1.77224300
B	2.75893300	0.33181500	-2.52524800	H	2.64972800	-4.38103500	-1.29294400
F	2.79058400	-1.05366300	-2.38279200	H	1.85443500	-3.27416200	-2.42787000
F	2.72679300	0.74043300	-3.83536200	H	2.74107500	-2.63167500	-1.05059600
F	1.70957700	0.87743400	-1.76955500	C	2.09252600	-2.74268700	4.43615900
F	4.00438300	0.85130000	-1.92266300	C	3.45489200	-2.07300600	4.32861300
H	3.12423400	4.13471800	4.75700100	C	0.99065600	-1.76549800	4.85843600
H	1.97804500	5.92863000	-1.47711500	H	4.22500200	-2.76965700	3.97447200
H	8.61081900	0.56528600	2.61954100	H	3.44824100	-1.21095800	3.66096000
C	5.86583000	3.00581000	-2.91652700	H	3.76433100	-1.70460900	5.31501500
H	5.74159500	1.98602700	-3.29419800	H	0.06848700	-2.30217300	5.11531100
H	5.19218700	3.10193700	-2.06108300	H	1.29900600	-1.17392100	5.72978500
H	5.51717700	3.70049900	-3.69206800	H	0.74422000	-1.06503500	4.04710200
H	7.90696700	3.04545200	-3.44947600	B	-1.14835000	1.86857900	-1.91221800
C	5.06363000	-1.36308400	-0.03162100	F	-0.16980000	1.88735600	-2.90016600
H	4.42451900	-1.04569000	-0.86872200	F	-0.66897700	2.53035100	-0.74395300
H	5.46377300	-0.40912400	0.37234800	F	-2.32068000	2.50146100	-2.35582300
O	4.60954000	-1.85652100	3.54668400	F	-1.44961800	0.52369400	-1.54907100
C	4.33699900	-1.14268100	4.65630800	O	-1.83095200	3.50205700	1.81773700
H	4.79370100	-1.64120000	5.54240000	C	-1.24509800	4.82590100	1.66889100
H	4.80532300	-0.13460300	4.65404200	H	-0.27715400	4.69572900	1.17067900
H	3.24985300	-1.01231000	4.86986200	H	-1.07024200	5.23916400	2.66977700
C	6.21449100	-2.18059100	-0.59084100	C	-2.20064700	5.65140100	0.86891500
H	5.86215900	-3.18271100	-0.87381600	C	-2.69484100	6.85925100	1.36337000
H	6.99013500	-2.32759900	0.17761300	C	-2.59538300	5.21416500	-0.40177100
C	6.78300600	-1.48454400	-1.81546600	C	-3.57029100	7.62965500	0.59834900
H	7.01072800	-0.43397400	-1.59614300	H	-2.39284800	7.19977300	2.35499900
H	7.70384800	-1.96027700	-2.17341700	C	-3.48077000	5.97577900	-1.15679800
H	6.05300400	-1.48778600	-2.63450000	H	-2.20451200	4.27719200	-0.79804900
C				C	-3.96817400	7.18632000	-0.66067300
H				H	-3.94799800	8.57242700	0.99139800
<b>8a'</b>				H	-3.77918500	5.62232000	-2.14310300
C	-4.28824500	1.24807200	-0.48753800	H	-4.65590200	7.78470300	-1.25679600
C	-4.27339500	-0.18299800	-0.87791400	H	4.09501300	2.85600300	4.11225900
C	-3.69529900	-1.05585200	0.16933000	H	2.30851600	2.00379700	-2.19433800
C	-2.55191600	0.83845200	1.14993900	H	2.18234400	-3.47838800	5.24984800
C	-3.45673100	1.72818000	0.45365800	H	0.25308200	-4.39766600	-1.00670100
H	-4.90232800	1.93395700	-1.06864000	H	-3.55699200	-0.22216600	-1.73286100
N	-1.46747900	1.19664700	1.82773200	C	-2.25532400	-1.49425100	2.16887400
C	-0.96970200	2.50056800	1.95586300	H	-1.17281500	-1.63590200	1.97877800
O	0.21429400	2.64274100	2.23446800	H	-2.29367700	-0.97036100	3.13753300
C	-2.85371800	-0.58959300	1.11997900	H	3.94865500	-2.11236300	0.09520000
C	4.15208300	-0.77546500	0.99607500	H	-3.40493900	2.79191700	0.63938200
C	1.96673300	-0.62068700	1.58901600	O	-5.52685400	-0.70558200	-1.29132000
C	3.68744600	-2.03727300	1.15939100	C	-5.92448500	-0.23155200	-2.55911800
N	3.10213600	0.08338100	1.27363100	H	-5.15463900	-0.43557700	-3.32044800
N	2.34806900	-1.93618200	1.51695800	H	-6.84311300	-0.76396700	-2.81736900
Cu	0.26719000	0.22585200	1.83356400	H	-6.13247400	0.84955100	-2.55703200
H	4.17550300	-2.99808400	1.06800900	C	-2.90329300	-2.86509300	2.30417400
H	5.13224300	-0.40624300	0.72729700	H	-2.66467200	-3.47786600	1.42077100
C	3.15632900	1.53252900	1.08960100	H	-3.99816400	-2.75803500	2.31479300
C	2.91322400	2.06221500	-0.19665400	C	-2.44421700	-3.57881700	3.56190400
C	3.45693500	2.37015700	2.18681000	H	-2.85630300	-4.59254600	3.63028900
C	2.88753300	3.45565200	-0.33044900	H	-1.35114600	-3.66446700	3.58947600
C	3.43361600	3.75146600	1.97535200	H	-2.75464200	-3.03035900	4.46121500
C	3.13201300	4.29964800	0.73871500	H			
H	2.65712900	3.86886900	-1.31205300	H			
H	3.65014700	4.40420800	2.82112200	H			
H	3.09584600	5.38036800	0.60798300	C	2.58028500	-3.72363400	2.67102600
C	1.58819300	-3.12359700	1.89073400	C	3.64941400	-3.46654800	1.80907700
C	0.96050800	-3.90757400	0.89285800	C	3.84755700	-2.21244100	1.25085000
C	1.61404800	-3.54837200	3.24016400	C	2.83832600	-1.18903800	1.47914200
C	0.39800800	-5.13057600	1.28071200	C	1.82537000	-1.46197400	2.47524000
C	1.05051900	-4.79192200	3.55013600	C	1.66837500	-2.71231400	3.01479400
C	0.45673900	-5.58949300	2.58626000	H	2.46010300	-4.72237400	3.08945400
H	-0.09023500	-5.73416800	0.51575600	H	4.36109900	-4.26066500	1.59733100
H	1.07250100	-5.12074200	4.58938800	H	1.16389600	-0.64788700	2.76094200
H	0.02669800	-6.55343500	2.85413200	H	0.87699700	-2.90597500	3.73492500
C	2.75044600	1.28544200	-1.49170100	N	2.86939000	-0.05721700	0.79680100

C	1.71763700	0.74219300	0.70542800	H	5.44940300	-2.36698600	3.91859100
O	1.74128100	1.95396700	0.80065300	H	4.66362400	-1.47453400	5.29489000
O	0.63850400	0.01515100	0.37806700	C	4.96356600	-1.92427100	0.32328600
C	-0.49632100	0.77677800	-0.09727200	H	5.41594900	-0.95530300	0.60730200
H	-0.09754000	1.63187400	-0.65770700	H	4.52158700	-1.71954500	-0.66225300
H	-1.04748400	1.16935600	0.76716500	C	6.04146300	-2.9850400	0.18941400
C	-1.34076300	-0.11593300	-0.94782100	H	6.48659900	-3.20093800	1.17421900
C	-0.75900200	-0.36278000	-1.97892100	H	5.59335300	-3.92709200	-0.15880100
C	-2.72154600	-0.17730800	-0.75181800	C	7.11403200	-2.53906600	-0.78615500
C	-1.55619700	-1.65378200	-2.79977900	H	7.58153900	-1.60681800	-0.44834300
H	0.31929700	-0.82785000	-2.12619500	H	7.90490100	-3.28985700	-0.90093300
C	-3.51994600	-0.96421900	-1.58063500	H	6.68800500	-2.33820100	-1.77728100
H	-3.17654700	0.39745600	0.05633500				
C	-2.93727500	-1.70394300	-2.60670200				
H	-1.09382800	-2.23118000	-3.59867500				
H	-4.59646800	-1.00289100	-1.41972300	C	-4.28919800	1.03429500	-0.86924200
H	-3.55780300	-2.32192300	-3.25406400	C	-4.39482000	-0.30053700	-0.96976400
C	7.05254000	4.26268900	0.22896600	C	-3.72298400	-1.14237400	-0.01789600
C	5.30343000	2.79922700	0.22494000	C	-2.53490000	0.72589900	0.93382500
C	5.98230300	4.91045900	0.73914300	C	-3.46656100	1.67308200	0.20039800
N	6.63370700	2.97787800	-0.08330400	H	-4.82368700	1.70459300	-1.53984500
N	4.92319500	4.01570800	0.73412200	H	-2.87082900	2.47548700	-0.25462000
Cu	4.24217600	1.17251200	-0.07067100	N	-1.49570900	1.11899700	1.64406600
H	5.86161200	5.92057400	1.10538000	C	-1.01301300	2.43042800	1.79504800
H	8.06988300	4.58377000	0.05349000	O	0.12492100	2.56684300	2.23227900
C	7.53427700	1.99763900	-0.67412000	C	-2.83937300	-0.68676000	0.92136100
C	8.33996800	1.20028700	0.17540400	C	4.16843000	-0.70080700	1.05518900
C	7.66470000	1.94101700	-2.08242900	C	1.96907200	-0.63006800	1.60998600
C	9.24866500	0.32317200	-0.42722100	C	3.74016100	-1.98045500	1.17470400
C	8.57269000	1.01380900	-2.61024400	N	3.08735500	0.11719200	1.33744100
C	9.36073100	0.21066900	-1.80348300	N	2.39166200	-1.93067800	1.50700900
H	9.87104300	-0.29625000	0.21871300	Cu	0.24260000	0.16974700	1.82012700
H	8.66507800	0.94726500	-3.69369200	H	4.26013600	-2.92279000	1.06800900
H	10.06194200	-0.49644000	-2.24392800	H	5.14126300	-0.29371600	0.81576100
C	3.62571900	4.43595800	1.24232600	C	3.09981000	1.57181600	1.19445100
C	3.35786700	4.30621900	2.62049600	C	2.86046900	2.12886900	-0.07990600
C	2.71982100	5.07454500	0.36988200	C	3.36095700	2.38745600	2.31891300
C	2.14863800	4.82250400	3.09925700	C	2.81211500	3.52497300	-0.17938100
C	1.52293200	5.56749500	0.91609800	C	3.30953600	3.77258800	2.14272600
C	1.23756700	5.44966400	2.26519300	C	3.02190700	4.34617000	0.91387400
H	1.93112700	4.71856400	4.16277100	H	2.59049700	3.95802400	-1.15443800
H	0.81948700	6.05145900	0.24550100	H	3.49534800	4.40788100	3.00888700
H	0.30581100	5.84713700	2.66477400	H	2.96910800	5.42913600	0.80916100
C	8.35178000	1.20627800	1.69937400	C	1.65996900	-3.14968200	1.83193800
C	8.83249000	2.52269200	2.31077900	C	1.09081900	-3.93269400	0.79871500
C	7.06548800	0.67848000	2.32979800	C	1.65503700	-3.60009300	3.17319300
H	9.79333400	2.82791400	1.87653800	C	0.55363600	-5.17924100	1.14546100
H	8.12778400	3.34663100	2.17320700	C	1.11711000	-4.86423300	3.44211300
H	8.97681100	2.39962700	3.39176300	C	0.58037600	-5.66029300	2.44421900
H	6.90194500	-0.37476300	2.06870600	H	0.11028600	-5.78309400	0.35384000
H	7.11530300	0.73810000	3.42543400	H	1.11446000	-5.21191300	4.47546000
H	6.17341000	1.22855400	2.01418000	H	0.16986700	-6.64111300	2.67936900
C	6.98481100	2.84068300	-3.10803900	C	2.73159400	1.38708400	-1.39896000
C	7.41394700	4.30554800	-2.99598900	C	4.11314500	1.07045700	-1.97764800
H	7.07977900	4.85591900	-3.88460600	C	1.84279500	0.16109400	-1.40825700
H	6.98355300	4.81316400	-2.12771000	H	4.75551100	1.95897400	-2.01720700
