

## Supplementary Information

New insights into the mechanism of synergetic photoredox/copper(I)-catalyzed  
carbocyanation of 1,3-dienes: a DFT study

Yanhong Liu,<sup>ab</sup> Aili Feng,<sup>a</sup> Rongxiu Zhu,<sup>a</sup> and Dongju Zhang<sup>\*a</sup>

<sup>a</sup>Key Lab of Colloid and Interface Chemistry, Ministry of Education, Institute of Theoretical  
Chemistry, School of chemistry and chemical engineering, Shandong University, Jinan  
250100, P. R. China

<sup>b</sup>School of Radiology, Shandong First Medical University & Shandong Academy of Medical  
Sciences, Taian 271016, P. R. China

Corresponding author:

\*E-mail: zhangdj@sdu.edu.cn

Tel: +86-531-88365833

## Table of Contents

I. Estimation of Barrier for Single Electron Transfer Process.....	S3
II. Energy Calibration Calculations.....	S5
III. Oxidative Quenching of PC* with NHP Ester.....	S7
IV Frontier Molecular Orbital Analyses for Two Quenching Processes of PC*.....	S7
V. Addition Reactions of Radical Species LCu(I) <sup>+</sup> ·2 <sup>-</sup> and 2 <sup>-</sup> with Substrate 1.....	S8
VI. Spin Densities Analyses.....	S8
VII. Addition Reactions of Radical Cy* with 1-Phenyl-1,3-Diene (1) .....	S9
VIII. <span style="float: right;">Distortion–Interaction</span> Analyses.....	S10
IX. <span style="float: right;">Non-Covalent</span> <span style="float: right;">Interactions</span> Analyses.....	S11
X. Formation of the Copper(II) Species.....	S12
XI. Extended Application of the Proposed Mechanism.....	S13
XII. Thermodynamic Data.....	S14
XIII. Cartesian Coordinates of all Structures Involved in This Work.....	S16

## I. Estimation of Barrier for Single Electron Transfer Process

According to the Marcus-Hush equation, the reorganization energy  $\lambda$  is decomposed into the inner-sphere nuclear reorganization energy  $\lambda_i$  and the outer-sphere solvent reorganization energy  $\lambda_o$ . The inner-sphere nuclear reorganization energy  $\lambda_i$  can be calculated from the equations (S1)-(S3):

$$\lambda_{i1} = \left| E^D(Q_P) - E^D(Q_R) \right| + \left| E^{D^+}(Q_P) - E^{D^+}(Q_R) \right| \quad (\text{S1})$$

$$\lambda_{i2} = \left| E^A(Q_P) - E^A(Q_R) \right| + \left| E^{A^-}(Q_P) - E^{A^-}(Q_R) \right| \quad (\text{S2})$$

$$\lambda_i = \frac{\lambda_{i1} + \lambda_{i2}}{2} \quad (\text{S3})$$

where  $\lambda_{i1}$  represents the reorganization energy of the electron-donating substrates (D),  $\lambda_{i2}$  is the reorganization energy of the electron-accepting substrates (A).  $Q_R$  and  $Q_P$  are the equilibrium geometries of the reactants and products, respectively.

In addition, the outer-sphere solvent reorganization energy  $\lambda_o$  can be obtained according to the equation (S4):

$$\lambda_o = \left( 332 \text{ kcal mol}^{-1} \right) \left( \frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R} \right) \left( \frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon} \right) \quad (\text{S4})$$

where  $a_1$  and  $a_2$  are the radii of the electron-donating substrates (D) and the electron-accepting substrates (A), respectively,  $R = a_1 + a_2$ ,  $\varepsilon_{op}$  and  $\varepsilon$  are the optical dielectric constant (2.087) and the static dielectric constant (10.125) of 1,2-dichloroethane (DCE), respectively. The radius of a molecule can be obtained by calculating the molecular volume via a Monte-Carlo integration as implemented in the Gaussian 16 program.

Therefore, the overall activation barrier of single electron transfer (SET) process can be calculated from the equations (S5) and (S6):

$$\lambda = \lambda_i + \lambda_o \quad (\text{S5})$$

$$\Delta G_{SET}^{\ddagger} = \frac{(\Delta G_r + \lambda)^2}{4\lambda} \quad (\text{S6})$$

where  $\Delta G_r$  is the reaction energy.

## II. Energy Calibration Calculations

**Table S1.** Relative Electronic and Gibbs Free Energies (in kcal mol<sup>-1</sup>) Calculated for Transition States (**TS9<sub>S</sub>**, **TS9<sub>R</sub>**, **TS10<sub>S</sub>**, and **TS10<sub>R</sub>**) Using the M06 Functional with Three Different Basis Sets [LANL2DZ(*f*)-6-311+G(d,p), SDD-6-311+G(d,p), Def2-TZVP)]<sup>a</sup>

Transition states	M06/LANL2DZ( <i>f</i> )-6-311+G(d,p)/PCM(DCE)		M06/SDD-6-311+G(d,p)/PCM(DCE)		M06/Def2-TZVP/PCM(DCE)	
	$\Delta\Delta E$	$\Delta\Delta G$	$\Delta\Delta E$	$\Delta\Delta G$	$\Delta\Delta E$	$\Delta\Delta G$
	<b>TS9<sub>S</sub></b>	0.0	0.0	0.0	0.0	0.0
<b>TS9<sub>R</sub></b>	2.2	1.9	2.5	2.1	2.4	2.0
<b>TS10<sub>S</sub></b>	3.1	2.9	3.1	2.8	2.9	2.6
<b>TS10<sub>R</sub></b>	7.3	6.0	7.3	6.0	6.9	5.6

<sup>a</sup>All energies reported in this table were obtained through single-point energy calculations using the PCM solvent model with 1,2-dichloroethane (DCE) as solvent.

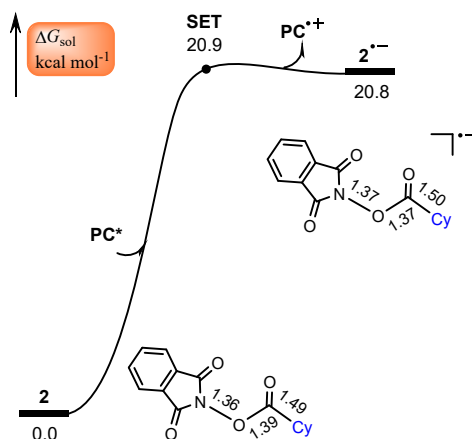
**Table S2.** Comparison of Relative Gibbs Free Energies for Two Key Transition States at Different Levels of Single-Point Energy Calculations: DLPNO-CCSD(T)/cc-PVTZ/SMD with tightPNO and RIJK vs. M06/LANL2DZ(*f*)+6-311+G(d,p)/PCM Levels<sup>a,b</sup>

Transition states	$\Delta\Delta G$	$\Delta\Delta G^b$
<b>TS9<sub>S</sub></b>	0.0	0.0
<b>TS9<sub>R</sub></b>	1.9	1.3

<sup>a</sup>The input file for the DLPNO-CCSD(T)/cc-PVTZ/SMD calculations was prepared using Multiwfn 3.8 software (T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580–592).

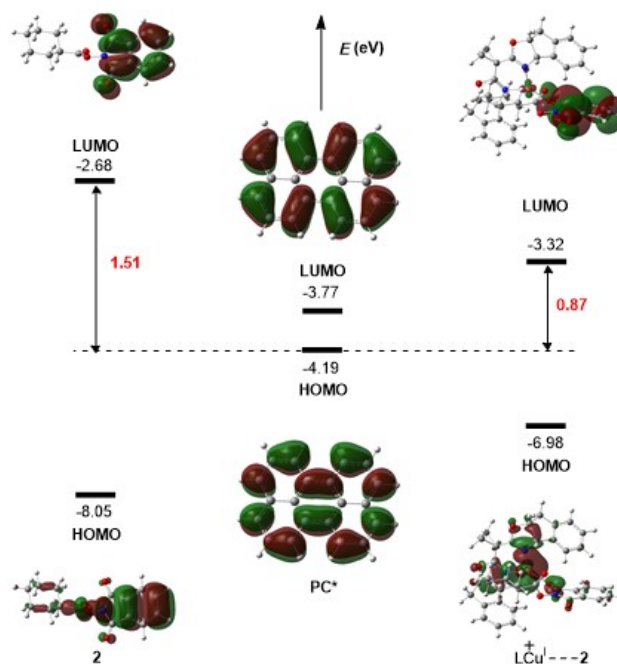
<sup>b</sup>The relative Gibbs free energies (in kcal mol<sup>-1</sup>) of the two key transition states calculated at the DLPNO-CCSD(T)/cc-PVTZ/SMD level are fairly consistent with those reported in the main body text.

### III. Oxidative Quenching of PC\* with NHP Ester



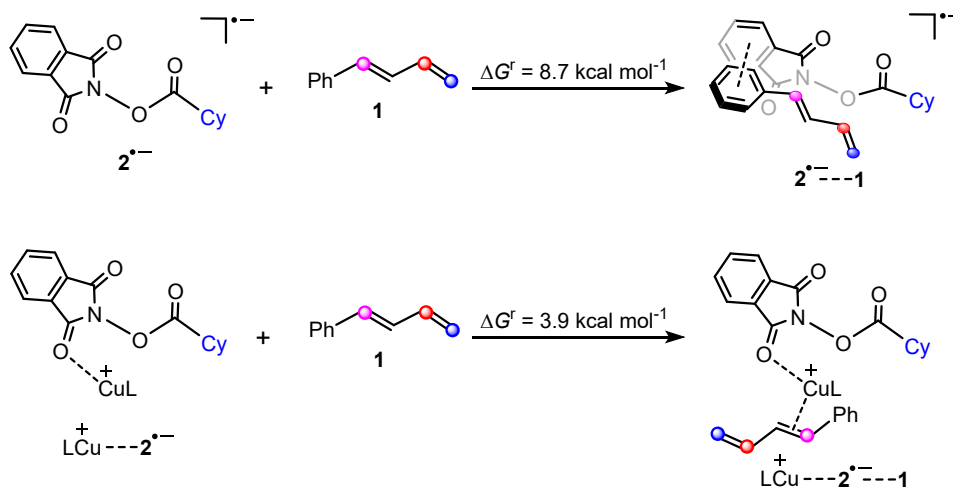
**Fig. S1.** Calculated Gibbs free energy profile for the oxidative quenching of photoexcited high-energy species PC\* with NHP ester **2**. Bond distances are in Å.

### IV. Frontier Molecular Orbital Analyses for Two Quenching Processes of PC\*



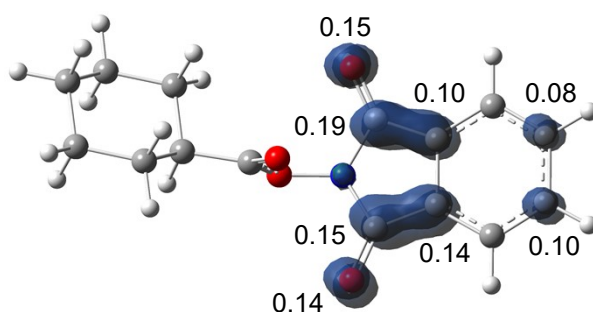
**Fig. S2.** Calculated HOMO–LUMO energy gaps of the electron donor-acceptor pairs involved in the oxidative quenching of photoexcited high-energy species PC\* with NHP ester **2** or its complex (LCu<sup>+</sup>...**2**) with the copper species LCu<sup>+</sup>.

## V. Addition Reactions of Radical Species $LCu(I)^+ \cdots 2^{\bullet-}$ and $2^{\bullet-}$ with Substrate **1**



**Fig. S3.** Calculated thermodynamics of the additions of both the radical species  $LCu(I)^+ \cdots 2^{\bullet-}$  and  $2^{\bullet-}$  to 1-phenyl-1,3-diene (**1**).

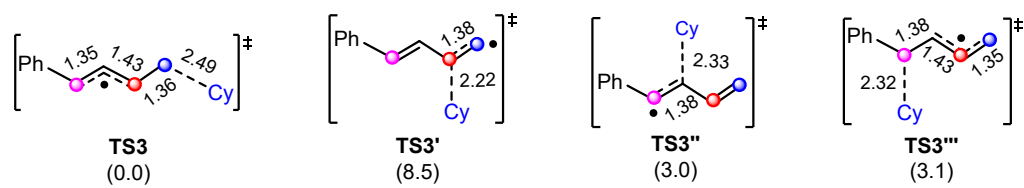
## VI. Spin Densities Analyses



**Fig. S4.** Calculated total spin isosurface and spin densities on atoms for intermediate  $2^{\bullet-}$ .



## VII. Addition Reactions of Radical Cy<sup>•</sup> with 1-Phenyl-1,3-Diene (**1**)



**Fig. S5.** Calculated relative Gibbs free energies of transition states for the additions of radical Cy<sup>•</sup> to 1-phenyl-1,3-diene (**1**) at four different C atoms. The relative Gibbs energies in parenthesis are in kcal/mol<sup>-1</sup>, and bond distances are in Å.

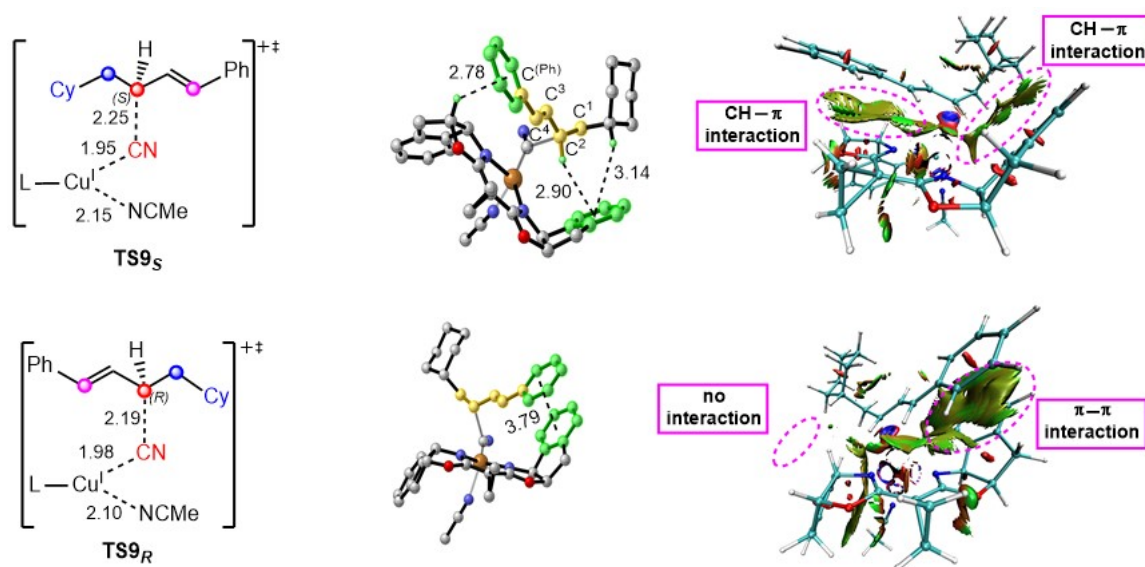
## VIII. Distortion–Interaction Analyses

**Table S3.** Distortion–Interaction Analyses for Key Transition States<sup>a</sup>

Transition states	$\Delta E^\ddagger$ <sup>b</sup>	$\Delta E_{\text{cat}}$ <sup>c</sup>	$\Delta E_{\text{sub}}$ <sup>c</sup>	$\Delta E_{\text{dist}}$ <sup>d</sup>	$\Delta E_{\text{int}}$ <sup>e</sup>
<b>TS9<sub>S</sub></b>	0.0	6.6	8.9	15.5	-15.5
<b>TS9<sub>R</sub></b>	2.2	7.1	8.4	15.5	-13.3
<b>TS10<sub>S</sub></b>	3.1	7.4	10.8	18.2	-15.0
<b>TS10<sub>R</sub></b>	7.3	7.4	12.2	19.6	-12.3

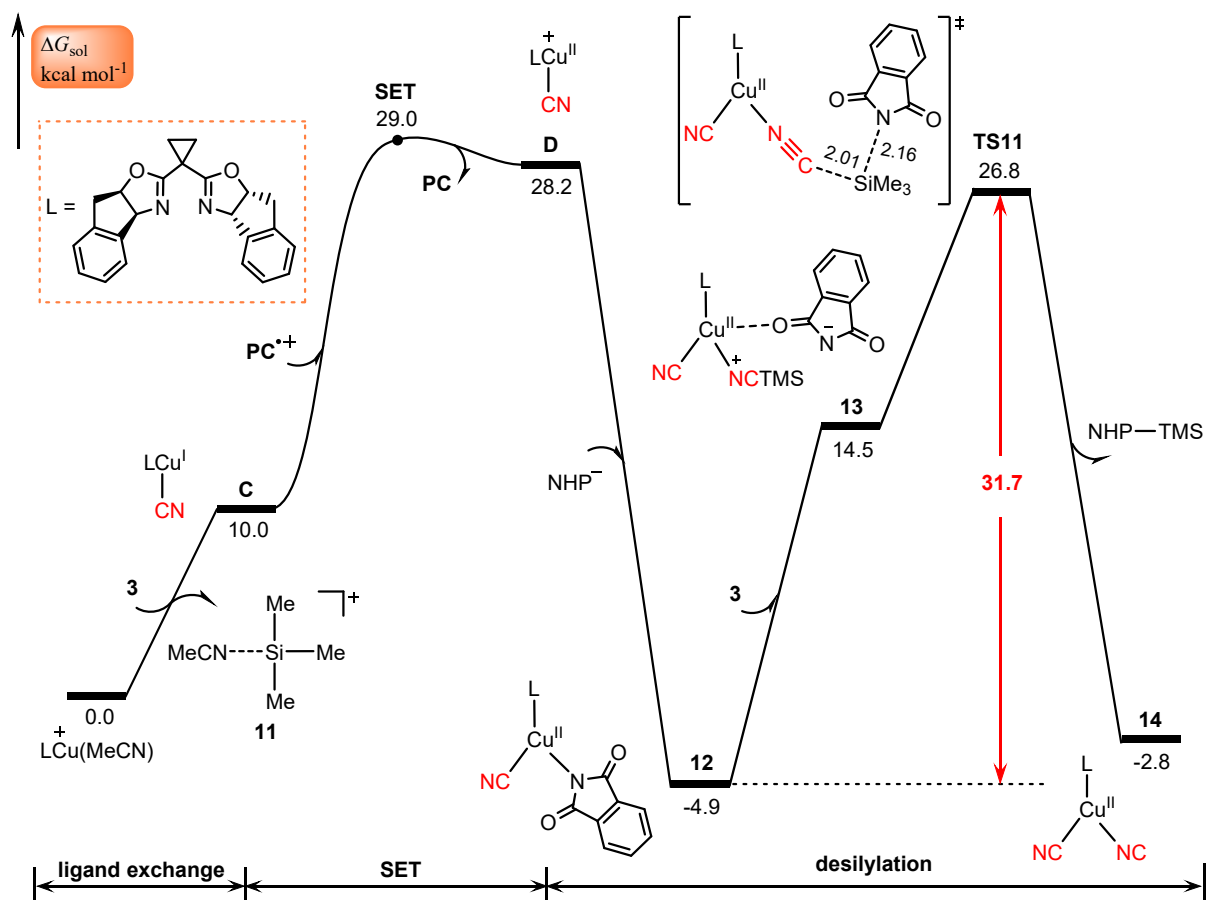
<sup>a</sup>All electronic energies are given in kcal mol<sup>-1</sup>. <sup>b</sup>The activation energy  $\Delta E^\ddagger$ . <sup>c</sup>The distortion energy of copper(I) fragment,  $\Delta E_{\text{cat}}$ , or and allyl cation fragment,  $\Delta E_{\text{sub}}$ , which describes the energy needed to distort the fragment from its geometry in the initial reactive complex to the corresponding geometry in the transition state. <sup>d</sup>The total distortion energy,  $\Delta E_{\text{dist}} = \Delta E_{\text{cat}} + \Delta E_{\text{sub}}$ . <sup>e</sup>The interaction energy  $\Delta E_{\text{int}} = \Delta E^\ddagger - \Delta E_{\text{dist}}$ .

## IX. Non-Covalent Interaction Analyses



**Fig. S6.** Non-covalent interactions (NCIs) analyses for  $TS9_S$  and  $TS9_R$ . The blue, green, and red surfaces represent the locations where the strong interaction, weak interaction, and steric effect occur, respectively. The bond distances are in Å.

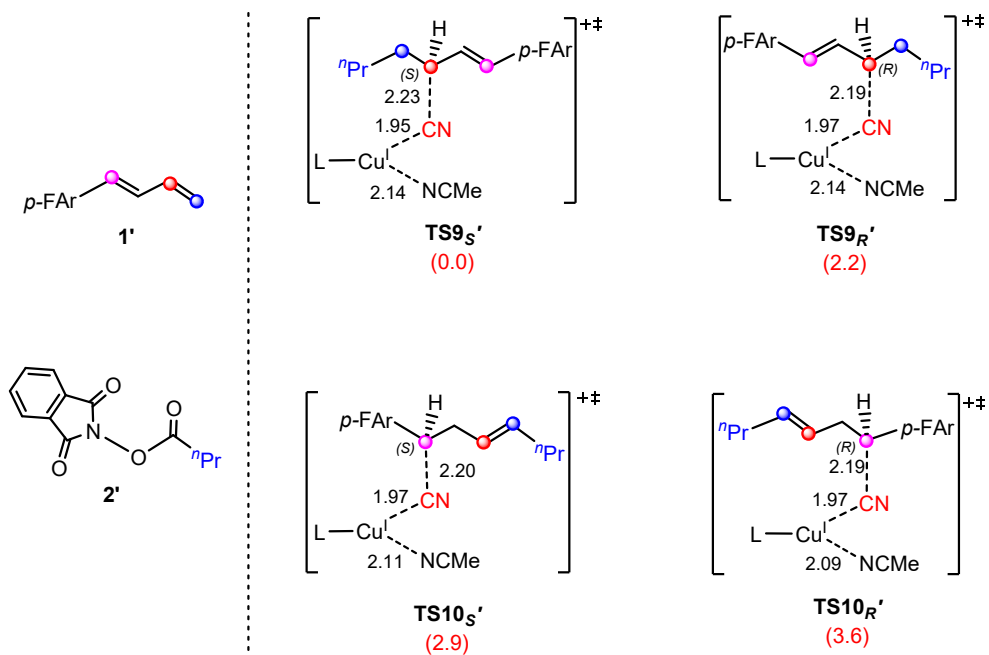
## X. Formation of the Copper(II) Species



**Fig. S7.** Calculated Gibbs free energy profile for the formation of the copper(II) species.

Bond distances are in Å.

## XI. Extended Application of the Proposed Mechanism



**Fig. S8.** Calculated relative Gibbs energies of the transition states involved in the regio- and enantioselectivity-determining transition states for the reaction of *p*-phenylmethyl-substituted 1,3-diene (**1'**) with *n*-propyl-substituted *N*-hydroxyphthalimide (NHP) ester (**2'**). Bond distances are in Å.

## XII. Thermodynamic Data

**Table S4.** Calculated Key Structures of Zero-Point Energy (*ZPE*) Corrections, Thermal Corrections to Enthalpies (*TCH*), Thermal Corrections to Gibbs Free Energies (*TCG*), Enthalpies (*H*), and Gibbs Free Energies (*G*), Electronic Energies (*E*) in 1,2-Dichloroethane (DCE) and the Imaginary Frequencies (*IF*,  $\text{cm}^{-1}$ ) of the Transition States. All Energies are Given in Hartree

Structures	<i>ZPE</i> (1)	<i>TCH</i> (2)	<i>TCG</i> (3)	<i>E</i> (DCE) (4)	<i>H</i> (DCE) (5)=(2)+(4)	<i>G</i> (DCE) (6)=(3)+(4)	<i>IF</i>
<b>1</b>	0.166285	0.17623	0.131546	-386.834	-386.657	-386.702	
<b>2</b>	0.280521	0.297908	0.235668	-935.926	-935.628	-935.69	
<b>3</b>	0.118651	0.12931	0.084783	-502.014	-501.885	-501.929	
<b>L</b>	0.382179	0.403137	0.330758	-1147.89	-1147.49	-1147.56	
<b>MeCN</b>	0.045308	0.049803	0.022378	-132.701	-132.651	-132.679	
<b>Cu(MeCN)<sub>4</sub><sup>+</sup></b>	0.185889	0.208231	0.125713	-726.933	-726.725	-726.807	
<b>LCu(MeCN)<sub>4</sub><sup>+</sup></b>	0.574319	0.61562	0.501255	-1874.87	-1874.26	-1874.37	
<b>LCu(MeCN)<sub>3</sub><sup>+</sup></b>	0.526586	0.563527	0.456345	-1742.15	-1741.59	-1741.7	
<b>LCu(MeCN)<sub>2</sub><sup>+</sup></b>	0.477457	0.510426	0.410808	-1609.44	-1608.93	-1609.03	
<b>LCu(MeCN)<sup>+</sup></b>	0.431664	0.459341	0.371256	-1476.73	-1476.27	-1476.36	
<b>B</b>	0.384259	0.407017	0.329103	-1343.98	-1343.58	-1343.65	
<b>Cu(MeCN)<sup>+</sup>...2</b>	0.329482	0.353167	0.276584	-1264.71	-1264.36	-1264.43	
<b>Cu(MeCN)<sub>2</sub><sup>+</sup>...2</b>	0.376758	0.405238	0.318246	-1397.44	-1397.04	-1397.12	
<b>LCu<sup>+</sup>...2</b>	0.667845	0.708006	0.597056	-2279.95	-2279.25	-2279.36	
<b>LCu<sup>+</sup>...2<sup>-</sup></b>	0.664425	0.705053	0.591622	-2280.09	-2279.38	-2279.5	
<b>2<sup>-</sup></b>	0.2778	0.295398	0.231848	-936.038	-935.742	-935.806	
<b>TS1</b>	0.274584	0.292172	0.228746	-936.009	-935.717	-935.78	-2009.94
<b>6</b>	0.27595	0.294389	0.228399	-936.055	-935.761	-935.827	
<b>TS2</b>	0.273067	0.291582	0.22508	-936.048	-935.757	-935.823	-618.83
<b>Cy<sup>*</sup></b>	0.154798	0.16177	0.125146	-235.077	-234.915	-234.952	
<b>TS3</b>	0.322417	0.338855	0.277512	-621.914	-621.575	-621.636	-239.23
<b>A</b>	0.326687	0.342549	0.28247	-621.977	-621.634	-621.694	
<b>PC</b>	0.253896	0.267868	0.213866	-768.978	-768.711	-768.765	
<b>PC*</b>	0.250197	0.26446	0.209819	-768.924	-768.66	-768.714	
<b>PC<sup>+</sup></b>	0.254487	0.268377	0.215023	-768.781	-768.513	-768.566	
<b>CO<sub>2</sub></b>	0.011904	0.015467	-0.0088	-188.561	-188.546	-188.57	
<b>NHP<sup>-</sup></b>	0.103176	0.111679	0.070525	-512.428	-512.316	-512.357	
<b>TS3'</b>	0.322894	0.33895	0.279329	-621.902	-621.563	-621.623	-516.77

