

## Supporting Information

# How Do Quantum Chemical Descriptors Shape the Hydrogen Atom Abstraction Reactivity in Cupric-superoxo Species? A Combined DFT and Machine Learning Perspective

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## Computational Methods

DFT computations employing the dispersion corrected Unrestricted Becke3LYP (B3LYP) hybrid functional was used in conjunction with a double  $\zeta$  quality LanL2DZ basis set with Los Alamos effective core potential for metal Cu and 6-31G(d) basis set for the rest of the atoms such as H, C, O, N. Molecular geometries were optimised without any constraints using G09 suite of programs<sup>1</sup>. At the same level of theory, frequency calculations have been performed to identify the nature of the species and to compute enthalpic and entropic corrections and therefore all the reported energies are free energies, unless otherwise stated. Further intrinsic reaction coordinates (IRC) were performed on selected geometries to affirm the correct nature of the transition state and polarizable continuum model (PCM) was employed to incorporate solvent effects and these calculations were performed using same functional at TZVP basis set for all atoms. Tetrahydrofuran was used as the solvent as employed in the experiments. Further analysis such as NBO (Natural bond orbital), AIM (Atoms in Molecules), Localized orbital locator (LOL), Energy decomposition analysis (EDA) and NCI (Non-covalent Interactions) were performed on the optimized geometries employing G09, and Multiwfn 3.7<sup>2</sup>. The iso surfaces of RDG were rendered by VMD 1.9.1 program.<sup>3</sup> Kinetic isotopic effect calculations were performed using Jacob Bigeleisen equation<sup>4</sup> and tunneling correction to the kinetic barrier were calculated using Pilgrim software employing age-McIver algorithm.<sup>5, 6</sup> For all examined reactions, the minimal energy path (MEP) was followed in mass-scaled coordinates (with scaling mass = 1 amu) and Hessian computations every 5 steps using the Page-McIver algorithm.<sup>6</sup> Machine learning studies were carried out utilizing the linear regression, Lasso, Adaboost<sup>7</sup>, Random Forest<sup>8</sup>, and extreme Gradient Boosting (XGBoost) models<sup>9 10 11</sup>. The EPR property calculations have been performed in Orca 4.2<sup>12</sup> version software. The starting coordinates for the EPR calculations have been obtained by DFT calculations in the Gaussian09 suite of programs as stated earlier.<sup>1</sup> The B3LYP hybrid functional<sup>13-15</sup> and def2-TZVP basis set has been used for all atoms for EPR property calculations. The DLPNO-CCSD(T) method, utilizing the cc-pVTZ basis set and incorporating the No Frozen Core and TIGHTPNO approximations, was employed to calculate precise energies. The optimized coordinates from DFT calculations conducted using the ORCA program were utilized in this process.<sup>16, 17</sup> Magnetic exchange interactions are calculated using B3LYP functional. The magnetic exchange interaction between Metal Cu(II) and O<sub>2</sub><sup>•-</sup> radical is described by the following spin Hamiltonian,  $\hat{H} = -J S_1 S_2$  here  $J$  is the isotropic exchange coupling constant.

Using the online SambVCA web programme, we derived percent buried volume (%BV) steric metrics to gauge the steric environment around each metal superoxo centre and substrate reactive C-H bond. We defined the negative z-axis as passing through the proximal oxygen centre and copper (for metal superoxo) and the xz plane as containing an additional atom bonded to the copper. We then centred the calculation on the proximal oxygen atom (for metal superoxo) We included hydrogen atoms in the computation, removed the distal oxygen atom from the calculation, and left all other variables at their default values (using Bondi radii scaled by 1.17, a sphere radius of 3.5 angstroms, and a mesh setting of 0.10 angstroms).<sup>18</sup>

Strength of H-bond interactions was quantified using the binding energy (BE), predicted based on the electron density at the bond critical point ( $\rho_{\text{BCP}}$ ) according to the following equation<sup>19</sup> i.e.,  $\text{B.E.} = [(-332.34 * \rho_{\text{BCP(a.u.)}} - 1.0661)] * 4.184 (\text{kJ/mol})$ .

For all reactions (each metal superoxo-substrate combination) assessed here, we calculated the free energies of proton coupled electron transfer ( $\Delta G_{PCET}$ ), free energy of proton transfer ( $\Delta G_{PT}$ ) free energy of electron transfer ( $\Delta G_{ET}$ ), and the asynchronicity ( $\eta$ ) and reorganization energy ( $\lambda$ ) according to the definition given by Srnec and coworkers. (See Figure S24) The effective acidity constant ( $\Delta P_{eff}^{k_a}$ ), effective reduction potential ( $\Delta E_{eff}^o$ ), and proton-coupled reduction potential ( $\Delta E^o(H)$ ) were also calculated using the methodology provided by Srnec and colleagues (See Figure S25). The methodology to calculate activation barriers of reactions from Valence bond theory ( $\Delta G_{VB}^\#$ ) is adapted from the work of Shaik and co-workers (See ESI Figure S23).

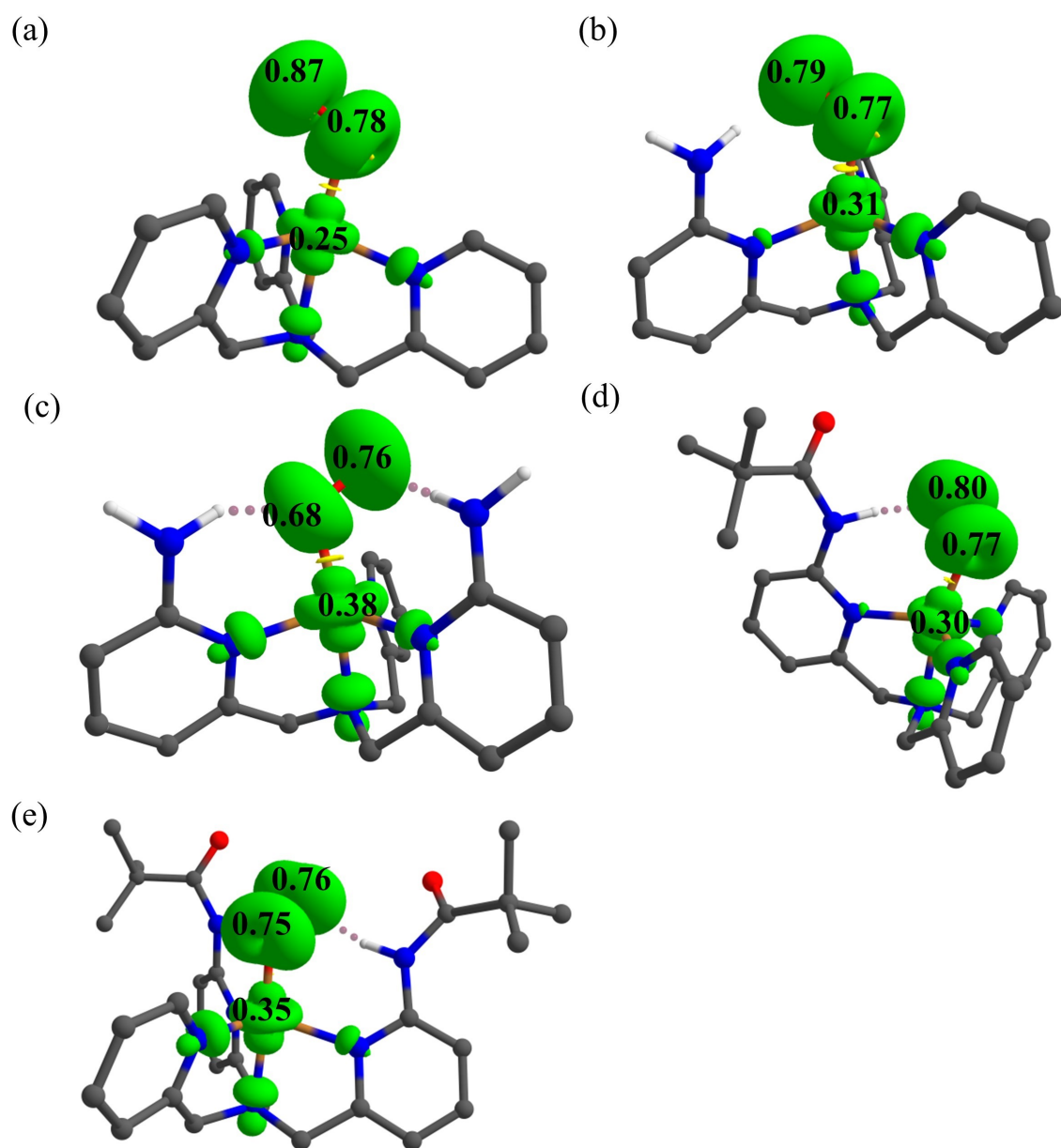


Figure S1: DFT computed spin density plots of triplet spin state ( $S=1$ ) of catalyst (a) **1a** (b) **2a** (c) **3a** (d) **4a** (e) **5a**

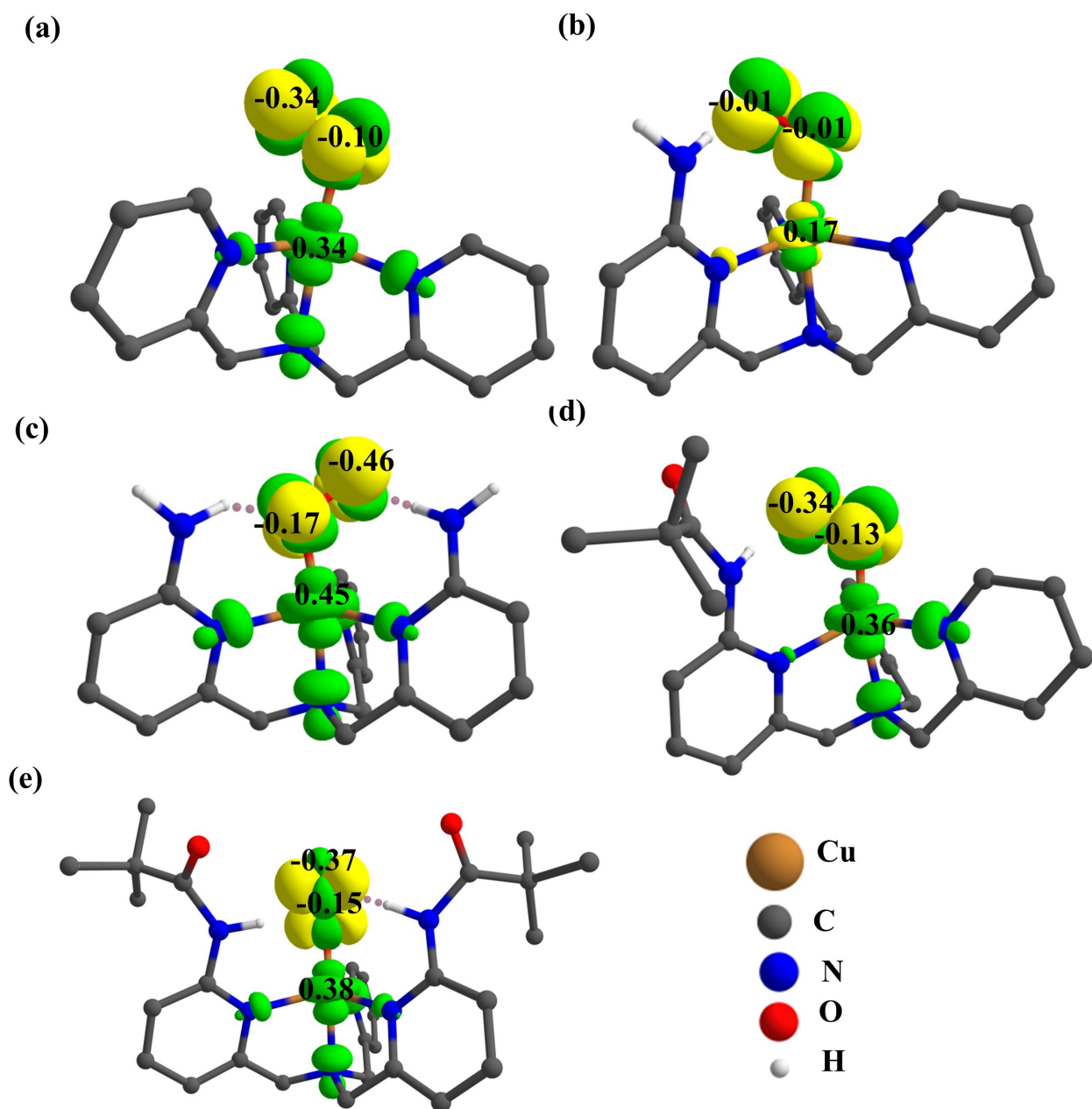


Figure S2: Spin density plots of S=0 of catalyst (a) **1a** (b) **2a** (c) **3a** (d) **4a** (e) **5a** (green and yellow colors are alpha and beta spin densities respectively).



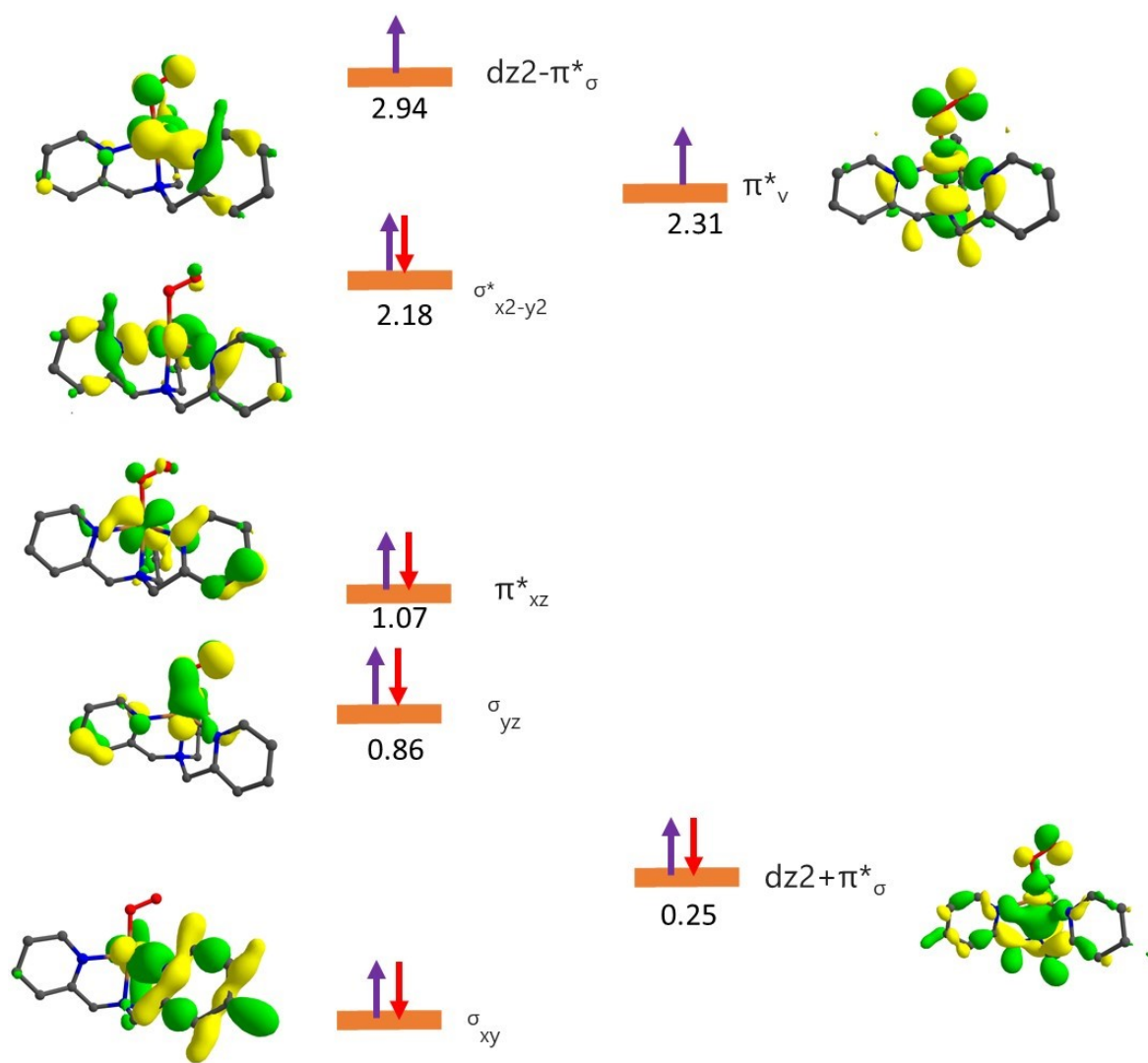


Figure S3: Frontier molecular orbital diagram of catalyst **1a** (Energy are given in eV)

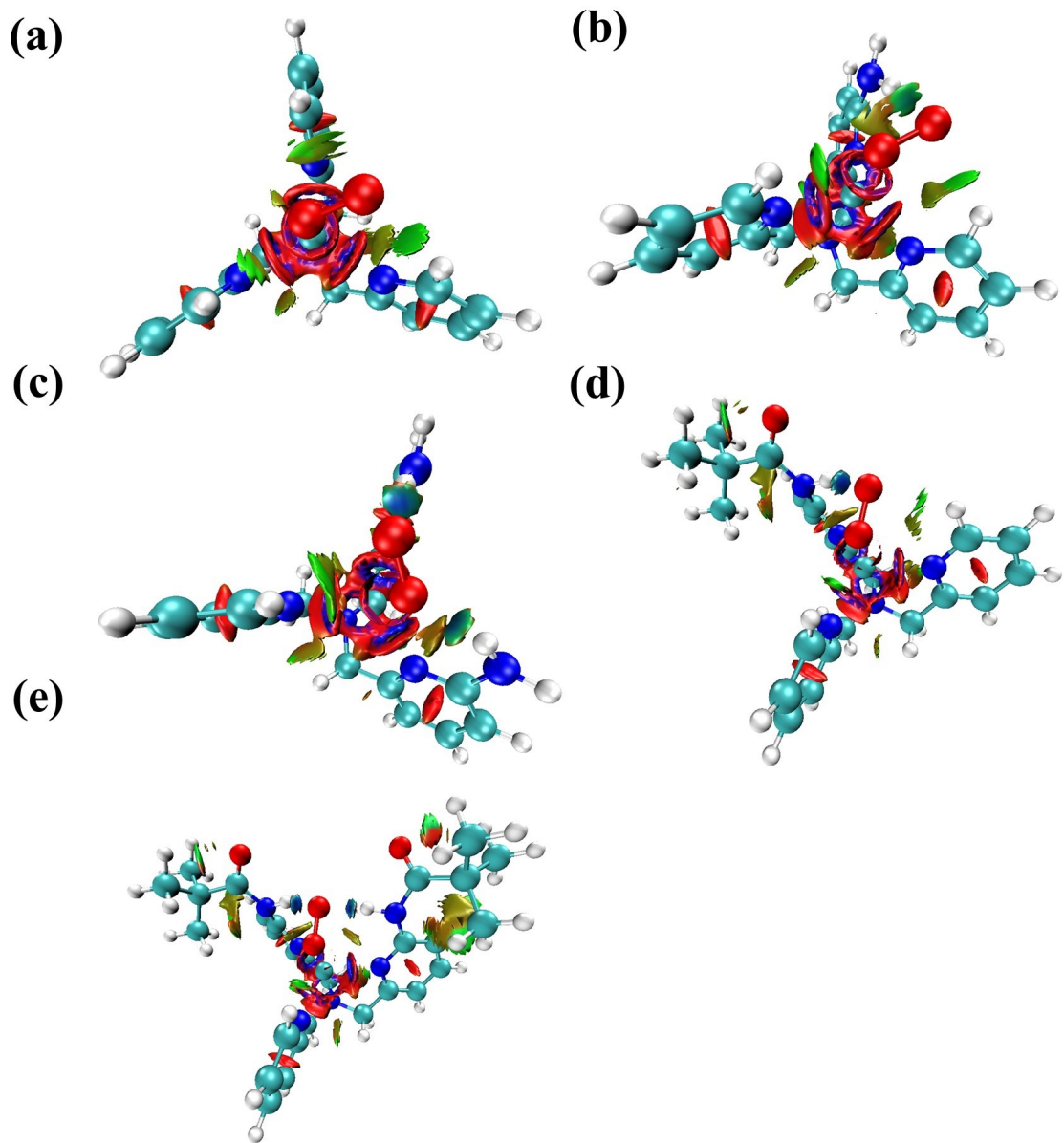


Figure S4: Non-covalent interaction (NCI) plots of complexes (a)1a (b)2a (c)3a (d)4a (e)5a

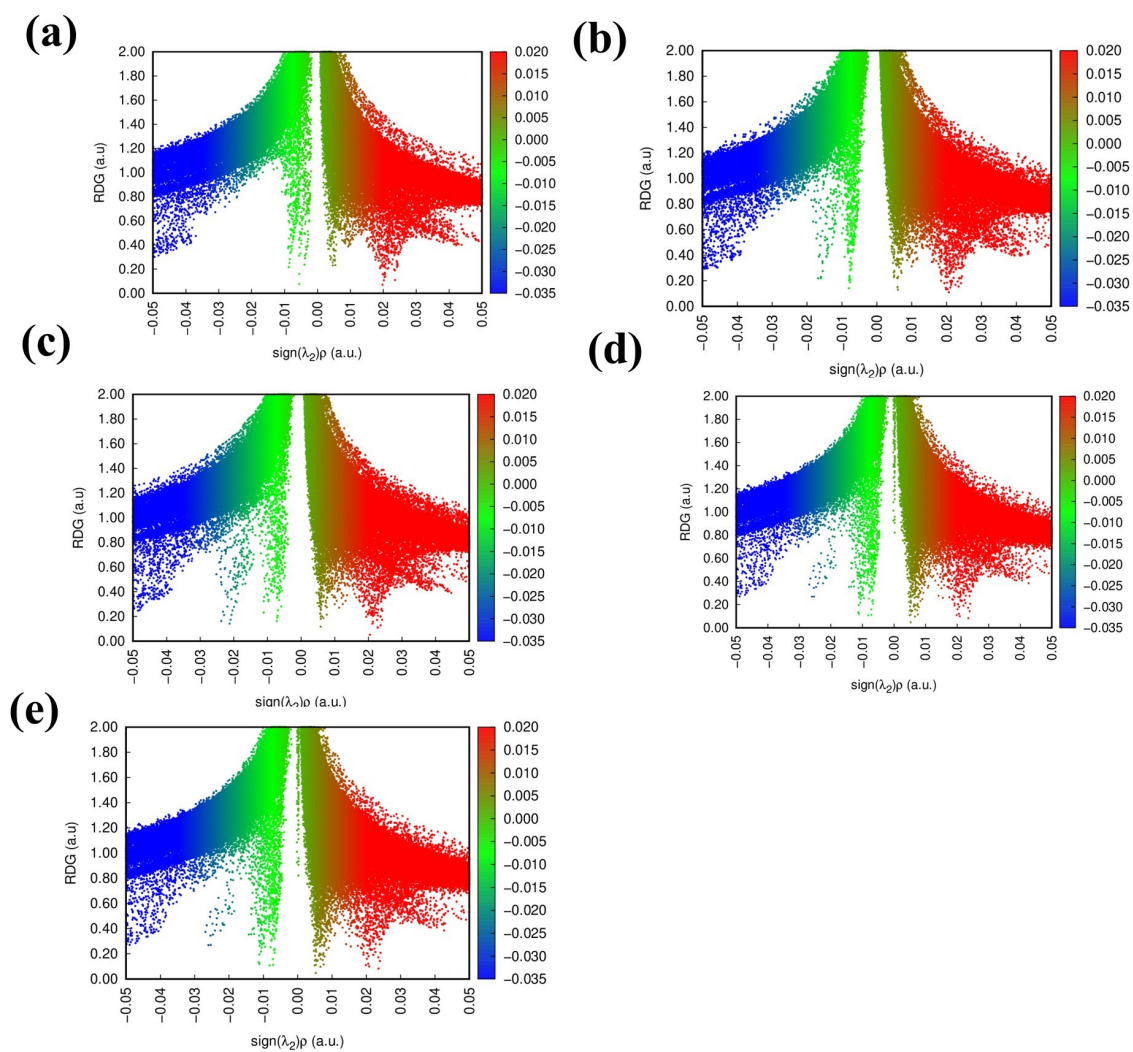


Figure S5: Reduced density gradient plots of complexes (a)1a (b)2a (c)3a (d)4a (e) 5a