H	8.50616600	4.40007900	-2.93441300	H	4.63189100	0.30544500	-1.38285500
C	4.19765000	3.56748400	3.64753500	H	4.01486300	0.67687400	-2.99723900
C	3.88152600	2.07534500	3.59008500	H	0.88806300	0.35960000	-0.91248500
C	5.70215800	3.80380000	3.63574300	H	1.60634000	-0.11999700	-2.44142800
H	2.81589000	1.88226700	3.76566400	H	2.31925900	-0.69957000	-0.93048100
H	4.12473100	1.65125400	2.60800900	C	3.70289300	1.91591400	3.72133900
H	4.45518400	1.51337100	4.33701000	C	2.50092500	1.31868200	4.44709700
H	5.96230900	4.86815200	3.57234300	C	4.96746500	1.06097700	3.79984400
H	6.14093500	3.40688700	4.56067400	H	1.68766700	2.05095300	4.50840500
H	6.19269800	3.28367700	2.80979500	H	2.09862100	0.44474000	3.92852300
C	2.84433800	5.19323300	-1.13954700	H	2.77309500	1.01114300	5.46618500
C	4.17498100	5.68075000	-1.69960600	H	5.81487200	1.58234000	3.33670000
C	2.40601500	3.88036800	-1.78399500	H	5.22759400	0.86595100	4.84840300
H	4.53747400	6.58012100	-1.18494500	H	4.86960200	0.08931000	3.30807100
H	4.95561100	4.91919700	-1.64484700	C	0.94737100	-3.54036500	-0.66214800
H	4.05376800	5.92950400	-2.76186400	C	-0.03723600	-2.38214400	-0.82732800
H	1.37370500	3.63022800	-1.51426200	C	2.26511200	-3.38165100	-1.41964500
H	2.48000000	3.92408600	-2.87819500	H	-1.04710900	-2.69880700	-0.53337000
H	3.01986200	3.03944900	-1.44349500	H	0.21842700	-1.51704000	-0.20602600
B	3.19550900	-0.21129200	-2.47521400	H	-0.08621700	-2.03112700	-1.86444900
F	2.75572400	-1.44087200	-1.98252000	H	2.86814000	-4.29562200	-1.33798200
F	3.23667200	-0.17008200	-3.84717300	H	2.06087100	-3.20911200	-2.48337400
F	2.39524800	0.83100300	-1.94566700	H	2.87820400	-2.54707900	-1.07332900
F	4.53694600	0.03013700	-1.94805000	C	2.07575700	-2.80599500	4.39822300
H	3.83803400	3.93797200	4.62023000	C	3.42198000	-2.09853700	4.34292400
H	2.10175900	5.95592200	-1.42109600	C	0.93503000	-1.86942300	4.80944100
H	9.13012900	0.47408200	1.96289900	H	4.22086800	-2.76826700	4.00052200
C	5.47360300	2.67595900	-3.21842300	H	3.41264300	-1.22486600	3.69078800
H	5.20115400	1.67022600	-3.54822200	H	3.69214200	-1.74051600	5.34461100
H	4.96433400	2.84547500	-2.26611400	H	0.02437600	-2.43821500	5.03565700
H	5.06982600	3.39655800	-3.94169600	H	1.20502800	-1.28358200	5.69716300
H	7.39238800	2.49865700	-4.07110500	H	0.68595600	-1.16312700	4.00389600
O	4.09334100	-0.87737700	3.44354700	B	-0.96980600	1.98585200	-2.00290900
C	4.52199200	-1.85298000	4.25905900	F	-0.05863300	1.88355100	-3.04693600
H	3.75280900	-2.66617200	4.38564300	F	-0.35457300	2.62767900	-0.88356900

F	-2.09728100	2.73335000	-2.38900800	O	-1.19392200	-1.17646700	-0.24209500
F	-1.38818500	0.69724000	-1.57605800	C	-1.09138700	-2.38693200	-0.97799300
O	-1.82011800	3.43456000	1.48789400	H	-1.65229800	-2.33480400	-1.91911500
C	-1.16353600	4.74003900	1.44242200	H	-0.02853900	-2.50618000	-1.18964700
H	-0.19986000	4.59515800	0.94328600	H	-1.43999900	-3.24163800	-0.38166300
H	-0.98484000	5.06434700	2.47457800	C	-3.08839100	-1.95803200	1.52488000
C	-2.07143300	5.65513600	0.69302500	H	-3.48346400	-2.97095800	1.42176000
C	-2.84848700	6.60640600	1.35611800	H	-2.05146800	-2.00677700	1.87948900
C	-2.19019500	5.51144600	-0.69422400	H	-3.69949300	-1.34089100	2.18092400
C	-3.73923100	7.40795900	0.64396000	C	-1.03437800	2.20303400	1.77463900
H	-2.76137400	6.71246700	2.43827900	O	-0.34112300	2.46419200	2.74210100
C	-3.08678800	6.30449700	-1.40364500	O	-1.61966600	3.19425300	1.01530700
H	-1.60419600	4.74774300	-1.20471700	C	-1.34353700	4.52363600	1.44621000
C	-3.86181600	7.25387300	-0.73612000	H	-0.26754300	4.72247200	1.32896200
H	-4.34196600	8.14916400	1.16710600	H	-1.55193900	4.60934900	2.52155400
H	-3.18235700	6.17357200	-2.48034900	C	-2.16657800	5.49226600	0.65006000
H	-4.56237700	7.87535200	-1.29253400	C	-2.92752400	5.10055900	-0.45369500
H	3.95061300	2.83867300	4.26768700	C	-2.16256000	6.84131200	1.02251300
H	2.25131000	2.10431000	-2.07743600	C	-3.66900400	6.04141600	-1.16816700
H	2.16373700	-3.55562700	5.19928100	H	-2.93488300	4.05350000	-0.74813100
H	0.46419100	-4.41076500	-1.13162400	C	-2.89987900	7.78002000	0.30838600
H	-5.01242400	-0.76407100	-1.73660600	H	-1.57412000	7.15610900	1.88568500
C	-2.22973900	-1.59038600	1.95767900	C	-3.65862900	7.38203900	-0.79241600
H	-1.14946700	-1.73876900	1.76216800	H	-4.25833600	5.72181200	-2.02680900
H	-2.25954700	-1.06838900	2.92824400	H	-2.88532600	8.82533100	0.61349700
H	-3.94324800	-2.20984300	-0.04807900	H	-4.23832400	8.11435200	-1.35234700
O	-4.31556500	2.22034500	1.22171800				
C	-4.97841600	3.39727300	0.80446500				
H	-5.40258300	3.84788100	1.70646600				
H	-4.27692400	4.10556200	0.33983000	N	-3.24835300	1.02567300	0.26182500
H	-5.79445400	3.18193200	0.09732200	N	-3.27842500	2.35163600	0.00861900
C	-2.88064700	-2.95915400	2.10304200	C	-2.38535800	2.97730700	-0.54704200
H	-2.664456200	-3.57238600	1.21413900	O	-4.10413700	0.37803300	1.07148000
H	-3.97477800	-2.84770100	2.13845300	C	-4.09098500	-1.05451500	0.99190700
C	-2.39835900	-3.67806400	3.34906600	C	-4.97190200	0.87868500	2.07718600
H	-2.80895000	-4.69213800	3.42138200	C	-5.05293100	-1.93215600	1.72945900
H	-1.30493300	-3.76321400	3.35618900	C	-5.84820300	0.09054200	2.86301400
H	-2.69205600	-3.13280300	4.25583300	C	-4.92404300	-1.25550400	2.71525100
				H	-6.48110200	0.60173800	3.58762900
				H	-6.62890100	-1.86898600	3.27209900
<b>4s</b>				H	-5.90537400	-2.73531400	0.72073200
C	-5.12035500	-0.11886200	1.60697500	C	-6.55506200	-2.06316700	0.15053000
C	-5.04793400	-1.37662600	0.89624600	H	-5.26444400	-3.28458300	0.02538900
C	-3.89402000	-1.78495300	0.34079400	H	-6.53821600	-3.44889800	1.25708400
C	-2.61222700	-1.00827200	0.44141800	H	-3.27772100	-1.78551000	0.26976000
C	-2.77262800	0.35170600	1.13115700	O	-2.18263900	-1.31674000	-0.55782700
C	-4.04952500	0.70320800	1.71387200	C	-2.56102400	-0.71051700	-1.37886700
H	-6.07199700	0.17803900	2.04663900	H	-1.49048000	-0.71949100	0.03298800
H	-5.95054500	-1.97874500	0.80522300	H	-1.72687800	-2.24520900	-0.90901600
H	-3.84561100	-2.72579300	-0.20809400	H	-4.46140000	2.98947900	0.36508500
H	-4.12839700	1.65989800	2.22857300	O	-4.53477400	4.36531200	0.00751200
N	-1.71614900	1.08528700	1.17971500	C	-3.69260600	4.90886000	0.45704200
O	-2.15277800	-0.68967700	-0.88390300	H	-4.40972000	4.46071300	-1.08141800
C	-1.56400300	-1.74418400	-1.60832700	C	-5.85007700	4.92767100	0.45834200
H	-2.20985500	-2.63498300	-1.67122400	C	-6.94985800	4.11427800	0.74565600
H	-1.40968000	-1.36011800	-2.61975200	C	-5.99458700	6.31510700	0.56508700
H	-0.59087400	-2.04119800	-1.19043800	C	-8.16544400	4.67833700	1.12977500
C	-1.71189000	2.29703700	1.85047500	C	-6.84464800	3.03390100	0.66698400
O	-1.38883500	2.44733300	3.01217400	H	-7.20927700	6.87949200	0.94265200
O	-2.02427700	3.30676200	1.00807700	C	-5.14057200	6.95894500	0.35000100
C	-1.90546200	4.62164800	1.57602600	H	-8.30145200	6.06112500	1.22846900
H	-0.89169500	4.72738800	1.98723100	C	-9.01030300	4.03118100	1.35287600
H	-2.59828200	4.71449000	2.42275900	H	-7.30185000	7.96177300	1.02121800
C	-2.18941000	5.64119600	0.51685000	H	-9.25166800	6.49936400	1.53001700
C	-1.96626600	5.37732100	-0.83691200	H	-4.42682100	-2.66790400	2.26196500
C	-2.64769500	6.90628300	0.89548300				
C	-2.19502700	6.36529900	-1.79191200				
H	-1.62500700	4.38900600	-1.13783700				
C	-2.86837500	7.89604300	-0.05851400				
H	-2.83519400	7.11701300	1.94932500	C	3.99491500	-3.88841600	0.59344400
C	-2.64276700	7.62747700	-1.40734200	C	4.88166400	-2.96146700	1.02333800
H	-2.02218200	6.14583800	-2.84455000	C	4.48985100	-1.51646700	1.02396700
H	-3.22595100	8.87648600	0.525264200	C	3.05516300	-1.19369800	0.61768000
H	-2.81984900	8.39782300	-2.15604200	C	2.21505300	-2.23743000	0.13618700
C	-1.58816200	-1.81290500	1.24323800	C	2.68498400	-3.51964600	0.12652100
H	-1.44299000	-2.81490700	0.82377400	H	4.27445000	-4.94201200	0.58223500
H	-0.63481400	-1.27219600	1.25744000	H	1.23240300	-1.99567500	-0.25138000
H	-1.93072600	-1.92957500	2.27764900	H	2.04187700	-4.30795800	-0.26306000
				N	2.80582400	0.09058200	0.74110600
				C	1.59378900	0.73914800	0.49199800
				O	1.59051000	1.92992300	0.23203400
				O	0.49758000	-0.00477000	0.67480300
				C	-0.73455600	0.67558200	0.31606000
				H	-0.60180700	1.07113800	-0.69725100
				H	-0.87473900	1.52132900	1.00037000
				C	-1.84597900	-0.31611300	0.40644600
				C	-1.96145900	-1.33496000	-0.54630700
				C	-2.78175900	-0.24035000	1.43912300
				C	-2.99505200	-2.26263600	-0.45917700
				H	-1.23401400	-1.38753900	-1.35794000
				C	-3.82147200	-1.16388400	1.52449600
				H	-2.69283300	0.55268600	2.18246200

C	-3.92786800	-2.17772100	0.57557600	C	3.79888700	0.28124000	1.62594000
H	-3.08098500	-3.04989000	-1.20670500	C	1.54505300	-0.02787200	1.48308600
H	-4.54846600	-1.09180500	2.33207000	C	3.57695400	-1.05249200	1.66936900