<b>TS3''</b>	0.322451	0.338685	0.278799	-621.91	-621.572	-621.632	-408.38
<b>TS3'''</b>	0.322663	0.338846	0.279729	-621.911	-621.572	-621.631	-447.62
<b>7</b>	0.611134	0.65324	0.537898	-2358.5	-2357.85	-2357.97	
<b>TS4</b>	0.611517	0.652168	0.542429	-2358.49	-2357.83	-2357.94	-82.55
<b>8</b>	0.391102	0.417026	0.334031	-1436.97	-1436.55	-1436.63	
<b>TS5</b>	0.390456	0.415898	0.333351	-1436.96	-1436.54	-1436.62	-151.3
<b>C</b>	0.391621	0.417343	0.333731	-1436.98	-1436.57	-1436.65	
<b>D</b>	0.392922	0.418015	0.337886	-1436.76	-1436.34	-1436.42	
<b>E</b>	0.724593	0.765718	0.651263	-2058.81	-2058.04	-2058.16	
<b>A<sup>+</sup></b>	0.329389	0.345204	0.285823	-621.799	-621.454	-621.513	
<b>A<sup>-</sup></b>	0.324832	0.340691	0.281672	-622.079	-621.739	-621.798	
<b>9</b>	0.391916	0.417492	0.334916	-1436.75	-1436.33	-1436.41	
<b>TS6</b>	0.39123	0.416349	0.335239	-1436.73	-1436.32	-1436.4	-211.13
<b>TS7<sub>S</sub></b>	0.721428	0.761744	0.64848	-2058.93	-2058.17	-2058.29	-372.36
<b>TS8<sub>S</sub></b>	0.720657	0.761457	0.645896	-2058.73	-2057.97	-2058.08	-355.24
<b>NHP-TMS</b>	0.21695	0.233568	0.174146	-921.534	-921.3	-921.359	
<b>10</b>	0.393835	0.418209	0.341663	-1436.48	-1436.07	-1436.14	
<b>TS9<sub>S</sub></b>	0.770916	0.81645	0.692062	-2191.5	-2190.69	-2190.81	-313.75
<b>TS9<sub>R</sub></b>	0.770066	0.815565	0.691418	-2191.5	-2190.68	-2190.81	-372.79
<b>TS9<sub>S</sub><sup>Z</sup></b>	0.771659	0.816604	0.694873	-2191.5	-2190.68	-2190.8	-322.37
<b>TS10<sub>S</sub></b>	0.770577	0.815528	0.691624	-2191.5	-2190.68	-2190.81	-362.91
<b>TS10<sub>R</sub></b>	0.769734	0.815555	0.689999	-2191.49	-2190.68	-2190.8	-374.4
<b>4<sub>S</sub></b>	0.339147	0.356782	0.293592	-714.816	-714.459	-714.522	
<b>4<sub>R</sub></b>	0.339147	0.356782	0.293592	-714.816	-714.459	-714.522	
<b>5<sub>S</sub></b>	0.339242	0.356776	0.293538	-714.812	-714.455	-714.519	
<b>5<sub>R</sub></b>	0.339171	0.356694	0.29371	-714.809	-714.452	-714.515	
<b><sup>3</sup>[LCu(MeCN)<sup>+</sup>]<sup>*</sup></b>	0.424088	0.4531	0.361356	-1476.59	-1476.14	-1476.23	
<b>11</b>	0.158247	0.170872	0.12101	-541.742	-541.571	-541.621	
<b>12</b>	0.497455	0.531956	0.430039	-1949.26	-1948.73	-1948.83	
<b>13</b>	0.619651	0.664213	0.544029	-2451.27	-2450.61	-2450.73	
<b>TS11</b>	0.619305	0.662826	0.54542	-2451.26	-2450.59	-2450.71	-87.03
<b>14</b>	0.400106	0.428399	0.340014	-1529.74	-1529.31	-1529.4	
<b>2<sup>+</sup>...1</b>	0.44607	0.473934	0.388013	-1322.88	-1322.41	-1322.49	
<b>LCu<sup>+</sup>...2<sup>-</sup>...1</b>	0.834382	0.884685	0.752245	-2666.94	-2666.06	-2666.19	
<b>TS9<sub>S</sub>'</b>	0.73214	0.777933	0.651721	-2114.12	-2113.35	-2113.47	-332.56
<b>TS9<sub>R</sub>'</b>	0.730768	0.776035	0.652293	-2114.12	-2113.35	-2113.47	-388.44
<b>TS10<sub>S</sub>'</b>	0.730772	0.776866	0.650083	-2114.12	-2113.34	-2113.47	-375.09
<b>TS10<sub>R</sub>'</b>	0.729802	0.776339	0.647999	-2114.12	-2113.34	-2113.47	-392.28

### XIII. Cartesian Coordinates of all Structures Involved in This Work

#### 1

C	2.28363700	1.39093400	-0.00020800
C	0.93315900	1.07309000	-0.00055600
C	0.51125400	-0.26620300	-0.00033100
C	1.49316500	-1.26742600	0.00016500
C	2.84586500	-0.94949900	0.00052500
C	3.24742700	0.38267300	0.00035400
H	2.58969600	2.43477700	-0.00041300
H	0.19622200	1.87421200	-0.00111600
H	1.18019700	-2.31093500	0.00030000
H	3.58843300	-1.74421800	0.00093800
H	4.30458200	0.63730100	0.00060800
C	-0.89247300	-0.66229400	-0.00062400
H	-1.06950900	-1.74134700	-0.00148300
C	-1.97020500	0.14442600	0.00015900
H	-1.85191000	1.23060000	0.00121900
C	-3.32816400	-0.35339800	-0.00023400
H	-3.44489400	-1.43964000	-0.00130700
C	-4.41472200	0.42923300	0.00062600
H	-4.32748700	1.51483400	0.00170300
H	-5.41899100	0.01520300	0.00028600

#### 2

C	2.76203800	0.77124300	-0.01667800
C	2.96612700	-0.60349600	-0.15065700
C	4.18055500	-1.18737500	0.15527400
C	5.19952600	-0.34524400	0.60742700
C	4.99520900	1.02882900	0.74232000
C	3.76445200	1.61132000	0.42969800
C	1.36771400	1.08689000	-0.39973900
C	1.71334200	-1.23289100	-0.62686300
H	4.32812600	-2.25895900	0.05064000
H	6.16837100	-0.76625200	0.86225100
H	5.80865100	1.65428000	1.09989400
H	3.59436500	2.67951600	0.53465700
O	1.41140300	-2.39231100	-0.76191800
O	0.72916000	2.10698600	-0.31385200
N	0.87699100	-0.13277500	-0.91380200
O	-0.46277300	-0.29781200	-1.11393400
C	-1.16394300	-0.44253800	0.08182700
O	-0.60549900	-0.53070900	1.13953600
C	-3.43874300	-1.07309000	0.89221500



H	-3.15003700	-2.12902300	0.96654900
C	-2.62883300	-0.38251100	-0.19989100
H	-2.81177100	-0.86326900	-1.17336200
C	-3.02083400	1.10381000	-0.31896300
H	-2.75768500	1.60532400	0.62637900
H	-2.43093900	1.58332200	-1.10988700
C	-4.51538700	1.23832700	-0.57961000
H	-4.78687800	2.29926400	-0.64227200
H	-4.74812400	0.79405700	-1.56030600
C	-5.33185900	0.53529500	0.49923300
H	-6.40399700	0.62309500	0.28360000
H	-5.16299000	1.03825900	1.46485600
C	-4.93143300	-0.93087800	0.62292800
H	-5.50312400	-1.42217600	1.41965300
H	-5.18241600	-1.45575700	-0.31263500
H	-3.18641000	-0.60762400	1.85681200

### 3

C	-0.84564400	1.60013700	-0.81436900
H	-0.47158100	1.66137500	-1.84159700
H	-1.93927500	1.66239000	-0.84698300
H	-0.47315100	2.46696200	-0.25876600
C	-0.84617400	-0.09497100	1.79238100
H	-1.93981600	-0.09763300	1.86194800
H	-0.47401100	-1.00983500	2.26493300
H	-0.47234000	0.76356200	2.35982200
C	-0.84474100	-1.50560800	-0.97848500
H	-0.47091100	-1.45911800	-2.00657100
H	-0.47097800	-2.42528100	-0.51660500
H	-1.93828000	-1.56577100	-1.01740200
Si	-0.32880400	0.00015000	-0.00014600
C	1.56325700	0.00020700	0.00033100
N	2.72762900	0.00037900	0.00058800

### L

C	-0.38227700	2.57136800	0.63325600
C	-0.00004300	1.23796200	0.00040100
C	0.38220100	2.57222000	-0.63067100
C	1.11621700	0.48258000	0.60917500
O	1.92671700	1.24460200	1.39344000
C	2.68881100	-0.94197300	1.13881500
C	2.92748100	0.36132800	1.93983600
H	2.63032300	-1.83826400	1.76944200
H	2.73377900	0.27646100	3.01435100

C	-1.11634600	0.48332900	-0.60924900
O	-1.92715200	1.24633600	-1.39224600
C	-2.68905500	-0.94060500	-1.14027000
C	-2.92800100	0.36370800	-1.93955100
H	-2.63075600	-1.83609700	-1.77205000
H	-2.73455800	0.28023600	-3.01422300
N	-1.41918800	-0.74058000	-0.43349700
N	1.41915400	-0.74108600	0.43190300
C	-4.75400900	0.04160600	-0.42744400
C	-3.85125700	-0.99235000	-0.18256400
C	-4.05481400	-1.88593500	0.86249700
C	-5.18435600	-1.73786600	1.66298000
C	-6.09216000	-0.70576100	1.41839500
C	-5.88245200	0.19008500	0.37286200
C	-4.33590900	0.86155400	-1.61648700
H	-3.33520500	-2.68002100	1.05439400
H	-5.36016200	-2.42749000	2.48550100
H	-6.96997000	-0.59985400	2.05203700
H	-6.59067300	0.99592800	0.18702500
C	3.85133000	-0.99249700	0.18142400
C	4.75395700	0.04119800	0.42787500
C	5.88267000	0.19069900	-0.37185600
C	6.09278400	-0.70386200	-1.41840600
C	5.18511200	-1.73571100	-1.66456000
C	4.05529500	-1.88480100	-0.86465300
C	4.33543100	0.85969400	1.61776600
H	6.59079800	0.99633700	-0.18478200
H	6.97081700	-0.59715400	-2.05160400
H	5.36123700	-2.42433500	-2.48785000
H	3.33579200	-2.67869000	-1.05775800
H	4.33631200	1.93990400	1.42871800
H	5.00433300	0.68946200	2.47177300
H	-5.00503600	0.69225100	-2.47050400
H	-4.33685200	1.94154100	-1.42617400
H	0.13342400	2.82415700	1.55384300
H	-1.43771300	2.82343900	0.59627900
H	1.43763600	2.82424800	-0.59332900
H	-0.13347800	2.82627900	-1.55091600

**MeCN**

C	0.00000000	0.00000000	-1.17477800
H	-1.02612300	0.00000000	-1.55187700
H	0.51306100	0.88864900	-1.55187700
H	0.51306100	-0.88864900	-1.55187700

C	0.00000000	0.00000000	0.27507100
N	0.00000000	0.00000000	1.43626700

**Cu(MeCN)<sub>4</sub><sup>+</sup>**

C	-2.79624400	-3.14141300	-1.99555300
H	-2.45920200	-4.15013600	-1.74423100
H	-2.77809000	-3.01906200	-3.08150100
H	-3.82095000	-3.00995100	-1.64032700
C	-1.93027800	-2.16451500	-1.37447400
N	-1.23357700	-1.38417300	-0.87800300
C	2.31707700	-1.99542900	3.50424800
H	3.03458500	-1.28749000	3.92756100
H	2.85712400	-2.87452400	3.14216800
H	1.61620300	-2.30225700	4.28533400
C	1.59965000	-1.37526100	2.41309300
N	1.02092100	-0.87706700	1.54256300
C	-2.56028500	3.53193700	1.62138800
H	-3.32862400	3.15936500	2.30434400
H	-3.04568600	4.05107100	0.79065300
H	-1.92012600	4.23747000	2.15759400
C	-1.76841000	2.43040000	1.12029800
N	-1.13336000	1.54792100	0.72117100
C	3.05375600	1.59638700	-3.12636700
H	3.61264300	0.76154400	-3.55689500
H	3.75484800	2.27866400	-2.63832700
H	2.53598500	2.12994600	-3.92805900
C	2.09706100	1.10657900	-2.16012200
N	1.33241500	0.71443900	-1.38368800
Cu	-0.00129200	0.00294500	-0.00164400

**LCu(MeCN)<sub>4</sub><sup>+</sup>**

C	2.22778100	-3.03013500	-3.53689000
H	1.96317300	-2.45617400	-4.42968600
H	2.06454100	-4.09273400	-3.73360300
H	3.28585000	-2.86621100	-3.30945300
C	-2.83443900	0.70643700	2.25370400
H	-3.24616900	1.63629100	1.84595000
H	-3.55789700	0.28897700	2.96068800
H	-2.69031500	-0.00305900	1.42823000
C	-1.56917500	0.96733400	2.91303100
N	-0.54997300	1.17671800	3.43096000
C	1.42266500	-2.59432700	-2.41783700
N	0.79532200	-2.22353800	-1.51639600
C	0.45799700	3.70123100	-0.57812200

C	-0.00026200	2.35939000	0.00021100
C	-0.45650300	3.70357000	0.57437900
C	-1.00186500	1.61726400	-0.78802900
O	-1.83081000	2.38996600	-1.50423600
C	-2.27713300	0.09903500	-1.78957000
C	-2.77373300	1.51500900	-2.16835000
H	-1.89200100	-0.48772500	-2.63483000
H	-2.71060300	1.74117000	-3.23494800
C	1.00079300	1.61746800	0.78926200
O	1.82892400	2.39000700	1.50654900
C	2.27653700	0.09904500	1.78993500
C	2.77276700	1.51496700	2.16928400
H	1.89123500	-0.48811800	2.63484100
H	2.71037100	1.74034300	3.23608600
N	1.16821100	0.35033700	0.85934200
N	-1.16852300	0.35010600	-0.85924600
Cu	0.00070800	-1.11079100	-0.00069900
C	4.47985300	0.37085300	0.91463500
C	3.43757500	-0.53898300	1.08530600
C	3.50659100	-1.82368900	0.55911900
C	4.63720300	-2.18863800	-0.16821800
C	5.67916500	-1.27720400	-0.35255000
C	5.61122400	0.00382700	0.19242600
C	4.18303700	1.68398700	1.58615400
H	2.68633600	-2.52602300	0.70723500
H	4.71181000	-3.18824600	-0.59106400
H	6.55762900	-1.57317400	-0.92147400
H	6.43083400	0.70614700	0.05232800
C	-3.43792100	-0.53939700	-1.08486100
C	-4.48056200	0.37003400	-0.91422700
C	-5.61172200	0.00268000	-0.19185000
C	-5.67918100	-1.27834500	0.35319100
C	-4.63693700	-2.18943400	0.16876100
C	-3.50647600	-1.82411100	-0.55862800
C	-4.18446500	1.68309900	-1.58616700
H	-6.43156600	0.70472600	-0.05174900
H	-6.55749100	-1.57458800	0.92220900
H	-4.71119000	-3.18907000	0.59159300
H	-2.68598300	-2.52615600	-0.70674800
H	-4.20408300	2.52981300	-0.88755800
H	-4.91584300	1.90929100	-2.37128800
H	4.91473800	1.91135300	2.37062700
H	4.20141900	2.53030300	0.88700400
H	0.06525600	3.93591000	-1.56246300

H	1.50247100	3.94458100	-0.40862900
H	-1.50065100	3.94782200	0.40428100
H	-0.06309000	3.94156800	1.55761100
C	2.83368600	0.70630200	-2.25333300
H	3.55642300	0.28751600	-2.96027300
H	2.68841400	-0.00270300	-1.42761900
H	3.24690800	1.63564900	-1.84596600
C	1.56869100	0.96901000	-2.91246000
N	0.54957000	1.17957700	-3.43007700
C	-2.22583700	-3.02846100	3.53682200
H	-3.28395200	-2.86405800	3.30989700
H	-1.96035500	-2.45395900	4.42901000
H	-2.06314000	-4.09100500	3.73427200
C	-1.42120100	-2.59403200	2.41688600
N	-0.79424200	-2.22434800	1.51472500

**LCu(MeCN)<sub>3</sub><sup>+</sup>**

C	-0.05615400	5.53021600	-0.64501100
H	0.35202800	5.93334500	0.28566100
H	-1.08046900	5.89118500	-0.76950300
H	0.55022800	5.88263300	-1.48353800
C	-3.34031200	-1.02017200	-2.49339800
H	-3.17470800	-1.80207300	-1.74453800
H	-3.50729300	-1.48877800	-3.46673900
H	-4.23131300	-0.45000000	-2.20577500
C	-2.19728600	-0.13309400	-2.54781100
N	-1.28404700	0.58574100	-2.57722500
C	-0.04432000	4.08591000	-0.59967800
N	-0.03432700	2.92799800	-0.56436400
C	0.54147400	-3.77330000	0.47364900
C	0.17261200	-2.40706100	-0.11301400
C	-0.26095500	-3.72938400	-0.75712900
C	-0.85884600	-1.64980300	0.62263600
O	-1.71037900	-2.40740000	1.32772000
C	-2.16172900	-0.11726600	1.56683800
C	-2.56566600	-1.51620900	2.09071300
H	-1.84391900	0.58148300	2.35157800
H	-2.33141800	-1.69065100	3.14427200
C	1.26356600	-1.67604300	-0.78572400
O	2.27038300	-2.44364600	-1.22238300
C	2.67729200	-0.16596800	-1.58761900
C	3.23449300	-1.57842600	-1.88117500
H	2.55661500	0.46371100	-2.47667900
H	3.24027200	-1.85970700	-2.93741800

N	1.36033000	-0.41294500	-0.98232500
N	-1.01174400	-0.37767800	0.68660600
Cu	-0.01399100	0.99631800	-0.45893300
C	4.66813100	-0.48805400	-0.30524500
C	3.62857400	0.40291700	-0.56997600
C	3.51198200	1.60332200	0.12255700
C	4.45692200	1.90286600	1.10070900
C	5.49645300	1.01149200	1.37391600
C	5.61116200	-0.18679600	0.67279800
C	4.59953800	-1.69127700	-1.20493900
H	2.68455200	2.28266000	-0.08234500
H	4.38160800	2.83267500	1.65966500
H	6.22526700	1.25615600	2.14305100
H	6.42464600	-0.87666100	0.88858300
C	-3.37256300	0.36298300	0.81527000
C	-4.41340800	-0.56097100	0.89837800
C	-5.62342200	-0.30912800	0.25898200
C	-5.77073100	0.87248400	-0.46477600
C	-4.72447700	1.79474500	-0.54712100
C	-3.51563300	1.54595100	0.09819200
C	-4.03848100	-1.74241000	1.74919400
H	-6.44263400	-1.02265100	0.32317200
H	-6.71215300	1.08182200	-0.96744900
H	-4.85841600	2.71353800	-1.11283000
H	-2.69483600	2.26070000	0.04385700
H	-4.17231800	-2.70414300	1.23854200
H	-4.64447400	-1.78607900	2.66239100
H	5.39750600	-1.66675700	-1.95785100
H	4.69700100	-2.64590000	-0.67524200
H	0.04469400	-4.02451900	1.40498700
H	1.58955900	-4.04287900	0.40230000
H	-1.32126300	-3.95508500	-0.69743700
H	0.21936600	-3.96203500	-1.70284500
C	1.96367700	-0.30508300	2.64247200
H	1.29807000	-1.14918500	2.85046400
H	2.74826300	-0.27732100	3.40382500
H	2.43299800	-0.44116600	1.65989900
C	1.21466700	0.93644800	2.64718100
N	0.61534300	1.93223900	2.65146400

**LCu(MeCN)<sub>2</sub><sup>+</sup>**

C	-2.51086500	-3.02595900	3.13012300
H	-2.39554600	-2.58910500	4.12549200
H	-2.33025800	-4.10239600	3.18888900

H	-3.53336500	-2.85290400	2.77784000
C	2.51049200	-3.02675300	-3.12975200
H	3.53298500	-2.85367300	-2.77745800
H	2.39521200	-2.58998000	-4.12516200
H	2.32987100	-4.10319100	-3.18843800
C	1.58451400	-2.41355100	-2.20417100
N	0.85926200	-1.91468000	-1.45037300
C	-1.58490200	-2.41286100	2.20445400
N	-0.85963400	-1.91408500	1.45060900
C	-0.35465300	4.05430600	0.64396100
C	-0.00001300	2.71083300	-0.00008300
C	0.35462000	4.05427900	-0.64419200
C	1.10723200	1.97052000	0.63465600
O	2.08995500	2.74850800	1.12070000
C	2.46385500	0.47172100	1.56021500
C	3.13558900	1.86193700	1.57905400
H	2.19269100	0.08258700	2.55101400
H	3.43075900	2.20555600	2.57246100
C	-1.10724700	1.97046400	-0.63479000
O	-2.09005400	2.74843500	-1.12069200
C	-2.46383900	0.47165500	-1.56036200
C	-3.13562000	1.86185800	-1.57918200
H	-2.19277000	0.08250700	-2.55118100
H	-3.43070800	2.20552100	-2.57259900
N	-1.22239500	0.70548000	-0.80247800
N	1.22247500	0.70552800	0.80221100
Cu	0.00010900	-0.75713100	0.00000900
C	-4.46056300	0.34536500	-0.26866100
C	-3.43419600	-0.40973300	-0.83467300
C	-3.38486500	-1.78946900	-0.68487700
C	-4.38356100	-2.41643900	0.05755900
C	-5.40920300	-1.66401600	0.63404900
C	-5.45732700	-0.28039600	0.47231600
C	-4.30937300	1.80783100	-0.58734300
H	-2.58052300	-2.36520400	-1.14211800
H	-4.37138300	-3.49760100	0.18030800
H	-6.18766600	-2.16619800	1.20438700
H	-6.26707300	0.29778400	0.91323700
C	3.43428700	-0.40965600	0.83462300
C	4.46061700	0.34547800	0.26858700
C	5.45745700	-0.28026800	-0.47229600
C	5.40944600	-1.66390700	-0.63391700
C	4.38384200	-2.41636300	-0.05740600
C	3.38506500	-1.78940700	0.68493900

C	4.30926000	1.80796400	0.58711000
H	6.26718000	0.29793500	-0.91322900
H	6.18797400	-2.16607300	-1.20417700
H	4.37177400	-3.49753900	-0.18003400
H	2.58074700	-2.36516100	1.14220300
H	4.06462100	2.39805400	-0.30642900
H	5.22392300	2.24083000	1.00745600
H	-5.22405900	2.24049600	-1.00785000
H	-4.06492700	2.39808600	0.30613700
H	0.20211600	4.29937400	1.54275100
H	-1.41215800	4.29699000	0.65616900
H	1.41212400	4.29696900	-0.65641300
H	-0.20214800	4.29930200	-1.54299500

**LCu(MeCN)<sup>+</sup>**

C	0.00383100	5.58898100	0.00163400
H	0.23245800	5.95795100	1.00514200
H	-0.97942800	5.96100700	-0.29883000
H	0.75662100	5.96348900	-0.69729700
C	0.00295900	4.14504800	0.00080200
N	0.00098700	2.98635300	0.00046300
C	0.35075500	-3.66777100	0.64402800
C	-0.00064400	-2.32068100	-0.00021000
C	-0.35255500	-3.66763700	-0.64444800
C	-1.11547800	-1.58228600	0.61728100
O	-2.10352400	-2.35234700	1.08136900
C	-2.56765300	-0.07826700	1.36533500
C	-3.06703300	-1.48968900	1.74532700
H	-2.46395900	0.60169100	2.21864100
H	-3.01363300	-1.72425300	2.81180600
C	1.11450500	-1.58275600	-0.61768200
O	2.10232700	-2.35318700	-1.08161100
C	2.56734700	-0.07928600	-1.36557800
C	3.06628500	-1.49090400	-1.74541300
H	2.46400400	0.60064700	-2.21894800
H	3.01300600	-1.72550000	-2.81189000
N	1.24166300	-0.31263400	-0.76608200
N	-1.24213700	-0.31210900	0.76566100
Cu	0.00014100	1.07557100	-0.00027100
C	4.59776000	-0.52414000	-0.18492300
C	3.56376800	0.39769100	-0.34397700
C	3.51564300	1.56307000	0.41186300
C	4.52137000	1.79649700	1.34567600
C	5.55585800	0.87397200	1.51235000



C	5.60254200	-0.28923300	0.74794100
C	4.45506200	-1.67609500	-1.14099800
H	2.70461700	2.27818700	0.27601000
H	4.50305900	2.70137300	1.94838300
H	6.33465900	1.06656800	2.24655100
H	6.41231300	-1.00420200	0.88022400
C	-3.56404700	0.39896000	0.34381500
C	-4.59835200	-0.52255300	0.18493700
C	-5.60309700	-0.28746800	-0.74791900
C	-5.55608200	0.87560900	-1.51250400
C	-4.52130300	1.79783600	-1.34599100
C	-3.51562100	1.56422100	-0.41218000
C	-4.45597300	-1.67442400	1.14116100
H	-6.41309100	-1.00220900	-0.88006900
H	-6.33484600	1.06834200	-2.24670600
H	-4.50273100	2.70261500	-1.94883600
H	-2.70435300	2.27908700	-0.27641200
H	-4.54980900	-2.65800100	0.66640900
H	-5.21823000	-1.63207300	1.92950300
H	5.21745900	-1.63416600	-1.92922900
H	4.54844800	-2.65964300	-0.66609400
H	-0.20955600	-3.90731800	1.54207900
H	1.40845400	-3.90873000	0.66217900
H	-1.41034200	-3.90820400	-0.66260400
H	0.20768900	-3.90738100	-1.54249100

## B

C	0.59240600	0.43180400	-3.26473400
C	0.00000000	0.00000000	-1.91300200
C	-0.59240600	-0.43180400	-3.26473400
C	0.78746700	-1.02931400	-1.19764100
O	1.30237000	-1.97326100	-1.98470000
C	1.83144400	-2.35169800	0.26908900
C	2.10377700	-2.86691700	-1.16230000
H	2.73769500	-2.12010800	0.83963100
H	3.13642400	-2.75341500	-1.50027400
C	-0.78746700	1.02931400	-1.19764100
O	-1.30237000	1.97326100	-1.98470000
C	-1.83144400	2.35169800	0.26908900
C	-2.10377700	2.86691700	-1.16230000
H	-2.73769500	2.12010800	0.83963100
H	-3.13642400	2.75341500	-1.50027400
N	-1.06092900	1.11475900	0.05996600
N	1.06092900	-1.11475900	0.05996600