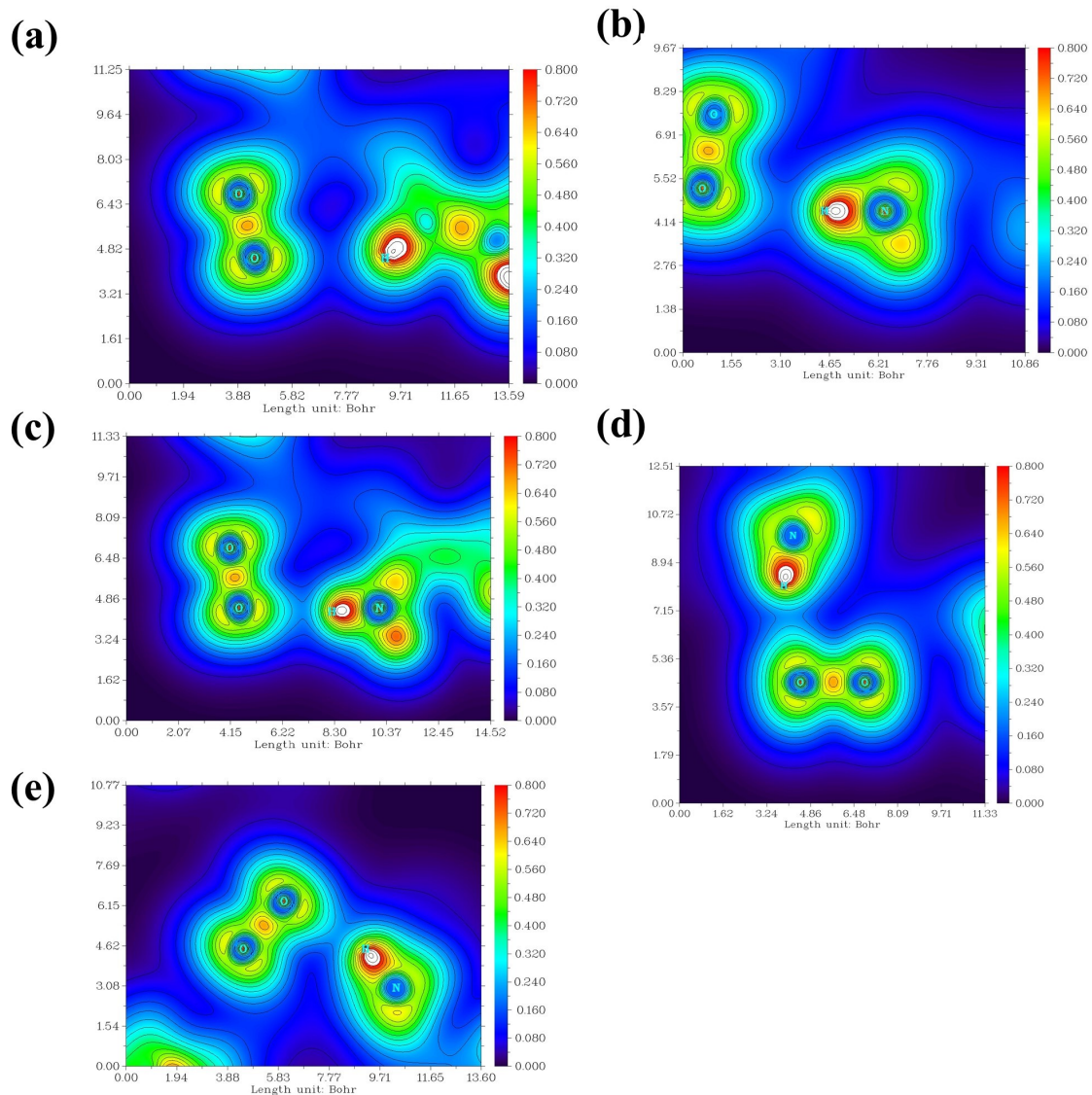


Figure S6: Localised orbital locator (LOL) of catalysts (a) **1a** (b) **2a** (c) **3a** (d) **4a** (e) **5a**

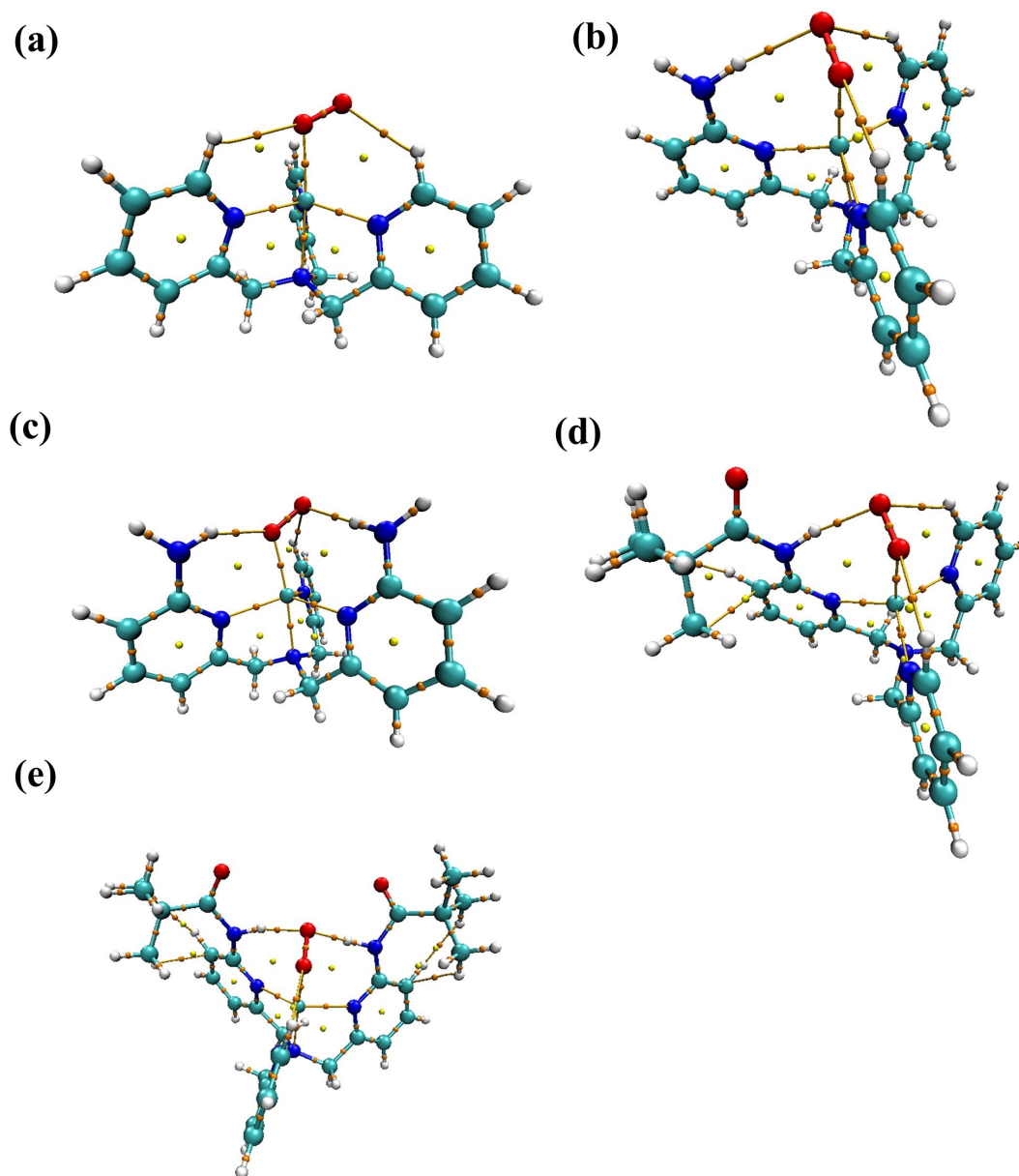


Figure S7: Molecular graphs of different catalysts along with their bond critical points (a) **1a** (b) **2a** (c) **3a** (d) **4a** (e) **5a** (Color code: yellow, ring critical point and green, cage critical point)

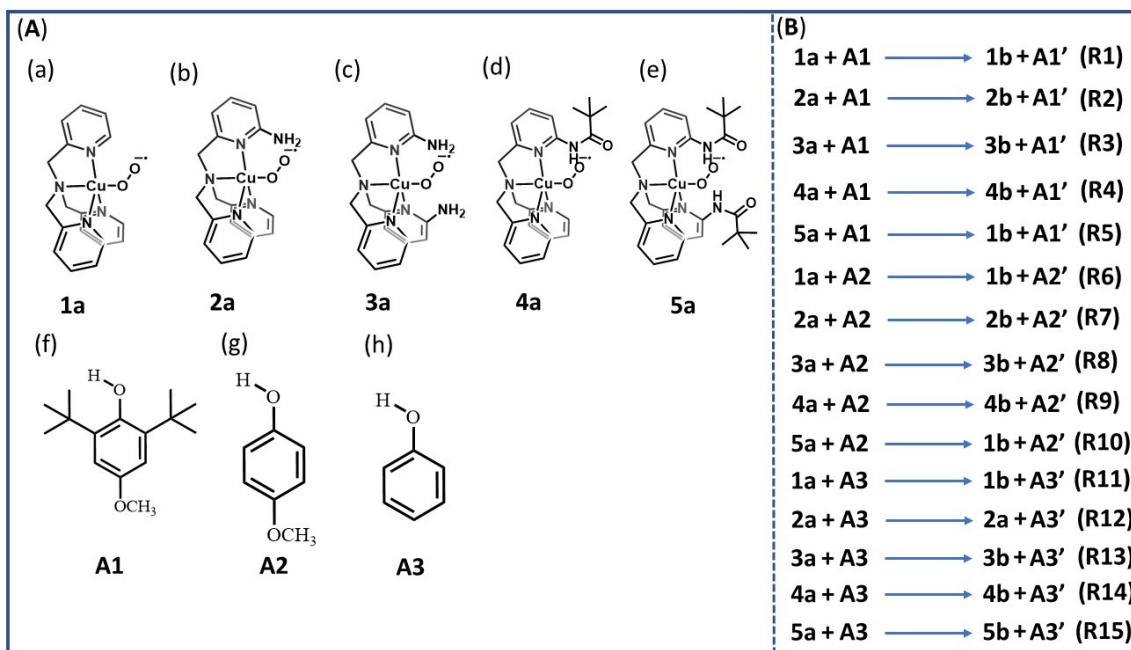


Figure S8: Different catalysts (**1a-5a**) and substrates (**A1-A3**) and reactions (**R1-R15**) under the study

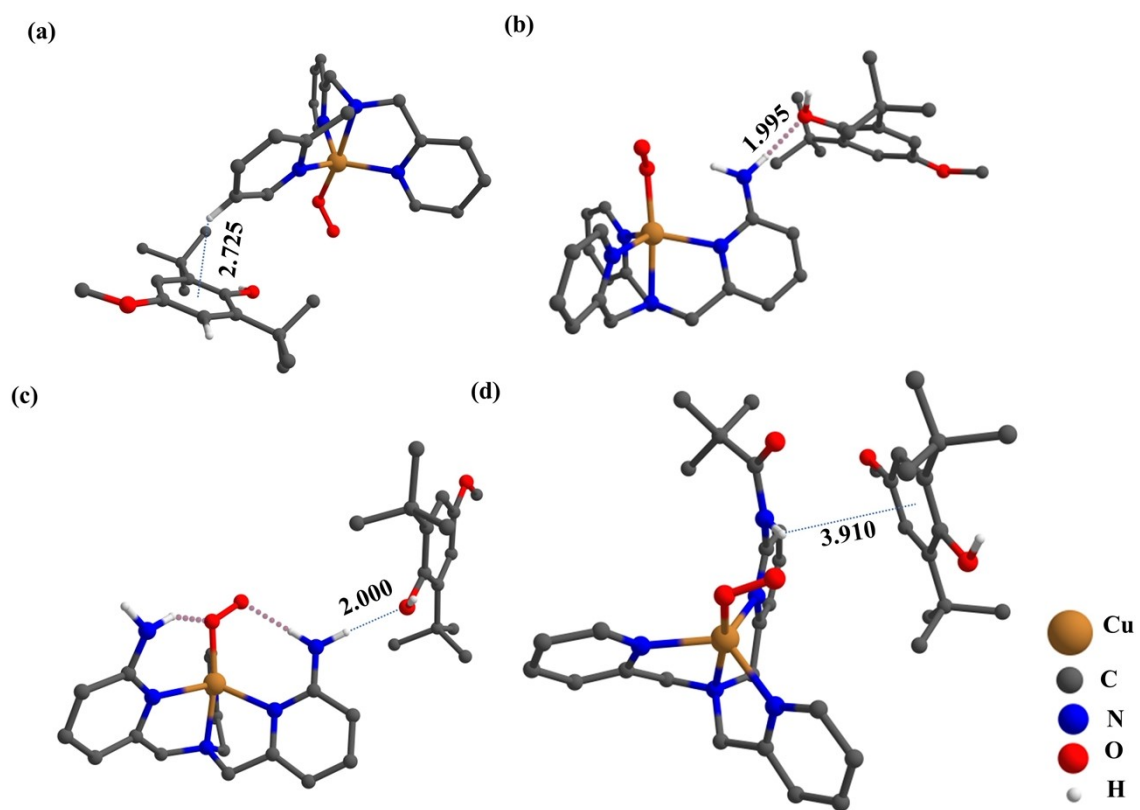


Figure S9: DFT Optimized Reactant complex structure's (a)  ${}^3\text{RC}_{\text{R1}}$  (b)  ${}^3\text{RC}_{\text{R2}}$  (c)  ${}^3\text{RC}_{\text{R3}}$  (d)  ${}^3\text{RC}_{\text{R4}}$  (bond distances are given in Å)

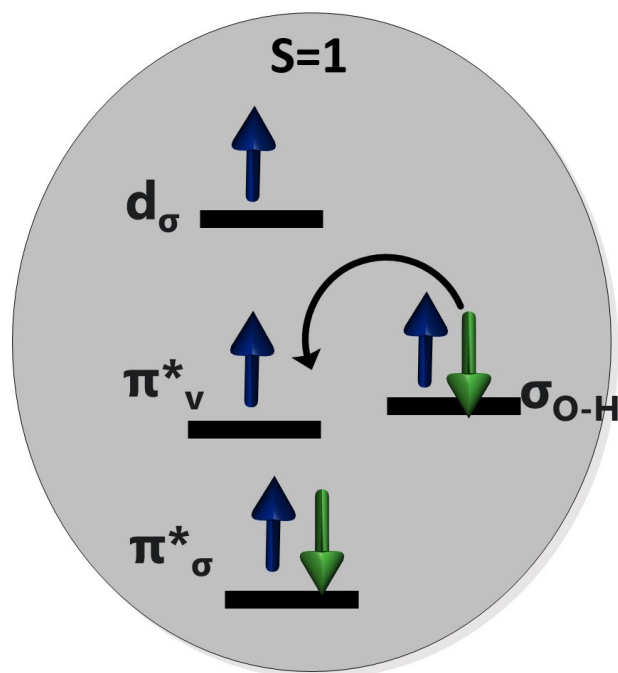


Figure S10: Orbital evolution diagram for HAT by copper superoxo catalysts **1a-5a**



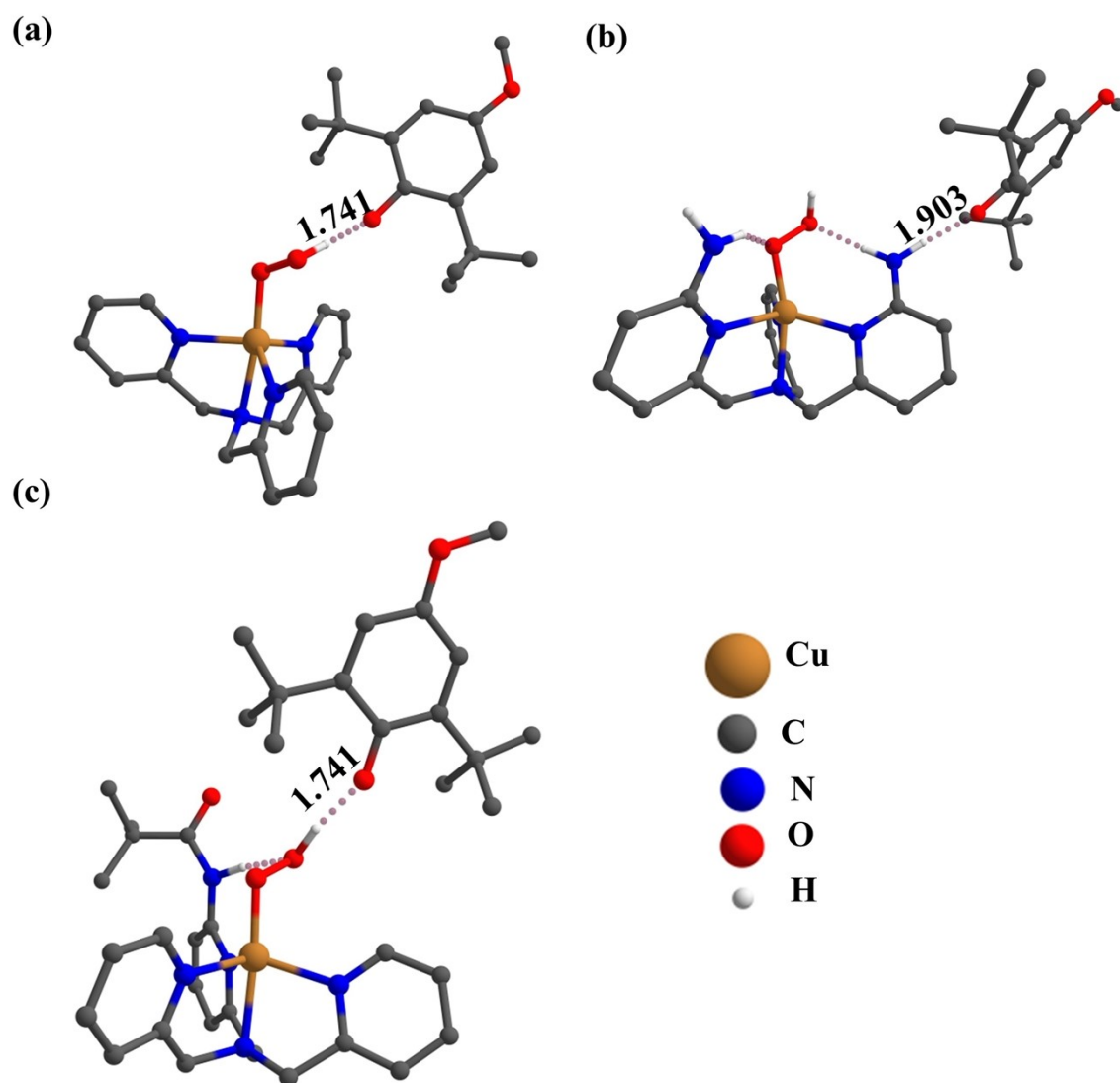


Figure S11: Product complex structures (a)  ${}^3\text{PC}_{\text{R1}}$  (b)  ${}^3\text{PC}_{\text{R3}}$  (c)  ${}^3\text{PC}_{\text{R4}}$  (bond distances are given in Å)

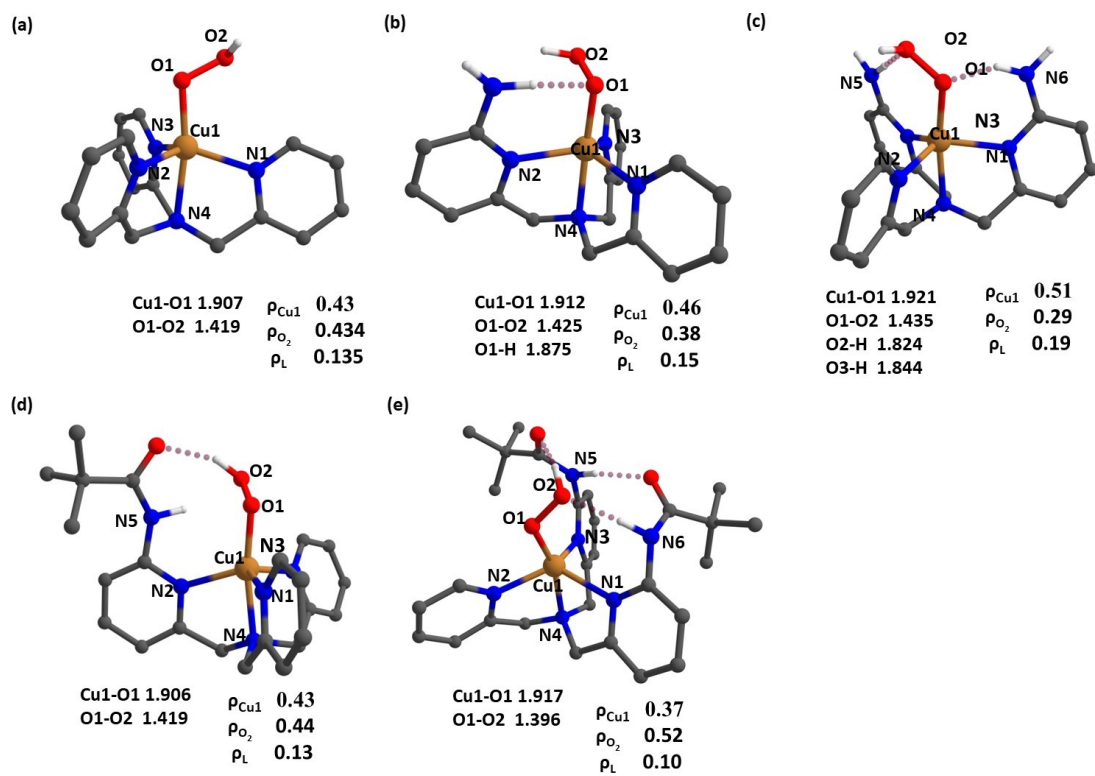


Figure S12: DFT optimized ground state geometries of catalysts (a) **1b** (b) **2b** (c) **3b** (d) **4b** (e) **5b**. (All bond distances are given in Å)