H	-4.73951700	-2.90114500	0.63824100	N	2.56240500	0.89974500	1.52632400
C	7.14076800	4.37807600	0.48703100	N	2.20501500	-1.23541500	1.57004100
C	5.36686200	2.95600000	0.35521900	Cu	-0.35658400	0.31748900	1.34689900
C	6.03193200	5.08057700	0.81853500	H	4.25544100	-1.88869800	1.76732800
N	6.72966100	3.08075500	0.20657300	H	4.71315200	0.85552400	1.68153700
N	4.95943600	4.20644700	0.73378400	C	2.41968200	2.34247800	1.35415100
Cu	4.22497800	1.41028500	0.18241200	C	2.49781500	2.88488800	0.05417800
H	5.89852600	6.11638300	1.09960600	C	2.24548700	3.17168100	2.48575000
H	8.17950800	4.67133700	0.42123700	C	2.27723900	4.25896500	-0.09289300
C	7.62924200	2.01082900	-0.20296800	C	2.03418500	4.53562700	2.26498600
C	8.22755700	1.18829400	0.78157300	C	2.02118400	5.07987600	0.99054800
C	7.91830500	1.83150600	-1.57734200	H	2.28831800	4.67231400	-1.10081600
C	9.04894500	0.14060600	0.34950800	H	1.86508600	5.17489400	3.13165000
C	8.75749900	0.76799300	-1.93386200	H	1.82630000	6.14212600	0.84538700
C	9.30764700	-0.08609500	-0.99233200	C	1.60247700	-2.55207700	1.68540100
H	9.49714500	-0.50544100	1.10499100	C	1.55532500	-3.40170600	0.55268100
H	8.97193400	0.61733400	-2.99171400	C	1.14806900	-2.99737700	2.94797900
H	9.94746500	-0.91142500	-1.30113500	C	1.00543200	-4.67891300	0.71404600
C	3.59559700	4.61334100	1.03037400	C	0.59714000	-4.28369500	3.03139500
C	3.11314200	4.50431900	2.35307600	C	0.51901700	-5.12366500	1.93418700
C	2.80450100	5.16697900	0.00006000	H	0.96305700	-5.33268900	-0.15724600
C	1.82126700	4.97327300	2.61585500	H	0.23540600	-4.62293100	4.00257600
C	1.52363600	5.61840300	0.33650200	H	0.09716000	-6.12310400	2.03124700
C	1.02788600	5.53009000	1.62640600	C	2.89876500	2.15816600	-1.21856000
H	1.44068400	4.88760200	3.63437300	C	4.42343600	2.05199400	-1.32222400
H	0.90331600	6.03730300	-0.45616800	C	2.24863000	0.81496000	-1.48357100
H	0.02742100	5.89183300	1.85930900	H	4.91274800	3.02255800	-1.17382000
C	8.08587700	1.31856600	2.29091700	H	4.82795100	1.35262800	-0.57784600
C	8.53556100	2.66251200	2.86206800	H	4.71237700	1.67244200	-2.31118600
C	6.71773600	0.86682200	2.79352900	H	1.16591600	0.84941000	-1.33636300
H	9.54218000	2.92030000	2.50824300	H	2.43577500	0.51249600	-2.52310200
H	7.87079700	3.49073800	2.60625200	H	2.66126900	0.02839800	-0.84622000
H	8.57122400	2.60511800	3.95753000	C	2.27885600	2.74465500	3.94355000
H	6.56716700	-0.19481200	2.56351600	C	1.01108000	2.00666300	4.34770300
H	6.63359200	1.00521200	3.87984100	C	3.56980700	2.04838900	4.37207000
H	5.89754200	1.41122200	2.31424200	H	0.12806600	2.63463200	4.18717700
C	7.41326800	2.67594600	-2.73824700	H	0.84719400	1.10268500	3.75386900
C	7.81583500	4.14879700	-2.67209200	H	1.03864000	1.71420600	5.40698200
H	7.59716700	4.63252800	-3.63248900	H	4.44947600	2.64072300	4.08710400
H	7.27931100	4.71149900	-1.90419200	H	3.58514900	1.93267800	5.46382300
H	8.89150100	4.25806300	-2.48004600	H	3.68928500	1.04945200	3.94413900
C	3.79845200	3.83465600	3.53483900	C	1.96997000	-3.05040200	-0.86777200
C	3.45057100	2.34429000	3.55153100	C	0.94020800	-2.11086900	-1.49694500
C	5.29402500	4.05411700	3.70862200	H	-0.01488700	-2.63253900	-1.62714300
H	2.36515000	2.19004300	3.59132700	H	0.73493400	-1.23495400	-0.87174800
H	3.81061200	1.84468000	2.64189600	H	1.27424700	-1.75171300	-2.47875200
H	3.90384200	1.84466500	4.41857900	C	1.12723700	-2.21978100	4.25562900
H	5.57215000	5.11270800	3.63248800	C	2.32468400	-1.33270400	4.55894100
H	5.60565000	3.69804200	4.69953500	C	-0.18931800	-1.45467000	4.38614700
H	5.88009700	3.49655800	2.97553100	H	3.27798900	-1.85589800	4.41055100
C	3.13529200	5.22367000	-1.48223900	H	2.33455600	-0.42717000	3.95057800
C	4.54623600	5.63337600	-1.87978600	H	2.28144100	-1.00544000	5.60558000
C	2.73545200	3.89925500	-2.13369100	H	-1.05188900	-2.13214400	4.32145000
H	4.88496400	6.53745700	-1.35707900	H	-0.24689000	-0.92121500	5.34353900
H	5.27309400	4.83968500	-1.69490300	H	-0.30244100	-0.70219800	3.59468700
H	4.57469400	5.83970000	-2.95747800	B	-1.04667000	2.35490300	-0.97711600
H	1.67364200	3.67685700	-1.98106800	F	-0.10366800	2.97028200	-1.78712600
H	2.93731400	3.90788000	-3.21201400	F	-0.62969400	2.41379200	0.39168200
H	3.28778200	3.05873600	-1.69953400	F	-2.29764300	2.95430700	-1.09088800
B	2.60786800	0.08705400	-2.75294300	F	-1.13881200	0.96455300	-1.31058500
F	3.12916100	-1.15554300	-3.12181200	C	-3.24360900	0.24257600	0.51897900
F	2.39896100	0.91262000	-3.83771800	C	-2.92055700	-0.82336500	-0.41252500
F	1.42827600	-0.09382000	-2.00332000	C	-4.27768200	1.11007000	0.12065300
F	3.59161400	0.72121900	-1.87750100	C	-3.51978300	-0.87076600	-1.74256300
H	3.32017700	4.27984500	4.42126800	C	-4.84185800	1.06010900	-1.15260600
H	2.46703200	6.00004900	-1.88648300	H	-4.55684700	1.91888000	0.78423600
H	8.80541100	0.58885000	2.69276200	C	-4.45926000	0.12841100	-2.09727400
C	5.93027900	2.46230200	-3.02165600	H	-5.57423800	1.81997600	-1.41871900
H	5.71424700	1.41911500	-3.27798300	H	-4.87214600	0.12327500	-3.10252500
H	5.29895400	2.70341500	-2.16293800	C	-2.96396300	-1.83154300	-2.74650200
H	5.60153700	3.08731800	-3.86207500	H	-2.72581100	-2.80430500	-2.30860400
H	7.94919700	2.27599800	-3.61231300	H	-3.65965400	-1.97111900	-3.57871900
O	5.40460600	-0.71323200	0.25503200	H	-2.02737800	-1.41606300	-3.13822000
C	5.64145900	-1.20567000	-1.07449900	O	-1.97667500	-1.74097400	-0.17832400
H	4.70878800	-1.43132700	-1.60310400	H	-4.07809300	-1.46323600	-0.75094100
H	6.15375700	-0.39246000	-1.59510000	O	-3.84964500	1.66382600	2.81153000
H	6.29493200	-2.08927700	-1.04987500	C	-3.92117800	2.67358900	3.82948200
C	6.25452200	-3.27934500	1.50341800	H	-3.63048800	2.23993400	4.79445200
H	6.47641400	-4.34804400	1.41900800	H	-4.98788100	2.92468600	3.86868500
H	7.01735900	-2.71909300	0.94445700	C	-3.07319400	3.87793900	3.51549000
H	6.37971500	-2.98722900	2.55680300	C	-2.56849000	4.10781300	2.23464400
H	4.61824900	-1.11361800	2.04429300	C	-2.76872700	4.78309300	4.53640200
				C	-1.76227800	5.21388600	1.97954700
				H	-2.76276300	3.40975600	1.42251700
				C	-1.97728800	5.89967200	4.27928800
				H	-3.14274900	4.60420400	5.54600800
				C	-1.46726100	6.11544300	2.99910600
				H	-1.35396800	5.34726700	0.97870000

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H	-1.74549800	6.59465900	5.08585300	H	5.60565000	3.69804200	4.69953500
H	-0.83294600	6.97934200	2.80073900	H	5.88009700	3.49655800	2.97553100
C	-1.98636900	-2.44617300	1.07920400	C	3.13529200	5.22367000	-1.48223900
H	-2.97505000	-2.39489600	1.54824100	C	4.54623600	5.63337600	-1.87978600
H	-1.72798500	-3.48159500	0.83716800	C	2.73545200	3.89925500	-2.13369100
H	-1.23957000	-2.01370200	1.75276900	H	4.88496400	6.53745700	-1.35707900
H	2.26858600	3.69251400	4.50331000	H	5.27309400	4.83968500	-1.69490300
H	2.57009600	2.82300700	-2.02883600	H	4.57469400	5.83970000	-2.95747800
H	1.12123100	-2.99852900	5.03448100	H	1.67364200	3.67685700	-1.98106800
C	3.42130600	-2.61923500	-1.07344200	H	2.93731400	3.90788000	-3.21201400
H	3.65108200	-1.62487600	-0.68506900	H	3.28778200	3.05873600	-1.69953400
H	4.11374800	-3.33181100	-0.60580900	B	2.60786800	0.08705400	-2.75294300
H	3.64201700	-2.60060700	-2.14815000	F	3.12916100	-1.15554300	-3.12181200
H	1.88829400	-4.00289600	-1.41349100	F	2.39896100	0.91262000	-3.83771800
H				F	1.42827600	-0.09382000	-2.00332000
H				F	3.59161400	0.72121900	-1.87750100
<b>6</b>				H	3.32017700	4.27984500	4.42126800
C	3.99491500	-3.88841600	0.59344400	H	2.46703200	6.00004900	-1.88648300
C	4.88166400	-2.96146700	1.02333800	H	8.80541100	0.58885000	2.69276200
C	4.48985100	-1.51646700	1.02396700	C	5.93027900	2.46230200	-3.02165600
C	3.05516300	-1.19369800	0.61768000	H	5.71424700	1.41911500	-3.27798300
C	2.21505300	-2.23743000	0.13618700	H	5.29895400	2.70341500	-2.16293800
C	2.68498400	-3.51964600	0.12652100	H	5.60153700	3.08731800	-3.86207500
H	4.27445000	-4.94201200	0.58223500	H	7.94919700	2.27599800	-3.61231300
H	1.23240300	-1.99567500	-0.25138000	O	5.40460600	-0.71323200	0.25503200
H	2.04187700	-4.30795800	-0.26306000	C	5.64145900	-1.20567000	-1.07449900
N	2.80582400	0.909058200	0.74110600	H	4.70878800	-1.43132700	-1.60310400
C	1.59378900	0.73914800	0.49199800	H	6.15375700	-0.39246000	-1.59510000
O	1.59051000	1.92992300	0.23203400	H	6.29493200	-2.08927700	-1.04987500
O	0.49758000	-0.00477000	0.67480300	C	6.25452200	-3.27934500	1.50341800
C	-0.73455600	0.67558200	0.31606000	H	6.47641400	-4.34804400	1.41900800
H	-0.60180700	1.07113800	-0.69725100	H	7.01735900	-2.71909300	0.94445700
H	-0.87473900	1.52132900	1.00037000	H	6.37971500	-2.98722900	2.55680300
C	-1.84597900	-0.31611300	0.40644600	H	4.61824900	-1.11361800	2.04429300
C	-1.96145900	-1.33496000	-0.54630700				
C	-2.78175900	-0.24035000	1.43912300				
C	-2.99505200	-2.26263600	-0.45917700				
H	-1.23401400	-1.38753900	-1.35794000				
C	-3.82147200	-1.16388400	1.52449600				