Cu	0.00000000	0.00000000	1.26074600
C	-0.80005000	4.49021600	0.02043600
C	-0.98352200	3.42216600	0.89647900
C	-0.38176300	3.40459800	2.14945600
C	0.42241800	4.47969700	2.51871200
C	0.61097800	5.55106700	1.64358500
C	0.00000000	5.56579800	0.39213600
C	-1.57733000	4.29818300	-1.25249500
H	-0.54209000	2.56967900	2.83222600
H	0.90284500	4.48769900	3.49398300
H	1.24033900	6.38503200	1.94494500
H	0.14783600	6.40560200	-0.28392100
C	0.98352200	-3.42216600	0.89647900
C	0.80005000	-4.49021600	0.02043600
C	0.00000000	-5.56579800	0.39213600
C	-0.61097800	-5.55106700	1.64358500
C	-0.42241800	-4.47969700	2.51871200
C	0.38176300	-3.40459800	2.14945600
C	1.57733000	-4.29818300	-1.25249500
H	-0.14783600	-6.40560200	-0.28392100
H	-1.24033900	-6.38503200	1.94494500
H	-0.90284500	-4.48769900	3.49398300
H	0.54209000	-2.56967900	2.83222600
H	0.97628200	-4.43533400	-2.15884100
H	2.41298800	-5.00580400	-1.31983700
H	-2.41298800	5.00580400	-1.31983700
H	-0.97628200	4.43533400	-2.15884100
H	1.55584100	-0.00703400	-3.50327500
H	0.47574000	1.48312300	-3.50495300
H	-0.47574000	-1.48312300	-3.50495300
H	-1.55584100	0.00703400	-3.50327500

**Cu(MeCN)<sup>+</sup>...2**

C	3.72777700	-0.70442200	-0.24420600
C	3.35640500	0.61616300	0.03155500
C	4.27890600	1.56297500	0.43361800
C	5.60761800	1.14444800	0.55240800
C	5.97932500	-0.17017500	0.27442800
C	5.03802300	-1.12200400	-0.13291800
C	2.52429100	-1.46880700	-0.62602600
C	1.90853800	0.73897200	-0.16126500
H	3.98099800	2.58480000	0.65048800
H	6.36433700	1.85566500	0.87044400
H	7.02053900	-0.46125200	0.37935300

H	5.31982400	-2.14890600	-0.34754800
O	1.18938800	1.71310400	0.06996100
O	2.33396200	-2.63080100	-0.85160600
N	1.49646200	-0.46732700	-0.67075000
O	0.18446700	-0.80749300	-0.78575200
C	-0.34131100	-1.30771400	0.42563800
O	0.31208600	-1.27877600	1.42748900
C	-2.58126900	-1.45248000	1.46177600
H	-2.07098800	-1.76683400	2.37873400
C	-1.73281300	-1.83196700	0.24017600
H	-1.60405200	-2.92973100	0.24890700
C	-2.42095600	-1.44229200	-1.06854100
H	-2.50563700	-0.34460900	-1.11629600
H	-1.81931700	-1.75268800	-1.92976000
C	-3.81295600	-2.06095400	-1.14067300
H	-4.30219600	-1.75936900	-2.07450500
H	-3.71595800	-3.15742200	-1.17777800
C	-4.66048700	-1.67302800	0.06434600
H	-5.65316500	-2.13481600	0.00001300
H	-4.82044100	-0.58213600	0.05728300
C	-3.97029800	-2.06834200	1.36403600
H	-4.57018600	-1.76829600	2.23163800
H	-3.88131600	-3.16515500	1.40827300
H	-2.66662700	-0.35345400	1.50188700
Cu	-0.66989300	1.93813000	-0.08832400
C	-5.03963400	2.80298200	-0.17499700
H	-5.19067400	3.87926100	-0.29327600
H	-5.49374400	2.47692100	0.76477500
H	-5.51594600	2.27750700	-1.00726400
C	-3.62888600	2.50995200	-0.15849600
N	-2.49666300	2.27256000	-0.14494300

**Cu(MeCN)<sub>2</sub><sup>+</sup>...2**

C	3.14451900	-1.49362000	-0.26673300
C	2.76798300	-0.36760800	-1.00269900
C	3.69029000	0.58418500	-1.39609800
C	5.02369700	0.36768400	-1.03622100
C	5.40144200	-0.76020600	-0.30570400
C	4.46003900	-1.71329100	0.09502900
C	1.93865900	-2.30172300	0.02639300
C	1.30437700	-0.39525600	-1.20146500
H	3.38592800	1.46145900	-1.96166700
H	5.78088700	1.09003800	-1.32877700
H	6.44647100	-0.89681500	-0.04175000

H	4.74455900	-2.59068800	0.66935200
O	0.54540800	0.44973400	-1.63279700
O	1.77675400	-3.27621700	0.71247300
N	0.91895500	-1.64472900	-0.70826900
O	-0.39334700	-1.98274600	-0.55906600
C	-1.04417300	-1.24799100	0.41631200
O	-0.46199100	-0.42966900	1.08400900
C	-3.21005800	-0.91016500	1.59087400
H	-2.74905500	-1.20008500	2.54273700
C	-2.49647400	-1.60227200	0.43306900
H	-2.56024900	-2.69645000	0.55266800
C	-3.13596400	-1.24263200	-0.92264600
H	-2.96163600	-0.17183500	-1.11643900
H	-2.64097100	-1.79220700	-1.73053600
C	-4.63119200	-1.53503600	-0.90906400
H	-5.07126500	-1.23278700	-1.86753500
H	-4.77916300	-2.62290600	-0.82434300
C	-5.33500700	-0.84410500	0.25222900
H	-6.40380800	-1.08986900	0.24994800
H	-5.26585200	0.24944500	0.12515200
C	-4.69849100	-1.23282300	1.58114800
H	-5.19532000	-0.72164700	2.41432200
H	-4.83810900	-2.31262300	1.74765200
H	-3.06586700	0.17762100	1.49205300
Cu	-0.17262900	1.87338400	0.27674300
C	3.96776900	2.05858300	2.00239000
H	4.34288300	1.03468600	2.09530000
H	3.97654700	2.53418200	2.98670400
H	4.61985600	2.61900500	1.32616100
C	2.62361400	2.04069600	1.47836800
N	1.54817500	2.02209700	1.05168800
C	-4.25866200	2.83058200	-1.31890000
H	-4.21190100	3.74000700	-1.92387700
H	-4.96569000	2.98263400	-0.49849000
H	-4.60393800	2.00276200	-1.94668100
C	-2.95173000	2.52457800	-0.79036600
N	-1.90662600	2.26001300	-0.36912300

### LCu<sup>+</sup>...2

C	4.17997100	-2.33727200	-0.08603600
C	3.75183300	-1.48877200	-1.11182400
C	4.63027400	-0.97517700	-2.04605500
C	5.97258300	-1.34857900	-1.92954000
C	6.40170800	-2.19177500	-0.90472200

C	5.50563000	-2.70110300	0.04088000
C	3.01710000	-2.70050400	0.75210100
C	2.31268000	-1.23464700	-0.94627600
H	4.28803800	-0.30570700	-2.83062200
H	6.69649000	-0.97115700	-2.64613700
H	7.45305200	-2.45751700	-0.84093200
H	5.83356500	-3.35443600	0.84459200
O	1.57768800	-0.52076900	-1.61830500
O	2.89824700	-3.42385000	1.70412400
N	1.95003600	-1.95504300	0.17362500
O	0.65688400	-2.13809100	0.55863000
C	0.33175300	-1.48009200	1.75191100
O	1.10629900	-0.75217600	2.30547700
C	-1.20916900	-1.93890600	3.65146800
H	-0.55150900	-2.73351700	4.02495000
C	-1.07569500	-1.81509400	2.13298600
H	-1.34892300	-2.76352600	1.64455400
C	-2.00640800	-0.71389400	1.59459200
H	-1.66605000	0.25577700	1.99483400
H	-1.91662900	-0.66310500	0.50028100
C	-3.45054000	-0.96810100	2.00469700
H	-4.08573800	-0.15188300	1.63224800
H	-3.80336700	-1.88977900	1.51449200
C	-3.58116300	-1.10759700	3.51661300
H	-4.62177400	-1.31788300	3.79238700
H	-3.31505000	-0.15068600	3.99330500
C	-2.65835400	-2.20151500	4.04186000
H	-2.73870100	-2.28439400	5.13235200
H	-2.97500000	-3.17258900	3.62937800
H	-0.86293600	-0.99867700	4.10652700
Cu	-0.05690600	0.47507200	-1.08652900
C	-3.68889900	3.17267600	0.42494100
C	-2.49221400	2.65253700	-0.38284800
C	-3.21341700	3.96292200	-0.71877400
C	-1.19284600	2.75776100	0.30656300
O	-1.05008100	3.85628100	1.06015000
C	0.75272200	2.38309000	1.32797600
C	0.31251700	3.83930700	1.54725500
H	0.67335600	1.73279500	2.21055200
H	0.28200100	4.14974600	2.59308900
C	-2.75658300	1.52833000	-1.29995900
O	-4.03722700	1.37527300	-1.64602400
C	-2.65750700	-0.24304000	-2.65129100
C	-4.12975500	0.21160800	-2.50900500

H	-2.27014200	-0.19687400	-3.67596700
H	-4.58936100	0.55145800	-3.43937200
N	-1.90716300	0.71305700	-1.81645900
N	-0.22881500	1.90586200	0.32707600
C	-3.87620700	-1.98367900	-1.56207000
C	-2.62749200	-1.62575800	-2.06697500
C	-1.52970000	-2.46949400	-1.94415000
C	-1.69350900	-3.68876200	-1.29163600
C	-2.94184100	-4.05243400	-0.78282600
C	-4.04120200	-3.20695800	-0.91962200
C	-4.90591300	-0.91931100	-1.82251100
H	-0.55668300	-2.17426200	-2.33776900
H	-0.84516400	-4.35903500	-1.17545400
H	-3.05878900	-5.00943400	-0.27956000
H	-5.01283700	-3.49829800	-0.52440700
C	2.15118600	2.49485800	0.81021700
C	2.42815200	3.80978100	0.43353300
C	3.68267700	4.13718300	-0.06723300
C	4.64715200	3.13578200	-0.17740800
C	4.37078500	1.82700100	0.22065100
C	3.11341800	1.49803500	0.72325600
C	1.24518500	4.70601200	0.68442200
H	3.91657900	5.16056600	-0.35411000
H	5.63533000	3.38275800	-0.55854300
H	5.14799500	1.06675900	0.15966300
H	2.88808700	0.49583700	1.08786400
H	0.73550700	4.97464100	-0.25163100
H	1.51827000	5.64531900	1.17655100
H	-5.71631100	-1.28580500	-2.46376300
H	-5.37715100	-0.55260500	-0.90131000
H	-3.45371800	3.51718500	1.42682100
H	-4.60333200	2.59836600	0.31875000
H	-2.64265300	4.86661000	-0.53026300
H	-3.79251500	3.94928600	-1.63708700

**LCu<sup>+</sup>...2<sup>-</sup>**

C	4.06659700	-2.45508100	-0.12554700
C	3.53500500	-1.69814000	-1.21497300
C	4.39041200	-1.19789500	-2.21150400
C	5.74185800	-1.46225500	-2.11358700
C	6.26852400	-2.21319000	-1.03293300
C	5.43798200	-2.70733800	-0.04150600
C	2.99546900	-2.83525500	0.77099600
C	2.13189200	-1.55489300	-1.03660100

H	3.98762600	-0.61309900	-3.03657500
H	6.42052700	-1.08514600	-2.87580300
H	7.33887700	-2.40011000	-0.98635300
H	5.83550500	-3.28136900	0.79373500
O	1.24244100	-0.96084400	-1.72620600
O	2.95224300	-3.48562000	1.81460000
N	1.86833900	-2.24532500	0.15262500
O	0.59386500	-2.42789600	0.61748900
C	0.26001400	-1.60572400	1.67360600
O	1.02490000	-0.81349200	2.15739000
C	-1.29703100	-2.03756600	3.57876100
H	-0.69819600	-2.89963600	3.89905000
C	-1.16921300	-1.83658600	2.06730700
H	-1.53691900	-2.72934800	1.53882500
C	-2.01435500	-0.63516500	1.61643400
H	-1.61179100	0.27546400	2.09068500
H	-1.91916300	-0.49744700	0.52982500
C	-3.47301200	-0.82510100	2.00779500
H	-4.06020200	0.04454000	1.67851000
H	-3.87568300	-1.69759900	1.46856400
C	-3.61211700	-1.04121400	3.51052000
H	-4.66323400	-1.20141000	3.78164900
H	-3.28482300	-0.13089200	4.03833000
C	-2.75890700	-2.21875500	3.97120600
H	-2.83984300	-2.35266400	5.05701600
H	-3.14209000	-3.14415000	3.51183300
H	-0.87789500	-1.15286800	4.08183400
Cu	0.11073500	0.40745200	-0.92482600
C	-3.43665700	3.28943600	0.56359500
C	-2.26187300	2.75949300	-0.26715100
C	-2.91734100	4.11600400	-0.53633700
C	-0.95871900	2.77379600	0.42264500
O	-0.75348600	3.84023600	1.21130000
C	0.98629800	2.27638800	1.39046600
C	0.60827900	3.73622900	1.69400800
H	0.91571200	1.58823200	2.24225200
H	0.58761600	3.98569200	2.75652000
C	-2.56688800	1.69326600	-1.24015500
O	-3.84232200	1.66303500	-1.65066800
C	-2.55989700	-0.04169900	-2.62057600
C	-3.95267200	0.63043000	-2.66502400
H	-2.06988500	-0.11366700	-3.59857900
H	-4.18403000	1.13844700	-3.60516600
N	-1.76170800	0.83117600	-1.74290000

N	-0.04188700	1.87482400	0.40638900
C	-4.17765600	-1.56898600	-1.74428700
C	-2.81792700	-1.38591400	-1.99362500
C	-1.88219300	-2.35399800	-1.64333100
C	-2.33090100	-3.51760200	-1.02287100
C	-3.69097100	-3.70490100	-0.76589100
C	-4.62297400	-2.73468200	-1.12788100
C	-4.99163200	-0.41347700	-2.25742100
H	-0.81960200	-2.19384600	-1.83101300
H	-1.61613600	-4.28597900	-0.73622400
H	-4.02619600	-4.61964400	-0.28197200
H	-5.68283800	-2.88721200	-0.93174200
C	2.36051900	2.35554700	0.80593100
C	2.69075700	3.67799500	0.50912600
C	3.92407300	3.97233500	-0.06069500
C	4.80670700	2.92705500	-0.33355100
C	4.47082400	1.60642800	-0.03189300
C	3.23887300	1.31076100	0.54914200
C	1.57491100	4.61676300	0.88415900
H	4.19958300	5.00047000	-0.28894200
H	5.77464200	3.14575200	-0.77940600
H	5.17070700	0.80055700	-0.24805300
H	2.96956700	0.28830600	0.81468500
H	1.05848500	5.00358600	-0.00559600
H	1.92008900	5.48763500	1.45201500
H	-5.59595000	-0.70750900	-3.12513600
H	-5.68742000	-0.00169200	-1.51642100
H	-3.19094300	3.56837200	1.58358700
H	-4.37770400	2.76736700	0.42432000
H	-2.30769800	4.98083300	-0.29571800
H	-3.49268100	4.17678500	-1.45476200

2-

C	2.74305800	0.79048000	-0.02202900
C	2.96617600	-0.61849300	-0.17267600
C	4.22069100	-1.16815500	0.12861100
C	5.22922400	-0.33467000	0.57067300
C	5.00724200	1.06292900	0.72225500
C	3.77896500	1.62171800	0.42996700
C	1.38455900	1.10096800	-0.36741900
C	1.75592900	-1.25541900	-0.61538400
H	4.38458300	-2.23951200	0.01572000
H	6.20789100	-0.74674500	0.80965100
H	5.82028600	1.69461000	1.07534500



H	3.60455800	2.69078900	0.54836500
O	1.43839800	-2.43489800	-0.81046600
O	0.70420200	2.13440000	-0.32140200
N	0.89181000	-0.14945200	-0.82929600
O	-0.45453600	-0.32298300	-1.03677500
C	-1.16944500	-0.45871000	0.12783800
O	-0.65987300	-0.55624000	1.21267600
C	-3.46902500	-1.03875900	0.92125500
H	-3.18736600	-2.09244600	1.04354500
C	-2.63612300	-0.39682000	-0.18231800
H	-2.80689300	-0.91815000	-1.13763700
C	-3.02448400	1.08043400	-0.37231100
H	-2.76865800	1.62527500	0.55133200
H	-2.42304400	1.52181400	-1.17596000
C	-4.51477300	1.21351400	-0.65629500
H	-4.78112000	2.27205900	-0.76834300
H	-4.74010800	0.72852900	-1.61972800
C	-5.34839500	0.56102100	0.44098400
H	-6.41822600	0.64691700	0.21152500
H	-5.18506800	1.10173900	1.38721800
C	-4.95769500	-0.90091500	0.62894600
H	-5.54359700	-1.35665200	1.43698400
H	-5.20094400	-1.46098700	-0.28849800
H	-3.22592200	-0.53803600	1.87071300

### TS1

C	2.56672600	-0.67742000	-0.35292400
C	2.69990400	0.64073500	0.14068500
C	3.89056600	1.33870800	0.08554200
C	4.98651300	0.72249100	-0.52889900
C	4.85202400	-0.57076900	-1.06478900
C	3.65977700	-1.28058600	-0.99678700
C	1.20253600	-1.12673000	-0.18810100
C	1.39698300	1.02352500	0.69623500
H	3.95712500	2.34574700	0.49414400
H	5.93722800	1.24361300	-0.60788800
H	5.71525700	-1.03103300	-1.54362900
H	3.57235700	-2.28236100	-1.41215600
O	1.09342700	2.00597500	1.34599800
O	0.66501000	-2.20688100	-0.49871600
N	0.49137700	-0.01324100	0.31924500
O	-2.28388600	-1.04846200	2.40954800
C	-1.63759100	-0.62051300	1.46726100
O	-0.34231100	-0.38487800	1.66641700

C	-3.61284000	-0.95860200	-0.03984600
H	-3.50993000	-2.04781700	0.05086100
C	-2.25402400	-0.28865800	0.12944500
H	-1.57341700	-0.64029100	-0.65862500
C	-2.39171400	1.23650000	0.00386500
H	-3.03162300	1.59247300	0.82907600
H	-1.41216400	1.71368400	0.13089400
C	-3.02533800	1.61668300	-1.32901200
H	-3.13276500	2.70704200	-1.39976500
H	-2.34855200	1.31389900	-2.14440500
C	-4.37384700	0.93096800	-1.51604400
H	-4.80725500	1.19256500	-2.49034300
H	-5.07444200	1.30216200	-0.75020900
C	-4.24111500	-0.58181600	-1.37669800
H	-5.22053400	-1.06572700	-1.48614900
H	-3.60990700	-0.96460500	-2.19516100
H	-4.27030200	-0.63977900	0.78307800

## 6

C	2.57583800	-0.49017300	-0.62419900
C	2.68890300	0.74055800	0.00691500
C	3.88374800	1.16301000	0.56319700
C	4.97584900	0.29716200	0.47181800
C	4.86072100	-0.94421300	-0.16121000
C	3.65077300	-1.35614100	-0.72413600
C	1.16512300	-0.59623100	-1.11026000
C	1.34609700	1.39369700	-0.08109400
H	3.96310900	2.13154300	1.05220900
H	5.93286900	0.58884500	0.89854200
H	5.73012000	-1.59574800	-0.21287800
H	3.55060700	-2.31943600	-1.21980500
O	1.06448700	2.49244600	0.37676200
O	0.69728900	-1.54739000	-1.72090500
N	0.47865900	0.56848300	-0.78646100
O	-1.67630700	-1.45635600	2.37967300
C	-1.29427900	-0.83314700	1.38283400
O	-0.05510000	-0.47634000	1.28320900
C	-3.54250400	-1.20393000	0.29890500
H	-3.34054200	-2.28071400	0.22357300
C	-2.23753400	-0.41868500	0.27372100
H	-1.71320400	-0.58934300	-0.67852200
C	-2.51201500	1.08630100	0.38020500
H	-2.98444800	1.28901700	1.35712300
H	-1.55998300	1.62906600	0.35187600

C	-3.43558200	1.54552800	-0.74009100
H	-3.63891700	2.62117700	-0.65247700
H	-2.91640800	1.40100300	-1.70232200
C	-4.73814900	0.75265100	-0.74237800
H	-5.38541700	1.07232500	-1.57010600
H	-5.28849200	0.96848300	0.18836400
C	-4.46969100	-0.74655000	-0.82237200
H	-5.41316100	-1.30780700	-0.79083900
H	-4.00201900	-0.97590900	-1.79386000
H	-4.03145900	-1.04979400	1.27329700

## TS2

C	-2.59562800	0.72996900	0.03054800
C	-2.54125300	-0.43709400	-0.71716600
C	-3.62070400	-1.29708600	-0.79984600
C	-4.77742400	-0.94615800	-0.09739700
C	-4.83252700	0.22878300	0.65686700
C	-3.73278700	1.08911700	0.73094100
C	-1.25566300	1.39058800	-0.12496400
C	-1.16670000	-0.48677100	-1.32068800
H	-3.56701700	-2.21012300	-1.38964400
H	-5.65014800	-1.59472800	-0.13390500
H	-5.74640000	0.47326700	1.19418200
H	-3.76491600	2.00532700	1.31734900
O	-0.74569500	-1.40951900	-2.01422600
O	-0.93375800	2.43866900	0.42989600
N	-0.47187300	0.64930400	-0.97762900
O	1.97122500	-1.21270000	2.63407200
C	1.32835700	-0.86896200	1.64847800
O	0.09644900	-0.73629200	1.43812400
C	2.40933700	1.05315600	0.45067000
H	1.45402500	1.59193400	0.49604200
C	2.15278800	-0.44125600	0.33683800
H	1.49036300	-0.62446200	-0.51792300
C	3.44198600	-1.23504400	0.24233100
H	4.03063300	-1.07239500	1.15591800
H	3.23581700	-2.31115900	0.17910800
C	4.23382500	-0.76345800	-0.97921000
H	5.16916700	-1.33366900	-1.05429600
H	3.65750900	-0.98010300	-1.89217700
C	4.51361100	0.73253600	-0.90365400
H	5.06911100	1.06296500	-1.79154500
H	5.16027000	0.93432000	-0.03430200
C	3.21914800	1.52366300	-0.75919700

H	3.42506900	2.59843700	-0.67101800
H	2.60212100	1.39021800	-1.66111200
H	2.97353800	1.25188400	1.37649300

**Cy**

C	1.25571500	-0.70657900	-0.24760300
C	1.27911500	0.76922000	0.16254000
C	0.00000100	1.45300000	-0.17528300
C	-1.27911200	0.76922200	0.16254000
C	-1.25571700	-0.70657700	-0.24760300
C	-0.00000100	-1.39637300	0.27325100
H	1.44610400	0.81163600	1.25868200
H	2.13561200	1.28587700	-0.28917900
H	1.27133700	-0.77571800	-1.34631400
H	2.15859600	-1.21453900	0.11565500
H	-1.44610200	0.81163800	1.25868200
H	-2.13561000	1.28588100	-0.28917800
H	-2.15859800	-1.21453500	0.11565500
H	-1.27133900	-0.77571500	-1.34631400
H	-0.00000100	-1.36433100	1.37571700
H	-0.00000200	-2.45726400	-0.00906600
H	0.00000200	2.51559000	-0.41139300

**TS3**

C	-3.24157000	0.73141900	0.80149700
C	-4.46506400	0.26354500	0.08534000
C	-4.21150700	-0.96065300	-0.79306100
C	-3.43968700	-2.02981800	-0.02865700
C	-2.09977200	-1.48445900	0.45151900
C	-2.28977500	-0.27048900	1.36011200
H	-5.16486600	-1.35742900	-1.16477000
H	-5.23578400	-0.00685900	0.83496900
H	-4.90584500	1.08260100	-0.50170900
H	-3.31896400	1.67944700	1.33526500
H	-4.03442600	-2.35342900	0.84204500
H	-3.29132100	-2.91897600	-0.65475200
H	-1.52769500	-2.25943100	0.97745000
H	-1.49943600	-1.19435200	-0.42581300
H	-2.66910000	-0.62463000	2.33900600
H	-1.32144100	0.20876000	1.57104400
H	-3.63001600	-0.66625800	-1.68099500
C	3.78898400	-1.66599800	-0.56802500
C	2.67661500	-0.83806500	-0.52968600
C	2.75983600	0.45715100	0.01081700

C	3.99847300	0.87550700	0.52323300
C	5.11207800	0.04556200	0.48539900
C	5.01432900	-1.22983700	-0.06399600
H	3.70000700	-2.66470900	-0.99038900
H	1.72609000	-1.20573200	-0.91304900
H	4.07889600	1.87417200	0.95161100
H	6.06056800	0.39688300	0.88592200
H	5.88337100	-1.88268700	-0.09448200
C	1.62733800	1.36840500	0.06303200
H	1.79538500	2.29895700	0.61216700
C	0.41196400	1.18269400	-0.50639400
H	0.21931000	0.27509600	-1.08573500
C	-0.67541400	2.11078700	-0.41498000
H	-0.50151600	3.02162400	0.16275100
C	-1.90146200	1.88359100	-0.95380600
H	-2.68363300	2.63702000	-0.93397000
H	-2.07178700	1.02389500	-1.60062600

## A

C	-4.65999100	0.89719400	1.31034500
C	-3.41578800	0.36614800	1.01184500
C	-3.16899100	-0.24810600	-0.23724700
C	-4.23664400	-0.29918700	-1.16120500
C	-5.47908800	0.23357200	-0.85717700
C	-5.70078300	0.83686900	0.38140500
H	-4.82439600	1.36506100	2.27879300
H	-2.62050700	0.42563100	1.75190000
H	-4.06638500	-0.76845300	-2.12971300
H	-6.28251200	0.18002600	-1.58867200
H	-6.67491600	1.25608900	0.62141100
C	-1.90226800	-0.80886000	-0.60195600
H	-1.84037300	-1.25699200	-1.59709000
C	-0.73823200	-0.83583200	0.18033700
H	-0.76491100	-0.39595400	1.18139900
C	0.44784300	-1.38361100	-0.23108700
H	0.49789200	-1.81852900	-1.23462000
C	1.69904800	-1.40430100	0.57407300
H	1.50896600	-0.98028900	1.57372600
H	2.02588300	-2.44570300	0.73299300
C	3.68639400	1.62150200	-0.85298100
C	2.53050600	0.84785900	-0.22996200
C	2.85387800	-0.63735300	-0.08074000
C	4.14822900	-0.81878200	0.70859500
C	5.30770200	-0.05116500	0.08430000

C	4.97249400	1.42962300	-0.05661600
H	2.31311800	1.25653900	0.77323800
H	1.61261200	0.97576900	-0.82028600
H	3.84475700	1.26206600	-1.88290000
H	3.43525800	2.68735800	-0.93071600
H	3.98247600	-0.45477500	1.73780500
H	4.38980000	-1.88819300	0.79191300
H	6.22082200	-0.18665100	0.67840200
H	5.51888400	-0.46868000	-0.91366200
H	4.84357700	1.86672000	0.94714900
H	5.80326900	1.96988500	-0.52900400
H	3.01082600	-1.05435700	-1.09362600