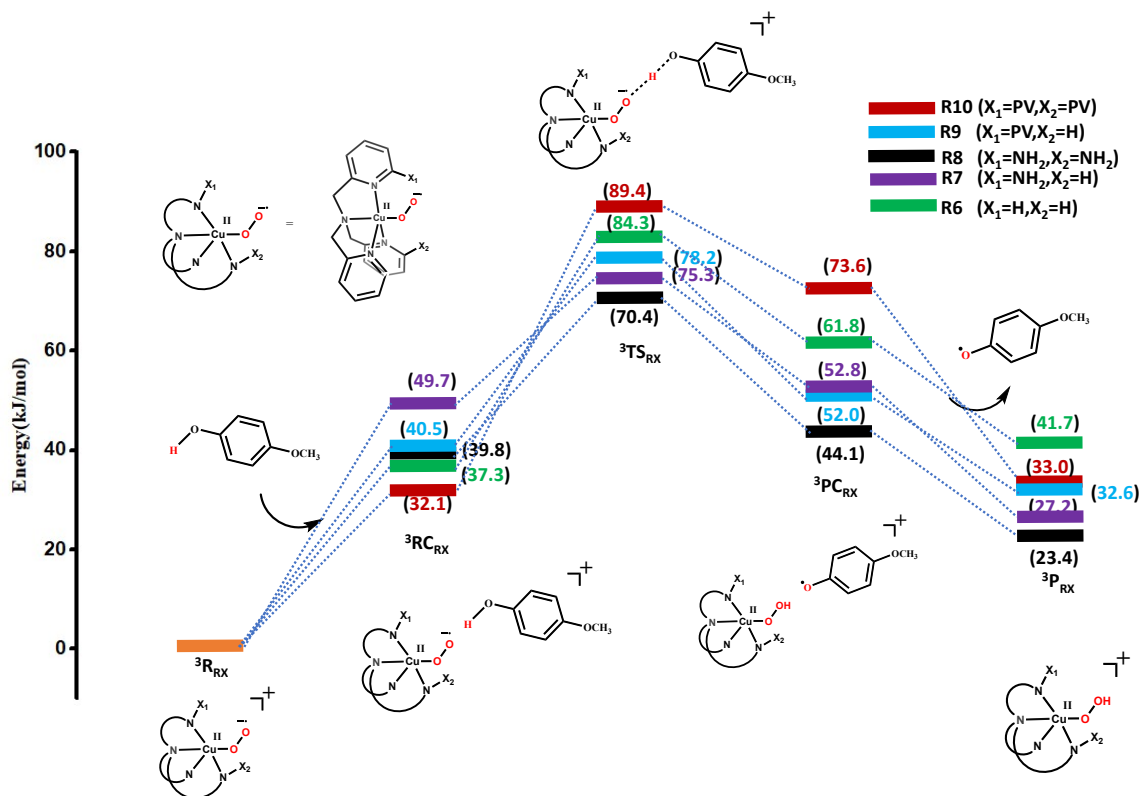


Figure S13: Energy profile for hydrogen atom abstraction (HAT) from p-methoxy phenol by **1a** (green; R1), **2a** (violet; R2), **3a** (black; R3), **4a** (blue; R4) and **5a** (brown; R5). (All energies are reported in kJ/mol and with reference to individual reactants shown in the orange color line)

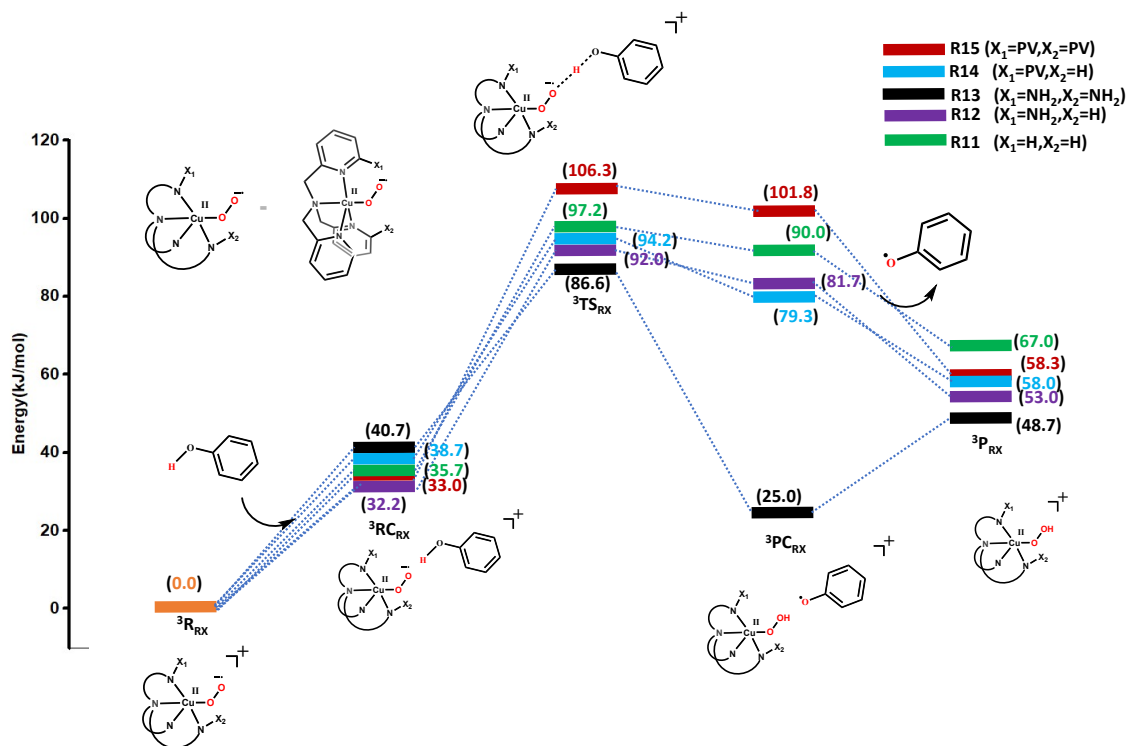


Figure S14: Energy profile for hydrogen atom abstraction (HAT) from phenol by **1a** (green; R1), **2a** (violet; R2), **3a** (black; R3), **4a** (blue; R4) and **5a** (brown; R5). (All energies are reported in kJ/mol and with reference to individual reactants shown in the orange color line)

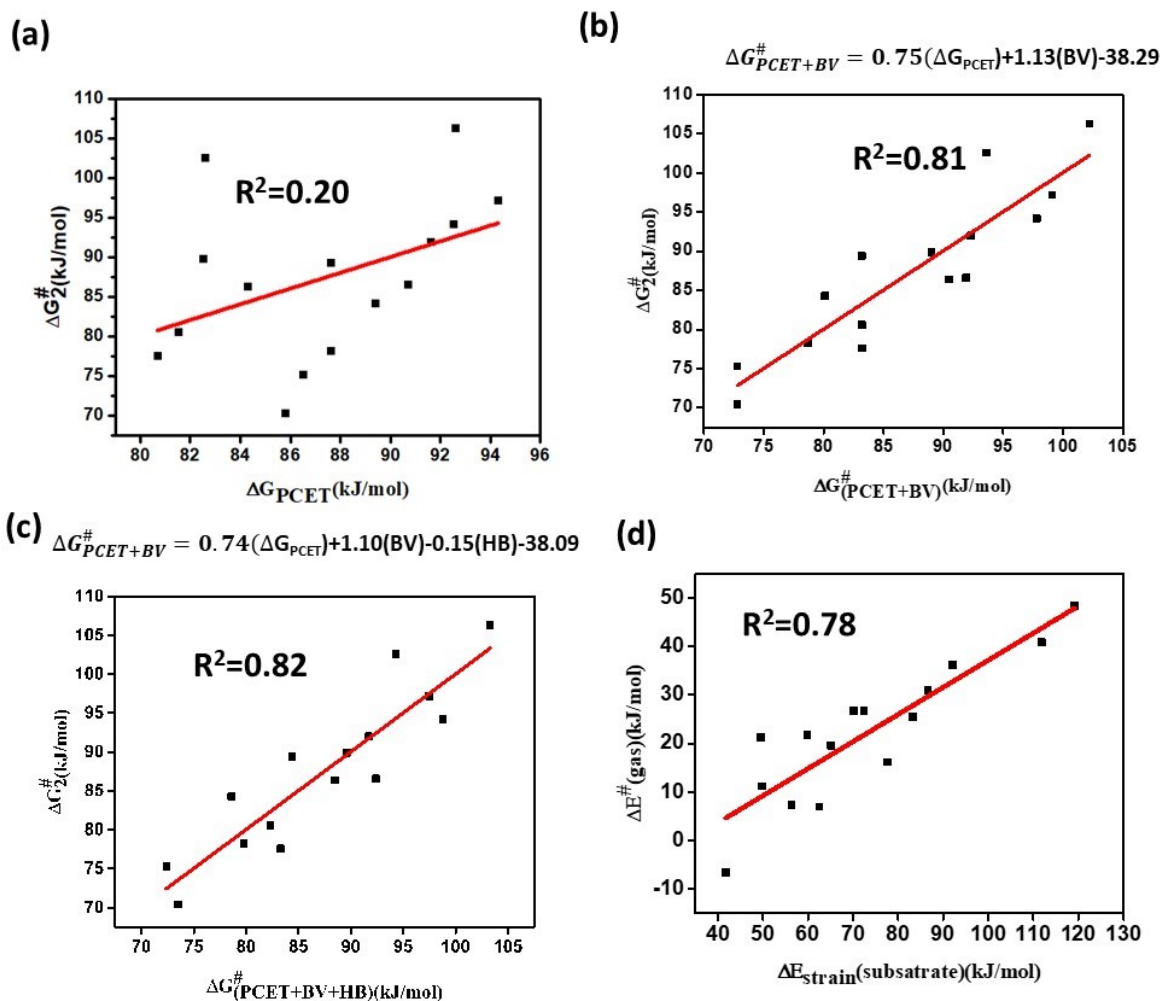


Figure S15: Plots of (a) Regression Analysis between  $\Delta G_{\text{P CET}}^{\ddagger}$  Vs  $\Delta G_{\text{P CET}}$  (b) Regression Analysis between  $\Delta G_{\text{P CET+BV}}^{\ddagger}$  vs  $\Delta G_{\text{P CET}}$  and BV (c) Regression Analysis between  $\Delta G_{\text{P CET+BV+HB}}^{\ddagger}$  vs  $\Delta G_{\text{P CET}}$  and Buried Volume (BV) and H-bonds strength (HB) (d) Regression Analysis between  $\Delta E_{\text{strain}}^{\ddagger}$  vs  $\Delta E_{\text{strain}}(\text{substrate})$

$\Delta G_{\text{P CET}}^{\ddagger}$  - free energy of reaction, BV - Buried volume, HB - H-bond strength,

### Energy decomposition analysis

To unravel the factors influencing the differences in the barrier of reactions **R1-R15** we employed the activation strain model and energy decomposition analysis (EDA). Therefore, the activation energy  $\Delta E^{\ddagger}$  of reactions can be decomposed into the strain energy  $\Delta E_{\text{strain}}$ , which corresponds to the deformation of the fragments ( $\Delta E_{\text{strain}} = \Delta E_{\text{strain}}(\text{substrate}) + \Delta E_{\text{strain}}(\text{catalyst})$ ) during the bond formation reaction. This is coupled with the mutual interaction  $\Delta E_{\text{int}}$  between the deformed fragments. The latter is subsequently broken down into steric repulsion  $\Delta E_{\text{steric}}$ , and bonding orbital interactions  $\Delta E_{\text{orb}}$ . As shown in the Figure S17(d), the strain energy associated with deforming the substrate increases, leading to an elevation in activation energy.

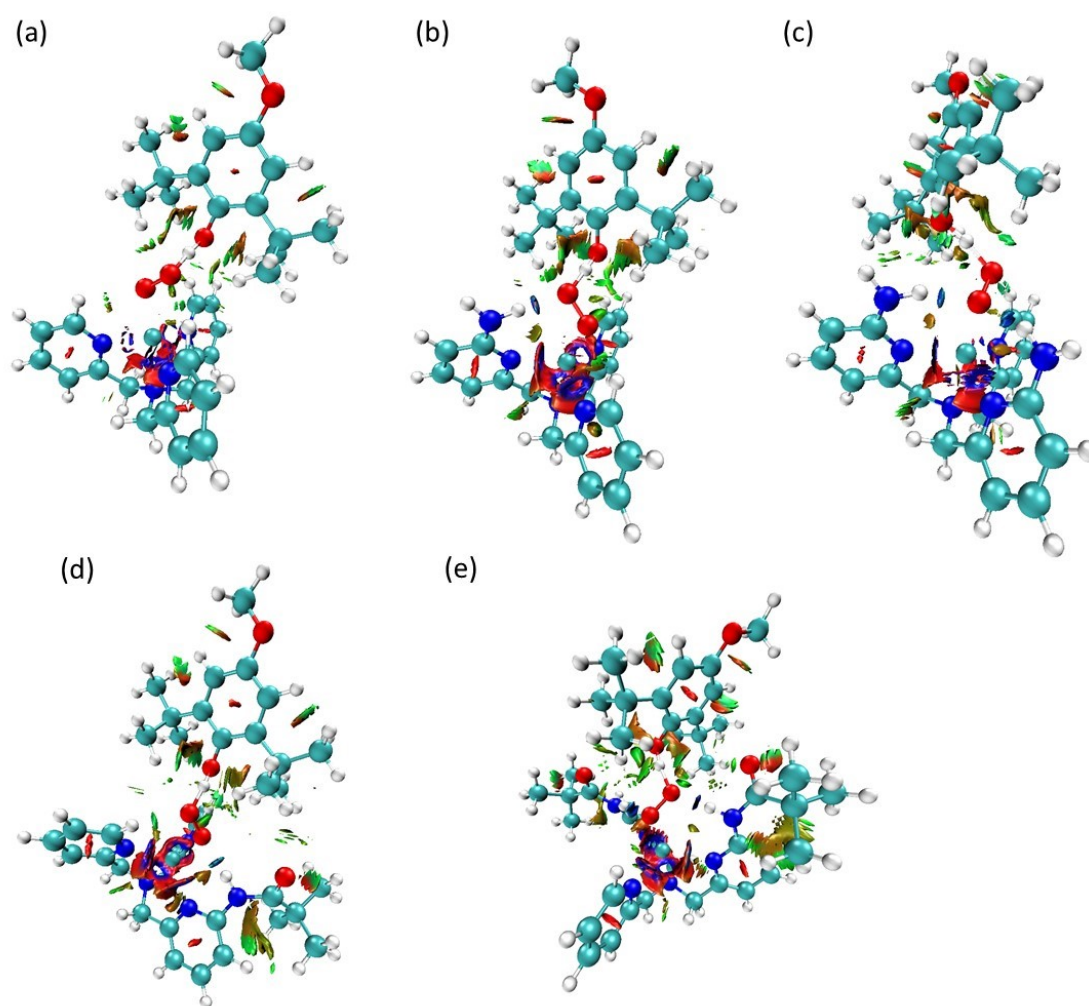


Figure S16: NCI plots of transition state structures (a)  ${}^3\text{TS}_{\text{R1}}$  (b)  ${}^3\text{TS}_{\text{R2}}$  (c)  ${}^3\text{TS}_{\text{R3}}$  (d)  ${}^3\text{TS}_{\text{R4}}$  (e)  ${}^3\text{TS}_{\text{R5}}$

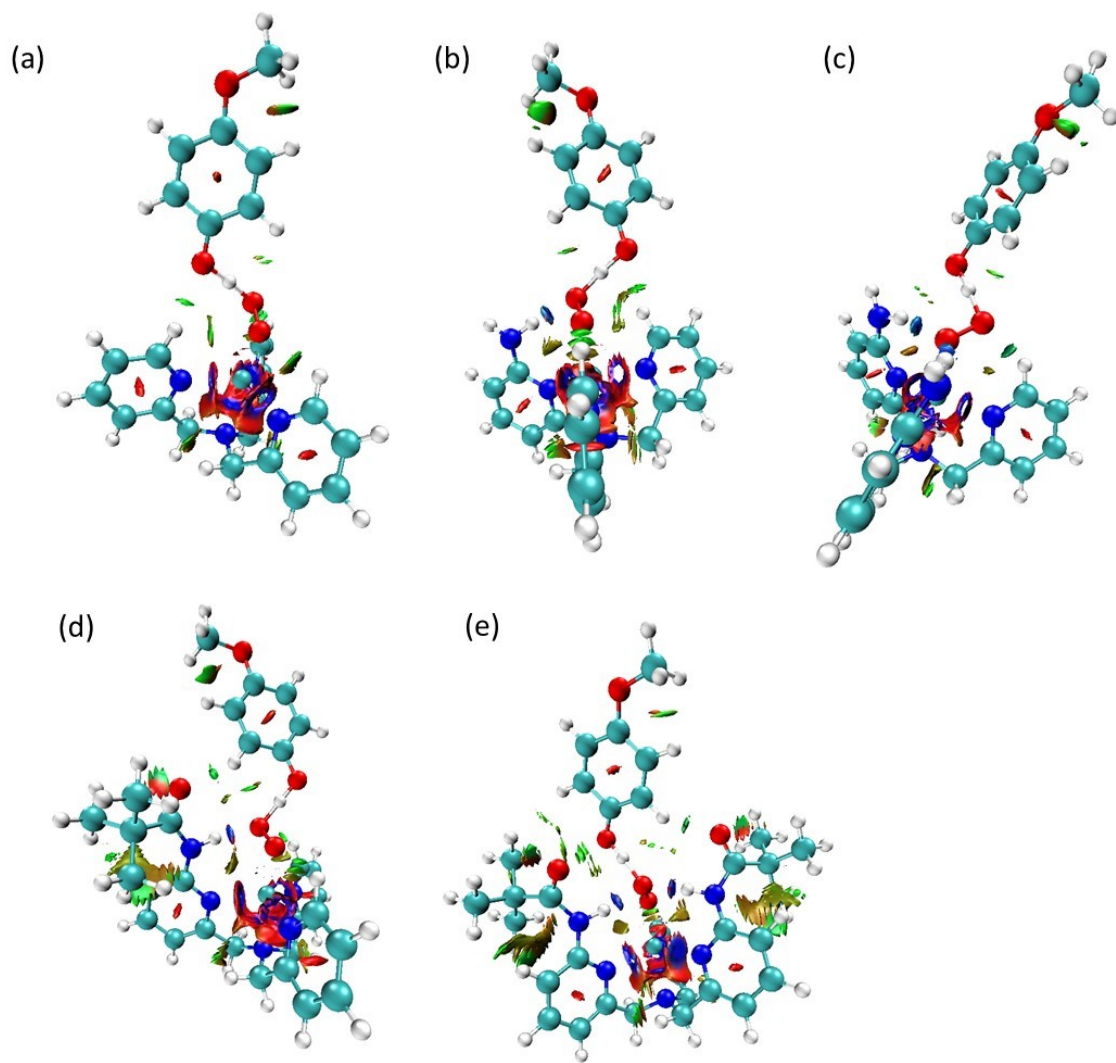


Figure S17: NCI plots of transition state structures (a)  ${}^3\text{TS}_{\text{R}6}$  (b)  ${}^3\text{TS}_{\text{R}7}$  (c)  ${}^3\text{TS}_{\text{R}8}$  (d)  ${}^3\text{TS}_{\text{R}9}$  (e)  ${}^3\text{TS}_{\text{R}10}$

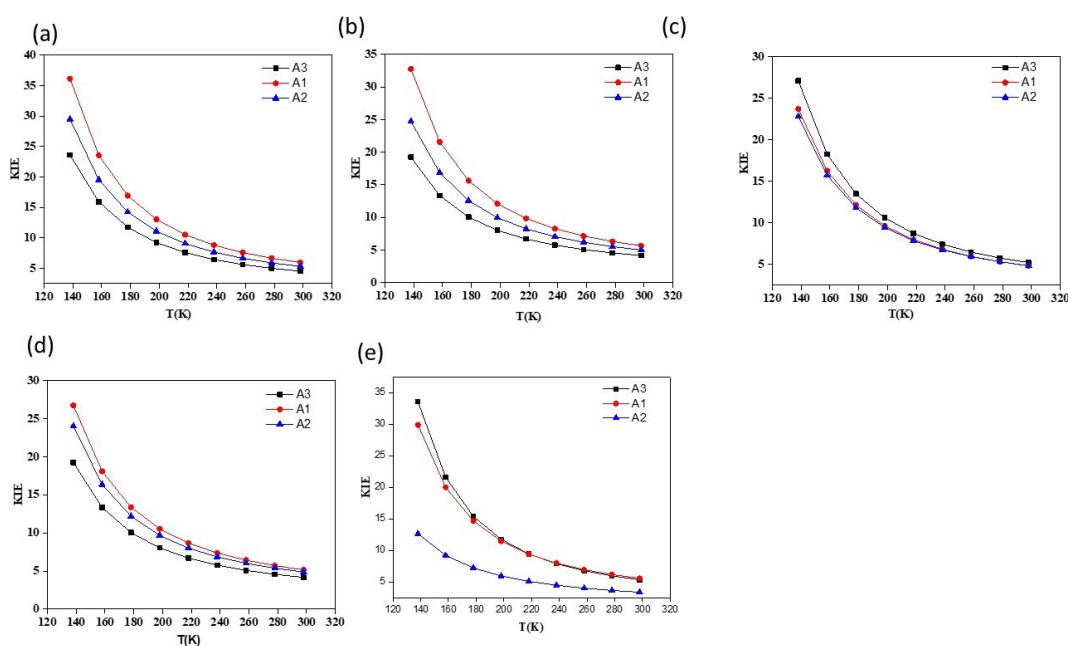


Figure S18: Temperature dependence of KIE of different catalysts with different substrates (a) **1a** (b) **2a** (c) **3a** (d) **4a** (e) **5a**

The Kinetic isotopic effects (KIE) of different reactions are calculated by using the B-M equation. The B-M equation assumes that isotope substitution has no effect on the PES, which works well for thermochemical reactions but not for photochemical activation. Translational, rotational, and vibrational motion are all treated separately in the B-M equation, and molecules are treated as rigid rotors and harmonic oscillators which neglect the vibrational anharmonicity. Another assumption is that a reaction's transition state is equivalent in all respects to the saddle point on the corresponding PES. When motion along the reaction coordinate causes a considerable change in vibrational entropy, this isn't true. The B-M equation also assumes that the reactant's internal energy is completely determined by the temperature  $T$  of the bulk solution, which is not the case when the reactant is freed by a very exothermic process. Further this equation is semiclassical i.e., it neglects the contribution from tunnelling. The B-M equation works well because the systematic mistakes caused by these approximations are effectively cancelled. <sup>20</sup>

At 138K the KIE for reactions R1 to R5 are 36.1,32.7,23.7,26.7 and 29.9 respectively. The reaction **R1** is thermoneutral ( ${}^3\text{RC}-{}^3\text{PC}$ ) and therefore it has high KIE i.e., 36.1. And also, **R4** and **R3** reactions are exothermic by 21 and 17 KJ/mol respectively. Therefore, their KIE are 26.7 and 23.7 respectively. The KIE has direct correlation with the symmetry of transition state which is measured by bond lengths difference of  $\text{O}_2\text{---H}$  and  $\text{H---O}_3$  in the transition state. The more this difference, the transition state has more asymmetry. (see bond lengths in the transition state). Surprisingly, **5a** has exception to this correlation which may attributed to the steric hindrance of two pivalimido groups. The KIE values of **R6**, **R7**, **R8**, **R9** and **R10** reactions are 29.4, 24.7, 22.8, 24.0 and 12.6 respectively. The KIE values of **R11**, **R12**, **R13**,



**R14** and **R15** reactions are 23.6, 19.2, 27.1, 19.2 and 33.5 respectively. There was no correlation between asymmetry of transition state and their KIE values for both **A2** and **A3**. In all cases, increase in the temperature causes the decrease in KIE and KIE is small at room temperature as expected. In the case of 1a, 2a and 4a, the KIE order as follows **A1** > **A2** > **A3** at all temperatures. However, for 3a and 5a, the KIE order is **A2** < **A1** < **A3**. This may be due to hydrogen bonding and steric hindrance. The difference in KIE of **A1**, **A2** and **A3** at any temperature, is large in the case of 1a, 2a and 4a and small in the case of 3a and 5a.