H	-2.69283300	0.55268600	2.18246200				
C	-3.92786800	-2.17772100	0.57557600				
H	-3.08098500	-3.04989000	-1.20670500				
H	-4.54846600	-1.09180500	2.33207000				
H	-4.73951700	-2.90114500	0.63824100				
C	7.14076800	4.37807600	0.48703100				
C	5.36686200	2.95600000	0.35521900				
C	6.03193200	5.08057700	0.81853500				
N	6.72966100	3.08075500	0.20657300				
N	4.95943600	4.20644700	0.73378400				
Cu	4.22497800	1.41028500	0.18241200				
H	5.89852600	6.11638300	1.09960600				
H	8.17950800	4.67133700	0.42123700				
C	7.62924200	2.01082900	-0.20296800				
C	8.22755700	1.18829400	0.78157300				
C	7.91830500	1.83150600	-1.57734200				
C	9.04894500	0.14060600	0.34950800				
C	8.75749900	0.76799300	-1.93386200				
C	9.30764700	-0.08609500	-0.99233200				
H	9.49714500	-0.50544100	1.10499100				
H	8.97193400	0.61733400	-2.99171400				
H	9.94746500	-0.91142500	-1.30113500				
C	3.59559700	4.61334100	1.03037400				
C	3.11314200	4.50431900	2.35307600				
C	2.80450100	5.16697900	0.00006000				
C	1.82126700	4.97327300	2.61585500				
C	1.52363600	5.61840300	0.33650200				
C	1.02788600	5.53009000	1.62640600				
H	1.44068400	4.88760200	3.63437300				
H	0.90331600	6.03730300	-0.45616800				
H	0.02742100	5.89183300	1.85930900				
C	8.08587700	1.31856600	2.29091700				
C	8.53556100	2.66251200	2.86206800				
C	6.71773600	0.86682200	2.79352900				
H	9.54218000	2.92030000	2.50824300				
H	7.87079700	3.49073800	2.60625200				
H	8.57122400	2.60511800	3.95753000				
H	6.56716700	-0.19481200	2.56351600				
H	6.63359200	1.00521200	3.87984100				
H	5.89754200	1.41122200	2.31424200				
C	7.41326800	2.67594600	-2.73824700				
C	7.81583500	4.14879700	-2.67209200				
H	7.59716700	4.63252800	-3.63248900				
H	7.27931100	4.71149900	-1.90419200				
H	8.89150100	4.25806300	-2.48004600				
C	3.79845200	3.83465600	3.53483900				
C	3.45057100	2.34429000	3.55153100				
C	5.29402500	4.05411700	3.70862200				
H	2.36515000	2.19004300	3.59132700				
H	3.81061200	1.84468000	2.64189600				
H	3.90384200	1.84466500	4.41857900				
H	5.57215000	5.11270800	3.63248800				

H	-5.93874800	-3.63255100	1.77844400	H	4.18268200	1.81154200	-0.21280900
O	-2.96618800	-1.58272400	0.29605800	C	0.92511100	3.30292600	1.25562700
C	-3.46864700	-1.50261900	-1.02605500	H	0.06760400	1.35450700	0.91612200
H	-4.52680100	-1.81240100	-1.07487300	C	2.05933200	4.10464600	1.13460700
H	-3.37319100	-0.48625200	-1.42963200	H	4.12280400	4.18125100	0.51685600
H	-2.86573900	-2.18983600	-1.62446500	H	0.00460700	3.71351300	1.67153400
O	-2.83433700	2.93880400	-0.95267000	H	2.02970100	5.14740800	1.44736300
C	-2.65901500	4.34847500	-1.13464000	H	-0.24643200	0.00520300	2.59641100
H	-3.49055500	4.88124300	-0.65330200				
H	-1.74740500	4.65491900	-0.60267300				
C	-2.57944600	4.66232300	-2.59737200				
C	-2.40974700	3.67511700	-3.56990600				
C	-2.65218000	6.00149000	-2.99488700				
C	-2.31533200	4.02470100	-4.91651300				
H	-2.35745900	2.63222400	-3.26594600				
C	-2.55234400	6.34998000	-4.33775300				
H	-2.78958100	6.77871000	-2.24172100				
C	-2.38420900	5.35979800	-5.30535500				
H	-2.18570200	3.24525500	-5.66595700				
H	-2.61042700	7.39711100	-4.63074600				
H	-2.31050300	5.62951100	-6.35763500				
H	-3.20701700	-1.00652200	2.18244100				
<b>6s-N</b>							
N	-0.95377300	-0.04328000	-1.39678600	H	-2.33023100	-4.39404800	2.00752500
C	-1.56152100	1.15754600	-1.07587100	H	-3.45780500	-5.45175300	1.12313200
O	-2.29977300	1.39756700	-0.13216200	O	-2.21617400	-1.78186200	1.08784700
C	-1.55792300	-1.17774400	-1.21336100	C	-1.83539100	-1.52360900	-0.25832700
C	-0.67840900	-2.41866400	-1.30381000	H	-2.10292500	-2.37127200	-0.90820500
C	-2.95350700	-1.38288200	-0.92195900	H	-2.31679000	-0.60958400	-0.62737000
C	-1.38500300	-3.73190700	-1.50912900	H	-0.74753200	-1.40495500	-0.25403700
C	-3.48396900	-2.63480500	-0.95851900	O	-4.09456800	2.52606600	0.78257200
H	-3.57560200	-0.51624200	-0.71901300	C	-4.66371800	3.75907900	1.18945500
C	-2.71440800	-3.80981700	-1.26950000	H	-5.65056000	3.88446900	0.71565000
H	-4.55074600	-2.75920500	-0.76708200	H	-4.85267200	3.73958000	2.27391500
H	-3.22354000	-4.77279900	-1.32329700	C	-3.74371800	4.88715900	0.82524400
C	-0.53824900	-4.90792600	-1.84432600	C	-2.55204600	4.68331300	0.12829100
H	-0.06692500	-4.79759900	-2.82938000	C	-4.08442800	6.18891400	1.21025600
H	0.29270400	-5.01186200	-1.13371900	C	-1.71511500	5.75823400	-0.16961800
H	-1.12143400	-5.83461100	-1.83996800	H	-2.28291100	3.67282800	-0.17166600
O	0.46331800	-2.27298100	-2.11801800	C	-3.25115300	7.26223400	0.91173000
C	0.14922300	-2.01815600	-3.47552700	H	-5.01396600	6.35937300	1.75711900
H	-0.57316900	-2.75333700	-3.86998800	C	-2.05827400	7.04973000	0.22066200
H	-0.25944900	-1.00740400	-3.60816000	H	-0.78355200	5.58048900	-0.70683200
H	1.08701700	-2.10719500	-4.02988600	H	-3.53264600	8.26854500	1.22041900
O	-1.09647500	2.10219900	-1.92551400	H	-1.40299700	7.88785300	-0.01308000
C	-1.39325800	3.46124700	-1.60411300	H	-3.46278800	-1.76890500	2.76446500
H	-2.31034600	3.75373700	-2.13616700	C	-6.05163500	-0.51457300	5.68053200
H	-1.60861100	3.52944400	-0.52957700	C	-5.17010200	-1.26737700	4.89615100
C	-0.23351100	4.33590300	-1.98723100	C	-3.87514700	-0.75351500	4.73178400
C	0.97307400	3.81292000	-2.44869300	C	-3.45341400	0.39657400	5.40164700
C	-0.36464200	5.72117200	-1.83930700	C	-4.35006100	1.11168200	6.18271800
C	2.03565200	4.66265300	-2.75123100	C	-5.66302600	0.66334700	6.30459600
H	1.07964400	2.73523900	-2.55518200	H	-7.07165000	-0.87926600	5.79750000
C	0.69738000	6.56823100	-2.13906300	H	-4.02003600	2.01696600	6.68371500
H	-1.30638900	6.13829200	-1.47842500	H	-6.38218000	1.22675800	6.89600500
C	1.90438300	6.04020400	-2.59777800	C	-5.60647400	-2.59292800	4.36481200
H	2.97707300	4.24014400	-3.10094400	H	-5.42546200	-3.37790200	5.11303600
H	0.58242700	7.64436200	-2.01643700	H	-6.67838300	-2.58883700	4.14228200
H	2.73736200	6.70095800	-2.83329000	H	-5.08021000	-2.90199500	3.46011400
H	-0.26094500	-2.48679200	-0.27760200	N	-2.93769800	-1.47292500	3.86422700
C	-2.49884200	-3.12132100	2.32760100	C	-1.68934600	-0.72667900	3.46913800
C	-1.11335400	-3.28064200	2.23112700	O	-0.59042500	-1.17771800	3.63150600
C	-0.31691200	-2.12508300	2.33532000	O	-2.60084400	-2.77689200	4.33920200
C	-0.89444900	-0.86653600	2.51867800	C	-2.10352400	-2.76507700	5.67874300
C	-2.27651300	-0.73172900	2.58008200	H	-1.84754400	-3.81035800	5.86218000
C	-3.07915800	-1.86678700	2.49615700	H	-1.20672400	-2.14327000	5.76428500
H	-3.13130500	-4.00475800	2.23883300	H	-2.87561000	-2.44115400	6.38838000
H	-2.71958800	0.25632800	2.68360300	O	-2.10396500	0.39627900	2.94895600
H	-4.16341300	-1.77320700	2.54352200	C	-1.18157500	1.19813700	2.16862100
C	-0.49883300	-4.62667700	2.01383100	H	-0.20422700	0.70300900	2.15617500
H	-0.20342900	-5.09464700	2.96139400	H	-1.63135400	1.17516500	1.16612000
H	-1.19922400	-5.30247200	1.50821300	C	-1.12235100	2.58616500	2.72300600
H	0.41811100	-4.55180800	1.41693000	C	0.02370800	3.35786000	2.51909200
N	1.09742500	-2.26734400	2.27259400	C	-2.22236900	3.15537400	3.37142200
C	1.98097000	-1.43763000	1.60194900	C	0.06351100	4.68643100	2.93517800
O	3.15548200	-1.30810600	1.87619000	H	0.88819100	2.91757500	2.02015500
O	1.66141400	-2.99174500	3.33464100	C	-2.17508500	4.47925400	3.79882200
C	1.78429400	-2.16861500	4.49692200	H	-3.12641200	2.56441300	3.52130700
H	2.19641300	-2.82968900	5.26300800	C	-1.03775400	5.25208100	3.57349200
H	2.47405500	-1.33792700	4.30833400	H	0.95711600	5.28251700	2.75557500
H	0.80177000	-1.79502500	4.81880500	H	-3.04613900	4.91847100	4.28543000
O	1.33822400	-0.86415700	0.55924000	H	-1.01454400	6.29501200	3.88506500
C	2.13514400	0.03028300	-0.24584800	H	-2.43215100	0.75528200	5.29767400
H	3.15484000	-0.36379700	-0.31474200				
H	1.64831200	-0.02781400	-1.22611400				
C	2.12309300	1.43182600	0.28706100	N	-1.52625300	-1.12516000	-1.84447300
C	3.26138900	2.23485100	0.18934800	C	-2.39034000	-0.08034800	-1.67313000
C	0.95627400	1.97784500	0.83017300	O	-3.60228400	-0.09712600	-1.79013700
C	3.22920200	3.56461900	0.60534800	C	-1.85430400	-2.43603700	-2.20844100

C	-0.81039300	-3.38027800	-2.17004800	C	-3.88792700	2.09317500	0.35813700
C	-3.13323900	-2.85104800	-2.59395600	H	-3.42100200	3.06391900	0.55604600
C	-1.02391200	-4.72693500	-2.47620400	H	-4.13232300	2.06187200	-0.71294500
C	-3.34551900	-4.18800400	-2.91766800	H	-4.83966100	2.05279600	0.89899700
H	-3.94314100	-2.13095300	-2.62533900	O	1.50568000	-1.63661000	1.64263000
C	-2.31287800	-5.11702400	-2.85434000	C	2.68750700	-2.43760000	1.88844500
H	-4.34368000	-4.50681800	-3.21360600	H	3.29514800	-2.44613100	0.97600200
H	-2.50120300	-6.164757800	-3.08876000	H	3.27317400	-1.95185100	2.67724800
C	0.09424800	-5.71856500	-2.37764300	C	2.22389500	-3.80379500	2.27706700
H	0.65044600	-5.80784500	-3.32147100	C	2.06134200	-4.79991500	1.31053400