**PC**

C	0.73490400	-1.24574500	0.00004900
C	1.43339500	-0.00003200	0.00000100
C	3.56164300	-1.22865400	0.00011100
C	2.87455100	-2.41597900	0.00021800
C	1.47090400	-2.42031400	0.00018500
C	-0.73490400	-1.24574500	-0.00004900
C	-3.56164200	-1.22865400	-0.00011100
C	-2.87455100	-2.41597900	-0.00021700
C	-1.47090400	-2.42031400	-0.00018400
H	4.64998800	-1.20936600	0.00012400
H	3.41029500	-3.36213900	0.00032300
H	0.96468300	-3.38171600	0.00028400
H	-4.64998800	-1.20936700	-0.00012300
H	-3.41029500	-3.36213900	-0.00032200
H	-0.96468200	-3.38171600	-0.00028200
C	2.86087700	0.00001600	0.00000200
C	-0.73487800	1.24565400	0.00004800
C	-1.43339500	-0.00003200	-0.00000100
C	-3.56157000	1.22873400	0.00010600
C	-2.87441400	2.41602600	0.00021200
C	-1.47076900	2.42027100	0.00018100
C	0.73487800	1.24565400	-0.00004900
C	3.56157000	1.22873400	-0.00010600
C	2.87441400	2.41602600	-0.00021300
C	1.47076900	2.42027100	-0.00018200
H	-4.64991700	1.20951100	0.00011700
H	-3.41009700	3.36222000	0.00031500
H	-0.96443300	3.38162600	0.00027900
H	4.64991700	1.20951200	-0.00011700
H	3.41009800	3.36222000	-0.00031700

H	0.96443300	3.38162600	-0.00028000
C	-2.86087700	0.00001600	-0.00000200

**PC\***

C	0.00002200	0.71147400	-1.23947800
C	0.00000000	1.41248600	0.00000000
C	0.00004600	3.54227700	-1.22633600
C	0.00009900	2.84609600	-2.43860700
C	0.00008700	1.47036400	-2.45501600
C	-0.00002200	-0.71147400	-1.23947800
C	-0.00004600	-3.54227700	-1.22633600
C	-0.00009900	-2.84609600	-2.43860700
C	-0.00008700	-1.47036400	-2.45501600
H	0.00004900	4.63062800	-1.21223200
H	0.00015400	3.39639800	-3.37655900
H	0.00015600	0.95887600	-3.41213100
H	-0.00004900	-4.63062800	-1.21223200
H	-0.00015400	-3.39639800	-3.37655900
H	-0.00015600	-0.95887600	-3.41213100
C	0.00000000	2.84762200	0.00000000
C	0.00002100	-0.71147400	1.23947900
C	0.00000000	-1.41248600	0.00000000
C	0.00004500	-3.54227800	1.22633500
C	0.00009800	-2.84609800	2.43860600
C	0.00008600	-1.47036600	2.45501700
C	-0.00002100	0.71147400	1.23947900
C	-0.00004500	3.54227800	1.22633500
C	-0.00009800	2.84609800	2.43860600
C	-0.00008600	1.47036600	2.45501700
H	0.00004700	-4.63062900	1.21223000
H	0.00015100	-3.39640100	3.37655800
H	0.00015600	-0.95888000	3.41213300
H	-0.00004700	4.63062900	1.21223000
H	-0.00015100	3.39640100	3.37655800
H	-0.00015600	0.95888000	3.41213300
C	0.00000000	-2.84762200	0.00000000

**PC<sup>+</sup>**

C	0.72231400	-1.23988100	0.00859100
C	1.41967600	-0.00000100	0.00000100
C	3.54441900	-1.22363500	0.02149500
C	2.85726400	-2.42533200	0.04145900
C	1.46834700	-2.43179200	0.03427300
C	-0.72231400	-1.23988100	-0.00859000

C	-3.54441900	-1.22363500	-0.02149500
C	-2.85726400	-2.42533200	-0.04145800
C	-1.46834700	-2.43179200	-0.03427300
H	4.63189200	-1.20750300	0.02494500
H	3.39942500	-3.36563500	0.06222000
H	0.96113700	-3.39102900	0.05369600
H	-4.63189200	-1.20750300	-0.02494500
H	-3.39942500	-3.36563500	-0.06221900
H	-0.96113700	-3.39102900	-0.05369400
C	2.84461000	0.00000000	0.00000200
C	-0.72231300	1.23987800	0.00858900
C	-1.41967600	-0.00000100	-0.00000100
C	-3.54441700	1.22363700	0.02148900
C	-2.85726000	2.42533300	0.04145400
C	-1.46834300	2.43179100	0.03427100
C	0.72231300	1.23987800	-0.00859000
C	3.54441700	1.22363700	-0.02148900
C	2.85726000	2.42533300	-0.04145400
C	1.46834300	2.43179100	-0.03427100
H	-4.63189100	1.20750700	0.02493700
H	-3.39942000	3.36563700	0.06221400
H	-0.96113100	3.39102600	0.05369400
H	4.63189100	1.20750700	-0.02493700
H	3.39942000	3.36563700	-0.06221500
H	0.96113100	3.39102700	-0.05369500
C	-2.84461000	0.00000000	-0.00000200

## CO<sub>2</sub>

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16475800
O	0.00000000	0.00000000	-1.16475800

## NHP-

C	0.14112100	0.69245000	0.00005500
C	0.14112100	-0.69245000	0.00010300
C	1.31797000	-1.41733700	0.00003300
C	2.51897500	-0.69800000	-0.00001000
C	2.51897500	0.69800100	-0.00000200
C	1.31797100	1.41733700	0.00002500
C	-1.31131400	1.10597100	-0.00010800
C	-1.31131400	-1.10597200	0.00038100
H	1.30666500	-2.50602700	0.00008800
H	3.46846600	-1.23006400	-0.00002900
H	3.46846600	1.23006200	-0.00004500



H	1.30666500	2.50602700	-0.00003400
O	-1.67297400	-2.28466500	-0.00039600
O	-1.67297500	2.28466500	0.00009200
N	-2.11195700	0.00000000	-0.00005900

**TS3'**

C	-2.69539500	0.36688600	0.87405100
C	-3.60703700	-0.19147200	-0.17370100
C	-2.93510500	-1.24759600	-1.04345800
C	-2.29153500	-2.32131800	-0.17505100
C	-1.22988500	-1.70720400	0.72899300
C	-1.80333900	-0.59172500	1.60302100
H	-3.66552800	-1.68656300	-1.73505000
H	-4.47256300	-0.65842600	0.33373500
H	-4.01835400	0.62365200	-0.78648500
H	-3.17059000	1.10979900	1.52002200
H	-3.07100000	-2.80023200	0.44105700
H	-1.85188200	-3.11307500	-0.79523200
H	-0.77264700	-2.47341700	1.36845400
H	-0.42179500	-1.30307900	0.10192200
H	-2.39975900	-1.05330800	2.41321500
H	-0.99105000	-0.04839100	2.11058300
H	-2.15964300	-0.77053800	-1.66455600
C	3.54374600	-0.84501800	-1.28639200
C	2.32238900	-0.22776900	-1.05560900
C	2.10466600	0.52548500	0.10976800
C	3.15532700	0.62499300	1.03327900
C	4.37805500	0.00564400	0.80362800
C	4.57947200	-0.73160200	-0.35973600
H	3.68967800	-1.42357300	-2.19607200
H	1.52277100	-0.33689000	-1.78654300
H	3.00071000	1.20239600	1.94426700
H	5.17676900	0.10009900	1.53607800
H	5.53474900	-1.21780500	-0.54312300
C	0.83992200	1.19440900	0.39988600
H	0.77418500	1.66462600	1.38543300
C	-0.22784500	1.28738700	-0.41321900
H	-0.18756900	0.86074100	-1.41968200
C	-1.46949700	1.95999000	-0.05680300
H	-1.46166800	2.44280000	0.92405500
C	-2.28816500	2.49136100	-1.03654300
H	-3.11746600	3.14928900	-0.78957300
H	-2.19198800	2.17718600	-2.07520200

**TS3''**

C	-1.92135400	-0.11795000	0.99517000
C	-2.97466400	-0.59529500	0.05079900
C	-2.45573100	-1.61341400	-0.96049300
C	-1.68365800	-2.72501300	-0.26024200
C	-0.49501400	-2.14971900	0.50027400
C	-0.93945000	-1.11113000	1.52775200
H	-3.29215300	-2.02179600	-1.54175300
H	-3.78111700	-1.07385600	0.64026500
H	-3.44969800	0.26353100	-0.44747300
H	-2.24575000	0.63817500	1.71376500
H	-2.35582500	-3.24304500	0.44422400
H	-1.34703700	-3.47798600	-0.98441400
H	0.07010200	-2.94620900	1.00116000
H	0.19644700	-1.68356300	-0.21800700
H	-1.42131400	-1.63983400	2.37281100
H	-0.07005300	-0.59281700	1.96066100
H	-1.78867800	-1.11436700	-1.68227100
C	2.98688000	-0.56213600	-1.41218900
C	1.81525900	0.12417800	-1.12840100
C	1.66479800	0.83296200	0.08175800
C	2.75217700	0.83203600	0.97725600
C	3.92317500	0.14571300	0.68988200
C	4.04833700	-0.55870900	-0.50674300
H	3.07885800	-1.09895400	-2.35415400
H	1.00658400	0.12555900	-1.85820200
H	2.65762300	1.38021700	1.91444000
H	4.74529800	0.15962200	1.40226900
H	4.96574200	-1.09563000	-0.73578500
C	0.47001800	1.56801100	0.42171200
H	0.54041400	2.20798000	1.30612000
C	-0.75470500	1.50019200	-0.21035800
H	-0.84670100	0.93537200	-1.14132500
C	-1.76415400	2.52715100	0.00703200
H	-1.65430400	3.11281300	0.92397700
C	-2.77452500	2.79392400	-0.82864000
H	-3.49695200	3.57902600	-0.62371600
H	-2.89584600	2.24095300	-1.76000900

**TS3'''**

C	-1.07179600	1.17166200	-0.98153300
C	-1.69780700	1.73980700	0.25151100
C	-0.68011900	2.09913600	1.32996700
C	0.43922200	2.95515600	0.74887500

C	1.15609800	2.21002800	-0.37026800
C	0.18767100	1.80754800	-1.48150400
H	-1.18041700	2.61738100	2.15817800
H	-2.23999900	2.66215000	-0.03530600
H	-2.46569500	1.05372500	0.63795600
H	-1.78576700	0.88891100	-1.75924700
H	0.00976300	3.89076000	0.35219700
H	1.15134400	3.24466700	1.53244300
H	1.96307600	2.82391000	-0.79072200
H	1.62864400	1.30995700	0.04752400
H	-0.09638700	2.71897800	-2.04407000
H	0.68662300	1.15750900	-2.21589200
H	-0.24812700	1.17699700	1.74921200
C	2.43229400	-1.29253400	1.47047200
C	1.08820800	-1.22597900	1.12850400
C	0.68810700	-1.18196000	-0.21619600
C	1.68621500	-1.23462900	-1.19913200
C	3.03276500	-1.30000600	-0.85839700
C	3.41345000	-1.32399000	0.47998000
H	2.71826200	-1.31982100	2.51975400
H	0.33868100	-1.19753700	1.91785900
H	1.39263200	-1.22439000	-2.24875900
H	3.78669300	-1.33664700	-1.64169700
H	4.46519000	-1.37246700	0.75175900
C	-0.71673100	-1.09744100	-0.63084400
H	-0.86801900	-1.16543900	-1.71098500
C	-1.79177300	-1.44113600	0.16801100
H	-1.65735300	-1.55902200	1.24620300
C	-3.12184300	-1.56656800	-0.33780900
H	-3.24155400	-1.43781900	-1.41788100
C	-4.21391300	-1.82758600	0.41290000
H	-5.20298000	-1.91870200	-0.02674700
H	-4.13489200	-1.96215500	1.49100700

7

C	-2.15368500	-2.22488700	1.52903300
O	-0.89999500	-2.94197800	1.33603000
C	-2.09873400	-1.13690300	0.43536700
H	-2.27064700	-0.12719400	0.82958800
C	-0.18477300	-2.25365400	0.43677800
N	-0.73519300	-1.23062200	-0.09962600
C	1.16065800	-2.79192100	0.15391800
C	1.25769800	-4.32186400	0.04667500
C	1.80317300	-3.65328600	1.23667800

H	0.31273000	-4.84979300	0.13133600
H	1.94468200	-4.69331500	-0.70703800
H	1.24805000	-3.71480000	2.16752500
H	2.88032900	-3.55423400	1.32937900
C	4.09554900	-1.70923100	-1.67711100
O	3.28777900	-2.59537600	-0.86281000
C	3.10416400	-0.59699300	-2.08771300
H	2.86563500	-0.58149400	-3.15842000
C	2.08388100	-2.03237500	-0.71179900
N	1.87705400	-0.93036100	-1.34226600
C	-4.82293700	-3.24973800	-0.91574300
C	-5.13174600	-2.65787400	-2.13808000
C	-4.45094600	-1.51838200	-2.57045100
C	-3.44622500	-0.95820000	-1.78501800
C	-3.14006900	-1.55503200	-0.56539800
C	-3.82108800	-2.69071500	-0.12855700
H	-5.35945300	-4.13607200	-0.58172600
H	-5.91300600	-3.08613500	-2.76190800
H	-4.70606700	-1.06650500	-3.52635600
H	-2.90444000	-0.07327200	-2.12122500
C	-3.34863800	-3.12885900	1.23141900
H	-3.05843400	-4.18567900	1.27155200
H	-4.13108100	-2.98984200	1.98805000
C	3.25232600	1.97109700	-1.76514800
C	3.73172100	0.67668500	-1.60525900
C	4.89437100	0.41577800	-0.88286500
C	5.60161400	1.46497700	-0.30433500
C	5.12435600	2.76580700	-0.45701800
C	3.95850300	3.02038500	-1.18223700
H	2.34051000	2.15886400	-2.33170500
H	6.51286700	1.27491600	0.25994400
H	5.66655000	3.59317400	-0.00531600
H	3.59465600	4.03967900	-1.28345900
C	5.21526200	-1.05378900	-0.85646800
H	5.22492700	-1.46529800	0.16212700
H	4.46713300	-2.30860000	-2.51066500
H	6.20116800	-1.26557200	-1.28680800
H	-2.13361900	-1.81212100	2.54249700
Cu	0.31747800	0.22478800	-1.15315800
N	-1.06752500	2.40196500	1.97372800
C	0.19779100	2.61416200	1.49194300
C	-1.08094900	1.20839600	2.62868800
O	-2.06198500	0.65901100	3.14504900
O	0.58187000	3.58392700	0.84000000

C	0.29351300	0.58866300	2.60479200
C	1.08585000	1.45375900	1.86455300
C	2.41993100	1.18606200	1.61850500
C	2.95040700	0.00912200	2.16131800
C	2.15807600	-0.85170400	2.92239200
C	0.80352100	-0.57557600	3.14841200
H	3.03588800	1.86661700	1.03119400
H	4.00284100	-0.22573100	2.00470500
H	2.60513000	-1.74640900	3.35208400
H	0.18062300	-1.24286000	3.74334100
Si	-3.39334900	3.18531000	-0.41417700
C	-4.25100600	1.98519800	0.72867200
H	-5.20123900	2.42031100	1.06129400
H	-3.63895800	1.75056600	1.60808200
H	-4.48079800	1.05412500	0.19268700
C	-4.35616700	3.37837600	-2.01098500
H	-5.32376700	3.85166200	-1.80794400
H	-4.55065800	2.40081400	-2.46856000
H	-3.82041300	4.00002800	-2.73611200
C	-2.85317700	4.80594200	0.32397200
H	-2.05012800	4.61110300	1.04190900
H	-3.69243700	5.28550000	0.83968800
H	-2.48860200	5.48837900	-0.45109800
C	-1.80984700	2.29064900	-0.99531300
N	-0.89941800	1.66285700	-1.35846900

#### TS4

C	-2.76455400	-1.54361700	1.61800400
O	-1.61124900	-2.43579800	1.62428700
C	-2.52711300	-0.70205500	0.34652100
H	-2.64061200	0.37710400	0.50495000
C	-0.75782500	-1.98562100	0.69462500
N	-1.13841700	-0.99989300	-0.02821300
C	0.51373500	-2.72840500	0.60155200
C	0.39323400	-4.25447800	0.77098000
C	0.98216800	-3.45836500	1.85602900
H	-0.62070500	-4.62540400	0.88410100
H	1.04897100	-4.84446700	0.13832100
H	0.38533800	-3.27341500	2.74372500
H	2.05709800	-3.49239900	2.00294400
C	3.56059700	-2.55196200	-1.35282400
O	2.70293100	-2.97236700	-0.25930800
C	2.79417700	-1.34649100	-1.94037600
H	2.62879100	-1.41528900	-3.02186300

C	1.55622600	-2.28961000	-0.34657400
N	1.48884300	-1.38472400	-1.25866800
C	-5.31522300	-2.84770900	-0.80943700
C	-5.43367200	-2.53807800	-2.16252600
C	-4.59734800	-1.58900900	-2.75317400
C	-3.62695100	-0.93680700	-1.99641100
C	-3.51049800	-1.25426800	-0.64817800
C	-4.34485000	-2.19918700	-0.05242200
H	-5.97195400	-3.58645900	-0.35348100
H	-6.18712200	-3.03983800	-2.76550400
H	-4.70648300	-1.35765300	-3.81026800
H	-2.96848500	-0.19293700	-2.44471200
C	-4.05295000	-2.33576400	1.41761700
H	-3.93465400	-3.37392100	1.74961000
H	-4.85870800	-1.90193700	2.02363500
C	3.32680600	1.19211000	-1.74579200
C	3.62243400	-0.15209000	-1.55348400
C	4.79331300	-0.54885800	-0.90684800
C	5.69731300	0.40505000	-0.45170900
C	5.41103600	1.75462700	-0.65241800
C	4.23286800	2.14641400	-1.29028300
H	2.39234000	1.50078100	-2.21456500
H	6.61330600	0.10399000	0.05343100
H	6.10868900	2.51060000	-0.29931200
H	4.00510300	3.20194900	-1.41263800
C	4.90309500	-2.04653900	-0.82986500
H	5.08929700	-2.41936300	0.18488000
H	3.64667300	-3.40835000	-2.02712700
H	5.72184900	-2.42110700	-1.45681100
H	-2.72146700	-0.96247900	2.54437600
Cu	0.02526000	-0.09994600	-1.50110200
N	-0.63673300	2.48743600	1.07953500
C	0.71061500	2.39997600	0.77343300
C	-0.93341800	1.59794600	2.08984000
O	-2.01366100	1.44210700	2.64894800
O	1.28818300	3.10733300	-0.04201100
C	0.30692700	0.81898800	2.40643900
C	1.31646000	1.30638400	1.58858900
C	2.59987700	0.79288100	1.63312600
C	2.84226500	-0.24592400	2.53745900
C	1.82991700	-0.72673300	3.37075900
C	0.53639200	-0.19498300	3.31738700
H	3.38758500	1.19005100	0.99678300
H	3.83912700	-0.67927200	2.60120600

H	2.05423600	-1.52524900	4.07509600
H	-0.25605600	-0.55904700	3.96881000
Si	-1.80176900	3.82431800	-0.08502200
C	-3.50006100	3.16367100	0.38313100
H	-4.17644400	4.01913900	0.50874400
H	-3.48125800	2.58273200	1.30987300
H	-3.90816400	2.53914900	-0.42285700
C	-2.15857100	4.97766900	-1.58487000
H	-2.76824700	5.83772100	-1.27387900
H	-2.69048200	4.45326000	-2.39121400
H	-1.22853300	5.37765000	-2.01263800
C	-1.15844400	5.14563700	1.12021600
H	-0.07973700	5.29299400	0.99099100
H	-1.32519700	4.82742800	2.15657300
H	-1.65613800	6.10841700	0.94857500
C	-1.17274600	2.42790700	-1.39245100
N	-0.81180000	1.53534800	-2.05968400

## 8

C	3.06202000	-1.28152000	-1.73769000
O	2.10439100	-2.16026200	-1.08809100
C	2.54010300	0.12291900	-1.35749600
H	2.43415200	0.80558700	-2.20875900
C	1.10345700	-1.39576500	-0.62855400
N	1.21548400	-0.12715300	-0.76793500
C	-0.01466500	-2.14154700	-0.02461900
C	0.32615800	-3.49486800	0.60594400
C	-0.37347700	-3.47489100	-0.68672900
H	1.38212400	-3.74366500	0.62409800
H	-0.23928200	-3.74392000	1.49826500
H	0.18905200	-3.70881700	-1.58500800
H	-1.43224000	-3.71093900	-0.71101500
C	-3.07640400	-1.29153700	1.72116200
O	-2.12641500	-2.16063700	1.04790000
C	-2.54745900	0.11703700	1.37137700
H	-2.42874000	0.77708300	2.23835300
C	-1.12257300	-1.39693300	0.59843500
N	-1.22815400	-0.12895300	0.76596900
C	5.56503300	-0.04694700	0.77514200
C	5.49661700	1.11514400	1.53995600
C	4.44946100	2.02219300	1.36716600
C	3.45106000	1.77757400	0.42770600
C	3.52330900	0.61272500	-0.32848600
C	4.56912800	-0.29475200	-0.16404300

H	6.38419600	-0.75065900	0.91191100
H	6.26807600	1.31836500	2.27937100
H	4.41409900	2.92587800	1.97120700
H	2.62643100	2.47756000	0.28898200
C	4.44854200	-1.44846900	-1.12151700
H	4.55044000	-2.43083400	-0.64540200
H	5.21714400	-1.39713200	-1.90343200
C	-3.45676500	1.82065900	-0.36754500
C	-3.53344400	0.63934000	0.36172000
C	-4.58676500	-0.25608400	0.18207200
C	-5.58720500	0.02264400	-0.74357200
C	-5.51470900	1.20257900	-1.48014600
C	-4.45871400	2.09665600	-1.29419000
H	-2.62366400	2.50863400	-0.22091100
H	-6.41268000	-0.67112800	-0.89204700
H	-6.28971400	1.43005600	-2.20860000
H	-4.41906300	3.01350700	-1.87752800
C	-4.46685000	-1.43553000	1.10771300
H	-4.57498200	-2.40401500	0.60534500
H	-3.03527000	-1.54604800	2.78383300
H	-5.23132900	-1.40271600	1.89450800
H	3.02431300	-1.51122700	-2.80627200
C	0.29058100	4.35269900	-0.13910700
N	0.13673400	3.18507800	-0.06848900
Cu	-0.03496400	1.31616800	0.02998700

### TS5

C	-3.08467400	1.24920100	-1.74135400
O	-2.14476500	2.11701500	-1.05022600
C	-2.56521500	-0.15861700	-1.37543900
H	-2.46583000	-0.83702700	-2.23102000
C	-1.13649600	1.35016400	-0.61130400
N	-1.23908000	0.08497800	-0.78983100
C	-0.02741600	2.09049900	0.01761900
C	-0.38804400	3.42374600	0.68013700
C	0.31629100	3.44529900	-0.60964900
H	-1.44694500	3.65922800	0.70090600
H	0.17089100	3.65721400	1.58066700
H	-0.24635800	3.69392300	-1.50390500
H	1.37201300	3.69514300	-0.62434600
C	3.04428600	1.25084100	1.75295000
O	2.07904100	2.11935000	1.10040100
C	2.54599700	-0.15807800	1.36095400
H	2.44225100	-0.84808600	2.20649600



C	1.09131200	1.34850100	0.62738400
N	1.22161100	0.07926000	0.76384000
C	-5.59643000	-0.00134100	0.74968900
C	-5.51792000	-1.15591700	1.52492900
C	-4.45896900	-2.05162300	1.36553000
C	-3.46060100	-1.80357000	0.42720600
C	-3.54513600	-0.64925700	-0.34305000
C	-4.60041600	0.24903600	-0.18862000
H	-6.42277500	0.69532800	0.87885300
H	-6.28940200	-1.36097200	2.26376200
H	-4.41362100	-2.94786000	1.97979200
H	-2.62512800	-2.49229500	0.29980900
C	-4.48352000	1.39882500	-1.15137700
H	-4.61010100	2.38233100	-0.68378200
H	-5.23609800	1.32929200	-1.94745900
C	3.49020300	-1.78560300	-0.43266200
C	3.54134100	-0.62642000	0.33367300
C	4.57445300	0.29771700	0.18166700
C	5.57821100	0.07240600	-0.75469400
C	5.53046400	-1.08392100	-1.52958500
C	4.49607400	-2.00785000	-1.36954000
H	2.67664500	-2.49992300	-0.30296700
H	6.38742000	0.78927500	-0.88178800
H	6.30808700	-1.26950200	-2.26714100
H	4.47638100	-2.90677600	-1.98121900
C	4.43234200	1.44173100	1.14771500
H	4.52411600	2.42927700	0.68048300
H	2.99424700	1.47422800	2.82222600
H	5.19612700	1.39401700	1.93451800
H	-3.02283600	1.50117900	-2.80387700
C	-0.17312500	-3.28175000	-0.49978600
N	0.27128300	-3.54714600	0.56807600
Cu	0.04696400	-1.34043700	-0.05828800

C			
C	-0.35198400	-3.47885500	-0.64540600
C	-0.00015700	-2.13535500	-0.00008700
C	0.35154200	-3.47891400	0.64518100
C	1.11179900	-1.38920800	-0.61319800
O	2.10579400	-2.15310300	-1.08521500
C	2.54712100	0.12859200	-1.35205800
C	3.05847400	-1.27602600	-1.74412300
H	2.43302400	0.81444500	-2.19963100
H	3.00508100	-1.50149100	-2.81288400

C	-1.11203900	-1.38913000	0.61306300
O	-2.10608300	-2.15296200	1.08504400
C	-2.54726000	0.12873100	1.35208000
C	-3.05870500	-1.27588000	1.74402500
H	-2.43307500	0.81448900	2.19971600
H	-3.00532400	-1.50144100	2.81276500
N	-1.22749400	-0.11928700	0.74863900
N	1.22732700	-0.11937700	-0.74868100
Cu	-0.00017300	1.33772700	0.00022600
C	0.00122700	3.22637000	-0.00027000
N	0.00229600	4.39940800	-0.00058100
C	-4.59098000	-0.30108300	0.18808200
C	-3.54661900	0.61138000	0.33488800
C	-3.49437400	1.77520100	-0.42408900
C	-4.50776300	2.01388000	-1.34853200
C	-5.55246000	1.10084800	-1.50370900
C	-5.60255700	-0.06002800	-0.73589900
C	-4.45214800	-1.45148300	1.14683800
H	-2.67223000	2.48014000	-0.30015900
H	-4.48608300	2.91707600	-1.95378500
H	-6.33633200	1.29887000	-2.23132400
H	-6.42013800	-0.76816700	-0.85829500
C	3.54649400	0.61106600	-0.33479100
C	4.59080200	-0.30147300	-0.18808000
C	5.60239100	-0.06057800	0.73592900
C	5.55236000	1.10021600	1.50386600
C	4.50771000	2.01331900	1.34878800
C	3.49430400	1.77480500	0.42432000
C	4.45190700	-1.45176900	-1.14695200
H	6.41993100	-0.76877900	0.85825000
H	6.33624300	1.29811600	2.23150400
H	4.48607900	2.91645000	1.95414300
H	2.67218500	2.47979100	0.30047100
H	4.55484200	-2.43594000	-0.67485400
H	5.21057100	-1.40208300	-1.93855900
H	-5.21080700	-1.40183000	1.93845200
H	-4.55514100	-2.43560300	0.67464500
H	0.20914500	-3.72019100	-1.54256100
H	-1.40951900	-3.72099000	-0.66313200
H	1.40905800	-3.72113600	0.66289700
H	-0.20960500	-3.72024500	1.54232600
<b>D</b>			
C	0.31113700	3.56857100	-1.04141800