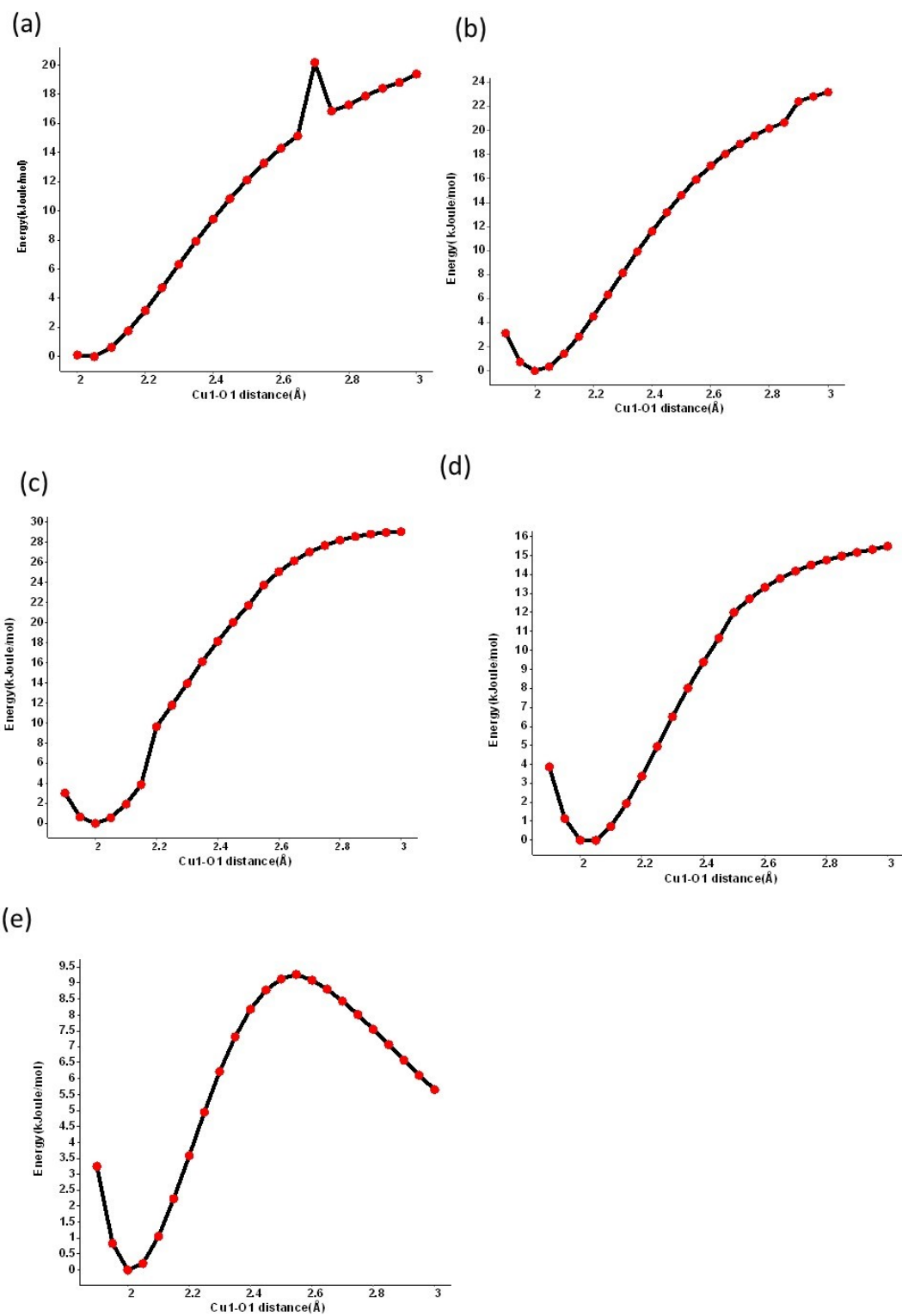


Figure S19: Relaxed scan of different catalysts by varying Cu1---O1 distance (a) **1a** (b) **2a** (c) **3a** (d) **4a** (e) **5a**.

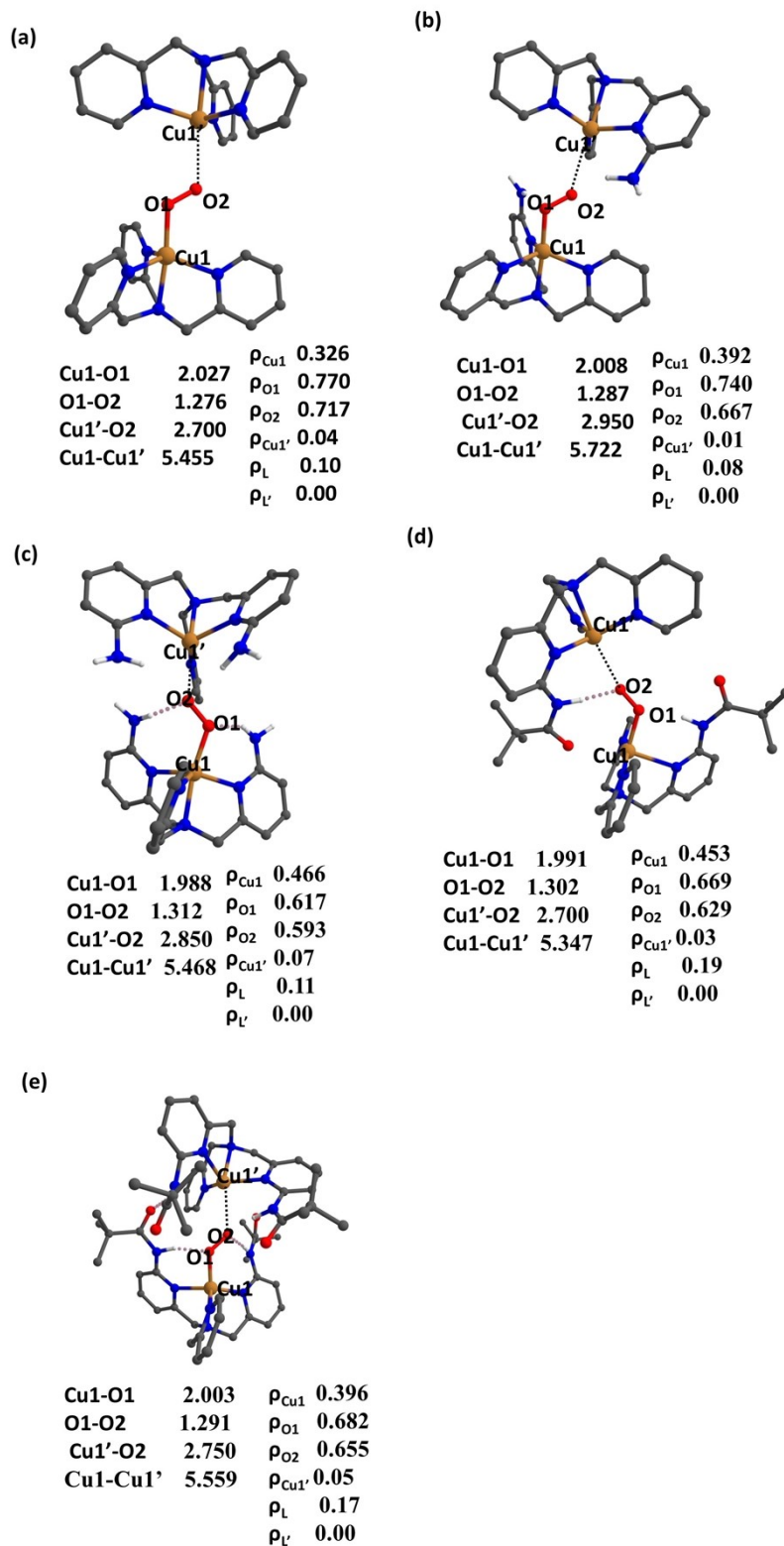


Figure S20: DFT optimized Transition state geometries of complexes (a)<sup>3</sup> (b)<sup>3</sup>  
(c) (d) (e) .

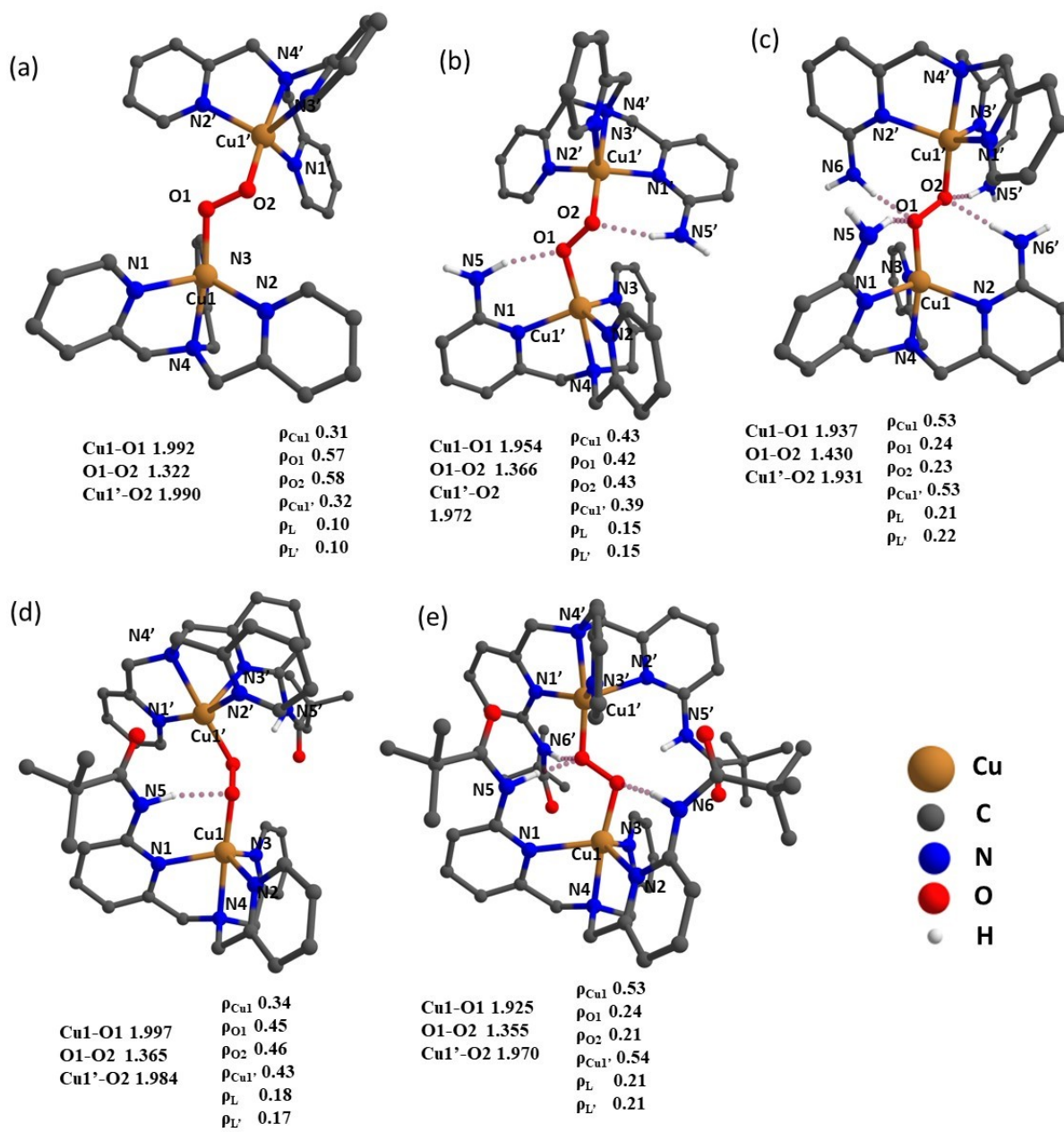


Figure S21: DFT optimized ground state geometries of complexes **1d-5d** (a) **1d** (b) **2d** (c) **3d** (d) **4d** (e) **5d**

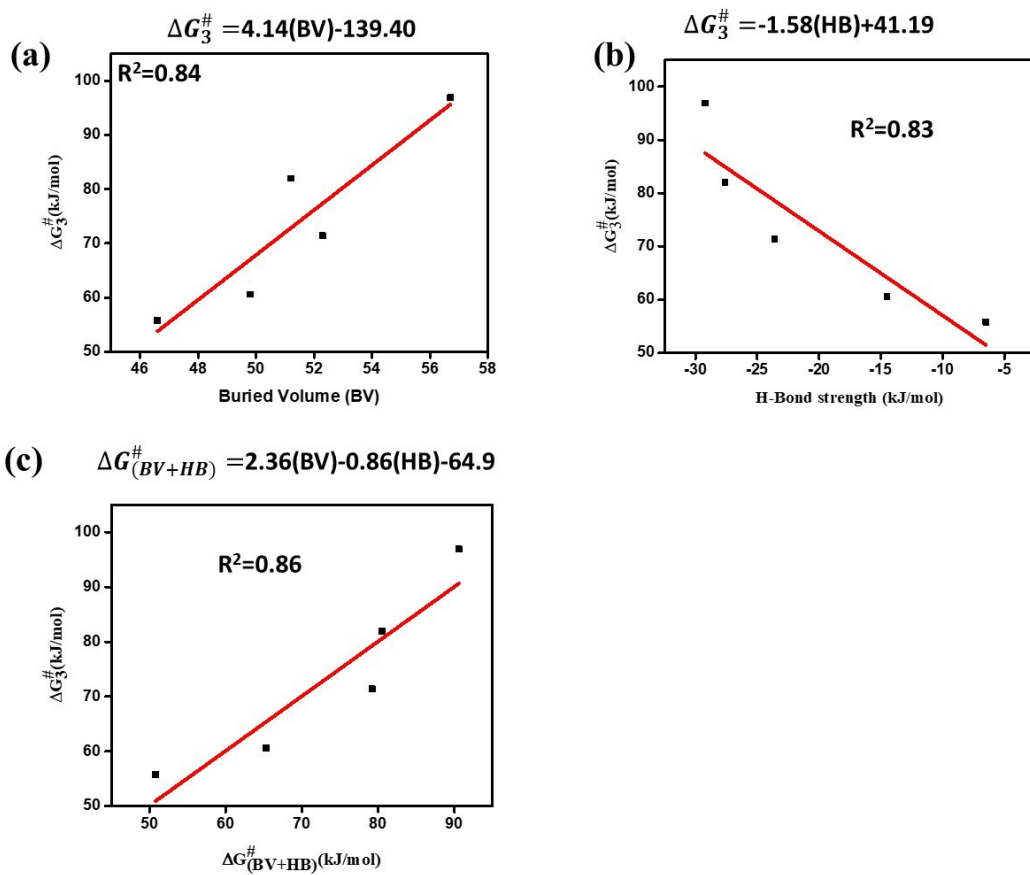


Figure S22: Plots of (a) Regression Analysis between  $\Delta G_3^\ddagger$  Vs  $\Delta G_{(BV+HB)}^\ddagger$  (b) Regression analysis between  $\Delta G_3^\ddagger$  Vs H-Bond strength (HB) (c) Regression Analysis between  $\Delta G_3^\ddagger$  Vs  $\Delta G_{(BV+HB)}^\ddagger$

## Valence Bond Diagrams for Modelling C-H Hydroxylation Mechanism

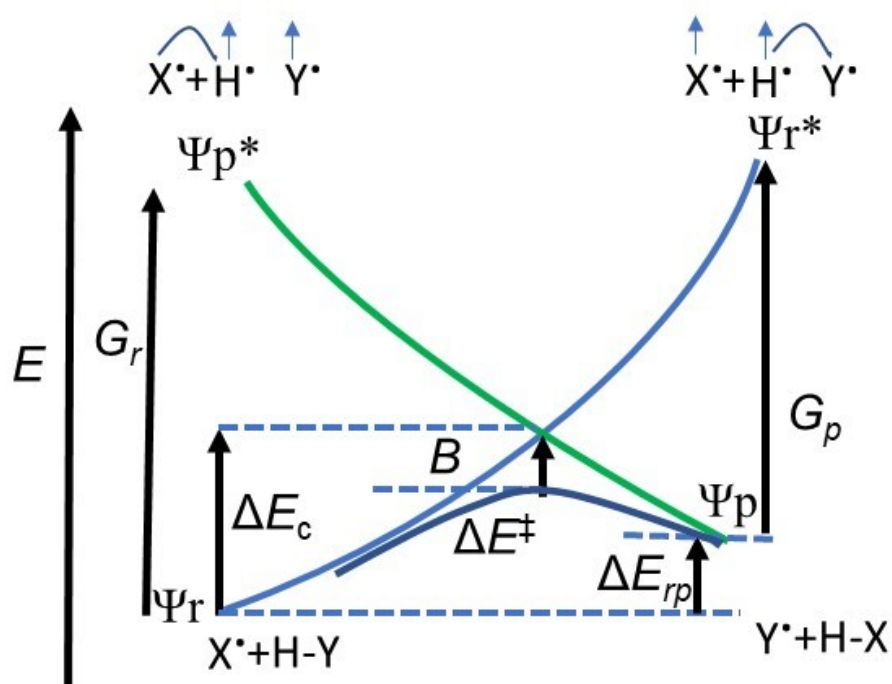
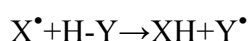


Figure S23: Valence Bond State Correlation Diagram (VBSCD) for the simple H-abstraction reaction  $X\cdot+H-Y\rightarrow XH+Y\cdot$  (where  $X\cdot = \{(X1)(X2)LCu(II) -O_2^{\cdot-}\}$ ,  $XH = \{(X1)(X2)LCu(II) -O_2^{\cdot-}\}$ ,  $H-Y$  is substrate and  $Y\cdot =$  substrate radical)

Above figure displays the VBSCD diagram for the hydrogen atom abstraction reactions by radical X from HY.



(where  $X\cdot = \{(X1)(X2)LCu(II) -O_2^{\cdot-}\}$  (**1a-5a**),  $XH = \{(X1)(X2)LCu(II) -O_2^{\cdot-}\}$  (**1b-5b**),  $H-Y$  is substrate (**A1-A3**) and  $Y\cdot =$  substrate radical (**A1'-A3'**))

The two curves have two main curves that represent the states of the reactants and product  $\Psi_r$  and  $\Psi_p$  which are represented in green and red, respectively, and two corresponding excited states,  $\Psi_r^*$  and  $\Psi_p^*$ . A unique bonding scheme is represented by each state curve: As a result, both  $\Psi_r$  and  $\Psi_p^*$  characterise the bonding pattern in the reactants, with  $\Psi_p^*$  representing the reactant-type bonding in the geometry of the products. The product-type bonding is involved in  $\Psi_p^*$ , but it occurs in the geometry of the reactants. These bonding characteristics cause the  $\Psi_r$  state to connect to  $\Psi_p^*$  and, at the same time,  $\Psi_r^*$  to connect to  $\Psi_p$  as we proceed along the reaction coordinate by shortening the O—H and R—O lengths and lengthening the O—H bond, which changes the geometry from reactants to products.  $\Psi_r$

The explicit barrier expression from the VB model is given by expression(1a)

$$\Delta E_{VB}^{\#} = f_0 G_0 + 0.5 \Delta E_{rp} + 0.5 \left( \frac{\Delta E_{rp}^2}{G_0} \right) - B \quad \rightarrow(1a)$$

This expression illustrates the relationship between the barrier and the two separate promotion gaps ( $G_r$  and  $G_p$ ), the  $f_0$  factor, which are shown in equation (1b) and the thermodynamic driving force,  $E_{rp}$ .

$$G_0 = 0.5(G_r + G_p), f_0 = 0.5(f_r + f_p) \quad \rightarrow(1b)$$

When ,  $\Delta E_{rp} \ll \ll G_0$ , the expression(1b) can be written as

$$\Delta E_{VB}^{\#} = f_0 G_0 + 0.5 \Delta E_{rp} - B \quad \rightarrow(1c)$$

It has previously been demonstrated that the promotion gap, which is proportional to the singlet-triplet promotion energy of the bonding electrons, may be represented as two times the vertical bond strength D based on semi-empirical VB equations. Equation (2) gives a good technique to approximating D. BDE is the corresponding bond dissociation energy and  $|RE_X \cdot|$  is absolute magnitude of the reorganization energy required to transform the X radical's geometry in the HX molecule from its optimal structure. The transition-state resonance energy B the from the semi-empirical VB analysis also approximated by equation (3). Both  $f_0=0.3$  and  $f_0=1/3$  will accurately forecast the trends in the barriers but 0.3 used here.

$$G_r = 2D_{H-Y} = 2[BDE_{H-Y} + |RE_Y \cdot|] \quad \rightarrow(2a)$$

$$G_p = 2D_{H-X} = 2[BDE_{H-X} + |RE_X \cdot|] \quad \rightarrow(2b)$$

$$B_{XHY} = \frac{1}{4}[BDE_{H-X} + BDE_{H-Y}] \quad \rightarrow(3)$$

Substituting the equations (2a),(2b) and (3) into the equations (1a),(1c), we may get

$$\Delta E_{VB}^{\#}(1) = 0.3G_0 + 0.5\Delta E_{rp} - B_{XHY} \quad \rightarrow(4a)$$

$$\Delta E_{VB}^{\#}(2) = 0.3G_0 + 0.5\Delta E_{rp} - B_{XHY} + 0.5 \left( \frac{\Delta E_{rp}^2}{G_0} \right) \quad \rightarrow(4b)$$