H	0.811442300	-5.43342400	-1.60325800	C	1.91776400	-4.09573100	3.60957300
H	-0.28979300	-6.71723900	-2.14250000	C	1.60390800	-6.06582300	1.66713900
O	0.42876600	-2.94475200	-1.73681300	H	2.29691900	-4.57686700	0.26953300
C	1.37503500	-2.74297700	-2.77915800	C	1.45951600	-5.35973700	3.97013500
H	1.51838400	-3.65615000	-3.37311100	H	2.04111900	-3.32176900	4.36774900
H	1.05339900	-1.92992800	-3.44939500	C	1.30246200	-6.34736700	2.99848900
H	2.31470000	-2.47408500	-2.28904000	H	1.48398400	-6.83462300	0.90565200
O	-1.66447200	1.02904400	-1.36061000	H	1.22718700	-5.57679600	5.01142600
C	-2.43569000	2.21990400	-1.13268500	H	0.94833700	-7.33782300	3.28014800
H	-3.29673400	2.21156000	-1.81339500				
H	-2.82303800	2.20182500	-0.10492900				
C	-1.53975300	3.39521900	-1.36275900				
C	-0.81844400	3.50418200	-2.55763800				
C	-1.40789500	4.39889800	-0.40097000				
C	0.02448900	4.58734800	-2.78023500				
H	-0.91351700	2.71978900	-3.30843000				
C	-0.57391800	5.49378200	-0.62758200				
H	-1.95666900	4.31269800	0.53814900				
C	0.15020100	5.58646000	-1.81365100				
H	0.58760500	4.65483900	-3.71008300				
H	-0.47839400	6.26864000	0.13220500				
H	0.81376700	6.43256700	-1.98520800				
C	-2.73548100	-0.12347000	2.01627400				
C	-1.76371800	-1.02922800	1.57304600				
C	-0.43453400	-0.57939300	1.54106800				
C	-0.09025300	0.70943600	1.95874500				
C	-1.07442500	1.59082000	2.38637700				
C	-2.40367700	1.16828700	2.41529200				
H	-3.77802100	-0.44226300	2.02828400				
H	-0.80215200	2.59754600	2.70212300				
H	-3.18711200	1.84820000	2.74956600				
C	-2.13590800	-2.41657200	1.15848300				
H	-2.24153100	-3.07353600	2.03206700				
H	-3.09165900	-2.42415600	0.62043500				
H	-1.37284500	-2.86713100	0.51605500				
N	0.59121200	-1.45667200	1.08808900				
C	1.58419800	-1.12881900	0.20095700				
O	2.68750500	-1.63257300	0.13778400				
O	0.86503300	-2.55863900	1.90840000				
C	1.63845900	-2.15296100	3.03984700				
H	1.80226300	-3.07083700	3.60913700				
H	2.59998900	-1.73267100	2.71947700				
H	1.08546300	-1.42863500	3.65467600				
O	1.10682600	-0.17313900	-0.64872700				
C	2.11842300	0.65001600	-1.28165500				
H	2.90026000	-0.00212200	-1.68808900				
H	1.57397500	1.13505800	-2.09865500				
C	2.65896100	1.63979500	-0.29580300				
C	3.82646800	1.36157400	0.42254900				
C	1.94274700	2.80694600	-0.01066700				
C	4.26616000	2.23392400	1.41611800				
H	4.37676100	0.44552000	0.21013000				
C	2.38300500	3.67974800	0.98025800				
H	1.02239800	3.01714100	-0.55752200				
C	3.54349100	3.39206100	1.69893100				
H	5.17394000	2.00701700	1.97325000				
H	1.81436600	4.58458500	1.19341200				
H	3.88679000	4.07276600	2.47685700				
H	0.95570300	1.01459300	1.92626900				
H	-0.56188400	-0.95803200	-1.55897700				
<b>P1</b>							
C	-2.99563500	0.96033800	0.76259600				
C	-1.60680500	1.09769900	0.73392500				
C	-0.74224700	0.06055600	1.14071900				
C	-1.29663000	-1.15322800	1.56019600				
C	-2.68102700	-1.30088900	1.57270500				
C	-3.52520000	-0.26359700	1.18887500				
H	-0.65568500	-1.96861800	1.87384100				
H	-3.10418300	-2.24752200	1.90430700				
H	-4.60428200	-0.39095700	1.22460100				
N	0.62255900	0.37403700	1.09386000				
C	1.76265900	-0.35049700	1.32607600				
O	2.87862200	0.13210000	1.24508100				
H	0.81266100	1.34415400	0.87123700				
O	-1.02060000	2.29577600	0.35636400				
C	-0.97787600	2.48841000	-1.05269800				
H	-1.98826100	2.51132100	-1.48356700				
H	-0.49137400	3.45263700	-1.21978400				
H	-0.39881600	1.69191600	-1.54246500				

C	-1.39331100	6.09626800	-4.34078700	C	-4.44312400	-1.77533900	0.58992200
H	-0.68765900	5.57191000	-2.37580500	C	-3.13189000	-1.29509500	0.91228500
C	-2.36169500	5.87711600	-5.32036200	C	-2.89896200	0.12281200	1.21762800
H	-4.13712000	4.77544100	-5.84499000	C	-4.04704800	1.00249900	1.09408400
H	-0.59050100	6.81155100	-4.51509500	H	-6.11801800	1.20180900	0.67891700
H	-2.32024800	6.42029700	-6.26341000	H	-6.46704100	-1.22168600	0.28416700
H	-3.94066800	1.06179900	1.40560900	H	-3.88027500	2.06561900	1.23689100
<b>TS<sub>7s-p1</sub></b>							
C	-5.73175800	-0.30128300	0.96128600	C	-1.74992000	-3.07512200	0.04805200
C	-5.81907000	-1.68413200	1.17090300	H	-2.27373300	-2.85679000	-0.88446400
C	-4.67878200	-2.46436000	1.35863300	H	-0.67201900	-2.98952000	-0.12052000
C	-3.42240100	-1.84341400	1.33145400	H	-1.98841200	-0.47249900	0.43335300
C	-3.30374100	-0.40069800	1.24072200	C	-4.70138600	-3.22661000	0.34433600
C	-4.51301100	0.33509500	0.97061200	H	-5.77414900	-3.43282600	0.40870700
H	-6.63664500	0.27718900	0.78419900	H	-4.36710300	-3.52790200	-0.65490700
N	-1.93566100	0.12770800	1.11958900	H	-4.18867100	-3.86222200	1.07531300
C	-1.69385100	1.46424600	1.26544300	C	-1.31325400	1.71807800	1.96847400
O	-0.72532100	2.02304100	0.78073000	O	-0.31827200	2.39553300	1.75044700
O	-2.59760700	2.12638700	2.07049900	C	3.84743000	-1.46754000	-0.51132700
C	-2.31812900	3.50980600	2.28861800	C	1.79832300	-0.61893900	0.02010000
H	-2.14513500	3.99919300	1.32080500	C	4.01841900	-0.16007600	-0.20814500
H	-1.37632600	3.59679100	2.84985600	N	2.49267000	-1.74402500	-0.37265500
C	-3.45941100	4.14064400	3.02958100	N	2.77087800	0.34195200	0.12532900
C	-3.47366400	5.53176600	3.18051700	Cu	-0.04187200	-0.22949700	0.40521600
C	-4.49823900	3.39212500	3.58721500	H	4.90290100	0.46143400	-0.19064800
C	-4.50111900	6.16172000	3.87523500	H	4.54955600	-2.22858400	-0.82287900
H	-2.66951000	6.12643000	2.74469800	C	1.92659000	-3.06269500	-0.61844700
C	-5.52995000	4.02406000	4.28095300	C	1.80266600	-3.97907600	0.45525100
H	-4.49826200	2.31003900	3.47447100	C	1.54968100	-3.42654200	-1.93373300
C	-5.53579000	5.40815700	4.42892600	C	1.22285100	-5.22529700	0.19070100
H	-4.49638800	7.24551900	3.98099400	C	0.96765500	-4.68799400	-2.11942500
H	-6.33367300	3.422667100	4.70946500	C	0.78853700	-5.58035500	-1.07603500
H	-6.34253500	5.89965700	4.96999600	H	1.11622500	-5.92855200	1.01673600
H	-2.86562900	-0.11609100	2.27896800	H	0.65298900	-4.96195600	-3.12606400
H	-6.79357500	-2.17182600	1.16644900	H	0.33094200	-6.55274200	-1.25192800
H	-4.44413200	1.40919100	0.82927500	C	2.57456000	1.72561000	0.52317000
C	-4.75979100	-3.94736800	1.54077900	C	2.80405100	2.09225000	1.86738300
H	-5.79882700	-4.29007300	1.50792200	C	2.22139700	2.68062000	-0.45313800
H	-4.19871100	-4.47905300	0.76292800	C	2.70706700	3.44807800	2.19670000
H	-4.32437400	-4.25912500	2.49732500	C	2.12783900	4.01680700	-0.04887900
O	-2.34532200	-2.63232800	1.53283200	C	2.37596700	4.40899400	1.25609600
C	-1.31615300	-2.64405800	0.52935200	H	2.87725200	3.73875100	3.23412700
H	-0.56636800	-3.34260200	0.90401000	H	1.84884100	4.76019400	-0.79653100
H	-1.73184500	-3.02181700	-0.41370700	H	2.30601200	5.45828800	1.54025600
H	-0.88620600	-1.64944800	0.38799400	C	2.24511200	-3.76578200	1.89475000
<b>TS<sub>6s-p1</sub></b>							
N	-2.83783800	1.30158700	1.08922800	H	4.30375500	-4.39078000	1.57532600
C	-2.08156800	2.38373300	0.67786400	H	4.11161600	-2.63307700	1.61738300
O	-1.11521700	2.81278700	1.27258800	H	4.02161000	-3.55728400	3.11497500
C	-3.82993400	0.66659000	0.42821900	H	0.34700500	-2.97779900	2.60856200
C	-3.89787800	-0.62938800	1.13876700	H	1.72290500	-2.66459800	3.68841100
C	-4.82651400	1.07108500	-0.47044000	C	1.51339300	-1.72595800	2.20222200
C	-5.18642700	-1.26715200	1.23145000	C	1.67675500	-2.58423200	-3.19405300
C	-6.03532500	0.40240200	-0.33355500	C	0.64122500	-1.46709600	-3.22796900
H	-4.72633100	1.95501500	-1.09341600	H	3.09143200	-2.12086300	-3.53573700
C	-6.23958200	-0.68501700	0.55313400	H	-0.37582600	-1.86911200	-3.18836200
H	-6.89341900	0.77151400	-0.89595300	H	0.73352700	-0.78337300	-2.37857800
H	-7.23794600	-1.11429400	0.63328300	H	0.72782500	-0.87427900	-4.14755100
C	-5.32287500	-2.55869200	1.96245300	H	3.80739200	-2.95297000	-3.49631400
H	-4.74591200	-3.35256500	1.46917000	H	3.10308100	-1.72056300	-4.55736200
H	-4.92119700	-2.48508400	2.97995900	H	3.46060400	-1.32832000	-2.88072700
H	-6.36728300	-2.88250900	2.01690600	C	3.00837900	1.16232200	3.05490300
O	-2.80170300	-1.51155400	0.90689800	C	1.64236000	0.74225500	3.60634900
C	-2.82686600	-2.07791700	-0.39382000	C	3.92382700	-0.04113100	2.88529400
H	-3.77462600	-2.60404700	-0.59323300	H	1.05750600	1.61474700	3.91881300
H	-2.68264100	-1.30920400	-1.16874400	H	1.04972600	0.22486500	2.83874100
H	-1.99588800	-2.79186500	-0.43499300	H	1.76034000	0.06741500	4.46490000
H	-3.09646400	0.22815700	1.92876900	H	4.89377000	0.22864500	2.44895700
O	-2.58630900	2.93813500	-0.45865100	H	4.11438000	-0.49500900	3.86695100
C	-1.89903300	4.12852300	-0.90279800	C	3.47805200	-0.81743900	2.26036500
H	-1.97205200	4.89511200	-0.12213200	C	1.83716600	2.41323500	-1.90009100
H	-0.83592800	3.88142300	-1.01988800	C	2.70330000	1.42969300	-2.67572500
C	-2.52877900	4.57352500	-2.18346800	H	0.35082900	2.06155900	-1.99878400