C	-0.00613200	2.33825300	-0.17908100
C	-0.39813300	3.76643900	0.22482100
C	-1.06513900	1.44692900	-0.66868400
O	-2.15064100	2.03274200	-1.14161300
C	-2.34587600	-0.31268400	-1.21459400
C	-3.02784700	0.99305500	-1.68463500
H	-2.19017900	-1.04786900	-2.01143400
H	-3.03963200	1.14117000	-2.76666600
C	1.09098000	1.72601000	0.57068700
O	2.12232600	2.49213200	0.87410400
C	2.43189500	0.29262700	1.65615400
C	3.15364200	1.64461500	1.47438700
H	2.26702700	-0.01444700	2.69413900
H	3.44624000	2.13605300	2.40229800
N	1.13806100	0.49915600	0.97959600
N	-1.03610100	0.15779400	-0.72380200
Cu	0.45639400	-0.98348500	-0.06111300
C	0.02474800	-2.61404600	-0.95323200
N	-0.26834600	-3.60318900	-1.50084600
C	4.17477400	-0.02519700	0.07121200
C	3.19210800	-0.67620000	0.80879200
C	2.84457800	-2.00930700	0.57556400
C	3.52066300	-2.69972800	-0.43961100
C	4.51941300	-2.06092000	-1.16734200
C	4.86031100	-0.72854500	-0.91419200
C	4.31275300	1.41470300	0.49348900
H	2.13389500	-2.52740700	1.22264900
H	3.26946800	-3.73614400	-0.64762400
H	5.04569800	-2.60602700	-1.94619100
H	5.64199700	-0.24608800	-1.49672700
C	-3.22579400	-0.80502700	-0.09660000
C	-4.35268900	0.00456200	0.03894700
C	-5.28199300	-0.25471100	1.04067200
C	-5.06532400	-1.32981500	1.89841400
C	-3.94102700	-2.14417600	1.75250600
C	-3.01136700	-1.88909400	0.74817000
C	-4.39753500	1.06893100	-1.02169800
H	-6.16452000	0.37189100	1.15168200
H	-5.78314400	-1.54112700	2.68736000
H	-3.79316300	-2.98551300	2.42490100
H	-2.14242900	-2.53356300	0.61983200
H	-4.58763800	2.07561800	-0.63229700
H	-5.18249800	0.86306900	-1.75977500
H	5.27498100	1.59764800	0.98579600

H	4.25179400	2.11639900	-0.34632300
H	-0.24804200	3.62987800	-1.96999800
H	1.36399500	3.82583200	-1.10033800
H	-1.46443800	3.96792900	0.20636200
H	0.14751800	4.16698400	1.07372000
<b>E</b>			
C	-2.16367400	3.97715700	0.08079900
C	-1.62968700	2.54183800	0.16153900
C	-2.52989500	3.15515600	1.24075700
C	-2.26608700	1.57139800	-0.74328500
O	-3.52624600	1.86387700	-1.08485300
C	-2.76320300	-0.08707200	-2.15125200
C	-4.03028800	0.73930600	-1.84461300
H	-2.39183400	-0.00232600	-3.18068900
H	-4.52254100	1.15097300	-2.72711300
C	-0.19987200	2.39519600	0.48756100
O	0.30473600	3.39249600	1.22192900
C	1.94028200	1.83244900	0.62389300
C	1.69326000	3.07662100	1.50691000
H	2.39495500	0.99376800	1.17062300
H	1.75914100	2.89649000	2.58416500
N	0.60014900	1.44814300	0.15019700
N	-1.75877700	0.50522300	-1.24518700
Cu	0.11706100	-0.28241400	-0.95792500
C	0.79151200	-0.85956500	-2.67164700
N	1.14681300	-1.21428500	-3.72925100
C	3.14804300	3.67586800	-0.29436800
C	2.80618300	2.33960900	-0.49691500
C	3.21981500	1.65402600	-1.63362700
C	3.98813600	2.33034900	-2.57711700
C	4.33320500	3.66856100	-2.37863200
C	3.91739600	4.34933300	-1.23748400
C	2.61362400	4.19004400	1.01355900
H	2.93362000	0.61458900	-1.79401000
H	4.31775700	1.81453400	-3.47570900
H	4.93191700	4.18489900	-3.12534100
H	4.18793100	5.39279700	-1.08767700
C	-3.12004800	-1.48816500	-1.75794400
C	-4.32854500	-1.51215900	-1.06143900
C	-4.80336600	-2.70997900	-0.53531600
C	-4.05325000	-3.87158400	-0.71519900
C	-2.85583800	-3.84569300	-1.43302900
C	-2.38262700	-2.64838700	-1.96782600

C	-4.95241700	-0.14509900	-0.99025500
H	-5.74660100	-2.74194700	0.00700300
H	-4.41406000	-4.81223600	-0.30635100
H	-2.29646700	-4.76570700	-1.58409600
H	-1.45831000	-2.61677100	-2.54539100
H	-4.98751200	0.24402800	0.03833200
H	-5.98382200	-0.13956100	-1.35941900
H	3.42114700	4.36035700	1.73659200
H	2.06738200	5.13624400	0.92389200
H	-2.90547100	4.15056900	-0.69157800
H	-1.41578900	4.75252000	0.20863400
H	-3.53162700	2.73584000	1.29429400
H	-2.04316000	3.34484300	2.19329100
C	-1.60883300	1.04535500	3.85293400
C	-0.91588500	0.26836300	2.94430500
C	-1.61235300	-0.62402900	2.09943500
C	-3.01663300	-0.71186000	2.20074300
C	-3.70473600	0.06924900	3.11402500
C	-3.00129700	0.94698400	3.93839800
H	-1.07139000	1.72978100	4.50350100
H	0.16774000	0.34006400	2.89362500
H	-3.55018500	-1.40761200	1.55183400
H	-4.78573000	-0.00470500	3.19004200
H	-3.53959600	1.56147800	4.65525400
C	-0.95342300	-1.43532300	1.12784600
H	-1.59306100	-2.06810300	0.50429700
C	0.42084200	-1.50465400	0.90455500
C	0.95667100	-2.23516700	-0.15847700
H	0.27710200	-2.87728400	-0.72654800
C	2.40787400	-2.43806000	-0.36377200
H	2.97258800	-1.58875800	0.04180200
H	2.61356200	-2.48913300	-1.43961700
C	2.87283700	-3.76794400	0.28587400
C	4.28910400	-4.11318700	-0.18736900
C	5.34728700	-3.19206300	0.41155700
C	5.28028900	-3.20314500	1.93525100
C	3.88583300	-2.83348400	2.43145600
C	2.82452100	-3.74306100	1.81671400
H	6.34258100	-3.50190100	0.06932600
H	4.50451200	-5.14752400	0.12229700
H	4.33216100	-4.09825600	-1.28447200
H	2.19059100	-4.55437700	-0.07262700
H	5.52912600	-4.21446000	2.29530600
H	6.03155800	-2.52575900	2.36025200

H	3.83726300	-2.90062900	3.52556800
H	3.68013100	-1.77842600	2.18584600
H	2.99891600	-4.77052400	2.17081800
H	1.82205700	-3.46884100	2.17505700
H	5.20737300	-2.16357500	0.04295200
H	1.10754700	-0.94301200	1.53765700

A<sup>+</sup>

C	-4.75178800	0.58358800	1.41453300
C	-3.47846500	0.16267700	1.09688000
C	-3.15795900	-0.17010900	-0.24295100
C	-4.15606600	-0.06453300	-1.24214500
C	-5.42836400	0.35950400	-0.91473000
C	-5.72323200	0.68207400	0.41137800
H	-5.00306000	0.83790000	2.43956500
H	-2.72541300	0.08326100	1.87559300
H	-3.90491100	-0.32020900	-2.26920000
H	-6.19376200	0.44283500	-1.67984200
H	-6.72502400	1.01483200	0.67057000
C	-1.87387200	-0.61027400	-0.63014700
H	-1.74649200	-0.85277400	-1.68773400
C	-0.74867800	-0.77198200	0.18404600
H	-0.78497200	-0.54576600	1.24833800
C	0.41987200	-1.22611600	-0.36383600
H	0.43681900	-1.43752600	-1.43733600
C	1.67066900	-1.43525900	0.37490700
H	1.53501100	-1.21369900	1.44260700
H	1.93892200	-2.50087400	0.28444400
C	3.73194000	1.72406600	-0.58689400
C	2.55335500	0.89374800	-0.09205600
C	2.83755300	-0.60401300	-0.19614500
C	4.12955300	-0.96147300	0.53465900
C	5.30470700	-0.13085800	0.03291000
C	5.01284700	1.36032400	0.15467100
H	2.34760100	1.13577400	0.96536100
H	1.64194600	1.15008500	-0.65233800
H	3.87382800	1.53929000	-1.66381700
H	3.51109900	2.79338100	-0.48008300
H	3.98399600	-0.77367300	1.61207800
H	4.33564000	-2.03532700	0.42757800
H	6.21480300	-0.39509800	0.58572900
H	5.49689000	-0.37735000	-1.02358900
H	4.90068300	1.62097100	1.21941000
H	5.85664900	1.94982100	-0.22506300

H 2.95730600 -0.86402800 -1.26275000

A-

C -4.48794700 1.27243700 1.08903500  
C -3.29035600 0.62421800 0.83853700  
C -3.14838500 -0.33636100 -0.21342500  
C -4.34002900 -0.56319400 -0.97271500  
C -5.52942200 0.09168800 -0.71062000  
C -5.63620200 1.02662800 0.32707500  
H -4.53031100 1.99469200 1.90650700  
H -2.42816500 0.85800900 1.46378100  
H -4.29338200 -1.28597700 -1.79042600  
H -6.40073000 -0.13102300 -1.32912100  
H -6.57268900 1.54063500 0.53250200  
C -1.95614100 -1.03070900 -0.51779100  
H -2.00056900 -1.72745300 -1.36228100  
C -0.72057700 -0.91695800 0.16325800  
H -0.69902400 -0.22029800 1.01430800  
C 0.45827900 -1.56348200 -0.07562500  
H 0.51737600 -2.26636300 -0.91536300  
C 1.70591100 -1.36691000 0.72462300  
H 1.46941200 -0.78005200 1.63151400  
H 2.10615100 -2.33112000 1.09414700  
C 3.63262400 1.50906000 -1.06241700  
C 2.49230600 0.78568200 -0.35597200  
C 2.85406700 -0.65366000 -0.00245700  
C 4.14010700 -0.68022100 0.82033900  
C 5.28881800 0.03731900 0.12057100  
C 4.90774500 1.47251300 -0.22672500  
H 2.24741800 1.31864500 0.58143600  
H 1.57638700 0.79430600 -0.96134400  
H 3.82533800 1.01909000 -2.03124900  
H 3.35132600 2.54633500 -1.28979200  
H 3.94207600 -0.18939100 1.79026900  
H 4.41467400 -1.72034900 1.05172700  
H 6.19451300 0.01794300 0.74204300  
H 5.53625800 -0.50214700 -0.80869900  
H 4.74015500 2.03482000 0.70686200  
H 5.73140400 1.97562500 -0.75116900  
H 3.04759600 -1.19422900 -0.94978700

9

C 3.08493300 1.45835800 1.62384800  
O 2.06308600 2.28381400 0.98289200

C	2.53613200	0.02004400	1.46330900
H	2.36721400	-0.50405900	2.41044900
C	1.09747200	1.49817600	0.55160100
N	1.23415500	0.23513000	0.79124500
C	-0.01140600	2.14901100	-0.14840200
C	0.31457800	3.43243900	-0.93085300
C	-0.40646400	3.55486700	0.33587000
H	1.36888000	3.68855800	-0.96101200
H	-0.23227800	3.54753800	-1.86133600
H	0.13010400	3.89830200	1.21489000
H	-1.47273500	3.75709000	0.31835100
C	-2.99044300	0.91830000	-1.82419600
O	-2.09544800	1.92871100	-1.24943100
C	-2.46153400	-0.39482800	-1.20484000
H	-2.31517300	-1.20434500	-1.92709000
C	-1.08364400	1.30441500	-0.67875400
N	-1.14953800	0.01402600	-0.66138200
C	5.47856900	-0.19817400	-0.76219200
C	5.40999600	-1.49226900	-1.27320200
C	4.40400000	-2.37076200	-0.86851300
C	3.44492100	-1.96082900	0.05504400
C	3.50817300	-0.66053500	0.54517800
C	4.51538200	0.21765500	0.15091800
H	6.27313900	0.47617200	-1.07449800
H	6.15495100	-1.82636000	-1.99105100
H	4.37413700	-3.38106500	-1.26767600
H	2.68051500	-2.66030300	0.39890300
C	4.40490000	1.54104200	0.85652700
H	4.40379600	2.40193100	0.17810800
H	5.23887700	1.69204100	1.55225300
C	-3.39176500	-1.71226800	0.84151700
C	-3.45794700	-0.71069100	-0.12087400
C	-4.52973100	0.18112700	-0.16165900
C	-5.55257800	0.08836100	0.77568400
C	-5.48502400	-0.90493600	1.74884100
C	-4.41507800	-1.80091400	1.78103800
H	-2.56128800	-2.41560700	0.85364200
H	-6.39148600	0.78072500	0.74956000
H	-6.27640300	-0.98746100	2.48995600
H	-4.38224900	-2.57546400	2.54313800
C	-4.40823800	1.13396900	-1.31723200
H	-4.57377000	2.18382700	-1.04990400
H	-2.87495500	0.99548400	-2.90760600
H	-5.12658100	0.89313300	-2.11072100



H	3.14660000	1.80598600	2.65609500
C	-0.70941800	-3.91634900	-0.86882100
N	-0.36528900	-2.84115100	-0.51694200
Cu	0.22474500	-1.18529700	0.04166900

### TS6

C	-2.92483400	0.95882100	-1.87128200
O	-2.03413900	1.93753200	-1.23500800
C	-2.45605400	-0.37835000	-1.25336300
H	-2.30243600	-1.18127500	-1.98115100
C	-1.05997800	1.28043600	-0.64053200
N	-1.15424400	-0.00902400	-0.65636400
C	0.00732600	2.08422600	-0.04446200
C	-0.38605600	3.45924700	0.52632700
C	0.35015800	3.41451800	-0.73605700
H	-1.45091800	3.66931400	0.51019300
H	0.14142500	3.73867100	1.43332500
H	-0.18650400	3.59089000	-1.66297300
H	1.40628000	3.66482500	-0.73897600
C	3.05150700	1.24207500	1.75786200
O	2.08162900	2.11976500	1.09669000
C	2.54122300	-0.17379500	1.39904500
H	2.41037700	-0.83462800	2.26272600
C	1.10272400	1.38046500	0.62161600
N	1.21901600	0.10343900	0.79299100
C	-5.60825400	0.16143000	0.61192800
C	-5.60267400	-0.84364600	1.57522800
C	-4.55669600	-1.76595200	1.63876400
C	-3.49558100	-1.69281400	0.74103300
C	-3.50047900	-0.67984100	-0.21173900
C	-4.54757300	0.23869700	-0.28377700
H	-6.42799900	0.87503400	0.56115200
H	-6.42376200	-0.91388800	2.28452900
H	-4.57243500	-2.54861800	2.39297700
H	-2.68424000	-2.41711000	0.77942400
C	-4.35789900	1.19940500	-1.42363600
H	-4.51336000	2.25013600	-1.15397900
H	-5.04540000	0.97939100	-2.24968500
C	3.46505300	-1.86160900	-0.34558800
C	3.52388900	-0.67679200	0.37970700
C	4.55113100	0.24494600	0.18508600
C	5.53873700	-0.00697600	-0.76125200
C	5.47729000	-1.18428200	-1.50257700
C	4.45097600	-2.10778100	-1.29720900

H	2.67517000	-2.59343900	-0.17181800
H	6.34564100	0.70489700	-0.92130700
H	6.24121000	-1.38879600	-2.24861200
H	4.42445700	-3.02502000	-1.87957400
C	4.42818800	1.41179900	1.12554400
H	4.51537300	2.38893100	0.63712300
H	3.00617100	1.48903300	2.82024400
H	5.20156600	1.37822800	1.90262800
H	-2.75701000	1.05411200	-2.94634600
C	-0.10281800	-3.37757800	0.34880100
N	-0.51674500	-3.01943000	-0.70754400
Cu	0.11877400	-1.26978900	0.07711300

### TS7<sub>s</sub>

C	-4.81456500	1.33332600	0.59315500
C	-3.43703500	0.65890200	0.53159800
C	-4.33350800	0.57678200	1.76058500
C	-3.34835800	-0.54755400	-0.31368200
O	-4.36682300	-1.40676800	-0.16289900
C	-2.81635900	-2.15011000	-1.76614200
C	-4.10608800	-2.55037300	-1.01047400
H	-2.95252600	-2.02039900	-2.84711600
H	-4.98224800	-2.67281300	-1.65092300
C	-2.26368300	1.54600700	0.63057100
O	-2.37296200	2.53428800	1.53472500
C	-0.32238300	2.58058900	0.40086200
C	-1.09399100	3.21788500	1.58060000
H	0.66249600	2.17702400	0.67811700
H	-0.66408500	3.00425400	2.56480200
N	-1.17734900	1.47388800	-0.03810500
N	-2.45150900	-0.84844600	-1.18168600
Cu	-0.66441800	0.02550100	-1.45071400
C	2.15235700	-0.07479300	-2.29681200
N	0.97466300	0.07547300	-2.40215700
C	-0.80759600	4.85577400	-0.14491500
C	-0.24598500	3.67476500	-0.62815600
C	0.26030500	3.59083700	-1.92063100
C	0.19644000	4.72002800	-2.73313900
C	-0.36371600	5.90611300	-2.25447900
C	-0.86792700	5.98274000	-0.95830500
C	-1.25575400	4.70805500	1.28373700
H	0.69067300	2.65649000	-2.28265300
H	0.58567000	4.67906400	-3.74795600
H	-0.40548900	6.78009900	-2.90081200

H	-1.30254900	6.91000300	-0.58879700
C	-1.82413600	-3.22609900	-1.42814800
C	-2.36308000	-4.13150100	-0.51625000
C	-1.58759300	-5.18143000	-0.03354500
C	-0.27221800	-5.30641300	-0.47464600
C	0.26225300	-4.39962400	-1.39179600
C	-0.51375400	-3.34915500	-1.87765600
C	-3.78885100	-3.79755000	-0.17461400
H	-2.00014100	-5.89263100	0.67973600
H	0.34474800	-6.12144500	-0.10327400
H	1.29126900	-4.51164400	-1.72669600
H	-0.09607000	-2.62255300	-2.57499800
H	-3.91923700	-3.57775100	0.89420000
H	-4.47210500	-4.62235400	-0.40950100
H	-0.62880600	5.30219700	1.96101000
H	-2.29062300	5.02903300	1.45303100
H	-5.57835800	0.89163800	-0.03977000
H	-4.79834900	2.41843500	0.62849000
H	-4.76199000	-0.39957900	1.96243500
H	-3.97884800	1.12990600	2.62417700
C	-0.39800100	0.38325600	3.71241000
C	0.50332600	0.11159400	2.69132200
C	0.27295200	-0.93571700	1.77606100
C	-0.89635500	-1.70478800	1.95324400
C	-1.79933200	-1.42388700	2.96830800
C	-1.56234300	-0.37318300	3.85575800
H	-0.18874500	1.19312600	4.41016700
H	1.40849500	0.71223400	2.60392800
H	-1.08784100	-2.53309100	1.26740000
H	-2.69887800	-2.03056500	3.06875600
H	-2.26842700	-0.15429600	4.65372100
C	1.16521400	-1.25475300	0.68394800
H	0.88371200	-2.13299600	0.09533600
C	2.31968400	-0.60656800	0.33067500
C	3.07025600	-0.92419600	-0.84143300
H	2.89532500	-1.93946100	-1.22155300
C	4.49924600	-0.46766000	-0.96321900
H	4.57000000	0.56790300	-0.59593000
H	4.76085800	-0.42207500	-2.03055300
C	5.51736300	-1.37472200	-0.25665900
C	6.95315100	-1.00648200	-0.64806300
C	7.40632700	0.31437700	-0.03140500
C	7.26739800	0.28283100	1.48732800
C	5.84337100	-0.07117600	1.90493600

C	5.39500800	-1.38518100	1.27130000
H	8.44558100	0.52534100	-0.31647600
H	7.62880000	-1.80437400	-0.29964900
H	7.04643500	-0.97226500	-1.74301100
H	5.32225200	-2.39962200	-0.61587600
H	7.95638800	-0.47741200	1.89164900
H	7.57236400	1.24321700	1.92371400
H	5.77119300	-0.13973500	2.99854300
H	5.16186700	0.74088800	1.60524200
H	6.03240800	-2.19517900	1.66162600
H	4.36467300	-1.62461200	1.56625500
H	6.80392500	1.14237700	-0.43622700
H	2.62972700	0.29184000	0.87577100

**TS8<sub>s</sub>**

C	-4.98167200	0.31843000	0.76492200
C	-3.49177100	-0.04201400	0.62606000
C	-4.30075900	-0.33153200	1.89061000
C	-3.18312700	-1.18704500	-0.24524800
O	-3.99346200	-2.23594700	-0.11364900
C	-2.34392000	-2.62097200	-1.74825800
C	-3.46858800	-3.30678100	-0.94130400
H	-2.56525500	-2.48751100	-2.81400300
H	-4.30111400	-3.66795400	-1.54704400
C	-2.54188100	1.08039300	0.69036800
O	-2.84358200	2.03530800	1.57097800
C	-0.91157300	2.55413400	0.35428700
C	-1.73897300	2.98561800	1.58484000
H	0.16424900	2.44726600	0.54900100
H	-1.23285000	2.85194000	2.54594200
N	-1.47021100	1.24071700	0.00136900
N	-2.24208600	-1.28912200	-1.11888400
Cu	-0.73569200	-0.07033600	-1.37483300
C	2.04244400	0.52805300	-2.19165500
N	0.85693600	0.54151800	-2.13410700
C	-2.02578200	4.60948800	-0.13868300
C	-1.23341000	3.59854000	-0.68245500
C	-0.87285200	3.60961900	-2.02550900
C	-1.32489900	4.65426200	-2.82783200
C	-2.12191900	5.66569000	-2.28900800
C	-2.47492900	5.65232700	-0.94197500
C	-2.25070600	4.39802900	1.33291700
H	-0.25232300	2.81438900	-2.43723900
H	-1.05623100	4.68220800	-3.88113000

H	-2.46969900	6.47387500	-2.92825500
H	-3.09559000	6.44362000	-0.52585800
C	-1.12205800	-3.45028600	-1.48903500
C	-1.37883400	-4.42083900	-0.52181600
C	-0.35422400	-5.25397800	-0.08306800
C	0.91874600	-5.10212800	-0.62872600
C	1.16711600	-4.13916000	-1.60850500
C	0.14300500	-3.30147900	-2.04718100
C	-2.81734500	-4.40075400	-0.08234700
H	-0.54246700	-6.01393000	0.67251500
H	1.72680200	-5.74875200	-0.29559400
H	2.16261300	-4.04775500	-2.03623900
H	0.33042900	-2.55009900	-2.81474600
H	-2.92439600	-4.15280900	0.98294200
H	-3.30586000	-5.37101000	-0.22616600
H	-1.67672500	5.11699800	1.93118500
H	-3.29796500	4.49685500	1.64093200
H	-5.65725100	-0.26907100	0.15078300
H	-5.19372200	1.38176400	0.81757100
H	-4.50077500	-1.38097500	2.08301900
H	-4.02770500	0.26780200	2.75360100
C	-0.29826700	0.40662600	3.69835400
C	0.58013900	0.29763100	2.63614800
C	0.48529100	-0.79019200	1.72469100
C	-0.53798600	-1.75249100	1.94908500
C	-1.40777400	-1.63430800	3.01398400
C	-1.29933500	-0.55100900	3.89628000
H	-0.20293200	1.23881300	4.39212200
H	1.35934000	1.04715700	2.51279100
H	-0.61038200	-2.60078000	1.26647400
H	-2.17373800	-2.39075100	3.17265800
H	-1.98336600	-0.46012800	4.73625400
C	1.36501000	-0.97166100	0.62808600
H	1.22796500	-1.87181200	0.02245900
C	2.48322500	-0.15518800	0.31865000
C	3.32512300	-0.38859600	-0.77454900
H	3.21155500	-1.35519500	-1.27514900
C	4.63953700	0.29722200	-0.95183400
H	4.57583100	1.32120100	-0.55788300
H	4.84717800	0.39007000	-2.02600800
C	5.78944400	-0.48610500	-0.29125000
C	7.15345100	0.02195400	-0.76811700
C	7.49895900	1.39472200	-0.19845700
C	7.44494200	1.37872700	1.32567700

C	6.08431600	0.90299900	1.82384600
C	5.73340900	-0.46363700	1.23995900
H	8.49405800	1.70288600	-0.54403300
H	7.92201500	-0.69663000	-0.44247300
H	7.18428400	0.03756400	-1.86638100
H	5.68655300	-1.53310200	-0.62069200
H	8.22188100	0.69422500	1.70360800
H	7.67812500	2.37118200	1.73223200
H	6.07224500	0.85224800	2.92013200
H	5.31764900	1.64385400	1.54563100
H	6.45676700	-1.20243000	1.61905500
H	4.74649200	-0.79613600	1.59560700
H	6.79512400	2.14979500	-0.58301600
H	2.67869000	0.73834500	0.91657300

### NHP-TMS

C	2.88397500	-0.85835300	1.58781300
H	2.45031700	-1.86140400	1.64963900
H	3.97510100	-0.95133100	1.64052800
H	2.55274300	-0.28337700	2.45987400
C	3.03653400	1.73833800	-0.06482100
H	4.13292800	1.69476600	-0.06789700
H	2.70954300	2.25907100	-0.96989300
H	2.71395700	2.32923100	0.79712000
C	2.90476700	-0.96446800	-1.51660000
H	2.54477500	-1.99698000	-1.48186400
H	2.51693300	-0.49286200	-2.42667300
H	3.99879500	-0.98216500	-1.58827000
Si	2.38314500	-0.00761200	0.00126300
C	-1.66704400	0.69946200	-0.00247800
C	-1.63632500	-0.68766300	-0.00370600
C	-2.79595400	-1.44166000	-0.00331700
C	-4.00669800	-0.74553200	-0.00231600
C	-4.03731400	0.65142700	-0.00120700
C	-2.85906100	1.40065400	-0.00093200
C	-0.26623000	1.19420100	-0.00047200
C	-0.21430800	-1.10749200	-0.00263800
H	-2.75941200	-2.52804600	-0.00359400
H	-4.94318900	-1.29733300	-0.00211800
H	-4.99775000	1.16050900	-0.00020900
H	-2.87106400	2.48757700	0.00056300
O	0.22455500	-2.24081700	0.00303100
O	0.10014200	2.35020000	0.00736400
N	0.56580900	0.06005300	-0.00628600