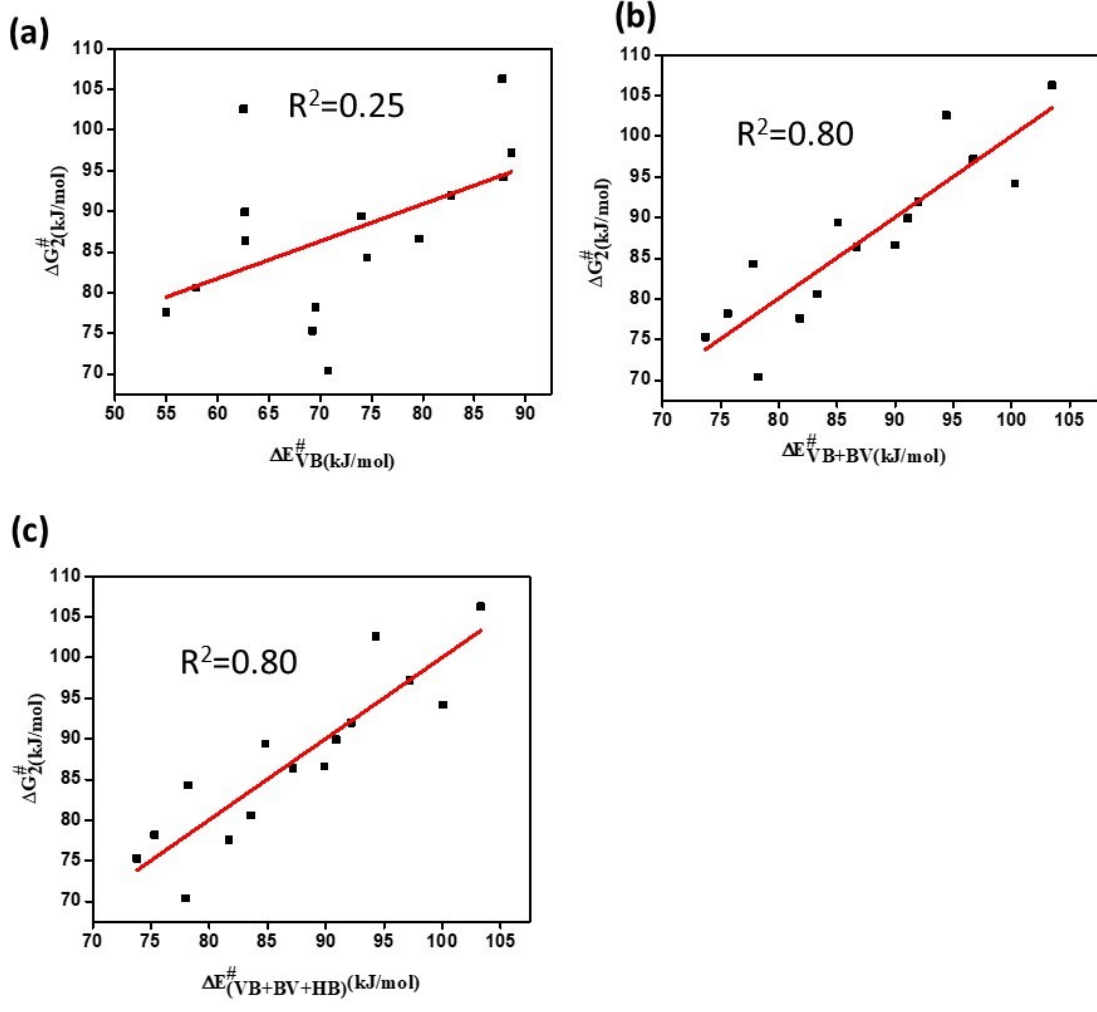


Figure S24: Plots of (a) Regression Analysis between  $\Delta G_2^\ddagger$  vs  $\Delta E_{VB}^\ddagger$  (b) Regression Analysis between  $\Delta G_2^\ddagger$  vs  $\Delta E_{VB+BV}^\ddagger$  (c) Regression Analysis between  $\Delta G_2^\ddagger$  vs  $\Delta E_{(VB+BV+HB)}^\ddagger$



## Dichotomy of Hydrogen atom transfer

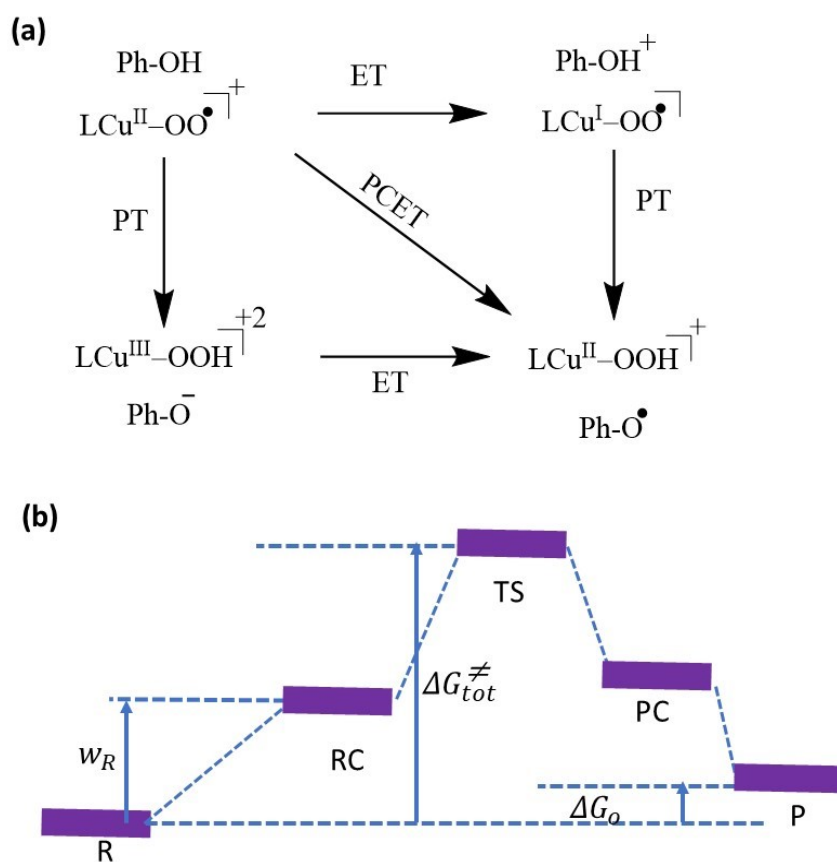


Figure S25: (a) Different Pathways for hydrogen atom abstraction from phenol by copper superoxo complex (b) HAA reaction Showing the formation of Reactant complex product complex.

For each metal superoxo-substrate combination assessed here, we tabulated the free energy of proton-coupled electron transfer ( $\Delta G_{PCET}$ , eqn(C)), free energies of proton transfer ( $\Delta G_{PT}$ , eqn(A)) and free energies of electron transfer ( $\Delta G_{ET}$ , eqn(B)), and the asynchronicity ( $\eta$ , eqn(E)) and reorganization energy ( $\lambda$ , eqn(D)) and frustration ( $\sigma$ , eqn(E)) as defined by Srnc and coworkers

$$\Delta G_{PT} = \left[ G_{(LCu^{III}-OOH)^{+2}} + G_{(Ph-O)^{-}} - G_{(Ph-OH)} - G_{(LCu^{II}-OO\cdot)^{+}} \right] \rightarrow (A)$$

$$\Delta G_{ET} = \left[ G_{(LCu^{I}-OO)} + G_{(Ph-OH)^{+}} - G_{(Ph-OH)} - G_{(LCu^{II}-OO\cdot)^{+}} \right] \rightarrow (B)$$

$$\Delta G_{PCET} = \left[ G_{(LCu^{II}-OOH)^+} + G_{(Ph-O)^-} - G_{(Ph-OH)} - G_{(LCu^{II}-OO)^+} \right] \rightarrow (C)$$

$$\frac{\lambda}{4} = \Delta G_{act}^{\ddagger} - w_R - \frac{\Delta G_o}{2} \rightarrow (D)$$

$$\eta = \frac{1}{\sqrt{2}} \left[ G_{(LCu^{III}-OOH)^{+2}} + G_{(Ph-O)^-} - G_{(LCu^I-OO)} - G_{(Ph-OH)^+} \right] \rightarrow (E)$$

$$\sigma = \Delta G_{PT} + \Delta G_{PT} \rightarrow (F)$$

Where,  $G_A$  is the free energy of species A (for example  $G_{(Ph-OH)}$  is free energy of substrate (A1-A3). Formation different species are shown in the Figure S24.  $\Delta G_{act}^{\ddagger}$  is activation obarrier of reaction and  $\Delta G_o$  is free energy of reaction.(shown in Figure S24 (b))

## Theoretical background on reduction potentials and acidity constants

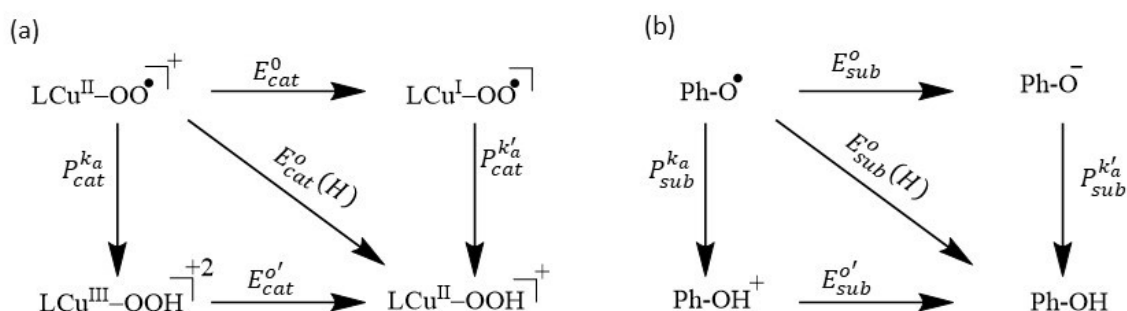


Figure S26: The thermodynamic cycles for (a) catalyst (b) substrate) connecting four structures that differ by one electron (horizontal arrows), one proton (vertical arrows), and a hydrogen atom (diagonal arrow), along with the associated thermodynamic quantities

There is a total of five thermodynamic quantities linked to this cycle. There is one electron reduction potential of these copper superoxo ( $E^o$ ) and the one-electron reduction potential of the protonated form of Cu(III)-OOH ( $E^o'$ ) and acidity constant of the copper superoxo ( $P^{ka}$ ) and the acidity constant of the reduced form of copper superoxo ( $P^{ka'}$ ). And further, both protonation and reduction processes are included in the proton-coupled reduction potential ( $E_H^o$ ), which measures a system's capacity to extract a hydrogen atom.

The acidity constant ( $P^{ka}$  and  $P^{ka'}$ ) is calculated according to the equation:

$$P^{ka} = \frac{\Delta G_{deprotonation} + G_{sol,H^+}}{RT \ln 10} \rightarrow (A1)$$

Where,  $\Delta G_{deprotonation} = G_{deprotonated} - G_{protonated}$

The effective acidity constant is defined by

$$\Delta P_{eff}^{ka} = \frac{\Delta P_a^k + \Delta P_a^{k'}}{2} \rightarrow (A2)$$

Where,

$$\Delta P_a^k = P_{cat}^{ka} - P_{sub}^{ka} \rightarrow (A3)$$

$$\Delta P_a^{k'} = P_{cat}^{ka'} - P_{sub}^{ka'} \rightarrow (A4)$$

Similarly, the one-electron reduction potential ( $E^\circ$  in V) is defined as a quantity reflecting Gibbs free energy change upon  $1e^-$   $-\Delta G_{\text{red/oxi}}/nF = -(G_{\text{red}} - G_{\text{oxi}})/nF$

proton-coupled reduction potential  $E^o(H)$  is defined by

$$E^o(H) = \Delta G_{\text{ox/red}} E_{\text{abs}}^o(\text{ref}) + G_{\text{sol,H}^+} \rightarrow (A5) \quad \text{where, } \Delta_{\text{Gox/red}} = G_{\text{ox}} - G_{\text{red}}$$

$E_{\text{abs}}^o[\text{reference}]$  is the absolute potential of a reference electrode, and  $G_{\text{sol,H}^+}$  is the free energy of solvation of a proton. The term  $G_{\text{sol,H}^+}$  incorporated into the context when the one-electron reduction of a solute is accompanied by its simultaneous protonation

Similar to acidity constants effective reduction potential were given by

$$\Delta E_{\text{eff}}^o = \frac{\Delta E^o + \Delta E^{\circ'}}{2} \rightarrow (A6)$$

Where,  $\Delta E^o = E_{\text{cat}}^o - E_{\text{sub}}^o \rightarrow (A7)$

$$\Delta E^{\circ'} = E_{\text{cat}}^{\circ'} - E_{\text{sub}}^{\circ'} \rightarrow (A8)$$

$$\Delta E^o(H) = E_{\text{cat}}^o(H) - E_{\text{sub}}^o(H) \rightarrow (A9)$$

$$\Delta G_2^\# = 0.980 (F09) - 0.1571 (F07) + 1.082 (F01) + 0.231 (F13) - 6.46$$

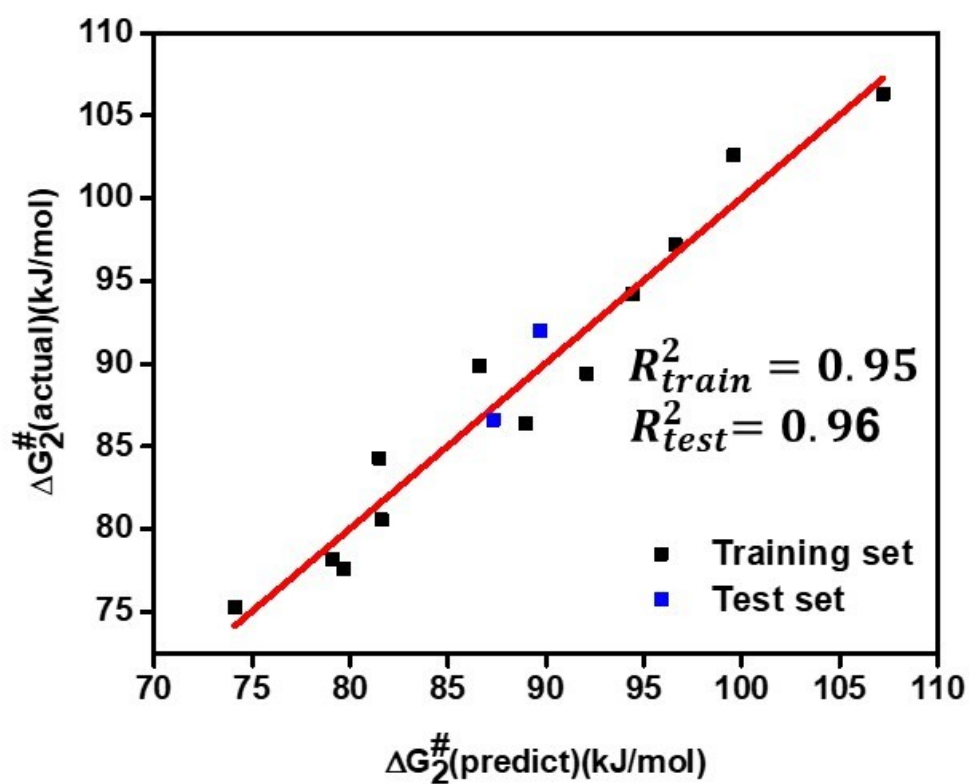


Figure S27: The Linear regression model performance for prediction of  $\Delta G_2^\#$

Table S1: Selected structural parameters of different catalysts used in this study **1a-5a**.

Complex	Cu- O1	Cu- O2	O1- O2	Cu- N1	Cu- N2	Cu- N3	Cu- N4	O2- H(N5)	O1- H(N6)
<sup>3</sup> <b>1a</b>	2.030	2.788	1.256	2.124	2.140	2.146	2.234	---	---
<sup>1</sup> <b>1a</b>	1.978	2.727	1.272	2.120	2.1434	2.148	2.209	---	---
<sup>3</sup> <b>2a</b>	2.010	2.785	1.266	2.156	2.187	2.121	2.200	---	2.0817
<sup>1</sup> <b>2a</b>	2.010	2.791	1.259	2.187	2.121	2.156	2.200	---	2.081
<sup>3</sup> <b>3a</b>	1.985	2.810	1.278	2.180	2.166	2.201	2.143	1.956	1.981
<sup>1</sup> <b>3a</b>	1.957	2.793	1.293	2.174	2.199	2.158	2.120	1.897	1.938
<sup>3</sup> <b>4a</b>	2.024	2.786	1.259	2.198	2.123	2.155	2.218	2.186	---
<sup>1</sup> <b>4a</b>	1.972	2.730	1.277	2.114	2.151	2.205	2.188	2.052	---
<sup>3</sup> <b>5a</b>	2.028	2.847	1.257	2.218	2.206	2.135	2.200	2.060	2.585
<sup>1</sup> <b>5a</b>	1.964	2.772	1.280	2.238	2.234	2.123	2.150	1.984	2.0988

Table S2: selected atoms spin densities of different catalysts used in this study **1a-5a**.

<b>Complex</b>	<b>Cu</b>	<b>O1</b>	<b>O2</b>	<b>O1 and O2</b>	<b>L(TMPA)</b>
<sup>3</sup> <b>1a</b>	0.25	0.785	0.872	1.65	0.09
<sup>1</sup> <b>1a</b>	0.339	-0.105	-0.338	-0.443	0.06
<sup>3</sup> <b>2a</b>	0.31	0.770	0.797	1.56	0.11
<sup>1</sup> <b>2a</b>	0.17	-0.011	-0.014	-0.025	-0.007
<sup>3</sup> <b>3a</b>	0.38	0.686	0.768	1.45	0.15
<sup>1</sup> <b>3a</b>	0.456	-0.176	-0.464	-0.64	0.10
<sup>3</sup> <b>4a</b>	0.25	0.785	0.834	1.71	0.08
<sup>1</sup> <b>4a</b>	0.366	-0.134	-0.346	-0.48	0.06
<sup>3</sup> <b>5a</b>	0.27	0.775	0.884	1.61	0.10
<sup>1</sup> <b>5a</b>	0.389	-0.148	-0.379	-0.527	0.09

Table S3: Variation of energy with change of dihedral angle catalysts used in this study **2a-5a**.

<b>Complex</b>	<b>N1-Cu-O1-O2</b>	<b>Energy</b>
<b>2a</b>	232	0.0
	340	1.5
	67	0.5
	226	0.1
	46	2.2
<b>3a</b>	54	0.0
	340	2.0
	67	0.3
	226	3.8
	46	0.2
<b>4a</b>	225	0.0
	340	2.5
	67	1.8
	226	0.1
	46	9.2
<b>5a</b>	229.79	0.0
	340	0.7
	67	1.2
	226	1.6
	46	23.8



Table S4: Electron density ( $\rho_{\text{BCP}}$ ), potential energy density ( $V$ ), localized orbital locator values (LOL), Wiberg bond indices (WBI) at BCP from natural bond orbital analysis, and binding energies (B.E) of important hydrogen bonds.

Complex	$\rho_{\text{BCP}}$ (a.u)	$V$ (a.u)	B.E=V/2 (kJ/mol)	B.E=(( 332.34* $\rho_{\text{BCP}}$ )- 1.0661)*4.184 (kJ/mol)	LOL	WBI
<b>1b</b>	0.009	-0.00495	-6.5	-16.66	0.139	0.006
<b>2b</b>	0.017	-0.01105	-14.5	-27.67	0.183	0.017
<b>3b</b>	0.024 and 0.0210	-0.01795 and - 0.01673	-23.6 and -22.0	-37.28 and - 34.03	0.218 and 0.193	0.030 and 0.017
<b>4b</b>	0.026	-0.02101	-27.6	-40.66	0.226	0.03
<b>5b</b>	0.026 and 0.027	-0.02221	-28.7 and -29.2	-41.18 and - 41.72	0.223 and 0.227	0.03 and 0.03

The electron density distribution is frequently used to characterize a variety of interactions within investigated systems, such as molecular aggregation, dimers, crystal structures, and hydrogen bonding.<sup>21</sup> Bader's "atoms in molecules" (AIM) theory, which is based on electron distribution calculations, is a potent technique for detecting and characterizing hydrogen bonding.<sup>22</sup> The electron density at X—O···H—Y BCP and its Laplacian well correlate with the hydrogen bond energy, according to several studies<sup>23 24 25</sup>. In 1998, Espinosa et al. showed that the binding energy (BE) of H-bond can be approximately estimated as the half value of  $V(r)$  (potential energy density) at the BCP for HBs of X—O···H—Y (X = C, N, O) namely  $BE \approx V_{\text{BCP}}/2$ . However, this relation is not valid given the fact that the BE can be predicted based on  $\rho_{\text{BCP}}$  at a much better accuracy compared to the  $V_{\text{BCP}}$ . The fitted equation for charged complexes is  $BE/\text{kcal/mol} = -332.34 \times \rho_{\text{BCP}}/\text{a. u.} - 1.0661$  with a MAPE of 10.0%.<sup>19</sup> We observed bond critical points (BCP) at H-bond interactions in **1a-5a**. The  $\rho$  value at BCP in **1a** is around 0.009 au implying that weaker hydrogen bonding interaction between hydrogen (attached to C) and  $\text{O}_2^{\bullet-}$  unit. (See Table S4) In complex **3a**, which has the two amino groups, has stronger hydrogen-bonded interactions between two amino groups hydrogens, and  $\text{O}_2^{\bullet-}$  atoms. ( $\rho$  values at O2-H(N5) and O2-H(N6) are 0.021 and 0.024 au respectively). The hydrogen bond interaction of the amino group H in **2a** is slightly lower than that of the pivalamido group H in **4a**. ( $\rho$  values at O2-H(N5) are 0.026 au and 0.017 au in **4a** and **2a** respectively) However, in complex **5a**, which has two pivalamido groups make the hydrogen bond with  $\text{O}_2^{\bullet-}$ , and this is slightly stronger than one pivalamido group ( $\rho$  values at O2-H(N6) and O2-H(N5) in **5a** are 0.026 au and 0.027 au). Binding energy values suggest that the strength of hydrogen bond interactions as follows **5a** > **4a** > **3a** > **2a** > **1a**.

Further NBO analysis was performed to get more insight into the hydrogen bond interactions. Wiberg bond index (WBI) of Cu-O and O-O also confirmed that electron transfer from copper center to dioxygen is little. The WBI of bonds O1-H3 or O2-H3 is around 0.006 implies weaker hydrogen bonding in **1a**. In complex **3a**, WBI values at O1-H2 and O2-H1 are 0.017 and 0.030 respectively. However, complex **5a**, the WBI of both hydrogen bonds are 0.03.

Further, localized orbital locator (LOL) analyses were conducted to examine the electron density localization associated with hydrogen bond interactions. Similar to ELF (electron localization function), Schmider and Becke defined another function for finding high localization zones called localized orbital locator (LOL). The LOL is given by equation (5).<sup>26</sup>

$$\text{LOL}(r) = \frac{\tau(r)}{1 + \tau(r)}$$

*where,*

$$\tau(r) = \frac{D_0(r)}{\left(\frac{1}{2}\right) \sum_i \eta_i |\nabla \varphi_i(r)|^2}$$

$D_0(r)$  is defined similar to ELF. Generally speaking, LOL and ELF are qualitatively comparable, but LOL communicates a more distinct and decisive picture than ELF.<sup>27</sup> The LOL values again support that the strength of hydrogen bond interactions as follows **5a** > **4a** > **3a** > **2a** > **1a**

Apart from AIM and NBO, we have also performed NCI analysis that is widely used to visualize hydrogen bond interactions. Noncovalent interaction analysis is a method for graphical representation of regions in real-space where non-covalent interactions occur, and it has been shown to be capable of differentiating hydrogen bonds, van der Waals interactions, and repulsive steric interactions.<sup>28</sup> The normalized and dimensionless reduced density gradient (RDG),  $s(\rho)$ , is used as a scalar function to characterize the deviations from a homogeneous electron distribution in the NCI approach. The reduced gradient function is defined by<sup>29</sup>

$$s(\rho) = \frac{|\nabla \rho|}{2\sqrt{3\pi^2\rho^4}}$$

The contributions to the Laplacian are the eigenvalues of electron density (second derivative) Hessian matrix as  $\nabla^2\rho = \lambda_1 + \lambda_2 + \lambda_3$ , where  $\lambda_1 < \lambda_2 < \lambda_3$ . the sign of second derivative helps in the identification of nature of interaction i.e., attractive, repulsive and Vander wall.<sup>30</sup> The colour codes were utilized to distinguish between different sorts of interactions in the 2D NCI and 3D NCI plots using an RGB colouring system. Strong attractive interactions, weak (van der Waals) interactions, and strong repulsive interactions were shown using blue, green, and red is surfaces.