C	-2.57207200	3.71610200	-3.28905000	H	3.77463900	1.64473100	-2.56614700
C	-3.06991100	5.85491400	-2.30106400	H	2.53124100	0.39600600	-2.36894700
C	-3.14287000	4.13504600	-4.48623600	H	2.45730400	1.48398000	-3.74390200
H	-2.15824200	2.71129600	-3.20136700	H	-0.27361500	2.81871600	-1.50821800
C	-3.63566100	6.28034000	-3.50220300	H	0.03218000	1.97133400	-3.04497000
H	-3.04709200	6.52573200	-1.44175200	B	0.12401200	1.10198800	-1.51583300
C	-3.67418400	5.42070000	-4.59658300	F	-2.72472200	-0.39449000	-2.24864900
H	-3.16979600	3.45923200	-5.33976100	F	-2.25038500	-0.08671400	-3.50956700
H	-4.05083400	7.28386300	-3.58032300	F	-1.60005200	-0.59019100	-1.35280300
H	-4.11630500	5.75041500	-5.53537500	F	-3.51647100	0.62405200	-1.72235700
<b>TS<sub>6-7</sub></b>							
C	-5.27970700	0.51573300	0.77906000	H	-3.43703500	-1.61840400	-2.25050200
C	-5.46957700	-0.85873000	0.53006300	O	-2.21140800	2.03486600	2.96242300

C	-4.22200000	4.52120500	2.77095200	H	3.60319400	-0.92572800	1.96432500
C	-2.20182300	4.98112800	1.53650700	C	2.08130700	2.44711500	-2.11902800
C	-4.94312600	5.33976700	1.90570600	C	3.06551200	1.60617300	-2.92580900
H	-4.72962700	4.01278600	3.59253800	C	0.63232800	1.97581100	-2.26990100
C	-2.92221200	5.80117100	0.67073400	H	4.09592100	1.96540300	-2.80203400
H	-1.13455800	4.81850200	1.38772600	H	3.04389500	0.54767800	-2.65836500
C	-4.29272000	5.98050300	0.85158800	H	2.81490300	1.66644000	-3.99254900
H	-6.01320300	5.47972800	2.05332900	H	-0.06168100	2.66364000	-1.77148000
H	-2.41210200	6.29753300	-0.15340000	H	0.35070500	1.89919100	-3.32804700
H	-4.85477500	6.61856300	0.17139800	H	0.47084500	0.98671500	-1.82088400
H	3.47874700	1.79342700	3.82507300	B	-2.25052300	-1.17051800	-2.30990900
H	1.96169800	3.38650200	-2.40044100	F	-2.06586100	-0.85345200	-3.64058700
H	2.02798800	-4.72503700	2.38896800	F	-0.98598200	-1.48514700	-1.69708300
H	1.40330100	-3.27616400	-4.00501200	F	-2.80903300	-0.09653100	-1.59725400
H	-3.27022000	-0.59584600	2.17456200	F	-3.07746200	-2.30917300	-2.16266500
O				O	-1.99324900	2.08738300	2.54110100
C				C	-1.76315800	3.41577400	3.04579500
<b>7</b>				H	-0.68399200	3.60952900	3.03827400
C	-5.09584400	0.38332900	0.42296900	H	-2.1261600	3.39077900	4.07909000
C	-5.25611100	-1.02049300	0.35228200	C	-2.51713400	4.42491800	2.23162500
C	-4.23870600	-1.94418600	0.53166000	C	-3.75880100	4.89693400	2.66623700
C	-2.95296300	-1.42228400	0.81315500	C	-2.01872300	4.86229900	0.99774100
C	-2.76795300	0.01149300	1.17710100	C	-4.49545500	5.78787900	1.88844500
C	-3.89058500	0.89606400	0.76619900	H	-4.15146900	4.55803400	3.62630000
H	-5.93510100	1.03233200	0.18446800	C	-2.75678300	5.74843600	0.21703200
H	-6.24637800	-1.41585700	0.12101000	H	-1.05336500	4.48688300	0.65670900
H	-3.72624200	1.96624100	0.85986500	C	-3.99572400	6.21324300	0.65942400
N	-1.42735100	0.49743600	0.98612000	H	-5.46013100	6.14987100	2.24174600
O	-1.83212700	-2.09222400	0.91468800	H	-2.36314600	6.07953400	-0.74306500
C	-1.61261200	-3.406171500	0.35636900	H	-4.56978700	6.90666300	0.04643600
H	-2.13046300	-3.50095800	-0.59751400	H	3.57211900	1.62921200	3.61969000
H	-0.53611100	-3.44021100	0.18331300	H	2.12023400	3.45237400	-2.56729100
H	-1.90607400	-4.17084900	1.08197800	H	2.16991900	-4.85828100	1.87529800
C	-4.56570600	-3.40311200	0.39298600	H	1.84190700	-3.15364400	-4.46605300
H	-5.64958900	-3.53807700	0.46780000	H	-2.96523800	-0.02123600	2.28303300
H	-4.25458900	-3.79946500	-0.57943400				
H	-4.10991900	-4.01631900	1.17652700				
C	-1.09198300	1.65450100	1.57439700				
O	-0.06962000	2.29275700	1.32950600				
C	4.05920100	-1.46411500	-0.81208100				
C	1.98885200	-0.64330300	-0.30703000				
C	4.21537300	-0.16856900	-0.45838700				
N	2.70252300	-1.74872100	-0.72193700				
N	2.95582300	0.31712600	-0.14500300				
Cu	0.10760000	-0.31140300	0.06038500				
H	5.09504200	0.45729400	-0.39787100				
H	4.77392000	-2.21132400	-1.12732900				
C	2.14296200	-3.04978700	-1.04794800				
C	1.97216800	-4.00987300	-0.02057100				
C	1.83054100	-3.35437800	-2.39464300				
C	1.38733900	-5.23598300	-0.36121900				
C	1.23055000	-4.59289900	-2.65508200				
C	0.98863100	-5.52292600	-1.65695900				
H	1.24592800	-5.97604200	0.42712600				
H	0.95633900	-4.82237900	-3.68410700				
H	0.51839000	-6.47649100	-1.89290400				
C	2.75924700	1.68699200	0.29437700				
C	2.96376600	2.00725300	1.65304100				
C	2.43080900	2.67472300	-0.65681000				
C	2.87274800	3.35283400	2.02444100				
C	2.33702300	3.99702200	-0.21219700				
C	2.56440300	4.34557400	1.10951700				
H	3.02441200	3.60844800	3.07409300				
H	2.07423500	4.76668300	-0.93892600				
H	2.49335200	5.38544500	1.42600700				
C	2.39957800	-3.87557400	1.43551800				
C	3.90756000	-3.70184100	1.61191700				
C	1.58631700	-2.86402200	2.23757400				
H	4.45750200	-4.48699600	0.07784100				
H	4.27089400	-2.73590200	1.25180700				
H	4.17185700	-3.76978400	2.67504500				
H	0.52242400	-3.13259000	2.25496200				
H	1.93806700	-2.82810900	3.27728100				
H	1.65264700	-1.85285200	1.82792300				
C	2.11126700	-2.49843200	-3.62427000				
C	1.22018900	-1.26846000	-3.73619900				
C	3.58721900	-2.15854800	-3.84334300				
H	0.17079000	-1.53468900	-3.87859200				
H	1.26394400	-0.65576900	-2.83268400				
H	1.53856200	-0.64733500	-4.58423300				
H	4.24165300	-3.02090200	-3.65780300				
H	3.73371500	-1.84947400	-4.88581800				
H	3.93017100	-1.32877900	-3.21819900				
C	3.12510200	1.03158900	2.80977600				
C	1.73904900	0.59696400	3.29601300				
C	4.03866000	-0.17206200	2.62410900				
H	1.14233900	1.46076700	3.61056400				
H	1.17592400	0.10282300	2.49133200				
H	1.82516300	-0.10200100	4.13924900				
H	5.02039600	0.10491300	2.22007900				
H	4.20248600	-0.65810900	3.59525800				

H	-0.34106900	-2.64665300	2.43287200	C	-5.27583100	6.75011500	-2.37223500
H	0.76091800	-2.17533600	3.74902400	H	-3.67823100	6.69153000	-0.92414700
H	0.91181000	-1.44836800	2.14140100	C	-5.88199300	6.09949800	-3.44471000
C	2.27263000	-2.97500300	-2.91059300	H	-5.83270700	4.38315500	-4.75080200
C	1.36869700	-1.80959900	-3.29780300	H	-5.67685100	7.69439200	-2.00689700
C	3.76261000	-2.64437600	-2.98762900	H	-6.75864800	6.53570800	-3.92199200
H	0.32917000	-2.12806600	-3.42934000	H	4.62360100	1.27095300	1.48840400
H	1.35192700	-1.02425700	-2.53807100	H	4.21740000	-1.48342900	1.50133200
H	1.70338300	-1.35664800	-4.24007200	C	2.35817500	2.70223500	0.79260800
H	4.37805500	-3.51000200	-2.70881700	C	1.90141800	3.35643500	1.95689400
H	4.02184700	-2.36801300	-4.01737300	C	2.64691400	3.42295400	-0.38882200
H	4.05456300	-1.80540000	-2.35169500	C	1.75011600	4.74767600	1.90839900
C	2.21605500	1.56845300	2.89090400	C	2.46269400	4.80897400	-0.36774200
C	0.72711500	1.25099800	3.05971100	C	2.02197300	5.47627100	0.76414400
C	3.08023800	0.34402500	3.15603600	H	1.39228900	5.25581600	2.80461000
H	0.12960000	2.17114200	3.03521700	H	2.67504700	5.36873700	-1.27834600
H	0.36473100	0.60774300	2.24549500	H	1.89175100	6.55737600	0.75240000
H	0.53932200	0.73879900	4.01331500	C	1.65529400	-2.19224300	0.65133900
H	4.14540300	0.54577900	2.98689900	C	1.00170700	-2.85728100	1.71655200
H	2.96211700	0.02947200	4.20152600	C	1.77294700	-2.79088700	-0.62276900
H	2.79736000	-0.50859800	2.53578000	C	0.43629000	-4.10942300	1.45812100
C	2.54765700	2.10053600	-2.30304500	C	1.19067200	-4.05385600	-0.80567200
C	3.52527300	0.99505800	-2.67975200	C	0.51810800	-4.70946300	0.20991300
C	1.11366000	1.76329900	-2.71737100	H	-0.07551200	-4.62112400	2.27347700
H	4.54320500	1.20311800	-2.32403100	H	1.27339700	-4.51638000	-1.78967100
H	3.22276400	0.02150500	-2.28852400	H	0.07234800	-5.68778900	0.03662200
H	3.56560100	0.89559700	-3.77208600	C	3.12122000	2.84236800	-1.71056800
H	0.43667100	2.61071200	-2.56481800	C	1.44064600	2.72022800	3.26040600
H	1.06193000	1.45959100	-3.77038700	C	2.39516400	-2.21016000	-1.88634600
H	0.71045700	0.93601300	-2.11970100	C	0.84413300	-2.34633700	3.13962600
B	-2.20648600	-0.03400300	-2.84427500	C	4.50512400	2.19804200	-1.63942100
F	-1.71571300	-0.00770600	-4.13434700	H	5.24535700	2.90191000	-1.23736700
F	-1.19531200	-0.69908000	-2.00441500	H	4.52747500	1.30012300	-1.01503400
F	-2.40397700	1.24823500	-2.32650800	H	4.83442500	1.90147500	-2.64361000
F	-3.36563200	-0.80582500	-2.72751800	C	3.61728100	-1.31666800	-1.74981600
O	-2.50575600	2.70110600	1.23316900	H	3.37194500	-0.33478000	-1.34082900
C	-2.23587200	4.09899400	1.43870800	H	4.39924200	-1.76388900	-1.12351600
H	-2.61568700	4.65725200	0.57286900	H	4.04651600	-1.14290000	-2.74483700
H	-1.14599600	4.23473500	1.46162300	C	-0.10319800	-1.15524100	3.23727500
C	-2.88754400	4.54558900	2.71006300	H	-0.20995100	-0.82772000	4.28019700
C	-2.90879800	3.72159900	3.83980900	H	0.24871700	-0.30202900	2.65211200
C	-3.44105700	5.82512400	2.79696000	H	-1.09601200	-1.41239100	2.84848000