**10**

C	0.52023600	3.50485800	-1.22037400
C	0.11819000	2.35504300	-0.27340000
C	-0.20013000	3.83702700	0.00428800
C	-0.96122400	1.47294700	-0.72445900
O	-2.05485600	2.04103000	-1.16143800
C	-2.27072700	-0.31491400	-1.20560400
C	-2.97064500	0.99371000	-1.64414000
H	-2.14395700	-1.04689300	-2.00939200
H	-3.04090700	1.13582000	-2.72378000
C	1.13422500	1.73808700	0.56061100
O	2.21855400	2.40508000	0.85702200
C	2.27528900	0.25001300	1.79331700
C	3.12930500	1.51990400	1.60485700
H	2.08716300	-0.05932400	2.82453200
H	3.38153300	2.05183900	2.52111000
N	1.02793900	0.53649500	1.07385800
N	-0.93220400	0.17442000	-0.78874400
Cu	0.52722600	-0.87934600	-0.11565100
C	0.10135800	-2.32777000	-1.22093900
N	-0.25087100	-3.19768800	-1.91362500
C	3.98349100	-0.24226200	0.22493300
C	2.90160100	-0.75917300	0.89573100
C	2.23536700	-1.96699700	0.50040700
C	2.84799000	-2.71439300	-0.57153900
C	3.97816400	-2.23311300	-1.19244900
C	4.54908200	-1.00438000	-0.80914200
C	4.33444000	1.13071300	0.73806000
H	1.63239200	-2.51281700	1.23612900
H	2.41933200	-3.66873400	-0.86110100
H	4.44211000	-2.80468800	-1.98916100
H	5.42821500	-0.64048900	-1.33635000
C	-3.08850400	-0.80148400	-0.04301500
C	-4.19271400	0.02550000	0.16326000
C	-5.05867800	-0.22069500	1.22264000
C	-4.80195300	-1.29948300	2.06451200
C	-3.70417500	-2.13437700	1.84504800
C	-2.84002100	-1.89412700	0.78144200
C	-4.29323500	1.08665300	-0.89572000
H	-5.92250500	0.41830600	1.39114100
H	-5.46954900	-1.50071600	2.89849300
H	-3.52856000	-2.98006200	2.50458300
H	-1.99656200	-2.55863300	0.59702900

H	-4.45009200	2.09674900	-0.50143400
H	-5.12244400	0.88343900	-1.58408100
H	5.24549500	1.10857800	1.34679400
H	4.50238900	1.85988300	-0.06061600
H	-0.01831500	3.50933500	-2.16349000
H	1.58851600	3.69071600	-1.27992100
H	-1.25630500	4.08329400	-0.04907800
H	0.34847100	4.26626400	0.83742600

### TS9<sub>s</sub>

C	-3.03117800	-0.71256100	3.41397400
C	-1.90206600	-0.42143800	2.41638500
C	-2.06157800	0.34340900	3.73446100
C	-0.82997400	-1.43101600	2.35716000
O	-0.50295000	-1.98029700	3.53799500
C	0.67907500	-2.95306800	1.76195800
C	0.66552000	-2.79796700	3.29384500
H	0.26891000	-3.90071200	1.38612400
H	0.52563500	-3.73004300	3.84397600
C	-2.28552900	0.29800100	1.18661100
O	-3.26851000	1.19194300	1.34949300
C	-2.52238500	1.09237900	-0.87185400
C	-3.45004000	1.88175000	0.08304500
H	-1.80392300	1.71840200	-1.41952300
H	-3.15161200	2.92239400	0.24988900
N	-1.77669500	0.18434700	0.01449800
N	-0.20864300	-1.86208600	1.32112600
Cu	-0.37292600	-1.25266100	-0.62542400
C	0.57086700	-0.50157900	-2.16379600
N	0.58131500	-0.26689000	-3.31575500
C	-4.79349200	0.65307600	-1.47127200
C	-3.46746700	0.34438400	-1.77171200
C	-3.14853400	-0.57352700	-2.76602300
C	-4.18578700	-1.20266800	-3.44974100
C	-5.51548500	-0.90866700	-3.14235800
C	-5.82823000	0.02443900	-2.15678900
C	-4.88473400	1.71844600	-0.41397400
H	-2.10726000	-0.79265500	-3.00063300
H	-3.95908600	-1.92252100	-4.23351000
H	-6.31604400	-1.40789100	-3.68360900
H	-6.86642600	0.25900100	-1.92891000
C	2.10655100	-2.73049800	1.37017500
C	2.83029100	-2.20931000	2.44348300
C	4.17995100	-1.91077500	2.29164800



C	4.78603300	-2.14362400	1.05745800
C	4.05666800	-2.66663300	-0.01227900
C	2.70290400	-2.96305400	0.13662000
C	1.96372300	-2.06067500	3.66508700
H	4.75774600	-1.51295000	3.12344700
H	5.84262700	-1.91907200	0.92465200
H	4.55141200	-2.85518100	-0.96305600
H	2.12707800	-3.37928200	-0.68990600
H	1.73711500	-1.00469200	3.87230200
H	2.43032100	-2.46475100	4.56970900
H	-5.25191400	2.66324500	-0.83442100
H	-5.55578800	1.46231900	0.41428500
H	-2.95945900	-1.66376400	3.93149700
H	-4.02312100	-0.42437900	3.08096700
H	-1.30146000	0.14248900	4.48307700
H	-2.37507000	1.37907200	3.63608800
C	-1.26651000	5.22585900	0.39842900
C	-0.49416600	4.13598100	0.03020500
C	-0.18299000	3.13758100	0.97192400
C	-0.65991200	3.27452300	2.28649600
C	-1.43185600	4.36683800	2.65302300
C	-1.73873000	5.34292200	1.70752100
H	-1.50629500	5.99002200	-0.33576600
H	-0.14117400	4.05114000	-0.99531000
H	-0.40660100	2.51144600	3.02140800
H	-1.79484000	4.45858700	3.67332300
H	-2.34621600	6.19924500	1.98863700
C	0.57507100	1.95645600	0.63462600
H	0.62483900	1.18601500	1.40876100
C	1.25148800	1.71324000	-0.52189900
C	1.95943200	0.50056100	-0.70334600
H	1.92623800	-0.21884900	0.12333300
C	3.14846000	0.40406200	-1.58784800
H	2.99228500	0.98852700	-2.50125600
H	3.30381000	-0.64143000	-1.88202500
C	4.40797700	0.87643400	-0.81368500
C	5.67243700	0.42421900	-1.55455200
C	5.90635400	1.20483900	-2.84410600
C	5.96711800	2.70396700	-2.56982000
C	4.71077000	3.18639900	-1.85151600
C	4.46811000	2.38850600	-0.57375800
H	6.83464800	0.86366600	-3.31951000
H	6.53097200	0.58262100	-0.88264300
H	5.62627000	-0.65521900	-1.75534700

H	4.39106500	0.36942900	0.16518500
H	6.84282700	2.91381600	-1.93423000
H	6.11657100	3.26147900	-3.50302900
H	4.79432700	4.25337100	-1.60882300
H	3.84575300	3.09797400	-2.52798900
H	5.30141300	2.57798100	0.12070900
H	3.56274700	2.74172700	-0.06243000
H	5.10007200	0.99384500	-3.56394000
H	1.27853500	2.44277400	-1.33270700
N	-1.24620000	-3.04102500	-1.43837500
C	-1.78876300	-3.86766600	-2.04218200
C	-2.46864000	-4.89697700	-2.79731300
H	-2.14536300	-5.88524200	-2.46012900
H	-3.54915600	-4.80741000	-2.65680600
H	-2.23884400	-4.79036200	-3.86080200

### TS9<sub>R</sub>

C	0.24932900	-4.36178500	-1.88066500
C	-0.00665700	-2.91682400	-1.43268100
C	-0.65993100	-3.52733000	-2.67840200
C	-0.86372900	-2.76685900	-0.23979100
O	-1.83031000	-3.69116100	-0.14807200
C	-1.80786000	-2.23967600	1.70458300
C	-2.57427000	-3.42346600	1.06342400
H	-1.29709900	-2.49741300	2.64231600
H	-2.54892900	-4.34136600	1.65534700
C	1.09247800	-1.96555100	-1.67703700
O	1.83693100	-2.24682500	-2.75818700
C	2.57480700	-0.30704000	-1.66812100
C	2.98691700	-1.37432300	-2.70169400
H	2.25977400	0.64962400	-2.10980700
H	3.14684800	-0.98856600	-3.71000100
N	1.41136600	-0.92436600	-0.99646300
N	-0.77064000	-1.90759500	0.70788000
Cu	0.85853200	-0.64508300	1.03412800
C	0.56620500	1.03490000	2.03222400
N	0.48028400	1.55560400	3.08330800
C	4.67587800	-1.20121100	-1.00663100
C	3.76190400	-0.17636600	-0.76379700
C	3.99541600	0.78227600	0.21388700
C	5.16308900	0.69850800	0.96859600
C	6.07651600	-0.33070200	0.73530700
C	5.84251000	-1.28436100	-0.25499800
C	4.21564800	-2.09614800	-2.12433300

H	3.28228300	1.59021200	0.38254200
H	5.36765200	1.44132900	1.73548900
H	6.98797400	-0.38286700	1.32684800
H	6.56846900	-2.07370800	-0.44162800
C	-2.85308900	-1.17887800	1.90488900
C	-4.07975200	-1.58312200	1.37882900
C	-5.19453300	-0.75995300	1.49084200
C	-5.06051400	0.47534600	2.11916600
C	-3.83221000	0.87582700	2.64729400
C	-2.71899400	0.04403400	2.55308900
C	-4.00008600	-2.94865000	0.75749000
H	-6.15498400	-1.07311300	1.08480200
H	-5.92377300	1.13229100	2.20406000
H	-3.74562000	1.83932400	3.14493300
H	-1.76161900	0.34759400	2.97317800
H	-4.16122000	-2.91452800	-0.33000200
H	-4.75154900	-3.63523000	1.16391800
H	4.99153200	-2.26270100	-2.87948100
H	3.91792100	-3.08807200	-1.75504800
H	-0.17720700	-5.12491800	-1.23830600
H	1.24663200	-4.55627400	-2.26191300
H	-1.72823600	-3.70562900	-2.59919300
H	-0.31014400	-3.13440700	-3.62787000
C	-5.45744700	1.35628600	-1.34581100
C	-4.17044100	1.60713000	-0.89964000
C	-3.12730800	0.71574500	-1.21035500
C	-3.41903400	-0.43124000	-1.97086200
C	-4.70956800	-0.68498100	-2.40711900
C	-5.73032500	0.21305500	-2.09723900
H	-6.25751900	2.05114600	-1.10438300
H	-3.96923300	2.49964000	-0.31133100
H	-2.60974500	-1.12016400	-2.21514400
H	-4.92267100	-1.57481400	-2.99373500
H	-6.74279700	0.02287400	-2.44441500
C	-1.76242400	0.93075200	-0.80782300
H	-1.04288500	0.19297000	-1.17514800
C	-1.24964800	1.93775200	-0.04187100
C	0.15233100	2.04419000	0.12766000
H	0.74922300	1.35591700	-0.47065300
C	0.81296100	3.33008600	0.48328700
H	1.74130700	3.13473800	1.03222200
H	0.16582700	3.91102000	1.15152400
C	1.18131400	4.11703800	-0.79778200
C	-0.02630600	4.70230300	-1.53753400

C	-0.68728300	5.84372100	-0.76938200
C	0.32244400	6.93656200	-0.43236000
C	1.51954200	6.37198500	0.32678500
C	2.17168700	5.23671600	-0.45562400
H	-1.51484300	6.25550400	-1.36061200
H	0.33086000	5.09090300	-2.50368800
H	-0.75915600	3.91920300	-1.77622200
H	1.69412600	3.40975100	-1.47175300
H	0.67937000	7.39221100	-1.37032800
H	-0.15626900	7.73912000	0.14277100
H	2.25771700	7.16059700	0.51977300
H	1.19394300	6.01125500	1.31493600
H	2.56623900	5.63952400	-1.40147600
H	3.02976900	4.82230000	0.09208000
H	-1.13940500	5.46550700	0.16133200
H	-1.88402300	2.68674800	0.43320300
N	2.34257400	-1.76992800	2.01164800
C	3.32829700	-2.19084800	2.45148600
C	4.56035700	-2.70969900	3.00410200
H	5.16262200	-3.16269400	2.21168800
H	5.13085700	-1.89650800	3.46187200
H	4.34315200	-3.46424100	3.76472200

**TS9<sub>s</sub><sup>Z</sup>**

C	3.51664300	2.85224700	0.29590200
C	2.20923300	2.05794100	0.49114000
C	2.65727800	3.15238800	1.45000100
C	1.13189800	2.39734400	-0.45655100
O	1.02599600	3.70417000	-0.72929300
C	-0.45446300	2.41556700	-2.02156900
C	-0.08955800	3.86636000	-1.63708400
H	-0.16498800	2.12568100	-3.04105900
H	0.26930300	4.47323000	-2.47041800
C	2.39026100	0.65834100	0.92028500
O	3.26080800	0.49235100	1.92492200
C	2.47679100	-1.55278300	1.08790200
C	3.32300800	-0.92660300	2.22297400
H	1.69209100	-2.23665300	1.43775700
H	2.90784300	-1.05619500	3.22756900
N	1.85386000	-0.39472800	0.42347300
N	0.33949600	1.60419800	-1.08134000
Cu	0.37563700	-0.40038800	-1.07373500
C	-0.34521600	-2.17768900	-1.20034000
N	-0.27668500	-3.31299800	-1.49367000

C	4.77780300	-2.10573200	0.73706400
C	3.49358400	-2.22888700	0.20497100
C	3.27481700	-2.88573400	-1.00199600
C	4.37136300	-3.40747000	-1.68430800
C	5.66023000	-3.27146100	-1.16453100
C	5.87180200	-2.62470800	0.05040100
C	4.75360000	-1.43935800	2.08399900
H	2.26654100	-2.99329300	-1.39952900
H	4.22243900	-3.92409300	-2.62966800
H	6.50652900	-3.68225000	-1.71022500
H	6.87584200	-2.53247300	0.46020100
C	-1.92914600	2.31683500	-1.77843700
C	-2.40348200	3.46083600	-1.13791400
C	-3.74548000	3.55350300	-0.78296100
C	-4.59912800	2.49494100	-1.08656300
C	-4.12466700	1.36447800	-1.75500100
C	-2.77858000	1.26590700	-2.10346700
C	-1.31188600	4.47443300	-0.93294100
H	-4.12612600	4.44278800	-0.28318600
H	-5.65143200	2.55817600	-0.82045000
H	-4.81484800	0.56487300	-2.01753900
H	-2.40107500	0.39455800	-2.64036900
H	-1.08713500	4.63144500	0.13197200
H	-1.57412400	5.45482600	-1.34584000
H	4.97681900	-2.15928500	2.88148300
H	5.47495000	-0.62079800	2.18969700
H	3.52330600	3.53391600	-0.54898600
H	4.42944500	2.28707700	0.46041900
H	2.05728400	4.05695700	1.43375800
H	2.97618700	2.80803300	2.42833900
C	-1.67074400	2.67932900	2.10832900
C	-1.75718200	1.30410400	1.94127000
C	-0.80053300	0.45372400	2.52413100
C	0.20204000	1.02803800	3.32875500
C	0.28876700	2.40205500	3.48717400
C	-0.64007900	3.23421200	2.86343900
H	-2.43425100	3.31653600	1.66808800
H	-2.61644200	0.89359500	1.41528700
H	0.92417500	0.37802000	3.82138600
H	1.07194200	2.82783600	4.10909700
H	-0.58218000	4.31217100	2.99632300
C	-0.80286200	-0.98887200	2.38653600
H	-0.32403300	-1.52029900	3.21227800
C	-1.32076900	-1.77723000	1.40312800

H	-1.28329500	-2.85771600	1.54933500
C	-1.88850000	-1.33909000	0.17050900
H	-1.84398500	-0.27414700	-0.06990500
C	-3.00572300	-2.08244500	-0.47049200
H	-2.85249600	-3.16230300	-0.36639600
H	-3.03778000	-1.85663500	-1.54338400
C	-4.35402400	-1.64089500	0.15999900
C	-5.51195300	-2.10045100	-0.73549600
C	-5.72065600	-3.61086200	-0.69185800
C	-5.93802400	-4.08936700	0.74001700
C	-4.79143900	-3.66021500	1.64974700
C	-4.57638700	-2.15056300	1.58796000
H	-6.57686300	-3.88355700	-1.32144900
H	-6.42873000	-1.60358900	-0.38123600
H	-5.34869400	-1.76243000	-1.76886100
H	-4.35963400	-0.53850700	0.17739500
H	-6.87634200	-3.65525500	1.12193100
H	-6.06381700	-5.17895300	0.76718600
H	-4.99251300	-3.96010900	2.68593700
H	-3.87142600	-4.18997100	1.35629300
H	-5.47711900	-1.65174300	1.97777300
H	-3.75291900	-1.84808300	2.24927700
H	-4.84844800	-4.12442700	-1.12549300
N	1.75431900	-0.32955500	-2.99013500
C	2.89790600	-0.18706800	-2.83496800
C	4.31354200	0.00425300	-2.60320300
H	4.58929800	1.04592900	-2.78917500
H	4.54159000	-0.25015900	-1.56042000
H	4.89977100	-0.64817900	-3.25592500

### TS10<sub>s</sub>

C	-2.80908900	-1.38325400	3.76603900
C	-1.99076000	-0.90325300	2.56698400
C	-1.67123800	-0.48504700	4.00963400
C	-1.08550900	-1.89466300	1.95788300
O	-0.66025600	-2.86152700	2.78752900
C	0.06642900	-3.20968600	0.58720200
C	0.31202700	-3.63437600	2.04603400
H	-0.55451700	-3.90417500	0.00416100
H	0.10815800	-4.68686200	2.25137100
C	-2.60980000	0.12765600	1.70976500
O	-3.48561800	0.92713400	2.33770000
C	-3.17315300	1.53557600	0.08638300
C	-4.01721600	1.84273100	1.34597500

H	-2.48249500	2.34195100	-0.20216000
H	-3.87424500	2.84972300	1.74594600
N	-2.37558100	0.36368500	0.47363800
N	-0.68641800	-1.95416200	0.73977600
Cu	-1.00177700	-0.60828500	-0.77288300
C	-0.08217200	0.73436000	-1.86512900
N	-0.06308300	1.32748100	-2.88054100
C	-5.46862800	1.18968600	-0.45834700
C	-4.17721000	1.21885900	-0.98092800
C	-3.93061900	0.95145400	-2.32231600
C	-5.01007500	0.64577200	-3.14796300
C	-6.30685200	0.61238900	-2.63052600
C	-6.54559300	0.88612000	-1.28525300
C	-5.48148100	1.52635300	1.00860600
H	-2.91285600	0.97977300	-2.71277600
H	-4.84412100	0.44312300	-4.20434600
H	-7.14156800	0.37780800	-3.28724000
H	-7.55966500	0.86582800	-0.89049800
C	1.43720700	-3.04514500	0.00776500
C	2.40061600	-3.09490900	1.01754400
C	3.75173800	-3.04381700	0.69073000
C	4.11564000	-2.93884000	-0.65247100
C	3.14703300	-2.86352300	-1.65493800
C	1.79238900	-2.91469100	-1.32934500
C	1.75782600	-3.22875500	2.37258700
H	4.51482500	-3.10139600	1.46492800
H	5.17036700	-2.91221100	-0.92285600
H	3.45258900	-2.77950600	-2.69525900
H	1.02609500	-2.87614400	-2.10303000
H	1.75528900	-2.26565900	2.90469400
H	2.26303200	-3.94983800	3.02295800
H	-6.13759300	2.37602200	1.23036200
H	-5.83519200	0.68932800	1.62422800
H	-2.70607000	-2.43445000	4.01289500
H	-3.81179000	-0.97320000	3.82910400
H	-0.75565500	-0.90060300	4.42037200
H	-1.87297400	0.55451600	4.25097100
C	-0.32800600	4.59285800	0.40593800
C	0.34112000	3.54291600	-0.20066000
C	0.43682400	2.30073300	0.44764800
C	-0.14752100	2.13909500	1.71230800
C	-0.80319500	3.19895800	2.32539300
C	-0.90003500	4.42349100	1.66889000
H	-0.41022800	5.54873700	-0.10381900

H	0.76257800	3.66722700	-1.19576900
H	-0.05761600	1.17824200	2.21886300
H	-1.24109400	3.07348300	3.31287700
H	-1.42210700	5.25125400	2.14204200
C	1.18751000	1.18816500	-0.10697200
C	2.41342200	1.35891300	-0.82275000
H	2.59171900	2.29010500	-1.36063700
C	3.36862400	0.40804400	-0.75816200
H	3.15349700	-0.50639400	-0.19605500
C	4.72499200	0.51240000	-1.34002600
H	4.83601100	1.46210100	-1.87877500
H	4.83764400	-0.29106700	-2.08714500
C	5.82164000	0.32199700	-0.27593000
C	7.20885500	0.24286700	-0.91662700
C	7.68180900	1.58930000	-1.45879400
C	7.64182500	2.66001800	-0.37245500
C	6.25497000	2.76992600	0.25400600
C	5.79371800	1.41905900	0.79309500
H	8.69799200	1.49132700	-1.86152100
H	7.92276900	-0.09698800	-0.15006300
H	7.21242500	-0.52065200	-1.70817600
H	5.61313000	-0.64260500	0.21652600
H	8.36539500	2.39432500	0.41567600
H	7.96172400	3.62939000	-0.77550000
H	6.25803200	3.51201700	1.06249500
H	5.53822000	3.14222600	-0.49594600
H	6.46568300	1.11772300	1.61166700
H	4.78824600	1.50053700	1.23053900
H	7.05015600	1.90086900	-2.30515800
H	1.09936400	0.24329600	0.43712200
N	-1.98135100	-1.85578300	-2.18543300
C	-2.74143300	-2.30677000	-2.93466900
C	-3.70749000	-2.84917700	-3.86401900
H	-3.87248800	-3.91068900	-3.66259200
H	-4.65567900	-2.31277500	-3.75384500
H	-3.34828900	-2.73156800	-4.88972300

### TS10<sub>R</sub>

C	-0.80977800	1.29144500	4.15642700
C	-0.76974000	0.93855600	2.67480500
C	-0.35982200	-0.05606100	3.77228800
C	-2.06648700	0.69372700	2.01067900
O	-3.09020900	0.41515400	2.83119400
C	-3.75389800	0.52924100	0.57656500



C	-4.27318300	0.24411700	2.00567700
H	-4.17323600	1.43947600	0.12635900
H	-5.00358500	0.97143200	2.36711600
C	0.33914200	1.50957200	1.87988400
O	1.38371400	1.94816200	2.59939900
C	1.74078100	2.17145600	0.28267200
C	2.33150900	2.52877400	1.66798600
H	2.31930600	1.42896400	-0.28713300
H	3.30023100	2.06736000	1.87785900
N	0.43287600	1.58001900	0.60320400
N	-2.31188400	0.73459500	0.75414700
Cu	-0.95727700	0.84557700	-0.79624400
C	-0.18720900	-0.46362700	-2.04130400
N	0.06660000	-0.76399900	-3.14965400
C	1.95315700	4.54148700	0.40523500
C	1.63479500	3.48013700	-0.43915300
C	1.27041000	3.69002500	-1.76322900
C	1.21136700	4.99821700	-2.23730500
C	1.51667100	6.06761300	-1.39253300
C	1.89403200	5.84781000	-0.06954400
C	2.35521100	4.06132000	1.77316700
H	1.04059400	2.84543900	-2.41248900
H	0.94165000	5.18852500	-3.27417900
H	1.47197700	7.08416300	-1.77655400
H	2.14549300	6.68572500	0.57773500
C	-4.09638400	-0.69823100	-0.21132300
C	-4.72617400	-1.64666800	0.59198300
C	-5.17194800	-2.83974800	0.03271900
C	-4.94675300	-3.07702300	-1.32155100
C	-4.28256700	-2.13797000	-2.11252200
C	-3.86068600	-0.93057500	-1.56165200
C	-4.80674400	-1.19502800	2.02634000
H	-5.67928200	-3.58384500	0.64473600
H	-5.28410900	-4.01099600	-1.76592200
H	-4.10457800	-2.34583500	-3.16487800
H	-3.35411000	-0.18103700	-2.16987300
H	-4.18372100	-1.81652200	2.68547400
H	-5.82550500	-1.24189300	2.42741900
H	3.34472900	4.43076000	2.06567100
H	1.65546500	4.39066800	2.55206200
H	-1.80103700	1.40299700	4.58259900
H	-0.06728500	2.01126500	4.48340900
H	-1.03635800	-0.89385800	3.91766100
H	0.70068800	-0.28959800	3.81578100

C	-2.25526300	-4.18350300	0.47833600
C	-1.48147100	-3.03324100	0.49307800
C	-0.49241600	-2.83146100	-0.48291400
C	-0.32726900	-3.77974900	-1.50629200
C	-1.12264400	-4.91157200	-1.53312600
C	-2.07804300	-5.12063700	-0.53554100
H	-3.00598900	-4.34176200	1.24847700
H	-1.61620100	-2.28930300	1.27830100
H	0.40539300	-3.60650400	-2.29133700
H	-1.00075600	-5.64073700	-2.32929800
H	-2.69498000	-6.01565900	-0.55801000
C	0.39978700	-1.70764900	-0.30529600
C	1.80368800	-1.76036500	-0.59247900
H	2.14809900	-2.39365900	-1.40798500
C	2.67237800	-1.11229300	0.21126500
H	2.24568600	-0.51300700	1.02231400
C	4.15554200	-1.11321600	0.13511100
H	4.54238300	-1.27901700	1.15214900
H	4.45646500	-0.07286500	-0.08946300
C	4.80523000	-2.06350400	-0.87042800
C	6.27160900	-1.69103400	-1.11651600
C	7.17005600	-2.00779000	0.07517700
C	7.06228900	-3.48003600	0.45721300
C	5.61513200	-3.86528400	0.74436100
C	4.70868600	-3.53369000	-0.43884500
H	8.20916200	-1.74694600	-0.16283000
H	6.62965000	-2.26287300	-1.98651100
H	6.34670000	-0.62905700	-1.38945800
H	4.27513000	-1.94398900	-1.82848000
H	7.43648300	-4.09354300	-0.37851700
H	7.70011300	-3.70499800	1.32147300
H	5.54028300	-4.93540300	0.97595100
H	5.27075500	-3.33669900	1.64726600
H	5.00524400	-4.15987000	-1.29435400
H	3.66886300	-3.80134500	-0.20528700
H	6.88915600	-1.38346400	0.93824400
H	0.12666300	-1.02941900	0.50427700
N	-1.81965900	2.39607400	-1.92446400
C	-2.16399200	3.36477100	-2.45800500
C	-2.56896100	4.58692400	-3.11572600
H	-1.80618000	5.35512900	-2.95334500
H	-2.68205100	4.41716100	-4.18950600
H	-3.52018000	4.93812700	-2.70732900