Table S5: Buried volume (BV) of different catalysts (**1a-5a**) and substrates (**A1-A3**) used in this study.

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<b>Catalyst/Substrate</b>	<b>%V<sub>buried</sub></b>
<b>1a</b>	46.6
<b>2a</b>	49.8
<b>3a</b>	52.3
<b>4a</b>	51.2
<b>5a</b>	56.7
<b>A1</b>	56.6
<b>A2</b>	30.4
<b>A3</b>	30.5

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Table S6: Selected structural parameters of reactant complex of reactions **R1-R15**.

Complex	Cu- O1	Cu- O2	O1- O2	Cu- N1	Cu- N2	Cu- N3	Cu- N4	O2- H(sub)	O3- H(sub)
<sup>3</sup> RC <sub>R1</sub>	2.038	2.831	1.254	2.131	2.139	2.138	2.241	4.135	0.965
<sup>3</sup> RC <sub>R2</sub>	2.023	2.841	1.266	2.163	2.150	2.148	2.196	5.774	0.968
<sup>3</sup> RC <sub>R3</sub>	1.986	2.814	1.277	2.185	2.171	2.190	2.147	5.592	0.968
<sup>3</sup> RC <sub>R4</sub>	2.029	2.797	1.258	2.190	2.125	2.155	2.221	4.861	0.965
<sup>3</sup> RC <sub>R5</sub>	---	---	---	---	---	---	---	---	---
<sup>3</sup> RC <sub>R6</sub>	1.999	2.765	1.267	2.138	2.124	2.139	2.211	2.147	0.972
<sup>3</sup> RC <sub>R7</sub>	1.989	2.783	1.278	2.160	2.189	2.126	2.184	2.183	0.972
<sup>3</sup> RC <sub>R8</sub>	1.982	2.793	1.279	2.189	2.169	2.189	2.143	2.625	0.970
<sup>3</sup> RC <sub>R9</sub>	1.996	2.731	1.275	2.227	2.117	2.165	2.183	2.766	0.971
<sup>3</sup> RC <sub>R10</sub>	2.115	2.995	1.240	2.173	2.211	2.177	2.265	3.021	0.989
<sup>3</sup> RC <sub>R11</sub>	1.999	2.767	2.138	2.138	2.124	2.138	2.209	2.140	0.972
<sup>3</sup> RC <sub>R12</sub>	1.995	2.825	1.276	2.147	2.191	2.126	2.174	2.093	0.973
<sup>3</sup> RC <sub>R13</sub>	1.982	2.795	1.279	2.191	2.185	2.169	2.141	2.632	0.970
<sup>3</sup> RC <sub>R14</sub>	1.998	2.724	1.274	2.166	2.116	2.231	2.185	2.791	0.971
<sup>3</sup> RC <sub>R15</sub>	---	---	---	---	---	---	---	---	---

Table S7: Selected structural parameters of transition states of all reactions **R1-R15**.

Complex	Cu- O1	Cu- O2	O1- O2	Cu- N1	Cu- N2	Cu- N3	Cu- N4	O2- H(N6)	O1- H(N6)	O2- H(sub)	H(sub)- O3
<sup>3</sup> TS <sub>R1</sub>	1.961	2.779	1.331	2.145	2.144	2.156	2.265	--	--	1.280	1.131
<sup>3</sup> TS <sub>R2</sub>	1.958	2.882	1.339	2.157	2.212	2.145	2.228	1.854	--	1.300	1.116
<sup>3</sup> TS <sub>R3</sub>	1.973	2.841	1.348	2.169	2.170	2.213	2.179	1.945	1.928	1.368	1.079
<sup>3</sup> TS <sub>R4</sub>	1.964	2.839	1.334	2.243	2.140	2.149	2.231	1.932	--	1.343	1.09
<sup>3</sup> TS <sub>R5</sub>	1.970	2.741	1.341	2.361	2.157	2.231	2.210	1.903	1.776	1.413	1.068
<sup>3</sup> TS <sub>R6</sub>	1.954	2.749	1.345	2.159	2.140	2.155	2.264	--	--	1.233	1.162
<sup>3</sup> TS <sub>R7</sub>	1.938	2.740	1.358	2.219	2.142	2.158	2.142	1.891	--	1.245	1.152
<sup>3</sup> TS <sub>R8</sub>	1.966	2.812	1.362	2.174	2.179	2.195	2.177	1.920	1.917	1.303	1.113
<sup>3</sup> TS <sub>R9</sub>	1.940	2.661	1.362	2.265	2.141	2.140	2.249	1.821	--	1.299	1.119
<sup>3</sup> TS <sub>R10</sub>	1.914	2.691	1.376	2.307	2.140	2.239	2.201	1.780	1.843	1.402	1.070
<sup>3</sup> TS <sub>R11</sub>	1.937	2.730	1.350	2.154	2.130	2.161	2.261	--	--	1.160	1.231
<sup>3</sup> TS <sub>R12</sub>	1.933	2.741	1.360	2.149	2.221	2.134	2.194	1.903	--	1.171	1.218
<sup>3</sup> TS <sub>R13</sub>	1.955	2.799	1.366	2.191	2.170	2.172	2.149	1.937	1.922	1.212	1.177
<sup>3</sup> TS <sub>R14</sub>	1.927	2.675	1.364	2.135	2.266	2.132	2.209	1.843	--	1.208	1.184
<sup>3</sup> TS <sub>R15</sub>	1.919	2.714	1.378	2.226	2.309	2.140	2.177	1.818	1.865	1.273	1.139

Table S8: Selected atom spin densities of transition states of all reactions **R1-R15**.

<b>Complex</b>	<b>Cu</b>	<b>O1</b>	<b>O2</b>	<b>H( sub)</b>	<b>O3</b>	<b>Sub</b>
${}^3\text{TS}_{\text{R1}}$	0.294	0.567	0.470	-0.032	0.167	0.58
${}^3\text{TS}_{\text{R2}}$	0.33	0.549	0.422	-0.029	0.154	0.58
${}^3\text{TS}_{\text{R3}}$	0.38	0.463	0.462	-0.027	0.143	0.57
${}^3\text{TS}_{\text{R4}}$	0.29	0.522	0.481	-0.027	0.140	0.61
${}^3\text{TS}_{\text{R5}}$	0.26	0.503	0.459	-0.17	0.133	0.70
${}^3\text{TS}_{\text{R6}}$	0.310	0.550	0.398	-0.021	0.212	0.65
${}^3\text{TS}_{\text{R7}}$	0.362	0.521	0.335	-0.016	0.208	0.67
${}^3\text{TS}_{\text{R8}}$	0.401	0.434	0.388	-0.018	0.191	0.63
${}^3\text{TS}_{\text{R9}}$	0.30	0.516	0.324	-0.012	0.214	0.77
${}^3\text{TS}_{\text{R10}}$	0.35	0.482	0.273	-0.011	0.204	0.79
${}^3\text{TS}_{\text{R11}}$	0.366	0.542	0.363	-0.021	0.252	0.62
${}^3\text{TS}_{\text{R12}}$	0.407	0.515	0.314	-0.017	0.248	0.59
${}^3\text{TS}_{\text{R13}}$	0.44	0.425	0.359	-0.020	.234	0.59
${}^3\text{TS}_{\text{R14}}$	0.36	0.512	0.303	-0.14	0.256	0.70
${}^3\text{TS}_{\text{R15}}$	0.39	0.478	0.252	-0.12	0.255	0.75

Table S9: Selected structural parameters of product complexes of all reactions **R1-R15**.

Complex	Cu- O1	Cu- O2	O1- O2	Cu- N1	Cu- N2	Cu- N3	Cu- N4	O2- H(N6)	O1- H(N6)	O2- H(sub)	H- O3
<sup>3</sup> PC <sub>R1</sub>	1.913	2.759	1.405	2.140	2.167	2.140	2.247	---	---	0.989	1.741
<sup>3</sup> PC <sub>R2</sub>	---	---	---	---	---	---	---	---	---	---	---
<sup>3</sup> PC <sub>R3</sub>	1.913	2.834	1.449	2.182	2.167	2.165	2.126	1.891	1.845	0.97	4.949
<sup>3</sup> PC <sub>R4</sub>	1.888	2.660	1.424	2.120	2.276	2.130	2.187	1.859	---	0.992	1.711
<sup>3</sup> PC <sub>R5</sub>	---	---	---	---	---	---	---	---	---	---	---
<sup>3</sup> PC <sub>R6</sub>	1.907	2.726	1.406	2.158	2.173	2.134	2.244	---	---	0.998	1.719
<sup>3</sup> PC <sub>R7</sub>	1.913	2.810	1.413	2.229	2.144	2.158	2.214	1.818	---	0.998	1.699
<sup>3</sup> PC <sub>R8</sub>	---	---	---	---	---	---	---	---	---	---	---
<sup>3</sup> PC <sub>R9</sub>	1.900	2.790	1.408	2.135	2.154	2.242	2.187	1.791	---	1.003	1.687
<sup>3</sup> PC <sub>R10</sub>	1.938	2.893	1.384	2.256	2.174	2.245	2.264	2.705	2.613	0.996	3.181
<sup>3</sup> PC <sub>R11</sub>	1.907	2.729	1.409	2.177	2.153	2.130	2.238	---	---	0.993	1.755
<sup>3</sup> PC <sub>R12</sub>	1.913	2.818	1.416	2.1560	2.229	2.142	2.2081	1.823	---	0.994	1.738
<sup>3</sup> PC <sub>R13</sub>	---	---	---	---	---	---	---	---	---	---	---
<sup>3</sup> PC <sub>R14</sub>	1.903	2.807	1.411	2.243	2.130	2.144	2.182	---	1.783	0.998	1.718
<sup>3</sup> PC <sub>R15</sub>	1.935	2.884	1.385	2.249	2.259	2.249	2.258	2.581	2.68	0.996	3.147

Table S10: Selected atom spin densities of product complexes of all reactions **R1-R15**.

Complex	Cu	O1	O2	O3	C(ben)
<sup>3</sup> PC <sub>R1</sub>	0.400	0.375	0.119	0.296	0.655
<sup>3</sup> PC <sub>R2</sub>	---	---	---	---	---
<sup>3</sup> PC <sub>R3</sub>	0.537	0.230	0.023	0.308	0.589
<sup>3</sup> PC <sub>R4</sub>	0.446	0.346	0.080	0.301	0.596
<sup>3</sup> PC <sub>R5</sub>	---	---	---	---	---
<sup>3</sup> PC <sub>R6</sub>	0.38	0.38	0.128	0.335	0.63
<sup>3</sup> PC <sub>R7</sub>	0.423	0.355	0.098	0.330	0.56
<sup>3</sup> PC <sub>R8</sub>	---	---	---	---	---
<sup>3</sup> PC <sub>R9</sub>	0.424	0.327	0.125	0.328	0.69
<sup>3</sup> PC <sub>R10</sub>	0.33	0.411	0.180		
<sup>3</sup> PC <sub>R11</sub>	0.40	0.375	0.20	0.38	0.693
<sup>3</sup> PC <sub>R12</sub>	0.443	0.347	0.09	0.379	0.69
<sup>3</sup> PC <sub>R13</sub>	---	---	---	---	---
<sup>3</sup> PC <sub>R14</sub>	0.43	0.324	0.116	0.380	0.68
<sup>3</sup> PC <sub>R15</sub>	---	---	---	---	---



Table S11: Selected structural parameters of **1b-5b**.

Complex	Cu-O1	Cu-O2	O1-O2	Cu-N1	Cu-N2	Cu-N3	Cu-N4	O2-H(N1/N2)	O1-H(N1/N2)	O2-H(N1/N2)
<sup>3</sup> <b>1b</b>	1.907	2.779	1.419	2.154	2.156	2.124	2.213	---	---	---
<sup>1</sup> <b>1a</b>	1.978	2.727	1.272	2.143	2.148	2.120	2.209	---	---	---
<sup>3</sup> <b>2b</b>	1.912	2.702	1.425	2.168	2.162	2.121	2.170	1.875	---	2.597
<sup>1</sup> <b>2b</b>	2.010	2.791	1.2592	2.146	2.128	2.181	2.219	2.120	---	---
<sup>3</sup> <b>3b</b>	1.921	2.866	1.435	2.159	2.254	2.153	2.134	1.824	1.844	---
<sup>1</sup> <b>3b</b>	1.957	2.793	1.293	2.128	2.1812	2.146	2.219	1.897	1.938	---
<sup>3</sup> <b>4b</b>	1.906	2.779	1.419	2.160	2.114	2.242	2.210	2.038	---	---
<sup>1</sup> <b>4b</b>	1.972	2.730	.277	2.151	2.205	2.114	2.188	2.052	---	---
<sup>3</sup> <b>5b</b>	1.917	2.874	1.396	2.265	2.189	2.1447	2.222	1.857	---	2.258
<sup>1</sup> <b>5b</b>	1.964	2.772	1.280	2.234	2.238	2.1237	2.150	1.984	---	2.0988

Table S12: Selected atom spin densities of different catalysts used in this study **1b-5b**.

<b>Complex</b>	<b>Cu</b>	<b>O1</b>	<b>O2</b>	<b>Ligand</b>
<b><sup>3</sup>1b</b>	0.435	0.347	0.087	0.135
<b><sup>1</sup>1b</b>	0.339	-0.105	-0.338	0.062
<b><sup>3</sup>2b</b>	0.466	0.304	0.082	0.153
<b><sup>1</sup>2b</b>	0.444	-0.172	-0.380	0.153
<b><sup>3</sup>3b</b>	0.510	0.246	0.046	0.194
<b><sup>1</sup>3b</b>	0.456	-0.176	-0.434	0.178
<b><sup>3</sup>4b</b>	0.427	0.357	0.089	0.128
<b><sup>1</sup>4b</b>	0.366	-0.134	-0.346	0.12
<b><sup>3</sup>5b</b>	0.375	0.382	0.135	0.103
<b><sup>1</sup>5b</b>	0.389	-0.148	-0.379	0.14

Table S13: Energy decomposition analysis for all reactions used in this study.

Reaction	$\Delta E^\#$ (gas)	$\Delta E_{steric}$	$\Delta E_{orb}$	$\Delta E_{int}$	$\Delta E_{strain}$	$\Delta E_{strain(catalyst)}$	$\Delta E_{strain(substrate)}$
<b>R1</b>	26.7	183.0	-239.4	-56.3	83.0	10.6	72.4
<b>R2</b>	19.5	166.7	-224.5	-57.8	77.3	12.2	65.1
<b>R3</b>	11.2	130.7	-177.7	-47.0	58.2	8.5	49.7
<b>R4</b>	21.7	150.4	-203.5	-53.1	74.7	14.9	59.8
<b>R5</b>	21.3	127.5	-185.9	-58.4	79.6	30.2	49.4
<b>R6</b>	25.5	201.7	-274.1	-72.3	97.8	14.6	83.2
<b>R7</b>	16.1	189.2	-266.7	-77.4	93.6	15.9	77.7
<b>R8</b>	7.3	152.8	-214.5	-61.7	69.0	12.6	56.3
<b>R9</b>	6.9	160.7	-242.2	-81.5	88.4	26.0	62.5
<b>R10</b>	-6.6	119.9	-199.6	-79.7	73.1	31.4	41.7
<b>R11</b>	48.3	259.7	-344.8	-85.0	133.4	14.2	119.1
<b>R12</b>	40.9	247.0	-332.8	-85.8	126.6	14.8	111.8
<b>R13</b>	30.9	212.7	-280.2	-67.5	98.4	11.8	86.6
<b>R14</b>	36.2	219.0	-298.5	-79.5	115.7	23.6	92.1
<b>R15</b>	26.7	185.1	-257.4	-72.3	99.1	29.0	70.1

Table S14: Wigner transmission coefficients of reactions R1-R15 at different temperatures.

T(K)	138K	158K	178K	198K	218K	238K	258K	278K	298K
<b>R1</b>	11.43	8.96	7.27	6.07	5.18	4.51	3.98	3.57	3.24
<b>R2</b>	9.44	7.44	6.07	5.10	4.38	3.84	3.41	3.08	2.81
<b>R3</b>	5.62	4.52	3.77	3.24	2.85	2.55	2.32	2.14	1.99
<b>R4</b>	6.64	5.30	4.39	3.74	3.26	2.90	2.61	2.39	2.21
<b>R5</b>	2.08	1.82	1.65	1.52	1.43	1.36	1.31	1.27	1.23
<b>R6</b>	13.94	10.87	8.77	7.28	6.18	5.35	4.70	4.19	3.77
<b>R7</b>	12.33	9.64	7.81	6.50	5.54	4.81	4.24	3.79	3.43
<b>R8</b>	9.76	7.68	6.26	5.25	4.51	3.94	3.51	3.16	2.88
<b>R9</b>	8.72	6.89	5.64	4.75	4.09	3.59	3.21	2.90	2.65
<b>R10</b>	2.20	1.91	1.72	1.58	1.48	1.40	1.34	1.30	1.26
<b>R11</b>	13.86	10.81	8.73	7.25	6.16	5.33	4.68	4.17	3.76
<b>R12</b>	13.53	10.56	8.53	7.09	6.02	5.21	4.58	4.09	3.69
<b>R13</b>	15.45	12.02	9.68	8.02	6.79	5.86	5.13	4.56	4.10
<b>R14</b>	14.07	10.97	8.86	7.35	6.24	5.39	4.74	4.22	3.80
<b>R15</b>	11.61	9.09	7.38	6.15	5.25	4.57	4.04	3.61	3.27

Table S15: Zero curvature tunneling (ZCT) transmission coefficients of reactions **R1-R15**.

<b>T(K)</b>	<b>298K</b>
<b>R1</b>	4.62
<b>R2</b>	3.99
<b>R3</b>	4.42
<b>R4</b>	3.5
<b>R5</b>	-
<b>R6</b>	3.17
<b>R7</b>	3.16
<b>R8</b>	2.11
<b>R9</b>	4.43
<b>R10</b>	-
<b>R11</b>	2.47
<b>R12</b>	3.83
<b>R13</b>	3.58
<b>R14</b>	2.87
<b>R15</b>	2.95

Table S16: Small curvature tunneling (SCT) transmission coefficients of reactions **R1-R15**.

<b>T(K)</b>	<b>298</b>
<b>R1</b>	140.73
<b>R2</b>	43.21
<b>R3</b>	13.58
<b>R4</b>	9.81
<b>R5</b>	-
<b>R6</b>	6.88
<b>R7</b>	19.00
<b>R8</b>	13.16
<b>R9</b>	29.78
<b>R10</b>	-
<b>R11</b>	6.71
<b>R12</b>	14.23
<b>R13</b>	17.95
<b>R14</b>	12.71
<b>R15</b>	6.32

Table S17: Wiberg bond index of transition states of reactions **R1-R15**.

<b>Reaction</b>	<b>O3-H<sub>sub</sub></b>	<b>O2-H<sub>sub</sub></b>	<b>(O3-H<sub>sub</sub>)-(O2-H<sub>sub</sub>)</b>
<b>R1</b>	0.44	0.33	0.11
<b>R2</b>	0.46	0.3	0.16
<b>R3</b>	0.5	0.25	0.25
<b>R4</b>	0.49	0.27	0.22
<b>R5</b>	0.51	0.23	0.28
<b>R6</b>	0.42	0.36	0.06
<b>R7</b>	0.43	0.35	0.08
<b>R8</b>	0.47	0.3	0.17
<b>R9</b>	0.46	0.3	0.16
<b>R10</b>	0.52	0.22	0.3
<b>R11</b>	0.35	0.43	-0.08
<b>R12</b>	0.36	0.42	-0.06
<b>R13</b>	0.4	0.38	0.02
<b>R14</b>	0.39	0.38	0.01
<b>R15</b>	0.44	0.32	0.12

Table S18:Natural charges of Transition states of reactions **R1-R15**.

<b>Reaction</b>	<b>O1</b>	<b>O2</b>	<b>H(sub)</b>	<b>N1</b>	<b>N2</b>	<b>Cu</b>	<b>O3*H+O2*H</b>
<b>R1</b>	-0.307	-0.324	0.453	--	--	0.809	-0.454359
<b>R2</b>	-0.322	-0.368	0.462	-0.75	--	0.837	-0.486486
<b>R3</b>	0.465	-0.342	-0.405	-0.745	-0.749	0.863	0.41391
<b>R4</b>	-0.351	-0.323	0.465	-0.613	--	0.814	-0.459885
<b>R5</b>	-0.356	-0.373	0.482	-0.614	-0.624	0.817	-0.498388
<b>R6</b>	-0.324	-0.36	0.45	--		0.823	-0.4347
<b>R7</b>	-0.35	-0.419	0.459	-0.749	--	0.851	-0.464967
<b>R8</b>	-0.431	-0.382	0.456	-0.743	-0.751	0.873	-0.447336
<b>R9</b>	-0.356	-0.442	0.468	-0.618	--	0.826	-0.47268
<b>R10</b>	-0.388	-0.502	0.486	-0.619	-0.617	0.857	-0.51516
<b>R11</b>	-0.32	-0.351	0.45	--		0.851	-0.42795
<b>R12</b>	-0.342	-0.4	0.457	-0.747	--	0.873	-0.451516
<b>R13</b>	-0.427	-0.362	0.449	-0.748	-0.74	0.895	-0.428346
<b>R14</b>	-0.347	-0.421	0.461	-0.617	--	0.858	-0.452702
<b>R15</b>	-0.382	-0.472	0.471	-0.616	-0.617	0.882	-0.477594



Table S19: Kinetic isotopic effect (KIE) of reactions **R1-R15**.

<b>T(K)</b>	<b>138K</b>	<b>158K</b>	<b>178K</b>	<b>198K</b>	<b>218K</b>	<b>238K</b>	<b>258K</b>	<b>278K</b>	<b>298K</b>
<b>R1</b>	36.1	23.6	16.9	13.0	10.5	8.8	7.6	6.7	6.0
<b>R2</b>	32.8	21.6	15.7	12.1	9.9	8.3	7.2	6.3	5.7
<b>R3</b>	23.7	16.3	12.2	9.6	8.0	6.8	6.0	5.3	4.8
<b>R4</b>	26.7	18.1	13.4	10.5	8.7	7.4	6.4	5.7	5.2
<b>R5</b>	29.9	20.0	14.7	11.5	9.4	8.0	6.9	6.2	5.6
<b>R6</b>	29.5	19.5	14.2	11.1	9.1	7.7	6.7	5.9	5.3
<b>R7</b>	24.7	16.9	12.6	10.0	8.3	7.1	6.2	5.5	5.0
<b>R8</b>	22.8	15.7	11.8	9.4	7.9	6.8	5.9	5.3	4.8
<b>R9</b>	24.0	16.4	12.2	9.7	8.0	6.9	6.0	5.4	4.9
<b>R10</b>	12.6	9.2	7.2	5.9	5.1	4.5	4.0	3.6	3.4
<b>R11</b>	23.6	15.9	11.8	9.2	7.6	6.5	5.6	5.0	4.5
<b>R12</b>	19.3	13.3	10.1	8.0	6.7	5.8	5.1	4.6	4.2
<b>R13</b>	27.1	18.3	13.5	10.6	8.7	7.4	6.5	5.8	5.2
<b>R14</b>	19.3	13.3	10.1	8.0	6.7	5.8	5.1	4.6	4.2
<b>R15</b>	33.6	21.6	15.4	11.8	9.4	7.9	6.8	5.9	5.3

Table S20: Kinetic isotopic effect (KIE) and Imaginary frequencies of transition states of all reactions **R1-R15** (\*wiberg bond order).