C	-3.46388300	4.17346600	5.03343900	C	-0.05206000	2.39659400	3.16423000
H	-2.49676200	2.71513050	3.77378200	H	-0.64139100	3.29863000	2.96294000
C	-3.99100000	6.28142500	3.99302100	H	-0.24901300	1.70704800	2.33397700
H	-3.44276600	6.46932500	1.91699800	H	-0.41602400	1.93838800	4.09356300
C	-4.00345500	5.45640700	5.11547200	H	1.54185100	3.52148300	4.00900700
H	-3.47630400	3.52023100	5.90467900	H	0.34855500	-3.17230500	3.67319700
H	-4.41931800	7.28121300	4.04475600	H	3.24218800	3.71775500	-2.36616400
H	-4.43709500	5.80956200	6.04956500	H	2.73000700	-3.09338700	-2.45282000
H	2.47263000	2.29669500	3.67576900	C	2.06966200	1.96287900	-2.38068200
H	2.84829600	2.98376300	-2.88798600	H	1.84993800	1.06533400	-1.79752900
H	1.31058700	-4.39109100	2.83114000	H	1.12046900	2.49564000	-2.51206500
H	2.11532700	-3.74813300	-3.67794800	H	2.41163800	1.63547900	-3.37152300
H	-2.76092700	0.35162200	1.43763300	C	1.30787400	-1.53849800	-2.72645500
H				H	0.52579800	-2.24798500	-3.02028300
H				H	0.81190800	-0.72601300	-2.18047600
H				H	1.72246600	-1.10499400	-3.64471500
<b>TS6-p1</b>				C	2.23537600	1.54266200	3.80583200
N	-2.44452800	1.52825200	0.64060000	C	2.07749400	0.62682800	3.23259100
C	-1.97102800	2.64047500	-0.04614300	H	3.31344000	1.74557100	3.83049700
O	-0.80279500	2.99204300	0.04514400	H	1.91301600	1.32983600	4.83375000
C	-3.40314000	0.64770800	0.25540800	H	2.16473300	-2.12585500	3.87687500
C	-2.94515700	-0.59131200	0.90227900	C	2.79908600	-3.02005400	3.82589700
C	-4.64814900	0.75789700	-0.36328700	H	2.73972600	-1.28424200	3.48129100
C	-3.93586300	-1.58226500	1.23351300	H	1.97011700	-1.91297500	4.93581400
C	-5.54825400	-0.24194300	-0.02917700	C	-3.53905000	-2.82527400	1.95765800
H	-4.92341200	1.61797200	-0.96665100	C	-2.61674200	-3.25263100	1.54241100
C	-5.22615500	-1.34471200	0.80606700	H	-3.32523200	-2.60961800	3.01418100
H	-6.57444900	-0.15454500	-0.38590900	H	-4.32572600	-3.58603600	1.92335600
H	-6.01497600	-2.05437600	1.05552400	H	-1.73522200	-1.11642200	0.30452700
C	-2.17801500	0.48757600	1.48626400	O	-1.98948900	-1.86621100	-0.89913200
C	3.55366500	-0.66362800	1.26302700	C	-1.00833500	-2.05393000	-1.34454800
C	1.60666100	0.30818200	0.59587700	H	-2.47378100	-2.82237600	-0.65750600
C	3.75585200	0.67528000	1.24005000	H	-2.60243100	-1.29059400	-1.60269700
N	2.23847800	-0.87901300	0.87382900	H			
N	2.56527400	1.26051000	0.83055400				
Cu	-0.17672800	0.54148700	-0.05291900				
B	-1.74109600	0.91079100	-3.21928500				
F	-1.36181800	2.15451200	-3.70465400				
F	-1.23081500	0.82352900	-1.81960400				
F	-3.12349300	0.79753200	-3.12800600				
F	-1.17244700	-0.13451000	-3.91796700				
O	-2.91748300	3.25723500	-0.75131300				
C	-2.43766000	4.37536900	-1.56331400				
H	-1.92564400	5.08115300	-0.89918900				
H	-1.71388100	3.96461200	-2.27519800				
C	-3.62756600	4.98009700	-2.22797900				
C	-4.23869200	4.33174400	-3.30761300				
C	-4.15474000	6.18806100	-1.76638100				
C	-5.36206100	4.89084000	-3.91014400				
H	-3.82349100	3.38969500	-3.66622500				
<b>5n</b>				C	-3.39782600	0.25553700	-2.00009500
				C	-3.04981600	-0.81032700	-2.75611600
				C	-1.64376200	-1.27181300	-2.80050500
				C	-0.74817500	-0.59602300	-1.82741200
				C	-1.10365700	0.59686700	-1.10944700
				C	-2.44347900	0.96610200	-1.21649200
				C	-4.42736300	0.61565500	-1.98876000
				C	-3.75881800	-1.32320600	-3.40498900
				C	-2.79254800	1.82280800	-0.65000800
				N	-0.10097900	1.16255200	-0.36714900
				O	0.42366700	-1.07675600	-1.53707600
				C	0.98077800	-2.26273100	-2.11703000
				H	0.20254500	-2.99666300	-2.35429600

H	1.54360500	-1.96582400	-3.00619900	C	-1.12047700	-1.16264700	-4.25560000
H	1.65219800	-2.65535900	-1.35153000	H	-1.72728700	-1.81603600	-4.89137700
C	-0.06490200	2.46120100	0.01676400	H	-1.19974000	-0.13176200	-4.60591100
O	0.89299000	2.95358800	0.61340300	H	-0.06932800	-1.44517400	-4.34293400
C	4.79611800	-1.20736900	2.33545700	C	-6.81754900	-5.20964100	-1.37785000
C	3.19804200	-0.05807100	1.16974200	C	-5.47290900	-5.12458200	-1.00778000
C	4.78822800	0.06066900	2.80353300	C	-4.89803400	-3.84515500	-0.92820700
N	3.82803800	-1.27739800	1.33963600	C	-5.64401200	-2.70185500	-1.22145300
N	3.81288100	0.74848600	2.09800200	C	-6.98468700	-2.81331700	-1.57123400
Cu	1.74773600	0.46539100	0.03154900	C	-7.57285400	-4.07323800	-1.65334400
H	5.37700500	0.54330300	3.57153600	H	-7.28019500	-6.19474200	-1.43855100
H	5.39707500	-2.06570500	2.60237500	H	-7.56306200	-1.91782000	-1.79194200
C	3.55888500	-2.50451400	0.60719400	H	-8.62059700	-4.17213900	-1.93177500
C	2.58955900	-3.41300700	1.10051100	C	-4.68119500	-6.35421100	-0.70503900
C	4.32618300	-2.81365400	-0.54341700	H	-4.08765800	-6.22628400	-0.20942700
C	2.38668900	-4.60585500	0.39453000	H	-5.33394000	-7.22306300	-0.57230200
C	4.06122500	-4.02194400	-1.20268900	H	-3.97485700	-6.58722300	-1.51230300
C	3.10334200	-4.91530700	-0.75071600	N	-3.52733000	-3.73253200	-0.55031000
H	1.64345100	-5.30722100	0.77473200	C	-2.99805300	-2.65950000	0.15762000
H	4.63954100	-4.25494100	-2.09632700	O	-1.84714900	-2.27769800	0.04760700
H	2.92495800	-5.85030300	-1.28063300	O	-2.65745400	-4.20664200	-1.57339400
C	3.52826400	2.14899600	2.36670500	C	-1.60761000	-4.99737200	-1.01669700
C	2.61202000	2.48467700	3.38602500	H	-1.08570100	-5.40879400	-1.88610600
C	4.23352400	3.14317900	1.65669300	H	-0.92138200	-4.37975700	-0.42385000
C	2.42414400	3.84063900	3.67414600	H	-2.01044700	-5.81379000	-0.40464000
C	3.99513400	4.47985300	1.99534700	O	-3.89031300	-2.21776800	1.06240400
C	3.10395600	4.83671800	2.99297100	C	-3.39661600	-1.25298100	2.01899400
H	1.71202700	4.10582500	4.45671400	H	-3.82284500	-1.59277500	2.97099800
H	4.52943500	5.25212700	1.44159100	H	-2.30431300	-1.32490500	2.07484800
H	2.93980800	5.88502000	3.23856100	C	-3.82027100	0.14820000	1.70198900
C	1.73896500	-3.25183000	2.35210600	C	-5.02905700	0.43395100	1.06223900
C	2.55376900	-3.28335600	3.64482100	C	-3.00057700	1.20277800	2.11196100
C	0.76176100	-2.08433300	2.28797100	C	-5.40091500	1.75658400	0.82660100
H	3.18632200	-4.17904600	3.69017900	H	-5.67334000	-0.38495600	0.74045200
H	3.20310700	-2.41033200	3.75719800	C	-3.38543900	2.52317400	1.90083300
H	1.88197700	-3.30105000	4.51259300	H	-2.04026800	0.98320700	2.57854600
H	0.12728300	-2.13536800	1.39406800	C	-4.58528200	2.80565700	1.25051900
H	0.10839300	-2.09103100	3.17228600	H	-6.33707700	1.97143400	0.31177000
H	1.27070000	-1.11956300	2.26090700	H	-2.73251400	3.33635700	2.21800800
C	5.42529400	-1.96360700	-1.16372600	H	-4.87202800	3.83925100	1.05872700
C	4.89490100	-0.67894400	-1.78856900	H	-5.16232100	-1.72701800	-1.16635200
C	6.64037200	-1.74754700	-0.26218600				
H	4.14623500	-0.88592000	-2.56072100				
H	4.41225600	-0.02272900	-1.06025600				
H	5.71225300	-0.11384900	-2.25552500				
H	7.01066800	-2.69876300	0.14296900				
H	7.45176700	-1.29367000	-0.84505900				
H	6.44118400	-1.07937600	0.57985100				
C	1.70702900	1.54007000	4.16064600				
C	0.41402100	1.31104200	3.37564600				
C	2.29698100	0.22812100	4.65895800				
H	-0.10406800	2.26074700	3.18995700				
H	0.61377400	0.86873100	2.38979700				
H	-0.25763500	0.64160900	3.93277600				
H	3.25261100	0.37466600	5.17787100				
H	1.60050400	-0.23985800	5.36753800				
H	2.45889200	-0.49170700	3.85480300				
C	5.15672200	2.93170600	0.46919700				
C	6.17414500	1.80274900	0.56466000				
C	4.31645500	2.82646100	-0.80306800				
H	6.71301900	1.80395700	1.52151800				
H	5.71385500	0.82144400	0.43411200				
H	6.91605400	1.90937000	-0.23741900				
H	3.70513600	3.72337300	-0.95519100				
H	4.94593500	2.68107000	-1.69032700				
H	3.61983900	1.98217000	-0.75214700				
B	1.83047000	0.97842500	-3.55226800				
F	2.52576400	1.98792900	-4.18304500				
F	2.29115200	0.84449800	-2.20038700				
F	0.44624500	1.24226400	-3.51430800				
F	2.05454900	-0.26715200	-4.19618400				
O	-1.15866700	3.21376600	-0.30807800				
C	-1.09661300	4.58495200	0.09053200				
H	-0.30341600	5.08576900	-0.48373100				
H	-0.80643300	4.65091100	1.14883100				
C	-2.44455900	5.19314500	-0.15028700				
C	-2.97630800	6.10425500	0.76520100				
C	-3.18928500	4.86547000	-1.28889000				
C	-4.22560700	6.68439000	0.55081600				
H	-2.40652800	6.35587000	1.66131200				
C	-4.44022400	5.43819300	-1.50145400				
H	-2.78385300	4.14721200	-2.00058200				
C	-4.96280100	6.34994200	-0.58353900				
H	-4.62673700	7.39157200	1.27545600				
H	-5.01140600	5.17247200	-2.39015200				
H	-5.94149300	6.79716200	-0.75134200				
H	1.42787500	2.10390600	5.06447600				
H	5.74065900	3.86277900	0.39936900				
H	1.11871500	-4.16160900	2.37523500				
H	5.79673600	-2.57604500	-1.99932600				
H	-1.64216300	-2.34056200	-2.52534500				

H	0.79495600	-3.43331800	3.10081200	C	-5.93209000	2.53470000	1.31830700
H	-0.23938000	-4.69945200	3.75771100	H	-4.91109000	0.92593800	2.32279800
H	-2.47511800	-3.57797400	0.95595300	C	-7.10736300	2.94855900	0.69568100