**4<sub>S</sub>**

C	-0.90372000	3.19016200	-0.47509800
N	-1.02140000	4.19533700	-1.04596100
C	4.03473900	-1.22104800	-1.23602500
C	2.86046300	-0.53420600	-0.96043300
C	2.68137300	0.10819800	0.27325900
C	3.70647700	0.02265800	1.22368800
C	4.88285400	-0.66439600	0.94796500
C	5.05199800	-1.28710200	-0.28481300
H	4.15648700	-1.71433000	-2.19770400
H	2.06869700	-0.50674000	-1.70723300
H	3.57298800	0.50831300	2.18964800
H	5.66780000	-0.71654500	1.69880600
H	5.96906100	-1.82884900	-0.50369200
C	1.46723200	0.85182600	0.61207100
H	1.36989400	1.13008900	1.66519300
C	0.49142600	1.21487000	-0.22650700
C	-0.76307600	1.90920100	0.22370400
H	-0.67953100	2.13615800	1.29806300
C	-2.03428000	1.06094800	-0.00051800
H	-2.14230900	0.88122300	-1.07997400
H	-2.89907100	1.67262500	0.29340900
C	-2.01514200	-0.25639500	0.79111900
C	-3.39519500	-0.58957900	1.36818600
C	-4.39253000	-1.00161600	0.29027600
C	-3.86700700	-2.19305100	-0.50318400
C	-2.50098500	-1.88666100	-1.10760100
C	-1.50751500	-1.44616300	-0.03612900
H	-5.36175900	-1.24010100	0.74695800
H	-3.28343100	-1.42390500	2.07878500
H	-3.77510000	0.26486600	1.94538800
H	-1.32427100	-0.11981100	1.63944400
H	-3.77444200	-3.05885300	0.17294400
H	-4.57942500	-2.48203300	-1.28662600
H	-2.10877600	-2.76368900	-1.63839400
H	-2.61226200	-1.09762600	-1.86853600
H	-1.33480500	-2.28994400	0.65065900
H	-0.53260500	-1.21183300	-0.48615900
H	-4.57665100	-0.15897300	-0.39558000
H	0.54663600	0.98672300	-1.29343100

**4<sub>R</sub>**

C	0.90371700	3.19015200	-0.47509900
N	1.02139400	4.19532500	-1.04596600

C	-4.03474300	-1.22105700	-1.23602100
C	-2.86046900	-0.53421000	-0.96043200
C	-2.68138300	0.10820200	0.27325600
C	-3.70648800	0.02266500	1.22368400
C	-4.88286200	-0.66439400	0.94796300
C	-5.05200300	-1.28710800	-0.28481000
H	-4.15648800	-1.71434500	-2.19769800
H	-2.06870300	-0.50674400	-1.70723200
H	-3.57300100	0.50832600	2.18964200
H	-5.66781000	-0.71654000	1.69880400
H	-5.96906500	-1.82885900	-0.50368700
C	-1.46724500	0.85183400	0.61206600
H	-1.36991300	1.13010900	1.66518500
C	-0.49143200	1.21486300	-0.22651100
C	0.76307000	1.90919200	0.22370300
H	0.67952400	2.13615100	1.29806200
C	2.03427600	1.06094000	-0.00051800
H	2.89906500	1.67262000	0.29340700
H	2.14230300	0.88121100	-1.07997300
C	2.01514300	-0.25640200	0.79112200
C	1.50753000	-1.44617300	-0.03612900
C	2.50100600	-1.88665600	-1.10760100
C	3.86703100	-2.19303000	-0.50318500
C	4.39253800	-1.00159300	0.29028300
C	3.39519600	-0.58957400	1.36819300
H	2.10880900	-2.76368800	-1.63839500
H	1.33482900	-2.28995700	0.65065700
H	0.53261800	-1.21185200	-0.48616000
H	1.32426700	-0.11982300	1.63944400
H	3.77447800	-3.05883700	0.17293800
H	4.57945400	-2.48199800	-1.28662900
H	5.36176900	-1.24007000	0.74696400
H	4.57665000	-0.15894400	-0.39556900
H	3.28344000	-1.42390500	2.07878500
H	3.77509000	0.26487200	1.94540000
H	2.61227200	-1.09761700	-1.86853400
H	-0.54663500	0.98670300	-1.29343200

### 5<sub>s</sub>

C	2.68584000	2.43071700	-0.27896200
N	3.29726900	3.24728000	-0.83457400
C	3.72836600	-1.63940500	-1.01857100
C	3.24608200	-0.33999100	-0.88459400
C	2.50286900	0.01729700	0.23812500

C	2.23761600	-0.93808900	1.21984800
C	2.72017600	-2.23437400	1.08644400
C	3.46825800	-2.58752000	-0.03450000
H	4.31133700	-1.90905000	-1.89605100
H	3.45606800	0.40054800	-1.65546400
H	1.64752000	-0.65784500	2.09275400
H	2.51544100	-2.97047200	1.86014100
H	3.84907800	-3.60054200	-0.13942000
C	1.89429500	1.40133800	0.39855400
C	0.47361500	1.41611600	-0.11599500
H	0.35623300	1.22424500	-1.18564900
C	-0.59118200	1.58838900	0.66521900
H	-0.43755500	1.75827800	1.73647800
C	-2.00564100	1.52414600	0.19713700
H	-2.01961200	1.36956900	-0.89084800
H	-2.49712300	2.49328100	0.37771700
C	-2.82093600	0.44103500	0.92187600
C	-4.28474600	0.44976600	0.47103000
C	-4.46628900	-0.08717700	-0.94700200
C	-3.86002500	-1.47936300	-1.09029300
C	-2.39292700	-1.49193500	-0.67171800
C	-2.22955000	-0.96135500	0.74914700
H	-5.53380200	-0.10726200	-1.20257900
H	-4.86531900	-0.18323400	1.16075800
H	-4.69812000	1.46506900	0.55554700
H	-2.79130900	0.69072000	1.99559000
H	-4.41834100	-2.17842700	-0.44597900
H	-3.97343600	-1.84486200	-2.11922100
H	-1.98186100	-2.50728700	-0.74254200
H	-1.80446500	-0.87568800	-1.37048600
H	-2.74810400	-1.64335800	1.44157900
H	-1.16963700	-0.96606000	1.04006600
H	-3.99486300	0.59325600	-1.67280600
H	1.88207400	1.66058800	1.46795700

### 5<sub>R</sub>

C	-2.46037800	2.44744900	-0.12933900
N	-2.90567700	3.36829900	-0.67987300
C	-2.76764400	-2.39144700	0.58762200
C	-2.12509200	-1.18104000	0.81362900
C	-2.61937200	-0.00081100	0.25320700
C	-3.76308600	-0.05062900	-0.54012500
C	-4.40508200	-1.26576000	-0.76961900
C	-3.91075600	-2.43728200	-0.20787000

H	-2.37423300	-3.30293900	1.03151600
H	-1.22646300	-1.14380000	1.42855500
H	-4.15979100	0.86174200	-0.98246400
H	-5.29609500	-1.29171000	-1.39252700
H	-4.41280800	-3.38472000	-0.38857300
C	-1.87286900	1.29410600	0.55544100
C	-0.40774700	1.18776000	0.20537400
H	-0.19477700	0.99143700	-0.84620000
C	0.56134800	1.26545800	1.11666400
H	0.26934700	1.45829400	2.15301200
C	2.03265500	1.12864600	0.88251600
H	2.43865300	0.46534100	1.66122700
H	2.49969700	2.10618700	1.09037300
C	2.46349900	0.65210400	-0.50499700
C	3.95988100	0.89073200	-0.73711500
C	4.84119700	-0.04268300	0.08754600
C	4.49764900	-1.50063800	-0.19789200
C	3.01769900	-1.77564700	0.04781000
C	2.13397300	-0.82629300	-0.75824200
H	5.89939200	0.15229300	-0.13001500
H	4.17776400	0.72301900	-1.80396000
H	4.20722200	1.94146000	-0.52965400
H	1.91877500	1.25968600	-1.24515100
H	4.73146000	-1.72124200	-1.25256600
H	5.12072700	-2.17185300	0.40748500
H	2.77336600	-2.81479400	-0.20874700
H	2.80095700	-1.67247100	1.12266000
H	2.28582200	-1.03298300	-1.82961800
H	1.07382900	-1.02805200	-0.55017800
H	4.70694200	0.16300700	1.16122400
H	-1.95529900	1.49984600	1.63505300

**<sup>3</sup>[LCu(MeCN)]\***

C	-0.10576500	5.59664500	-0.10249700
H	-0.22554000	5.99183400	0.90969900
H	-0.95016000	5.92467000	-0.71464500
H	0.82029800	5.98778800	-0.53214700
C	-0.06238100	4.15379100	-0.06501000
N	-0.02939500	2.99585400	-0.03687600
C	0.40954400	-3.66233200	0.59528500
C	0.04108400	-2.31310000	-0.03533400
C	-0.30863200	-3.65788100	-0.68489600
C	-1.07052800	-1.58713000	0.60267400
O	-2.04672100	-2.36868300	1.07317000

C	-2.52712400	-0.10183600	1.37728300
C	-3.00516700	-1.51931100	1.76108700
H	-2.42339800	0.57888000	2.22993300
H	-2.92775000	-1.75807500	2.82521000
C	1.14324600	-1.56174600	-0.66003800
O	2.13131000	-2.32021700	-1.14231100
C	2.58537600	-0.04178900	-1.40295300
C	3.09267700	-1.44522300	-1.79559900
H	2.46245200	0.65514900	-2.24531700
H	3.04500900	-1.67162500	-2.86433300
N	1.25625400	-0.28908700	-0.79805200
N	-1.20505500	-0.31913100	0.76330500
Cu	0.01605900	1.08525300	-0.01279300
C	4.58544600	-0.50395900	-0.18629800
C	3.55849400	0.40955200	-0.37545500
C	3.43357100	1.63575500	0.48262500
C	4.37331500	1.80993600	1.49692900
C	5.39744700	0.90229700	1.69475400
C	5.52399400	-0.32229200	0.81412100
C	4.47824000	-1.62616800	-1.18354600
H	2.67381300	2.38065400	0.25974400
H	4.31563800	2.69108600	2.13297500
H	6.13727200	1.05965200	2.47414000
H	6.32291500	-1.03561800	0.99491500
C	-3.54057100	0.36273700	0.36613300
C	-4.56789600	-0.56943700	0.22349500
C	-5.58599500	-0.34889200	-0.69818800
C	-5.55989500	0.81095700	-1.46850300
C	-4.53255500	1.74422300	-1.31819100
C	-3.51333300	1.52498100	-0.39556700
C	-4.40292000	-1.71572000	1.18263500
H	-6.38998100	-1.07260300	-0.81772600
H	-6.34887400	0.99251100	-2.19461200
H	-4.52989500	2.64632600	-1.92535100
H	-2.70757600	2.24842600	-0.27315100
H	-4.49952600	-2.70229900	0.71477700
H	-5.15131600	-1.67303800	1.98421500
H	5.24936500	-1.54078500	-1.95943100
H	4.58597100	-2.62139300	-0.73698500
H	-0.13956400	-3.91120600	1.49781900
H	1.46894100	-3.89617100	0.60024600
H	-1.36461400	-3.90663300	-0.69323100
H	0.24344200	-3.88646100	-1.59093500

**11**

C	-1.36396000	1.79721400	-0.21995700
H	-0.95137000	2.18168700	-1.15803700
H	-2.45085400	1.92999400	-0.24814600
H	-0.97093600	2.39342000	0.60966700
C	-1.35886700	-0.70981100	1.66748000
H	-2.44557500	-0.76539500	1.79388700
H	-0.95353500	-1.72116300	1.77295700
H	-0.95660100	-0.08254600	2.46927700
C	-1.35815300	-1.09098400	-1.44704300
H	-0.95770400	-0.67551300	-2.37713500
H	-0.94981100	-2.09659800	-1.30545300
H	-2.44469500	-1.17868000	-1.55497100
Si	-0.96445200	0.00005700	-0.00001100
N	0.89859900	0.00331800	-0.00093700
C	2.05253000	0.00191000	-0.00089100
C	3.48593100	0.00026700	0.00065700
H	3.85086000	0.08523300	-1.02706700
H	3.84978700	0.84726400	0.58933400
H	3.84768300	-0.93330100	0.44092300

**12**

C	2.14175200	-2.30252100	-2.07779700
O	0.83453600	-2.94050700	-1.98781600
C	2.07731000	-1.24593400	-0.95401300
H	2.38468600	-0.24163800	-1.26513200
C	0.08741600	-2.21854800	-1.15576400
N	0.65468500	-1.22445600	-0.57182600
C	-1.30476000	-2.66115100	-1.01657800
C	-1.57811900	-4.15879600	-1.19283900
C	-1.97301000	-3.24117700	-2.26827900
H	-0.69424300	-4.77373200	-1.32871800
H	-2.34729400	-4.56329100	-0.54255700
H	-1.36837100	-3.20228800	-3.16884000
H	-3.02279500	-2.99257200	-2.38603300
C	-4.11860200	-1.57602400	0.99543000
O	-3.43758100	-2.33859000	-0.04457700
C	-3.08053900	-0.49098900	1.34825100
H	-2.90054000	-0.37292900	2.42192200
C	-2.17073000	-1.93478300	-0.08122500
N	-1.84462900	-0.96339800	0.69584200
C	4.34748400	-3.72533800	0.60033100
C	4.51834300	-3.25126200	1.89872400
C	3.90210500	-2.06961300	2.31349300



C	3.10084400	-1.34268200	1.43597200
C	2.93101700	-1.82580500	0.14264900
C	3.54587000	-3.00411500	-0.27820500
H	4.83154800	-4.64594700	0.27959800
H	5.14023600	-3.80720600	2.59669900
H	4.05092400	-1.71120300	3.32930900
H	2.63511100	-0.40827300	1.75377000
C	3.24223400	-3.29600700	-1.72156700
H	2.91545500	-4.32579600	-1.90710300
H	4.12081700	-3.12481900	-2.35653900
C	-3.00098100	1.99734900	0.57205100
C	-3.61522400	0.75464800	0.68940600
C	-4.87156400	0.51796500	0.13142400
C	-5.53365900	1.52868100	-0.55684300
C	-4.92056400	2.77266000	-0.68187300
C	-3.66369200	3.00606000	-0.12163500
H	-2.02157200	2.17946200	1.01425000
H	-6.51467200	1.35004900	-0.99327100
H	-5.42586600	3.57075300	-1.22091400
H	-3.19745000	3.98261600	-0.22860000
C	-5.34604800	-0.87928700	0.41955600
H	-5.72062600	-1.41126900	-0.46264500
H	-4.33970500	-2.28136000	1.80074500
H	-6.15828900	-0.88084400	1.15754400
H	2.21771000	-1.89402900	-3.08885000
C	-0.45166700	0.74966000	2.60225300
N	-0.73451400	1.16488000	3.65866200
Cu	-0.09289000	0.04287000	0.80211400
N	1.06757200	1.53572600	0.24881900
C	2.07065700	2.22775300	0.89722900
C	0.71841200	2.17224400	-0.92393800
O	-0.16565800	1.81336200	-1.69012500
O	2.58638100	1.93075100	1.96334300
C	1.60439100	3.36440900	-1.07652400
C	2.43019300	3.40159100	0.04014900
C	3.37740600	4.39380700	0.20731100
C	3.47079800	5.36495500	-0.79451500
C	2.63936400	5.32787900	-1.91549300
C	1.68558900	4.31834000	-2.07337900
H	4.01985600	4.41428400	1.08442600
H	4.20214700	6.16417800	-0.70135400
H	2.73852400	6.09866900	-2.67603900
H	1.03285700	4.28074300	-2.94261000

## 13

C	-2.13098200	-1.96828200	1.22249900
O	-0.89610200	-2.69400000	0.94865800
C	-2.12891900	-0.91108100	0.10801900
H	-2.39203200	0.07968000	0.48364500
C	-0.16755500	-1.94102900	0.12861700
N	-0.72571200	-0.88673100	-0.35856800
C	1.18855200	-2.43546800	-0.11870300
C	1.35226500	-3.95995300	-0.18660700
C	1.84193200	-3.25148300	1.00126700
H	0.42603200	-4.52172900	-0.11582600
H	2.07059500	-4.31101500	-0.92044000
H	1.26632400	-3.29966000	1.92100500
H	2.90999300	-3.09479700	1.11770200
C	4.01546100	-1.28307700	-2.05710700
O	3.29497100	-2.14699900	-1.13189200
C	3.12444000	-0.02558800	-2.10414800
H	2.91626400	0.33735100	-3.11522600
C	2.08695300	-1.62395100	-0.94443600
N	1.85637000	-0.47846800	-1.48467300
C	-4.68058600	-3.26854400	-1.18363700
C	-4.93120200	-2.82676700	-2.48020700
C	-4.26052100	-1.71607800	-2.99246500
C	-3.33197400	-1.02898400	-2.21454900
C	-3.08526600	-1.46925700	-0.91732300
C	-3.75302700	-2.58440100	-0.40601800
H	-5.19958000	-4.13867000	-0.78596800
H	-5.65228600	-3.35423600	-3.10030000
H	-4.46147900	-1.38506500	-4.00860200
H	-2.80477600	-0.16907400	-2.62041800
C	-3.34310800	-2.86151800	1.01308600
H	-3.10666800	-3.91304100	1.21291200
H	-4.13341600	-2.57375900	1.71918500
C	3.46030100	2.24725600	-0.86071300
C	3.86696000	0.97608900	-1.25367700
C	5.09781100	0.45860500	-0.84523900
C	5.93015900	1.19742500	-0.01106400
C	5.51743600	2.46176700	0.40072100
C	4.29586300	2.98500300	-0.02649800
H	2.50015600	2.64502600	-1.17965200
H	6.88821500	0.79442500	0.31227000
H	6.15514200	3.05031600	1.05648400
H	3.99078100	3.97665500	0.29904000
C	5.35764700	-0.88856800	-1.45755800

H	5.70776000	-1.64450800	-0.74499600
H	4.08727400	-1.83043500	-3.00114300
H	6.11653200	-0.82370400	-2.24774500
H	-2.04223500	-1.56261400	2.23643900
C	0.75564400	1.74286200	-2.92554400
N	1.13614500	2.39468900	-3.81873000
Cu	0.14161900	0.61719000	-1.43433700
N	-0.95757800	1.48591700	1.97793800
C	0.27466700	1.36991300	1.43079200
C	-1.00274400	0.67178200	3.08354800
O	-1.99321100	0.44790800	3.77756600
O	0.66391000	1.88422900	0.36580700
C	0.34083800	0.01830500	3.29459300
C	1.14171100	0.46387500	2.25374000
C	2.45529500	0.05804500	2.10879600
C	2.95724300	-0.82264400	3.07443200
C	2.15182800	-1.27963700	4.12015500
C	0.81786900	-0.86908900	4.24065900
H	3.06286000	0.41225300	1.27460100
H	3.98919700	-1.16268800	3.01011200
H	2.57064300	-1.96803500	4.85101200
H	0.18415700	-1.22573500	5.05029600
Si	-3.92585600	2.90000400	0.30628100
C	-4.51879100	1.44151100	1.31296100
H	-5.42270100	1.73721100	1.85904100
H	-3.75921900	1.13477000	2.04532100
H	-4.78272000	0.58747200	0.67617300
C	-5.20330300	3.49210900	-0.92088100
H	-6.07143600	3.89419500	-0.38662000
H	-5.54873400	2.66782100	-1.55449900
H	-4.80526700	4.28222900	-1.56559300
C	-3.14056200	4.24031100	1.32983200
H	-2.75777200	5.05665200	0.70954300
H	-2.31288400	3.79594000	1.89377000
H	-3.87011200	4.65330600	2.03510200
C	-2.51188200	2.20420800	-0.78223900
N	-1.66105600	1.67942200	-1.37318500

### TS11

C	-2.61485000	-1.43844000	1.75349800
O	-1.42995000	-2.28235400	1.89630900
C	-2.38605400	-0.77230000	0.38372100
H	-2.53168500	0.31224400	0.40324000
C	-0.57418900	-1.94620000	0.94160700

N	-0.96997700	-1.07386300	0.07759800
C	0.71751300	-2.64006200	0.98100800
C	0.67318900	-4.14041500	1.33219800
C	1.18777700	-3.19127400	2.32454200
H	-0.32336700	-4.55098400	1.46251600
H	1.37421400	-4.75969800	0.78106000
H	0.55838400	-2.93344600	3.17039200
H	2.25910600	-3.14144900	2.49269400
C	3.78317700	-2.41206600	-0.93324000
O	2.94159400	-2.78786600	0.19698000
C	2.92833300	-1.35005600	-1.65734400
H	2.80497400	-1.53197300	-2.73004000
C	1.74661300	-2.24111500	0.01711100
N	1.61117800	-1.46177900	-0.99921900
C	-5.05216900	-3.18723100	-0.49425800
C	-5.16261700	-3.08066300	-1.87840100
C	-4.36760400	-2.18060500	-2.58909100
C	-3.44525000	-1.37661400	-1.92406000
C	-3.33111900	-1.49377700	-0.54216300
C	-4.12964000	-2.38801900	0.17202000
H	-5.67785200	-3.88634000	0.05733400
H	-5.87791100	-3.70282600	-2.41123900
H	-4.46993800	-2.10432500	-3.66881400
H	-2.83154900	-0.66590900	-2.47614500
C	-3.86605600	-2.30078800	1.64982900
H	-3.71586700	-3.27361500	2.13226700
H	-4.69890800	-1.81463200	2.17336600
C	3.19419000	1.23961700	-1.66452800
C	3.61615200	-0.04734200	-1.35172300
C	4.79881900	-0.26745500	-0.64450500
C	5.58520600	0.80811000	-0.24646000
C	5.17053900	2.10026300	-0.56542000
C	3.98246100	2.31577000	-1.26542200
H	2.25900900	1.40945500	-2.19716800
H	6.50991600	0.64435100	0.30368600
H	5.77512300	2.95052300	-0.25848600
H	3.65440000	3.32858400	-1.48258500
C	5.06025300	-1.73451900	-0.44723300
H	5.27390100	-2.00652400	0.59348000
H	3.95485700	-3.32795600	-1.50420900
H	5.91730400	-2.07253900	-1.04288100
H	-2.60294100	-0.73749600	2.59433700
C	0.56582200	-0.35171400	-3.43832300
N	0.93496100	-0.29840200	-4.54623800

Cu	-0.01967700	-0.46418000	-1.57238800
N	-0.89355100	2.60593000	1.14608100
C	0.44569000	2.53796000	0.80357200
C	-1.12753000	1.78711900	2.22927100
O	-2.19864900	1.58764000	2.79343900
O	0.96252000	3.14742500	-0.12426000
C	0.16356600	1.12616300	2.60792500
C	1.12982100	1.58030600	1.72209300
C	2.43742600	1.13305700	1.77848200
C	2.75038900	0.20012700	2.77272700
C	1.78217200	-0.24332300	3.67651400
C	0.46222000	0.21576500	3.60479800
H	3.18832000	1.49976100	1.08182600
H	3.76803500	-0.17982800	2.84940100
H	2.06211200	-0.95815200	4.44750500
H	-0.30029400	-0.12974100	4.30058500
Si	-2.15397300	3.75266600	-0.18882700
C	-3.79964200	3.16034200	0.49674100
H	-4.47029900	4.02778100	0.54939000
H	-3.70712600	2.71015800	1.48901900
H	-4.26281300	2.43187500	-0.18169900
C	-2.62716800	4.60491200	-1.84359600
H	-3.24738100	5.49214200	-1.65427400
H	-3.18626800	3.93344400	-2.50996100
H	-1.73609500	4.94245600	-2.39062600
C	-1.43671800	5.25450700	0.71717300
H	-0.37867700	5.39068200	0.46757500
H	-1.50945300	5.12277400	1.80253400
H	-1.97573000	6.16324700	0.42090800
C	-1.53020300	2.15459900	-1.23759400
N	-1.21353100	1.14457900	-1.73118200

#### 14

C	3.03752500	1.35180700	1.72981500
O	2.09411900	2.24839000	1.07083500
C	2.53222100	-0.04240400	1.30381500
H	2.41093100	-0.75287500	2.12735500
C	1.10278100	1.50734300	0.58602000
N	1.21015400	0.23175700	0.70726200
C	0.00048600	2.25425600	-0.02935300
C	0.35364000	3.59041600	-0.69347900
C	-0.34826500	3.61061000	0.59475400
H	1.41286900	3.82535700	-0.71661300
H	-0.20617000	3.81441100	-1.59607500

H	0.21304500	3.85805100	1.49028200
H	-1.40639500	3.85073800	0.61093600
C	-3.05483100	1.31584600	-1.73876200
O	-2.10226600	2.22369800	-1.10915400
C	-2.54636600	-0.06966500	-1.29050700
H	-2.43921300	-0.79553500	-2.10343100
C	-1.10533900	1.49395100	-0.62049400
N	-1.21553700	0.21524500	-0.71807700
C	5.58314600	0.22301600	-0.78111100
C	5.53509700	-0.90809100	-1.59193100
C	4.49378800	-1.82929800	-1.46805200
C	3.48067600	-1.62898400	-0.53399200
C	3.52862900	-0.49237400	0.26692400
C	4.57198500	0.42656000	0.15165300
H	6.39890200	0.93717800	-0.87685600
H	6.31812600	-1.07689400	-2.32760700
H	4.47457800	-2.71122300	-2.10377800
H	2.67200000	-2.35058100	-0.42335700
C	4.43562800	1.54014100	1.15276500
H	4.55039700	2.54147200	0.72161000
H	5.18509600	1.45208700	1.94958500
C	-3.47088800	-1.61449500	0.59570800
C	-3.52864000	-0.49645900	-0.23048100
C	-4.57019800	0.42530800	-0.12283100
C	-5.57004800	0.24312700	0.82627800
C	-5.51236400	-0.86953800	1.66146400
C	-4.47247100	-1.79345500	1.54625900
H	-2.66362600	-2.34034700	0.49686700
H	-6.38440400	0.95960500	0.91584500
H	-6.28660100	-1.02190300	2.40987100
H	-4.44515100	-2.66060800	2.20152800
C	-4.44535500	1.51762700	-1.14851200
H	-4.55339800	2.52755400	-0.73620400
H	-2.99308400	1.50222200	-2.81392900
H	-5.20462900	1.41444600	-1.93407400
H	2.96362100	1.56030300	2.80023200
C	1.12273500	-3.33045800	2.01292500
N	0.70305500	-2.53109500	1.25316600
Cu	0.00540000	-1.21243200	-0.00571200
C	-0.68061000	-2.57983000	-1.24872400
N	-1.11854000	-3.37581800	-1.98533900