<b>Reaction</b>	<b>KIE</b>	<b>(O3-H<sub>sub</sub>)- (O2-H<sub>sub</sub>)*</b>	<b>Imaginary Frequency</b>
<b>R1</b>	6.0	0.11	-1517.45
<b>R2</b>	5.7	0.16	-1364.88
<b>R3</b>	4.8	0.25	-1009.35
<b>R4</b>	5.2	0.22	-1116.04
<b>R5</b>	5.6	0.28	-488.38
<b>R6</b>	5.3	0.06	-1689.78
<b>R7</b>	5.0	0.08	-1581.59
<b>R8</b>	4.8	0.17	-1390.45
<b>R9</b>	4.9	0.16	-1305.14
<b>R10</b>	3.4	0.3	-514.44
<b>R11</b>	4.5	-0.08	-1685.11
<b>R12</b>	4.2	-0.06	-1662.94
<b>R13</b>	5.2	0.02	-1785.67
<b>R14</b>	4.2	0.01	-1698.61
<b>R15</b>	5.3	0.12	-1530.20

Table S21: Structural parameters of different catalysts used in this study **1d-5d** (OSS=Open shell singlet and CSS=closed shell singlet).

Complex	Cu1-O1	Cu1-O2	O1-O2	Cu1'-O2	Cu1'-O1	Cu1-Cu1'	Cu1-N1	Cu1-N2	Cu1-N3	Cu1-N4	Cu1'-N1'	Cu1'-N2'	Cu1'-N3'	Cu1'-N4'
<b><sup>3</sup>1d</b>	1.992	2.859	1.322	1.990	2.857	4.532	2.164	2.143	2.161	2.232	2.160	2.164	2.143	2.227
<b><sup>1</sup>1d<sub>CSS</sub></b>	1.947	2.750	1.335	1.947	2.750	4.574	2.107	2.152	2.162	2.220	2.162	2.107	2.152	2.220
<b><sup>1</sup>1d<sub>OSS</sub></b>	1.951	2.819	1.350	1.951	2.819	4.451	2.161	2.153	2.149	2.216	2.149	2.161	2.153	2.216
<b><sup>3</sup>2d</b>	1.954	2.873	1.366	1.972	2.840	4.489	2.178	2.128	2.204	2.168	2.180	2.179	2.169	2.190
<b><sup>1</sup>2d<sub>OSS</sub></b>	1.949	2.812	1.399	1.936	2.835	4.562	2.179	2.162	2.160	2.177	2.167	2.173	2.145	2.157
<b><sup>1</sup>2d<sub>CSS</sub></b>	1.975	2.851	1.347	1.977	2.837	4.709	2.150	2.151	2.162	2.190	2.135	2.170	2.172	2.188
<b><sup>3</sup>3d</b>	1.937	2.852	1.430	1.931	2.795	4.594	2.188	2.196	2.176	2.110	2.153	2.249	2.206	2.119
<b><sup>1</sup>3d<sub>CSS</sub></b>	1.956	2.820	1.362	1.956	2.813	4.655	2.192	2.241	2.174	2.155	2.185	2.156	2.247	2.143
<b><sup>1</sup>3d<sub>OSS</sub></b>	1.926	2.810	1.430	1.928	2.822	4.606	2.227	2.192	2.168	2.121	2.218	2.166	2.176	2.109
<b><sup>3</sup>4d</b>	1.997	2.965	1.365	1.984	2.811	4.608	2.184	2.133	2.187	2.228	2.045	2.084	2.487	2.179
<b><sup>1</sup>4d<sub>CSS</sub></b>	1.990	2.954	1.344	1.981	2.781	4.682	2.085	2.269	2.150	2.219	2.466	2.050	2.061	2.197
<b><sup>1</sup>4d<sub>OSS</sub></b>	1.961	2.938	1.397	1.963	2.777	4.586	2.172	2.110	2.207	2.208	2.044	2.491	2.064	2.172
<b><sup>3</sup>5d</b>	1.925	2.743	1.434	1.916	2.858	4.566	2.136	2.316	2.220	2.109	2.088	2.399	2.213	2.088
<b><sup>1</sup>5d<sub>CSS</sub></b>	1.961	2.856	1.355	1.970	2.892	4.713	2.233	2.120	2.261	2.145	2.281	2.264	2.125	2.139
<b><sup>1</sup>5d<sub>OSS</sub></b>	1.917	2.728	1.426	1.910	2.848	4.555	2.125	2.343	2.221	2.110	2.382	2.202	2.100	2.088

Table S22: Selected atom spin densities of different complexes **1d-5d**.

<b>Complex</b>	<b>Cu1</b>	<b>O1</b>	<b>O2</b>	<b>Cu1'</b>	<b>L</b>	<b>L'</b>
<b><sup>3</sup>1d</b>	0.315	0.579	0.580	0.318	0.103	0.103
<b><sup>1</sup>1d<sub>CSS</sub></b>	0.00	0.00	0.00	0.00	0.00	0.00
<b><sup>1</sup>1d<sub>OSS</sub></b>	0.376	0.155	-0.155	-0.376	0.14	-0.12
<b><sup>3</sup>2d</b>	0.433	0.428	0.433	0.398	0.157	0.157
<b><sup>1</sup>2d<sub>CSS</sub></b>	0.00	0.00	0.00	0.00	0.00	0.00
<b><sup>1</sup>2d<sub>OSS</sub></b>	0.451	0.199	-0.151	-0.481	0.16	-0.17
<b><sup>3</sup>3d</b>	0.529	0.240	0.235	0.537	0.213	0.228
<b><sup>1</sup>3d<sub>CSS</sub></b>	0.00	0.00	0.00	0.00	0.00	0.00
<b><sup>1</sup>3d<sub>OSS</sub></b>	0.532	0.165	-0.152	-0.535	0.213	-0.22
<b><sup>3</sup>4d</b>	0.345	0.455	0.468	0.436	0.179	0.17
<b><sup>1</sup>4d<sub>CSS</sub></b>	0.00	0.00	0.00	0.00	0.00	0.00
<b><sup>1</sup>4d<sub>OSS</sub></b>	0.484	0.112	-0.253	-0.408	0.198	-0.139
<b><sup>3</sup>5d</b>	0.538	0.242	0.211	0.545	0.217	0.217
<b><sup>1</sup>5d<sub>CSS</sub></b>	0.00	0.00	0.00	0.00	0.00	0.00
<b><sup>1</sup>5d<sub>OSS</sub></b>	0.525	0.174	-0.146	-0.534	0.23	-0.22

Table S23: Energetics of different spin states of complexes **1d-5d**

Complex	S=1	S=0(closed shell singlet)	S=0(open shell singlet)
<b>1d</b>	0.0	59.4	78.8
<b>2d</b>	0.0	64.3	73.0
<b>3d</b>	0.0	80.4	92.5
<b>4d</b>	0.0	68.9	77.2
<b>5d</b>	0.0	64.5	90.5

Table S24: Selected structural parameters of transition state of dimerisation.

Complex	Cu1'- O2	Cu1'- O1	O1-O2	Cu1- O1	Cu1- O2	Cu1'- Cu1	Cu1'- N1'	Cu1'- N2'	Cu1'- N3'	Cu1'- N4'	Cu1- N1	Cu1- N2	Cu1- N3	Cu1- N4
${}^3TS_{1d}^{1a}$	2.700	3.510	1.276	2.027	2.856	5.455	2.105	2.109	2.110	2.273	2.139	2.141	2.147	2.200
${}^3TS_{2d}^{2a}$	2.950	3.948	1.287	2.008	2.816	5.722	2.110	2.104	2.101	2.253	2.138	2.187	2.149	2.154
${}^3TS_{3d}^{3a}$	2.850	3.727	1.312	1.988	2.906	5.468	2.114	2.140	2.155	2.229	2.181	2.192	2.172	2.111
${}^3TS_{4d}^{4a}$	2.700	3.766	1.302	1.991	2.809	5.347	2.089	2.138	2.130	2.266	2.448	2.083	2.061	2.138
${}^3TS_{5d}^{5a}$	2.750	3.670	1.291	2.003	2.914	5.559	2.122	2.164	2.122	2.263	2.128	2.246	2.128	2.124

Table S25: Selected atom spin densities of transition state of dimeristaion.

<b>Complex</b>	<b>Cu1'</b>	<b>O1</b>	<b>O2</b>	<b>Cu1</b>	<b>L'</b>	<b>L</b>
${}^3TS_{1d}^{1a}$	0.04	0.770	0.717	0.326	0.00	0.10
${}^3TS_{2d}^{2a}$	0.01	0.740	0.667	0.392	0.00	0.08
${}^3TS_{3d}^{3a}$	0.07	0.617	0.593	0.466	0.00	0.11
${}^3TS_{4d}^{4a}$	0.03	0.669	0.629	0.453	0.00	0.19
${}^3TS_{5d}^{5a}$	0.05	0.682	0.655	0.396	0.00	0.17

Table S26: Free energies and activation free energies of all reaction **R1-R15**

<b>Reaction</b>	$\Delta G_1^0$ (kJ/mol)	$\Delta G_2^0$ (kJ/mol)	$\Delta G_3^0$ (kJ/mol)	$\Delta G_2^\#$ (kJ/mol)	$\Delta G_3^\#$ (kJ/mol)	$\Delta G_2^\# - \Delta G_3^\#$ (kJ/mol)
<b>R1</b>	-5.1	16.0	41.6	86.4	55.8	30.6
<b>R2</b>	-12.9	1.5	39.9	80.6	60.6	20
<b>R3</b>	-13.0	-2.3	37.9	77.6	71.4	6.2
<b>R4</b>	-20.8	6.9	75.6	89.9	82	7.9
<b>R5</b>	-23.4	7.3	94.1	102.6	96.9	5.7
<b>R6</b>	-5.1	41.8	41.6	84.3	55.8	28.5
<b>R7</b>	-12.9	27.2	39.9	75.3	60.6	14.7
<b>R8</b>	-13.0	23.4	37.9	70.4	71.4	-1
<b>R9</b>	-20.8	32.6	75.6	78.2	82	-3.8
<b>R10</b>	-23.4	33.0	94.1	89.4	96.9	-7.5
<b>R11</b>	-5.1	67.1	41.6	97.2	55.8	41.4
<b>R12</b>	-12.9	52.6	39.9	92.0	60.6	31.4
<b>R13</b>	-13.0	48.8	37.9	86.6	71.4	15.2
<b>R14</b>	-20.8	57.9	75.6	94.2	82	12.2
<b>R15</b>	-23.4	58.4	94.1	106.3	96.9	9.4



Table S27: Vertical bond strength (D) and bond dissociation energies (BDE) of different reactions **R1-R15** (See Figure S26 and related data for description of all variables used here).

Reaction	$D_{H-X}(\text{kJ/mol})$	$D_{H-Y}(\text{kJ/mol})$	$BDE_{H-X}(\text{kJ/mol})$	$BDE_{H-Y}(\text{kJ/mol})$	$G_r(\text{kJ/mol})$	$G_p(\text{kJ/mol})$	$B_{XHY}(\text{kJ/mol})$	$\Delta E_{rp}(\text{kJ/mol})$	$\Delta E_{VB}^\#(1)(\text{kJ/mol})$	$\Delta E_{VB}^\#(2)(\text{kJ/mol})$
<b>R1</b>	337.5	363.5	305.2	318.0	727.0	675.0	155.8	16.0	62.5	62.7
<b>R2</b>	360.4	363.5	322.2	318.0	727.0	720.9	160.0	1.5	57.9	57.9
<b>R3</b>	357.6	363.5	322.8	318.0	727.0	715.2	160.2	-2.3	55.0	55.0
<b>R4</b>	362.7	363.5	316.7	318.0	727.0	725.3	158.7	6.9	62.6	62.6
<b>R5</b>	371.6	363.5	328.8	318.0	727.0	743.3	161.7	7.3	62.5	62.5
<b>R6</b>	337.5	378.7	305.2	344.4	757.4	675.0	162.4	41.8	73.3	74.5
<b>R7</b>	360.4	378.7	322.2	344.4	757.4	720.9	166.7	27.2	68.7	69.2
<b>R8</b>	357.6	378.7	322.8	344.4	757.4	715.2	166.8	23.4	70.4	70.8
<b>R9</b>	362.7	378.7	316.7	344.4	757.4	725.3	165.3	32.6	68.8	69.5
<b>R10</b>	371.6	378.7	328.8	344.4	757.4	743.3	168.3	33.0	73.3	74.0
<b>R11</b>	337.5	400.1	305.2	371.9	800.2	675.0	169.3	67.1	85.6	88.6
<b>R12</b>	360.4	400.1	322.2	371.9	800.2	720.9	173.5	52.6	80.9	82.8
<b>R13</b>	357.6	400.1	322.8	371.9	800.2	715.2	173.7	48.8	78.0	79.6
<b>R14</b>	362.7	400.1	316.7	371.9	800.2	725.3	172.1	57.9	85.7	87.9
<b>R15</b>	371.6	400.1	328.8	371.9	800.2	743.3	175.2	58.4	85.5	87.7

Table S28: Different Descriptors and target variables used in the regression model.

Feature index	Feature name
F01	$BV_{tot}$
F02	$\Sigma E$ ( kJ/mol)
F03	$\Delta E_{BDE}$ ( KJ/mol)
F04	$E_{FMO}$ ( eV)
F05	$\eta$ ( meV)
F06	$\lambda$ ( meV),
F07	$\Delta G_{ET}$ (kJ/mol)
F08	$\Delta G_{PT}$ (kJ/mol)
F09	$\Delta G_{PCET}$ (kJ/mol)
F10	$\Delta P_{eff}^{ka}$
F11	$\Delta E_{eff}^o$ [meV]
F12	$\Delta E^o(H)$ [meV]
F13	HB (kJ/mol)
F14	$J$ (cm <sup>-1</sup> )
F15	$\sigma$ (kJ/mol)
T02	$\Delta G_2^\#$ (kJ/mol)
T01	$\Delta G_{tot}^\#$ (kJ/mol)

F01 -  $BV_{tot}$  =%V Buried volume of catalyst+%V Buried volume of substrate,

F02-  $\Sigma E$  ( kJ/mol)=  $E_{BDE}^{catalyst} + E_{BDE}^{substrate}$  (where,  $E_{BDE}^{Cu-OOH}$   $E_{BDE}^{substrate}$  are BDE of copper hydroperoxo complex and BDE of substrate respectively )

F02- $\Delta E_{BDE}$  ( KJ/mol)= $E_{BDE}^{catalyst} - E_{BDE}^{substrate}$  (where,  $E_{BDE}^{Cu-OOH}$   $E_{BDE}^{substrate}$  are BDE of copper hydroperoxo complex and BDE of substrate respectively )

F04 -  $E_{FMO}$  ( eV) =  $E_{LUMO}$  (Alpha orbital) of catalyst +  $E_{HOMO}$  (Alpha orbital) of substrate

For details of F05-F09, See Figure S24 and related data.

For details of F10-F12 See Figure S26 and related data.

F13-HB (HB=strenth of H-bond interaction)

F14-  $J$  (cm<sup>-1</sup>) ( $J$ =Exchange coupling constant)

F15 -  $\sigma$  (kJ/mol) ( $\sigma = \Delta G_{PT} + \Delta G_{ET}$ )

T01-  $\Delta G_{tot}^\#$  (kJ/mol) ( $\Delta G_{tot}^\# = \Delta G_2^\# - \Delta G_3^\#$ )

Table S29: Different Descriptors values and target variables values at 298 K values used in the regression model .

<b>F00</b>	<b>F01</b>	<b>F02</b>	<b>F03</b>	<b>F04</b>	<b>F05</b>	<b>F06</b>	<b>F07</b>	<b>F08</b>	<b>F09</b>	<b>F10</b>	<b>F11</b>	<b>F12</b>	<b>F13</b>	<b>F14</b>	<b>F15</b>	<b>T02</b>	<b>T01</b>
<b>R1</b>	103.2	623.2	-12.8	-9.4	684.1	1339	193.5	286.9	16	-9.6	400.6	-166.3	-6.5	1697.4	480.4	86.4	30.6
<b>R2</b>	106.4	640.2	4.2	-9.4	976.5	1606.4	160.1	293.4	1.5	-11.8	682.5	-15.9	-14.5	1423.8	453.5	80.6	20
<b>R3</b>	108.9	640.8	4.8	-9.4	1058.5	1523.5	152.7	297.1	-2.3	-30.4	760.5	23.9	-23.6	1094.4	449.8	77.6	6.2
<b>R4</b>	107.8	634.7	-1.3	-9.5	809.2	1131.7	152.1	262.5	6.8	-10.3	536.6	-71.2	-27.6	1572.4	414.6	89.9	7.9
<b>R5</b>	113.3	646.8	10.8	-9.4	1027.5	1324.5	125.8	266	7.3	-12.9	688.7	-75.6	-17	1578.3	391.8	102.6	5.7
<b>R6</b>	77	649.6	-39.3	-9.6	482.1	1084.1	221.3	287.1	41.7	-9.4	124.5	-432.8	-6.5	1697.4	508.4	84.3	28.5
<b>R7</b>	80.2	666.6	-22.3	-9.6	774.5	497.5	187.9	293.6	27.2	-10	406.4	-282.4	-14.5	1423.8	481.5	75.3	14.7
<b>R8</b>	82.7	667.2	-21.7	-9.5	856.5	783.5	180.5	297.4	23.4	-12.3	484.4	-242.6	-23.6	1094.4	477.9	70.4	-1
<b>R9</b>	81.6	661.1	-27.7	-9.6	607.1	887.2	179.9	262.7	32.6	-10.1	260.5	-337.7	-27.6	1572.4	442.6	78.2	-3.8
<b>R10</b>	87.1	673.3	-15.6	-9.6	825.4	1691.4	153.6	266.2	33	-12.8	412.6	-342.1	-17	1578.3	419.8	89.4	-7.5
<b>R11</b>	77.1	677	-66.7	-10.2	-35.4	1160.8	283.6	278.7	67	-5.5	-372.8	-695.5	-6.5	1697.4	562.3	97.2	41.4
<b>R12</b>	80.3	694	-49.7	-10.2	256.9	1380.5	250.2	285.2	53	-7.7	-90.9	-545.1	-14.5	1423.8	535.4	92	31.4
<b>R13</b>	82.8	694.6	-49.1	-10.2	338.9	893.4	242.7	289	48.7	-8.3	-13	-600.5	-23.6	1094.4	531.7	86.6	15.2
<b>R14</b>	81.7	688.5	-55.2	-10.3	89.6	1098.6	242.1	254.3	58	-6.1	-236.9	-600.5	-27.6	1572.4	496.4	94.2	12.2
<b>R15</b>	87.2	700.7	-43	-10.2	307.9	1830.3	215.8	257.9	58.3	-8.8	-84.7	-604.8	-17	1578.3	473.7	106.3	9.4

Table S30: Different Regression models (to predict T01 using feature combination {F13+F09+F08+F07}) performance metrics for Target variable T01.

Regression Method (F13+F09+F08+F07)	R <sup>2</sup>		Mean Absolute Error (MAE)		Root Mean Square Error (RMSE)		R <sup>2</sup> Cross-validation 4
	Train	Test	Train	Test	Train	Test	
<b>Linear regression</b>	0.97	0.90	1.84	3.20	2.183	4.01	0.82
<b>Lasso</b>	0.97	0.91	1.92	3.15	2.22	3.91	0.85
<b>Ridge</b>	0.97	0.91	1.92	3.15	2.22	3.91	0.85
<b>Elastic net</b>	0.97	0.91	1.90	3.15	2.211	3.911	0.85

Table S31: Linear Regression model (to predict T01 using feature combination {F13+F09+F08+F07}) features coefficients and their p-values.

Features	Coefficient <sup>#</sup>	p-value	Coefficient*
F09	-0.8226	0.000	-18.7055
F08	-0.3075	0.023	-4.5758
F07	0.5055	0.000	21.8389
F13	1.0751	0.000	8.3484

# feature scaling was not performed

\* Feature scaling was performed using either min-max scaling or standard scaling techniques (both gave same coefficient values)

Normalization, also referred to as min-max scaling, reshapes features to a range spanning from 0 to 1. It involves subtracting the minimum value of the feature and dividing by the range (the maximum value minus the minimum value). Standardization alters features to possess a mean of 0 and a standard deviation of 1 by subtracting the mean and dividing by the standard deviation of the feature.

Table S32: Different Regression models features (to predict T02 using feature combination {F09+F07+F01}) performance metrics for Target variable T02.

Regression Method(F09+F07+F01)	R <sup>2</sup>		Mean Absolute Error (MAE)		Root Mean Square Error (RMSE)		R <sup>2</sup> Cross-validation 4
	Train	Test	Train	Test	Train	Test	
Linear regression	0.92	0.90	2.20	2.77	2.616	2.868	0.36
Lasso	0.92	0.89	2.16	2.90	2.627	3.034	0.34
Ridge	0.92	0.90	2.20	2.78	2.616	2.88	0.36
Elastic net	0.92	0.890	2.16	2.90	2.62	3.031	0.36

Table S33: Linear Regression model features (to predict T02 using feature combination {F09+F07+F01}) coefficients and their p-values.

Features	Coefficient <sup>#</sup>	p-value	Coefficient <sup>*</sup>
F01	1.0715	0	14.39113
F07	-0.1249	0.02	-5.3942
F09	0.9374	0	21.31591

# feature scaling was not performed

\* Feature scaling was performed using either min-max scaling or standard scaling techniques (both gave same coefficient values)

Table S34: Selected bond lengths of optimised catalyst **1a** and analogue complex crystal

Complex	Cu-O1	Cu-O2	O1-O2
[TMG <sub>3</sub> trenCu(O <sub>2</sub> )] <sup>+</sup> <sub>31</sub>	1.927	2.842	1.280
{ <sup>(X1)(X2)</sup> LCu(II)-O <sub>2</sub> <sup>•-</sup> }	2.030	2.788	1.256
[X1=H, X2=H ( <b>1a</b> )] structre [Å]			

Table S35: Singlet-triplet gaps of **1a-5a** with different functionals (single point calculations with different functionals were performed on on B3-LYP optimized geometries of catalysts **1a-5a**)

Complex	$\Delta G_{S-T}$					
	PBE/BSII/ /B3LYP/B S1	BP86/BSII //B3LYP/B S1	PBE0/BSII //B3LYP/B S1	TPSSH/BSI I//B3LYP/B S1	$\omega$ - B97X/BSII //B3LYP/B S1	B3LYP/BSI I//B3LYP/B S1
<b>1a</b>	22.3	24.1	113.7	103.4	126.3	100.5
<b>2a</b>	22.3	24.1	110.0	86.2	120.3	96.2
<b>3a</b>	18.6	26.4	117.6	88.3	137.6	100.8
<b>4a</b>	20.0	21.5	107.7	80.9	122.0	93.5
<b>5a</b>	24.3	30.4	121.2	90.8	134.6	105.8

$\Delta G_{S-T} = G_S - G_T$ ;  $G_T$  and  $G_{S_m}$  are Gibbs free energy of triplet and singlet species respectively.