H	-2.33956700	-3.74772400	2.72746700	H	-9.12112900	2.40873400	0.13927000
H	-1.54719300	-2.41428200	1.87837300	H	-5.06222300	3.18987600	1.35216500
C	2.56238700	-1.80996800	-1.71702600	H	-7.16484000	3.93963800	0.24673600
C	1.73841300	-0.58046300	-2.08676500	H	-7.90061300	-1.52257700	-0.60872500
C	3.78472900	-1.49928700	-0.85324600				
H	1.04197100	-0.78776200	-2.90614100				
H	1.13167700	-0.21617800	-1.25330100	<b>6n</b>			
H	2.39144000	0.24191800	-2.40771100	C	-3.18518400	-0.54812900	-2.39345900
H	4.34694300	-2.41173200	-0.61197100	C	-2.68105600	-1.74075700	-2.90160100
H	4.45664200	-0.83082200	-1.40635700	C	-1.40638900	-2.18783500	-2.50393300
H	3.54209600	-0.99676500	0.08627900	C	-0.64945800	-1.38457400	-1.64155600
C	-1.30162300	-0.00874200	4.27637900	C	-1.14158500	-0.16204500	-1.10512600
C	-2.61148300	-0.32661600	3.55026500	C	-2.45992900	0.20049400	-1.46994500
C	-0.45937800	-1.26116300	4.46382600	H	-4.17913200	-0.21107500	-2.68984600
H	-3.30541700	0.51948600	3.62745000	H	-3.26290600	-2.33921900	-3.60417500
H	-2.44664400	-0.49807500	2.47675000	H	-2.87153500	1.13406100	-1.09167500
H	-3.09140000	-1.22008100	3.97465500	N	-0.35488900	0.51059400	-0.20894500
H	0.51250000	-1.04836800	4.92612700	O	0.63180800	-1.75195300	-1.30374700
H	-0.99281800	-1.96447300	5.11757600	C	1.56242100	-1.78560900	-2.40666300
H	-0.27882400	-1.78216200	3.52175000	H	1.81083100	-2.82683300	-2.64517900
C	1.38821800	2.58075400	0.60759400	H	1.15135200	-1.26107500	-3.27379900
C	2.63695500	1.71973700	0.47205300	H	2.45949700	-1.25409600	-2.08198200
C	0.45948300	2.43629900	-0.59894800	C	-0.35426700	1.86688800	-0.07820500
H	3.26555300	1.75429000	1.37211200	O	0.16774100	2.45621300	0.87158000
H	2.39804300	0.67545800	0.26376500	C	5.04587800	-1.29546300	1.96063400
H	3.24047900	2.07735900	-0.37232100	C	3.12496800	-0.35942700	1.15893800
H	-0.33869200	3.18702100	-0.57284800	C	4.80184900	-0.18427800	2.69268500
H	1.00544500	2.54139700	-1.54505100	N	4.02548200	-1.39688900	1.02359300
H	-0.03310600	1.45650000	-0.61694700	N	3.63410400	0.37729700	2.19798700
B	-1.50200300	0.52457500	-3.75671300	Cu	1.47697600	-0.04235900	0.25582100
F	-1.37152100	1.86844500	-4.07862200	H	5.34047600	0.26732000	3.51212300
F	-1.23108100	0.34449000	-2.35748800	H	5.84788700	-2.01950700	2.00527200
F	-2.81291500	0.06302700	-4.01063100	C	3.97222400	-2.45698400	0.02868400
F	-0.58861400	-0.26996800	-4.47800600	C	3.21446500	-3.62384200	0.28730200
O	-3.63221000	2.43784300	-1.04707600	C	4.73368000	-2.32666000	-1.15960700
C	-3.43803800	3.84900900	-0.96810700	C	3.20016900	-4.62486100	-0.69198800
H	-2.66890300	4.10239800	-1.71216000	C	4.68276600	-3.37692300	-2.08456600
H	-3.05394300	4.11180900	0.02590500	C	3.92105600	-4.51349200	-1.86932900
C	-4.73265300	4.54399200	-1.26869100	H	2.61111700	-5.52207500	-0.50007400
C	-5.11202400	5.67319900	-0.53997000	H	5.25583900	-3.27603400	-3.00597800
C	-5.57695700	4.07672000	-2.28340800	H	3.89365000	-5.30932900	-2.61246200
C	-6.30959300	6.33217400	-0.81616600	C	3.05526500	1.58436200	2.76380100
H	-4.46365600	6.03466100	0.25996100	C	2.17191700	1.47657900	3.85887600
C	-6.77731100	4.72813200	-2.55491800	C	3.43935500	2.84269900	2.25161100
H	-5.28158200	3.19676000	-2.85467400	C	1.69436000	2.65945100	4.43360800
C	-7.14786800	5.85808300	-1.82338300	C	2.91991200	3.98387100	2.87237000
H	-6.59203300	7.21082700	-0.23755300	C	2.06003300	3.90601000	3.95474500
H	-7.42608800	4.35522500	-3.34704500	H	1.00515400	2.58044600	5.27565700
H	-8.08598700	6.36781600	-2.03995300	H	3.20290000	4.95766500	2.47208700
H	-1.57224300	0.32873800	5.28949300	H	1.67280500	4.81198500	4.41888800
H	1.73917700	3.62461800	0.62050600	C	2.44279400	-3.95494300	1.55764300
H	-0.95484100	-5.39144400	1.54639700	C	3.32649900	-4.01987400	2.80269400
H	2.97924300	-2.19025700	-2.66178000	C	1.16736000	-3.13648100	1.74190500
H	-5.37362100	-2.62477900	-1.25216400	H	4.15848200	-4.71968100	2.65107700
C	-4.41406500	-3.47887300	-3.21667300	H	3.75464400	-3.05391300	3.08110700
H	-5.34005800	-3.97655100	-3.53221500	H	2.74184700	-4.37460900	3.66167800
H	-3.80666600	-3.32246800	-4.11602500	H	0.48825600	-3.27356000	0.89128500
H	-3.865652400	-4.16283900	-2.55952300	H	0.64229900	-3.44455500	2.65841900
C	-8.89873800	-5.01682100	-1.82083000	H	1.35595800	-2.05998200	1.81101000
C	-7.60349700	-4.85836800	-1.29632000	C	5.58835600	-1.13599600	-1.57424900
C	7.29909900	-3.58142200	-0.78377800	C	4.75487900	0.10703000	-1.88001900
C	-8.20288200	-2.52086900	-0.90758800	C	6.78759800	-0.85193300	-0.66852300
C	-9.46526000	-2.72006200	-1.44212800	H	4.10852400	-0.03407000	-2.75283600
C	-9.82605600	-3.98807600	-1.88651500	H	4.09645300	0.38631900	-1.05197700
H	-9.16347100	-5.99893100	-2.21107800	H	5.40521000	0.96612000	-2.09058100
H	-10.15036100	-1.87871300	-1.52416700	H	7.34880400	-1.76979800	-0.44661500
H	-10.81157100	-4.16920700	-2.31048700	H	7.46962100	-0.15943700	-1.17801700
C	-6.69232400	-6.05135400	-1.39892100	H	6.51590400	-0.38561700	0.28207400
H	-6.46230900	-6.50728600	-0.42947700	C	1.55645000	0.20694400	4.42699800
H	-7.18220500	-6.82324200	-2.00106800	C	0.25817500	-0.08768700	3.67234500
H	-5.73621000	-5.81125500	-1.87262300	C	2.41829900	-1.04158800	4.52086200
N	-5.96241400	-3.19714900	-0.29004500	H	-0.45302100	0.74144000	3.78404900
C	-5.79567700	-2.28082300	0.90254200	H	0.43775700	-0.20766700	2.59439700
O	-4.68876200	-1.96920900	1.23639400	H	-0.20993500	-1.01127700	4.04381100
O	-5.07285900	-4.28877200	-0.09695900	H	3.38862100	-0.84970800	4.99469500
C	-5.27862400	-4.93371500	1.16262000	H	1.89827800	-1.80066300	5.12075800
H	-4.69803000	-5.85594700	1.08664900	H	2.60060200	-1.48594100	3.54047500
H	-4.88572900	-4.32444100	1.98492300	C	4.28093400	3.10566600	1.01468200
H	-6.34003800	-5.16803500	1.32065900	C	5.55229200	2.28293700	0.85080900
O	-6.94979300	-2.00625500	1.46690600	C	3.39244700	3.02490600	-0.22620000
C	-6.89589300	-0.93551400	2.49144800	H	6.15163200	2.25069900	1.77067100
H	-7.77683700	-1.16165400	3.09757700	H	5.34096100	1.25643200	0.54448600
H	-5.98499100	-1.08268000	3.07880700	H	6.17421600	2.72380300	0.06094300
C	-6.95522300	0.40852400	1.84998000	H	2.55480500	3.72884700	-0.16299900
C	-8.13370000	0.82843100	1.21879200	H	3.95855600	3.23675000	-1.14251800
C	-5.84796200	1.26091800	1.87781200	B	2.95123200	2.02898800	-0.33965700
C	-8.20499900	2.08789600	0.63351400	F	1.28125700	1.46338900	-3.39973900
H	-8.99841700	0.16160500	1.19564000	F	1.06165300	2.84045100	-3.50132800

F	1.71620800	1.16092200	-2.06496100
F	0.08788400	0.75545600	-3.64746900
F	2.27995500	1.03621400	-4.28626900
O	-0.94688400	2.52195500	-1.10874300
C	-0.80542500	3.94536500	-1.16389300
H	0.05108900	4.15067200	-1.82033300
H	-0.58000000	4.33734600	-0.16349300
C	-2.07948700	4.50665000	-1.71672700
C	-2.66457000	5.64432100	-1.15726700
C	-2.70167200	3.88768200	-2.80808300
C	-3.85020200	6.16465800	-1.67647400
H	-2.18599500	6.12650200	-0.30239200
C	-3.89107200	4.39928900	-3.31899200
H	-2.23568800	3.00589700	-3.24899100
C	-4.46929600	5.53865100	-2.75606200
H	-4.29281400	7.05639700	-1.23283800
H	-4.36590400	3.91197900	-4.17009200
H	-5.39676800	5.94020700	-3.16285600
H	1.27752500	0.46703600	5.46049700
H	4.60634000	4.15289900	1.11672000
H	2.10245200	-4.99031600	1.39980200
H	6.03119000	-1.44866100	-2.53176700
H	-2.54122900	-2.31597100	-0.61379300
C	-0.85046300	-3.47749500	-3.02877900
H	-1.64970700	-4.12840600	-3.40403800
H	-0.15900200	-3.31086500	-3.86490200
H	-0.28747000	-4.01843800	-2.25580100
C	-6.38190900	-3.29445400	-1.72809300
C	-5.09486400	-3.48813800	-1.20770800
C	-4.61140100	-2.47322800	-0.36466300
C	-5.32459500	-1.29934500	-0.13277200
C	-6.58994700	-1.14091100	-0.68159400
C	-7.12985800	-2.15246500	-1.46849200
H	-6.78470700	-4.06522100	-2.38417300
H	-7.13407800	-0.21527700	-0.50442000
H	-8.12052500	-2.04257100	-1.90507600
H	-4.30668200	-5.48506800	-0.86364900
H	-4.80929000	-5.14127800	-2.52083100
H	-3.29261100	-4.47709400	-1.88948900
N	-3.21602800	-2.54894000	0.15547100
C	-2.76548600	-1.69224300	1.36134300
O	-1.60488200	-1.44923800	1.47900700
O	-2.78882500	-3.89804000	0.47269900
C	-3.50071700	-4.44328100	1.58296500
H	-3.19615000	-5.49176100	1.58479200
H	-3.20344500	-3.97102300	2.52684900
H	-4.58633400	-4.36544800	1.44008000
O	-3.78561200	-1.48409100	2.16025900
C	-3.56826700	-0.40413000	3.17202500
H	-4.28115700	-0.67649600	3.95330600
H	-2.53981200	-0.49616900	3.53474900
C	-3.85351800	0.90648900	2.52684300
C	-5.18087300	1.30746400	2.32042400
C	-2.80799000	1.69732500	2.04099200
C	-5.45882400	2.47202700	1.61284100
H	-5.99582800	0.68771600	2.70064000
C	-3.09131400	2.87853500	1.35746500
H	-1.76959700	1.39045400	2.17356200
C	-4.41136800	3.25696400	1.12550100
H	-6.49216200	2.77172300	1.44296300
H	-2.26713300	3.49100000	0.99822900
H	-4.62159300	4.16348300	0.55876000
H	-4.88535900	-0.48217600	0.42758700
C	-4.33245600	-4.70685300	-1.63591200