**2\*...1**

C	-2.58196600	-0.89950900	0.94714100
---	-------------	-------------	------------

C	-2.89037800	-1.96637000	0.03931400
C	-4.19612900	-2.11341300	-0.45148200
C	-5.17053000	-1.22257700	-0.04319900
C	-4.86184200	-0.16391400	0.85626900
C	-3.57994800	0.00010400	1.34270600
C	-1.18174000	-0.92932600	1.26635800
C	-1.70035200	-2.72292400	-0.24363600
H	-4.42685500	-2.92124300	-1.14552900
H	-6.18854500	-1.32556800	-0.41475400
H	-5.64662100	0.53167200	1.14906600
H	-3.32711000	0.82630700	2.00728200
O	-1.45337500	-3.67366900	-0.99561100
O	-0.43093300	-0.18691000	1.91234100
N	-0.74884700	-2.11493700	0.61583300
O	0.59245500	-2.39405400	0.53674100
C	1.25052400	-1.64080900	-0.39919300
O	0.69209500	-0.96543700	-1.22515200
C	3.53286000	-1.39017300	-1.40816900
H	3.28208000	-2.07423100	-2.22906600
C	2.72706400	-1.74317300	-0.16396300
H	2.95557700	-2.77349300	0.15178900
C	3.06946400	-0.79819800	1.00264900
H	2.74135100	0.21859000	0.73154100
H	2.48792500	-1.08076900	1.88809600
C	4.56553100	-0.80006200	1.28769200
H	4.78913100	-0.08139000	2.08716300
H	4.85983100	-1.79342700	1.66284500
C	5.37841400	-0.47742000	0.03818300
H	6.45245000	-0.52581900	0.25882500
H	5.17042900	0.56043400	-0.26965900
C	5.02662300	-1.41917200	-1.10832400
H	5.59735600	-1.16031900	-2.00898900
H	5.32006700	-2.44598100	-0.83601800
H	3.23824500	-0.38341600	-1.74294000
C	-2.62807900	3.90686600	-0.16928900
C	-1.25446600	3.72375800	-0.09213400
C	-0.65568300	2.56277200	-0.60663500
C	-1.48038700	1.59572700	-1.20082100
C	-2.85539600	1.77942400	-1.27393900
C	-3.43511800	2.93668800	-0.76375000
H	-3.07351800	4.81453400	0.23318400
H	-0.63652200	4.49686900	0.36167200
H	-1.02802700	0.67645300	-1.57352700
H	-3.48034500	1.00156000	-1.70822100

H	-4.51292600	3.07734500	-0.81580500
C	0.78363000	2.33178300	-0.56964900
H	1.12683200	1.46683700	-1.14472100
C	1.70793700	3.05023000	0.09700000
H	1.41167700	3.89259300	0.72718100
C	3.12218000	2.75156500	0.03729300
H	3.40916700	1.95083600	-0.65117300
C	4.07059100	3.37200300	0.75139000
H	3.82148300	4.17190800	1.44747100
H	5.12004600	3.10153700	0.66605900

**LCu<sup>+</sup>...2<sup>-</sup>...1**

C	3.83333000	2.37813200	1.94463000
C	3.12832100	1.17565500	2.25629900
C	3.80170200	0.08622900	2.83470300
C	5.15088600	0.21336700	3.09852100
C	5.85090000	1.40740000	2.79074500
C	5.19928900	2.48539900	2.21487900
C	2.92733200	3.32678600	1.33157000
C	1.77557300	1.31503700	1.84768200
H	3.26217600	-0.83297500	3.06108700
H	5.69237900	-0.61612200	3.54841600
H	6.91407000	1.47163900	3.01048900
H	5.73203200	3.40292600	1.97088900
O	0.79073700	0.51064000	1.88595000
O	3.07156300	4.46021300	0.87586100
N	1.69721300	2.62504600	1.35707800
O	0.55378700	3.11816000	0.78517300
C	0.53099000	2.99448600	-0.58893000
O	1.43869500	2.51234500	-1.21518100
C	-0.51075900	4.48920700	-2.29116200
H	0.09599100	5.33519500	-1.94412500
C	-0.76354000	3.51058600	-1.14130700
H	-1.31028000	4.01790500	-0.33242900
C	-1.61472100	2.32784700	-1.62899000
H	-1.04905600	1.78057600	-2.40065100
H	-1.79223500	1.62599800	-0.80356100
C	-2.93385500	2.82149400	-2.20662400
H	-3.53138600	1.96452600	-2.54711900
H	-3.51305900	3.30650200	-1.40416100
C	-2.69836500	3.80947800	-3.34295300
H	-3.65315200	4.17772400	-3.73919400
H	-2.19174400	3.29030800	-4.17258800
C	-1.82988000	4.97529200	-2.88076200



H	-1.63528600	5.66596100	-3.71052300
H	-2.37471100	5.55032300	-2.11517000
H	0.07831200	3.96901500	-3.06212100
Cu	0.06115600	-0.19716300	0.21126300
C	-2.76220300	-2.52630200	-2.99016500
C	-1.81232400	-2.06084600	-1.88936800
C	-2.03485300	-3.54344300	-2.21376100
C	-0.53237300	-1.47297800	-2.33981900
O	-0.14357900	-1.85414900	-3.56396600
C	1.33545400	-0.28648600	-2.61992300
C	1.09390700	-1.16184800	-3.87032500
H	1.29760800	0.79476500	-2.80107900
H	0.90636200	-0.59371600	-4.78469900
C	-2.43491500	-1.58339200	-0.63650500
O	-3.72125100	-1.93604200	-0.46718700
C	-2.88854000	-0.68107200	1.33984500
C	-4.15371500	-1.39567100	0.80973800
H	-2.51275700	-1.07995800	2.29048200
H	-4.47072200	-2.24795500	1.41742800
N	-1.87992600	-0.91618800	0.30166700
N	0.21872300	-0.63486800	-1.72237000
C	-4.57876300	0.96714700	0.99165600
C	-3.26978200	0.76678200	1.42433100
C	-2.45675100	1.82611300	1.81170500
C	-2.98476400	3.11431100	1.76977800
C	-4.30098300	3.32406900	1.34970200
C	-5.10573300	2.25521900	0.95873700
C	-5.24571000	-0.33338300	0.62821900
H	-1.42021300	1.64602900	2.10466600
H	-2.36704200	3.96149200	2.06237000
H	-4.70234000	4.33494900	1.32531000
H	-6.12858900	2.42880900	0.62888300
C	2.66275600	-0.73581800	-2.08766800
C	3.17227300	-1.79179900	-2.84056000
C	4.38018800	-2.38157800	-2.47986000
C	5.05764300	-1.90336500	-1.35902400
C	4.54686000	-0.83720000	-0.61509200
C	3.34302900	-0.23923500	-0.98146200
C	2.27524700	-2.13074900	-3.99962100
H	4.79040000	-3.20570200	-3.06182200
H	6.00086900	-2.35967700	-1.06672500
H	5.08882700	-0.46238300	0.25222500
H	2.95198100	0.61487400	-0.42967100
H	1.91726000	-3.16803500	-3.96619700

H	2.78611400	-2.00330500	-4.96165100
H	-6.10480900	-0.54256300	1.27753600
H	-5.62356300	-0.34573200	-0.40178700
H	-2.43770100	-2.32039000	-4.00436500
H	-3.81693900	-2.37580400	-2.78650500
H	-1.19062300	-4.05359700	-2.67068000
H	-2.57310200	-4.10679000	-1.45607900
C	-2.60767400	-3.73307200	3.45389500
C	-1.68026600	-3.79592400	2.42281500
C	-0.54654900	-2.96740700	2.42511600
C	-0.38547500	-2.06522600	3.48629900
C	-1.31417200	-2.00406100	4.52018200
C	-2.42853500	-2.83883000	4.50999600
H	-3.47932800	-4.38400000	3.43476400
H	-1.84336400	-4.49472400	1.60309200
H	0.46677700	-1.38784100	3.46953200
H	-1.16983200	-1.29615300	5.33311300
H	-3.15696900	-2.79124700	5.31582600
C	0.45827100	-3.00394800	1.36642700
H	1.25647700	-2.25661400	1.44723200
C	0.49850700	-3.87462100	0.33868000
H	-0.26999700	-4.64680800	0.24564000
C	1.53339000	-3.88361700	-0.66910600
H	2.31424100	-3.12290300	-0.58101500
C	1.58525100	-4.77333400	-1.67132000
H	0.83022500	-5.55238900	-1.77694700
H	2.39606300	-4.77067300	-2.39561800

### TS9<sub>s</sub>'

C	-1.72759500	-0.25227300	3.85244500
C	-0.94415000	-0.03408700	2.55215100
C	-1.16165400	1.07709800	3.58513300
C	0.39839500	-0.64114000	2.51049800
O	1.04324000	-0.65512000	3.68793500
C	2.26425400	-1.74251400	2.00642400
C	2.38063000	-1.13475900	3.41791400
H	2.17726200	-2.83762000	1.97995700
H	2.62568000	-1.85347000	4.20171500
C	-1.74114100	0.04898700	1.31322800
O	-2.93846200	0.62908200	1.46344800
C	-2.55818800	-0.06790000	-0.74969500
C	-3.58040500	0.65574000	0.16226700
H	-2.20647100	0.53402800	-1.59977300
H	-3.73856500	1.71066400	-0.08060400

N	-1.41549400	-0.34397100	0.13712400
N	0.99901100	-1.17261800	1.50936100
Cu	0.33551300	-1.38314200	-0.41718900
C	0.70019800	-0.96306900	-2.28698100
N	0.48120000	-1.13699300	-3.42873200
C	-4.53291300	-1.40569500	-0.61355800
C	-3.26166900	-1.32601200	-1.17972000
C	-2.77611300	-2.33398100	-2.00593400
C	-3.58218500	-3.44410500	-2.24507100
C	-4.84941100	-3.53702100	-1.66598400
C	-5.33530000	-2.51697700	-0.85169300
C	-4.86717400	-0.17115600	0.17675800
H	-1.78744100	-2.24950300	-2.45693600
H	-3.22806500	-4.24008500	-2.89671900
H	-5.46810600	-4.40948900	-1.86342600
H	-6.32957300	-2.58605000	-0.41417300
C	3.46882800	-1.23292500	1.27544300
C	4.09827000	-0.22828000	2.01136100
C	5.24183800	0.38669200	1.51349000
C	5.74206100	-0.02101800	0.27735000
C	5.10969600	-1.02866300	-0.45366900
C	3.96062100	-1.64291700	0.04207200
C	3.39090500	0.01984000	3.31586400
H	5.74729500	1.16398800	2.08315700
H	6.64365200	0.44261100	-0.11841900
H	5.52439000	-1.34625000	-1.40841700
H	3.46460400	-2.43689300	-0.51678900
H	2.85250400	0.97821400	3.30715400
H	4.07490100	0.05181600	4.17052600
H	-5.69153900	0.38572100	-0.28564300
H	-5.17350100	-0.38431400	1.20794800
H	-1.24157800	-0.88932000	4.58424900
H	-2.79590800	-0.39618900	3.72815300
H	-0.27331000	1.38356300	4.12907400
H	-1.83720700	1.87053200	3.27971600
C	-2.78503800	4.42532800	-1.33951600
C	-1.71291900	3.56547200	-1.47942000
C	-0.97781800	3.15299900	-0.35035600
C	-1.35919500	3.64441300	0.90904700
C	-2.43269800	4.51057300	1.04096700
C	-3.16718500	4.91172900	-0.07901400
H	-3.34939100	4.73262600	-2.21833100
H	-1.44836700	3.19469000	-2.46753200
H	-0.78286200	3.35275200	1.78659200

H	-2.71034000	4.88564800	2.02418100
C	0.11714300	2.22161200	-0.43518300
H	0.49644900	1.84162100	0.51770400
C	0.73475700	1.77873100	-1.56623500
C	1.77691900	0.82487500	-1.49275900
H	2.06105400	0.48455100	-0.49137800
C	2.85841000	0.76661900	-2.50978700
H	2.45402100	0.91246900	-3.51863200
H	3.36068900	-0.20816900	-2.47814500
H	0.44870900	2.14238800	-2.55409100
N	0.02123400	-3.49901000	-0.43131800
C	-0.34487100	-4.58544700	-0.59820200
C	-0.80767100	-5.93950100	-0.80796400
H	-0.19090700	-6.63972700	-0.23882900
H	-1.84641000	-6.03104200	-0.47893700
H	-0.74718200	-6.19344600	-1.86962400
C	3.87310500	1.87032400	-2.17487600
H	3.39110100	2.85525700	-2.26695700
H	4.19117100	1.77348700	-1.12384200
C	5.09531800	1.80307900	-3.07953700
H	5.57469000	0.81912400	-2.96314700
H	4.77394900	1.86278400	-4.12946300
C	6.09063200	2.90774100	-2.76939700
H	6.97297500	2.85275400	-3.41542000
H	5.63677500	3.89702800	-2.90680700
H	6.43354200	2.84567000	-1.72846400
C	-4.34021900	5.82948900	0.04810900
H	-4.27435500	6.65428200	-0.67029800
H	-5.27544300	5.29780000	-0.16687100
H	-4.41746800	6.25164200	1.05409500

**TS9<sub>R</sub>'**

C	-0.08079400	-4.26774600	-0.46083600
C	-0.16417000	-2.73962800	-0.49114900
C	-1.00093400	-3.63590700	-1.41702600
C	-0.89791700	-2.10569300	0.62306600
O	-1.81336600	-2.90309300	1.19485300
C	-1.70164900	-0.79271200	2.22782900
C	-2.51943700	-2.10516400	2.17167000
H	-1.10043100	-0.67412500	3.14049700
H	-2.51691700	-2.67317400	3.10444000
C	0.97975500	-2.04415500	-1.11216900
O	1.59180400	-2.74283000	-2.07721400
C	2.61719900	-0.65969100	-1.71183200

C	2.75394700	-1.98716700	-2.49435000
H	2.42472700	0.21251300	-2.35218400
H	2.68393800	-1.87910100	-3.57858900
N	1.44670100	-0.87924000	-0.84044100
N	-0.76762600	-0.91926700	1.09123200
Cu	0.95382100	0.25876900	0.82927600
C	0.76025400	2.18473200	1.18538900
N	0.73064000	3.01652400	2.01584900
C	4.68075900	-1.67937100	-1.08809300
C	3.89563300	-0.53859000	-0.93495100
C	4.30375900	0.51311600	-0.12300200
C	5.52082000	0.40918400	0.54485000
C	6.31035000	-0.73299100	0.39624800
C	5.89713400	-1.78361400	-0.42025800
C	4.05395900	-2.66370400	-2.03676000
H	3.67692000	1.39653400	-0.00182400
H	5.86012600	1.22344600	1.18153200
H	7.26111600	-0.80066600	0.92053300
H	6.52016100	-2.66796000	-0.53893000
C	-2.73024400	0.29246700	2.07604000
C	-3.98360300	-0.24875400	1.78781900
C	-5.08723300	0.58165200	1.63383400
C	-4.91737100	1.95826400	1.76359100
C	-3.66313800	2.49611400	2.05462300
C	-2.55824200	1.66380200	2.22101500
C	-3.93070700	-1.74652700	1.68922200
H	-6.06603100	0.16387800	1.40095100
H	-5.77185000	2.62030200	1.63890100
H	-3.54919500	3.57251200	2.16269100
H	-1.57969300	2.07930100	2.45619600
H	-4.05714700	-2.08220800	0.64885900
H	-4.71024500	-2.24050200	2.27960600
H	4.70969800	-2.88483100	-2.88696100
H	3.82889600	-3.62496800	-1.55750900
H	-0.49422800	-4.73728200	0.42515600
H	0.84610900	-4.68857100	-0.83552200
H	-2.06607500	-3.65688100	-1.19947600
H	-0.72814000	-3.60894300	-2.46740600
C	-5.44538200	1.26797800	-1.72073100
C	-4.14566300	1.68032600	-1.49540400
C	-3.09199300	0.74811900	-1.52288100
C	-3.39520300	-0.59668200	-1.79650200
C	-4.70100400	-1.00500200	-2.00620000
C	-5.74941600	-0.07897100	-1.96441500

H	-6.25439500	1.99648200	-1.69627300
H	-3.93928500	2.73114700	-1.30335400
H	-2.58017800	-1.32027000	-1.83918800
H	-4.91859600	-2.05232300	-2.21016200
C	-1.71437200	1.09602200	-1.30959400
H	-1.00348200	0.28087800	-1.46982900
C	-1.17786100	2.29627900	-0.94856200
C	0.23145800	2.44085300	-0.92509900
H	0.79571700	1.58492500	-1.29801100
H	-1.79461500	3.15820200	-0.69330300
N	2.28050900	-0.58440900	2.27883000
C	3.23872000	-0.99839100	2.78261800
C	4.43482200	-1.51284600	3.41265500
H	4.79763000	-2.38754200	2.86540900
H	5.21372200	-0.74490100	3.40592700
H	4.22223000	-1.79832400	4.44633100
C	0.89010000	3.76407700	-1.09673500
H	0.42323800	4.51354500	-0.44451800
H	0.62299600	4.05562100	-2.12991200
C	2.40289000	3.75700400	-0.96549000
H	2.82077300	2.99280100	-1.64254500
H	2.67126700	3.45290900	0.05726800
C	3.04109600	5.10172100	-1.27255800
H	2.62089800	5.86297600	-0.59892700
H	2.77161400	5.41423100	-2.29243200
C	-7.16873600	-0.51030000	-2.14979800
H	-7.68478700	-0.55459200	-1.18158500
H	-7.72459600	0.19818700	-2.77332200
H	-7.23555100	-1.50283800	-2.60527100
C	4.55252000	5.05018500	-1.12299400
H	5.01865400	6.01893100	-1.33014800
H	4.83415900	4.75440500	-0.10415100
H	4.99033900	4.31435900	-1.80982900

### TS10s'

C	-1.99218200	-0.87804900	4.04382700
C	-1.29878900	-0.53147300	2.72479300
C	-1.06632400	0.26342300	4.01671700
C	-0.20796300	-1.43422400	2.31340300
O	0.42179600	-2.05580300	3.32459700
C	1.19404000	-2.77680300	1.23333900
C	1.53554600	-2.76451400	2.73388100
H	0.73794400	-3.70926600	0.87175600
H	1.57023600	-3.75161200	3.19841500

C	-2.12556900	0.11709300	1.68826900
O	-3.11666100	0.89040800	2.15841300
C	-2.99251200	0.92574700	-0.19161500
C	-3.85067200	1.38625000	1.01004100
H	-2.47205100	1.74227900	-0.71542000
H	-3.91133600	2.47224900	1.12472600
N	-1.97778200	0.05436300	0.41845900
N	0.18504400	-1.71038700	1.12369100
Cu	-0.45481300	-0.89640500	-0.64896000
C	0.13908600	0.31855100	-2.07526500
N	0.00471600	0.62666700	-3.20257700
C	-5.18314900	0.02504600	-0.45883500
C	-3.93956100	0.16687600	-1.07179600
C	-3.68065500	-0.38237100	-2.32217400
C	-4.69707100	-1.08877100	-2.96101300
C	-5.94554400	-1.23472200	-2.35243300
C	-6.19805000	-0.67742900	-1.10048400
C	-5.22429600	0.71204600	0.87972300
H	-2.70141900	-0.25842000	-2.78587800
H	-4.52293300	-1.51849200	-3.94551900
H	-6.73278800	-1.78260600	-2.86537700
H	-7.17569200	-0.78907600	-0.63510800
C	2.49092300	-2.47254100	0.55087300
C	3.44512500	-2.05520000	1.48090000
C	4.74516600	-1.78345700	1.06609000
C	5.06692800	-1.93614800	-0.28308900
C	4.10325400	-2.33801100	-1.20997700
C	2.79943200	-2.60716900	-0.79705600
C	2.85791000	-1.99125000	2.86645600
H	5.50397200	-1.47032500	1.78101400
H	6.08336700	-1.73589000	-0.61918700
H	4.37530200	-2.44939300	-2.25702700
H	2.04201200	-2.93960700	-1.50634700
H	2.64385400	-0.95222100	3.15825500
H	3.51717700	-2.40796900	3.63459200
H	-6.03943900	1.44205800	0.94416300
H	-5.37308500	0.00403900	1.70526100
H	-1.66598000	-1.80150800	4.51096600
H	-3.05846100	-0.67816500	4.06726600
H	-0.08102400	0.14460000	4.45831100
H	-1.47839100	1.26785900	4.03293900
C	-0.92013200	4.49862200	-0.84551500
C	-0.04214800	3.49491100	-1.20550000
C	0.31513100	2.49956200	-0.27935100

C	-0.23030600	2.55235800	1.01181300
C	-1.09622900	3.57470400	1.37159600
C	-1.46622200	4.55542000	0.44697900
H	-1.20121400	5.25763500	-1.57315500
H	0.34600400	3.45291100	-2.22076800
H	0.05697200	1.79647800	1.74266200
H	-1.49865100	3.61591200	2.38276000
C	1.27723500	1.45949200	-0.58179400
C	2.43679800	1.68342800	-1.39273800
H	2.40455100	2.45635000	-2.16000800
C	3.57452200	1.00227200	-1.15187800
H	3.56783600	0.23358500	-0.37244000
C	4.87248000	1.24206700	-1.82375900
H	4.76582800	1.99620000	-2.61526200
H	5.18842200	0.30536800	-2.31287100
H	1.39810500	0.69488400	0.19072800
N	-1.12940300	-2.60950400	-1.67344400
C	-1.72632200	-3.38061500	-2.29903300
C	-2.48512900	-4.33381300	-3.07732100
H	-2.39646200	-5.33232600	-2.64156600
H	-3.53872400	-4.03903500	-3.08452800
H	-2.11460800	-4.35812000	-4.10536300
C	5.96165300	1.65872600	-0.83198100
H	5.99511700	0.93759200	0.00110500
H	5.69354300	2.62798900	-0.38541000
C	7.33283500	1.74795500	-1.48337400
H	7.59831000	0.76068600	-1.89193700
H	7.28117300	2.42856000	-2.34618500
C	8.40388900	2.21630800	-0.51361900
H	8.48375300	1.53543800	0.34317500
H	9.38873300	2.27015000	-0.98926300
H	8.16913400	3.21313200	-0.11986600
C	-2.44232800	5.62874500	0.80712100
H	-3.42232900	5.42425100	0.35658300
H	-2.58293600	5.70186700	1.88949200
H	-2.11814500	6.60464000	0.42982800

**TS10<sub>R</sub>'**

C	-0.53095500	-2.08920600	3.86917200
C	-0.32427700	-1.44767100	2.50235400
C	0.09889700	-0.76077500	3.81020000
C	0.76843900	-1.98690700	1.66711400
O	1.65899000	-2.75430000	2.31295800
C	2.10778500	-2.60835900	0.00764900



C	2.64912700	-3.17562900	1.34015600
H	1.74996600	-3.37650800	-0.69188000
H	2.67484600	-4.26664900	1.38048100
C	-1.52465800	-0.89822700	1.83670700
O	-2.55606200	-0.64852700	2.65583000
C	-3.04685300	-0.10954600	0.42029000
C	-3.64098600	-0.11791300	1.85103700
H	-2.99716200	0.88489100	-0.04716900
H	-3.87224600	0.87205500	2.25492500
N	-1.67488000	-0.61064300	0.59582300
N	0.95035300	-1.80135800	0.41285000
Cu	-0.20073300	-0.70125200	-0.90005500
C	0.15847300	0.99099300	-1.84097500
N	0.21102400	1.56044900	-2.86869500
C	-4.88901500	-1.62748700	0.45698100
C	-3.90839600	-1.06256200	-0.35531300
C	-3.79452700	-1.40345500	-1.69752800
C	-4.67727700	-2.34221000	-2.22370900
C	-5.65784500	-2.91832200	-1.41291400
C	-5.77363600	-2.56272300	-0.07124400
C	-4.84476900	-1.06641700	1.85189600
H	-3.02700400	-0.94413600	-2.31981500
H	-4.60934700	-2.62295000	-3.27257200
H	-6.34461900	-3.64770600	-1.83626300
H	-6.54656300	-3.00809100	0.55217500
C	3.24485000	-1.81522000	-0.56344800
C	4.33874900	-1.82467500	0.30042100
C	5.52396400	-1.19979200	-0.07248600
C	5.58515200	-0.54753000	-1.30245500
C	4.47585100	-0.51314000	-2.14944500
C	3.29445800	-1.15467300	-1.78590700
C	4.02443000	-2.54107400	1.58625300
H	6.38969800	-1.21196100	0.58845600
H	6.50726100	-0.05455200	-1.60470900
H	4.53837700	0.00924400	-3.10107800
H	2.42712500	-1.14865100	-2.44676600
H	3.96545100	-1.84165800	2.43330800
H	4.77909800	-3.28947600	1.85231700
H	-5.76680000	-0.52576300	2.09769800
H	-4.71986200	-1.83763700	2.62169100
H	0.09463100	-2.94934900	4.08026300
H	-1.56181300	-2.15826700	4.19874800
H	1.17140800	-0.68457700	3.96891700
H	-0.48420200	0.11220900	4.08999500

C	4.15565300	1.60163300	0.91970100
C	2.79842300	1.35180800	0.84325000
C	1.97546300	2.13067800	0.01177400
C	2.56068900	3.13520900	-0.77694800
C	3.92399000	3.35437600	-0.71926300
C	4.74219900	2.59976200	0.13440400
H	4.78142400	1.00319400	1.57970900
H	2.35117900	0.56153700	1.44604700
H	1.94319300	3.71934800	-1.45573100
H	4.37597600	4.12167600	-1.34455700
C	0.55059300	1.92556300	0.09477800
C	-0.42270000	2.97758000	-0.02958600
H	-0.23018800	3.79891400	-0.71776600
C	-1.51025000	2.97208000	0.76527600
H	-1.62698800	2.12635900	1.44977700
C	-2.56509200	4.01315300	0.83910600
H	-2.60635800	4.38459800	1.87656700
H	-3.53824600	3.50929400	0.69943500
H	0.24834300	1.10935900	0.75304700
N	-0.56152000	-2.16905900	-2.34854200
C	-0.84968900	-2.99969900	-3.10274700
C	-1.22195400	-4.03560800	-4.04022600
H	-0.44588900	-4.80454000	-4.07725200
H	-2.16390600	-4.49463900	-3.72748500
H	-1.34709500	-3.60794000	-5.03844600
C	-2.44236500	5.17663600	-0.13001300
H	-1.48715700	5.69959700	0.03290800
H	-2.41399100	4.79803400	-1.16349500
C	-3.58927900	6.16517500	0.01722700
H	-4.54267100	5.63871900	-0.13948600
H	-3.61579800	6.53539200	1.05308100
C	-3.47657800	7.33231100	-0.94856500
H	-3.47987800	6.98394300	-1.98895600
H	-4.30405200	8.03983700	-0.83178500
H	-2.54139800	7.88411800	-0.79080100
C	6.21293500	2.85262900	0.20985200
H	6.45881400	3.45992000	1.09029000
H	6.76922300	1.91282700	0.30269500
H	6.57611300	3.38856800	-0.67222000