BSII refers to TZVP(for all atoms) and BSI refers to [LanL2Dz (Cu),6-31G\*(others)] All functionals dispersion corrected)

Table S36: Singlet-triplet gaps for **1a-5a** (single point calculations with different functionals were performed on with respective functional optimized geometries of catalysts **1a-5a**)

Complex	$\Delta G_{S-T}$					
	PBE/BSII/ /PBE/BSI	BP86/BSII/ /BP86/BSI	PBE0/BSII/ /PBE0/BSI	TPSSH/BSII/ /TPSSH/BSI	$\omega$ - B97X/ BSII// $\omega$ - B97X/ BSI	B3LYP/BSII/ /B3LYP/BSI
<b>1a</b>	22.1	24.9	118.6	88.0	125.5	100.5
<b>2a</b>	19.4	18.2	103.7	78.0	109.7	96.2
<b>3a</b>	22.5	16.4	116.2	80.4	113.8	100.8
<b>4a</b>	18.2	18.7	103.7	79.1	18.0	93.5
<b>5a</b>	23.0	30.5	126.4	91.9	144.5	105.8

$\Delta G_{S-T} = G_S - G_T$ ;  $G_T$  and  $G_S$  are Gibbs free energy of triplet and singlet species respectively.



Table S37: Activation energies of reactions **R1-R5** (single point calculations with different functionals were performed on B3-LYP optimized geometries and transition states)

Reaction	$\Delta G_2^\ddagger$					
	PBE/BSII/ /B3LYP/B S1	BP86/BSII //B3LYP/B S1	PBE0/BSII //B3LYP/B S1	TPSSH/BSI I//B3LYP/B S1	$\omega$ B97X/BSI I//B3LYP/B S1	B3LYP/BSI I//B3LYP/B S1
<b>R1</b>	50.9	59.2	88.3	80.5	125.2	86.4
<b>R2</b>	46.6	54.5	82.4	72.3	118.0	80.6
<b>R3</b>	41.6	49.9	79.1	68.3	82.6	77.6
<b>R4</b>	51.9	63.1	91.7	80.6	126.3	89.9
<b>R5</b>	62.9	75.6	105.7	92.2	121.2	102.6

BSII refers to TZVP(for all atoms) and BSI refers to [LanL2Dz (Cu),6-31G\*(others)]

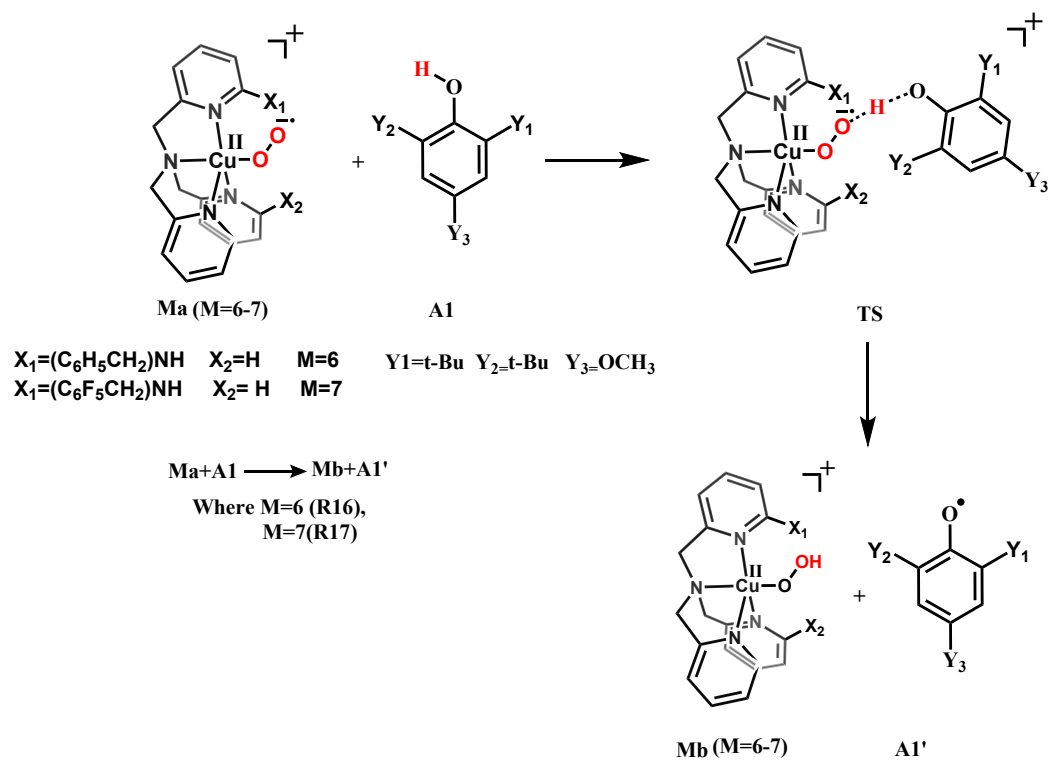


Figure S28: Different catalyst structures (**6a-7a**) which was not seen during model

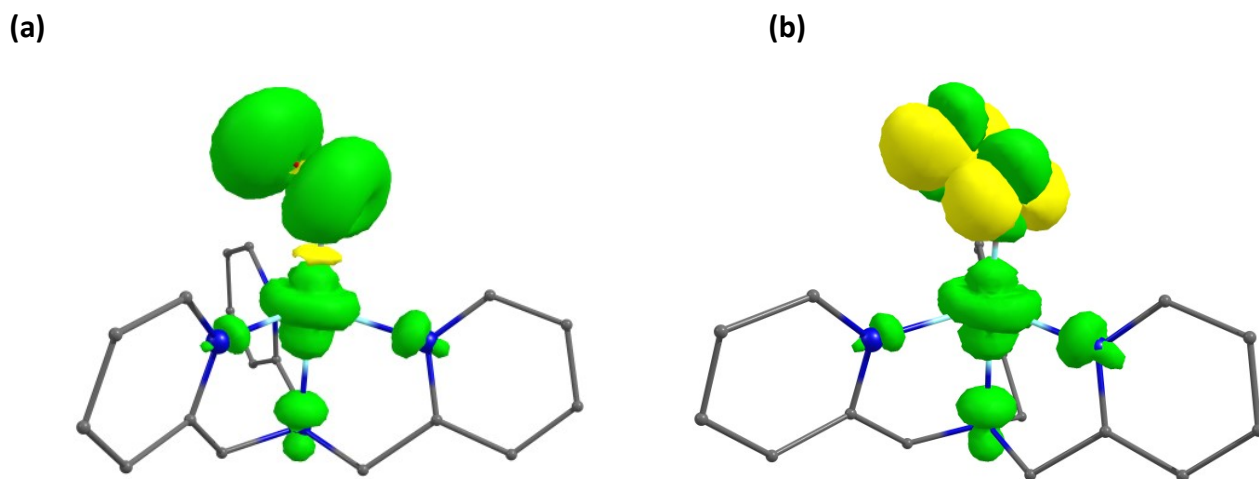


Figure S29: spin density plots of catalyst structures (**1a**) computed at DLPNO-CCSD(T) level

Table S38: Free energies and activation free energies of two unseen HAT reactions **R16-R17**.

Reaction	$\Delta G_1^0$ (kJ/mol)	$\Delta G_2^0$ (kJ/mol)	$\Delta G_3^0$ (kJ/mol)	$\Delta G_2^\#$ (kJ/mol)	$\Delta G_3^\#$ (kJ/mol)	$\Delta G_{2-3}^\#$ (kJ/mol)
R16	-10.7	-0.9	40.9	81.2	71.4	9.8
R17	-4.9	-0.8	42.7	90.0	86.2	3.8

Table S39: Different Descriptors values for reactions **R16-R17**.

Features	Reaction	
	<b>R6</b>	<b>R7</b>
F13	-39.8	-40.7
F08	275.9	294.1
F07	168.2	164.8
F09	-0.9	-0.8

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## Coordinates

### <sup>3</sup>1a

Cu	0.019014000	-0.012897000	-0.706634000
C	2.950340000	-0.855255000	-1.320470000
H	2.567989000	-0.935319000	-2.333947000
C	4.261549000	-1.205035000	-1.008089000
H	4.927473000	-1.566033000	-1.784462000
C	4.682979000	-1.086595000	0.315862000
H	5.694937000	-1.358073000	0.600903000
C	3.783493000	-0.617599000	1.274052000
H	4.080493000	-0.515148000	2.313435000
C	2.490707000	-0.273013000	0.879971000
C	1.493495000	0.331366000	1.856857000
H	1.755713000	0.051840000	2.888548000
H	1.577313000	1.423335000	1.794455000
C	-0.263696000	-1.392763000	1.909812000
H	-0.547962000	-1.462463000	2.970740000
H	0.628934000	-2.016771000	1.779360000
C	-1.371109000	-1.957341000	1.032785000
C	-2.293481000	-2.879495000	1.526556000
H	-2.265062000	-3.170322000	2.572373000
C	-3.243592000	-3.420434000	0.659293000
H	-3.968951000	-4.142229000	1.022503000
C	-3.251000000	-3.013851000	-0.674096000
H	-3.974793000	-3.404193000	-1.381428000
C	-2.306719000	-2.077259000	-1.088148000
C	-0.875135000	0.992360000	1.958447000
H	-0.704340000	1.312215000	2.997456000
H	-1.864988000	0.521096000	1.931517000
C	-0.904079000	2.201058000	1.034842000
C	-1.218179000	3.473944000	1.510961000
H	-1.387163000	3.631313000	2.572008000
C	-1.316749000	4.532024000	0.606597000
H	-1.562538000	5.530338000	0.955845000
C	-1.091084000	4.287711000	-0.747403000
H	-1.156842000	5.080364000	-1.484926000
C	-0.767466000	2.991950000	-1.142293000
N	2.085346000	-0.400112000	-0.399569000

N	0.102799000	-0.019636000	1.525938000
N	-1.385574000	-1.563633000	-0.257140000
N	-0.675138000	1.971762000	-0.273899000
O	0.125267000	0.010927000	-2.734168000
O	-0.994292000	0.020109000	-3.304332000
H	-2.277537000	-1.713949000	-2.111179000
H	-0.575577000	2.750429000	-2.183334000

**'1a**

Cu	0.027681000	-0.014310000	-0.704570000
C	2.958673000	-0.828452000	-1.324895000
H	2.571356000	-0.909751000	-2.336355000
C	4.274983000	-1.161688000	-1.015144000
H	4.944094000	-1.512836000	-1.793245000
C	4.697877000	-1.039740000	0.308161000
H	5.714026000	-1.298854000	0.589800000
C	3.796175000	-0.583154000	1.270799000
H	4.095646000	-0.478073000	2.309182000
C	2.498692000	-0.254812000	0.879813000
C	1.490660000	0.337465000	1.851328000
H	1.740510000	0.053624000	2.884363000
H	1.565318000	1.430332000	1.795460000
C	-0.251112000	-1.402430000	1.894696000
H	-0.528609000	-1.466425000	2.957265000
H	0.646001000	-2.019293000	1.761988000
C	-1.358458000	-1.973065000	1.023246000
C	-2.271439000	-2.906182000	1.512695000
H	-2.238106000	-3.206493000	2.555670000
C	-3.219650000	-3.445990000	0.642055000
H	-3.938403000	-4.176731000	1.000536000
C	-3.234621000	-3.027382000	-0.687590000
H	-3.957994000	-3.417195000	-1.395623000
C	-2.299401000	-2.079517000	-1.097445000
C	-0.883933000	0.977283000	1.948835000
H	-0.708647000	1.287202000	2.989571000
H	-1.869298000	0.497068000	1.922155000
C	-0.924726000	2.190609000	1.033103000
C	-1.257186000	3.458399000	1.509347000
H	-1.432393000	3.614020000	2.569630000

C	-1.366546000	4.514422000	0.603303000
H	-1.626785000	5.509489000	0.951367000
C	-1.133985000	4.273348000	-0.750228000
H	-1.209145000	5.065366000	-1.487506000
C	-0.791440000	2.982290000	-1.145229000
N	2.093160000	-0.386296000	-0.398670000
N	0.103484000	-0.024695000	1.503529000
N	-1.380454000	-1.568737000	-0.262690000
N	-0.688325000	1.965706000	-0.274434000
O	0.139929000	0.020015000	-2.679392000
O	-1.008162000	0.019435000	-3.227683000
H	-2.273080000	-1.702363000	-2.115434000
H	-0.593839000	2.740039000	-2.184936000

**<sup>3</sup>2a**

Cu	-0.064526000	0.023364000	0.622260000
C	-0.084974000	3.035434000	1.385879000
H	-0.181842000	2.635592000	2.390883000
C	-0.110297000	4.405582000	1.139293000
H	-0.224288000	5.103476000	1.961740000
C	0.005226000	4.845734000	-0.178934000
H	-0.018745000	5.905953000	-0.412190000
C	0.146504000	3.904122000	-1.198940000
H	0.235016000	4.215062000	-2.235508000
C	0.177871000	2.549004000	-0.871064000
C	0.415844000	1.474297000	-1.918767000
H	0.104924000	1.831335000	-2.911756000
H	1.494233000	1.282192000	-1.973790000
C	-1.683668000	0.193336000	-1.844041000
H	-1.892331000	-0.004694000	-2.906255000
H	-2.065497000	1.198269000	-1.625695000
C	-2.424688000	-0.802613000	-0.966939000
C	-3.580776000	-1.447571000	-1.405164000
H	-3.946227000	-1.282996000	-2.414294000
C	-4.255225000	-2.298653000	-0.528829000
H	-5.158902000	-2.809148000	-0.847926000
C	-3.747445000	-2.487994000	0.755827000
H	-4.237285000	-3.144048000	1.467307000
C	-2.579963000	-1.818089000	1.114061000



H	-2.136110000	-1.938014000	2.097867000
C	0.463284000	-0.980908000	-2.099268000
H	0.673106000	-0.876822000	-3.173746000
H	-0.213769000	-1.835450000	-1.984286000
C	1.743199000	-1.275564000	-1.340253000
C	2.877612000	-1.707548000	-2.005630000
H	2.884985000	-1.789743000	-3.087037000
C	4.008388000	-2.044092000	-1.242272000
H	4.915006000	-2.390206000	-1.729598000
C	3.958776000	-1.938456000	0.130914000
H	4.812729000	-2.198592000	0.748294000
C	2.766485000	-1.479418000	0.743699000
N	0.057558000	2.130107000	0.404634000
N	-0.237150000	0.201866000	-1.563753000
N	-1.934963000	-0.992994000	0.274419000
N	1.683225000	-1.141076000	0.009090000
N	2.693857000	-1.331048000	2.097415000
H	1.781158000	-1.310823000	2.535351000
O	-0.201896000	0.157638000	2.623349000
O	-0.148219000	-0.952767000	3.230225000
H	3.431405000	-1.735492000	2.656454000
<b>!2a</b>			
Cu	-0.065924000	0.006579000	0.624237000
C	-0.137000000	3.022282000	1.396020000
H	-0.223771000	2.619209000	2.400899000
C	-0.191113000	4.392731000	1.155626000
H	-0.318457000	5.084851000	1.981015000
C	-0.086502000	4.839978000	-0.161043000
H	-0.132787000	5.900242000	-0.390685000
C	0.073121000	3.904581000	-1.183780000
H	0.154153000	4.220662000	-2.219434000
C	0.132996000	2.548776000	-0.861373000
C	0.393182000	1.486677000	-1.917590000
H	0.083029000	1.850873000	-2.908563000
H	1.475048000	1.313705000	-1.968414000
C	-1.683670000	0.168568000	-1.857715000
H	-1.893515000	-0.038112000	-2.918377000
H	-2.081715000	1.168143000	-1.643602000
C	-2.410702000	-0.833342000	-0.974984000

C	-3.559591000	-1.493490000	-1.410026000
H	-3.926204000	-1.337149000	-2.420046000
C	-4.225254000	-2.348344000	-0.530846000
H	-5.122929000	-2.870227000	-0.848471000
C	-3.716460000	-2.526449000	0.755012000
H	-4.199519000	-3.184443000	1.469332000
C	-2.556423000	-1.842355000	1.110450000
H	-2.111808000	-1.952495000	2.095607000
C	0.484473000	-0.967634000	-2.108183000
H	0.698766000	-0.864702000	-3.182265000
H	-0.177308000	-1.834353000	-1.994318000
C	1.767581000	-1.239022000	-1.344341000
C	2.910862000	-1.649294000	-2.008873000
H	2.920125000	-1.730558000	-3.090344000
C	4.047689000	-1.964190000	-1.245979000
H	4.960635000	-2.293472000	-1.733137000
C	3.996004000	-1.858105000	0.127205000
H	4.854946000	-2.101229000	0.744647000
C	2.795647000	-1.420778000	0.739507000
N	0.022588000	2.122521000	0.412921000
N	-0.239344000	0.201761000	-1.579716000
N	-1.919853000	-1.014264000	0.267602000
N	1.705251000	-1.106006000	0.005354000
N	2.726648000	-1.269295000	2.094574000
H	1.819391000	-1.269230000	2.542835000
O	-0.158576000	0.1111707000	2.629430000
O	-0.168711000	-0.996587000	3.227179000
H	3.475927000	-1.659984000	2.647914000

**<sup>3</sup>a**

Cu	-0.009463000	0.088869000	0.550146000
C	1.822902000	2.594010000	1.194653000
H	1.523199000	2.394473000	2.218021000
C	2.627572000	3.684396000	0.874073000
H	2.965565000	4.357389000	1.654685000
C	2.973927000	3.886359000	-0.461512000
H	3.592615000	4.730222000	-0.751622000
C	2.510098000	2.989678000	-1.424459000

H	2.760385000	3.118404000	-2.473124000
C	1.719167000	1.914050000	-1.021773000
C	1.250728000	0.852548000	-2.000101000
H	1.193617000	1.263394000	-3.018655000
H	1.994722000	0.047561000	-2.020348000
C	-1.187099000	1.129303000	-1.880226000
H	-1.433726000	1.121303000	-2.951872000
H	-0.890962000	2.153588000	-1.623185000
C	-2.400149000	0.741891000	-1.058805000
C	-3.675921000	0.846115000	-1.582687000
H	-3.827648000	1.169842000	-2.606522000
C	-4.762486000	0.525467000	-0.750976000
H	-5.779131000	0.602457000	-1.124748000
C	-4.531527000	0.108374000	0.541295000
H	-5.350032000	-0.150009000	1.205555000
C	-3.196593000	0.007664000	1.008282000
C	-0.214191000	-1.122571000	-2.083844000
H	-0.019280000	-1.188672000	-3.163877000
H	-1.266881000	-1.385213000	-1.929983000
C	0.653456000	-2.112106000	-1.330763000
C	1.143211000	-3.238179000	-1.968169000
H	0.959256000	-3.397359000	-3.025086000
C	1.868103000	-4.169835000	-1.205877000
H	2.258543000	-5.071133000	-1.668993000
C	2.091753000	-3.927638000	0.131052000
H	2.656286000	-4.622896000	0.744187000
C	1.586307000	-2.736730000	0.712711000
N	1.378221000	1.728852000	0.268872000
N	-0.033361000	0.255546000	-1.586729000
N	-2.150529000	0.326783000	0.209932000
N	0.862278000	-1.851981000	-0.014165000
N	1.801782000	-2.469766000	2.025333000
H	1.619216000	-1.546542000	2.403005000
O	-0.131859000	0.276011000	2.523234000
O	0.944378000	0.110749000	3.193469000
H	2.439269000	-3.054295000	2.544514000
N	-2.938276000	-0.451541000	2.262745000
H	-2.028012000	-0.281321000	2.671783000
H	-3.709078000	-0.534487000	2.909259000

**13a**

Cu	-0.026563000	0.086297000	0.539238000
C	1.632771000	2.698683000	1.182995000
H	1.342330000	2.480976000	2.205367000
C	2.368937000	3.835749000	0.859358000
H	2.662855000	4.531299000	1.637980000
C	2.705487000	4.054477000	-0.476182000
H	3.270788000	4.934707000	-0.767146000
C	2.303033000	3.127522000	-1.438515000
H	2.549124000	3.268337000	-2.486579000
C	1.580511000	2.006155000	-1.033336000
C	1.183501000	0.907897000	-2.001344000
H	1.091370000	1.302105000	-3.023280000
H	1.978967000	0.154121000	-2.017319000
C	-1.268653000	1.022348000	-1.889943000
H	-1.505556000	0.977298000	-2.962364000
H	-1.040911000	2.067996000	-1.650399000
C	-2.454758000	0.570349000	-1.064433000
C	-3.735946000	0.589886000	-1.583043000
H	-3.912466000	0.888592000	-2.610450000
C	-4.796936000	0.217831000	-0.738441000
H	-5.818322000	0.227393000	-1.106992000
C	-4.535275000	-0.161333000	0.559064000
H	-5.333929000	-0.454500000	1.232962000
C	-3.194190000	-0.174502000	1.022228000
C	-0.147884000	-1.163121000	-2.066111000
H	0.042208000	-1.216786000	-3.147275000
H	-1.178526000	-1.496694000	-1.901777000
C	0.796545000	-2.079123000	-1.314501000
C	1.356182000	-3.178230000	-1.939461000
H	1.168914000	-3.371966000	-2.989979000
C	2.158124000	-4.039587000	-1.169711000
H	2.604276000	-4.920709000	-1.621206000
C	2.386332000	-3.753703000	0.157079000
H	3.010296000	-4.393240000	0.773226000
C	1.807400000	-2.588506000	0.726078000
N	1.247114000	1.806370000	0.256840000
N	-0.059639000	0.229739000	-1.576501000
N	-2.173704000	0.189894000	0.208500000

N	1.005172000	-1.777525000	-0.006894000
N	2.036389000	-2.268916000	2.020193000
H	1.752593000	-1.369697000	2.401723000
O	-0.167430000	0.246428000	2.485306000
O	0.931874000	0.163019000	3.162254000
H	2.693674000	-2.814624000	2.556031000
N	-2.902841000	-0.587174000	2.282700000
H	-1.997758000	-0.362010000	2.680894000
H	-3.663672000	-0.714255000	2.933638000

**<sup>3</sup>4a**

Cu	0.829764000	0.027513000	-0.441331000
C	0.866289000	2.981859000	-1.391416000
H	0.467421000	2.548346000	-2.303796000
C	1.156134000	4.340384000	-1.294495000
H	0.981729000	4.994762000	-2.141740000
C	1.678418000	4.824720000	-0.095503000
H	1.925437000	5.876230000	0.015457000
C	1.886796000	3.937845000	0.961625000
H	2.295588000	4.283349000	1.906331000
C	1.558598000	2.593096000	0.792757000
C	1.679545000	1.588401000	1.927100000
H	2.424078000	1.929021000	2.661996000
H	0.715459000	1.543814000	2.447920000
C	3.382503000	0.042038000	1.048395000
H	4.024374000	-0.146443000	1.922149000
H	3.727008000	0.980390000	0.596714000
C	3.542472000	-1.072235000	0.026530000
C	4.695678000	-1.853883000	-0.032214000
H	5.490067000	-1.707806000	0.693482000
C	4.810322000	-2.818063000	-1.034654000
H	5.700422000	-3.436437000	-1.100653000
C	3.763956000	-2.979107000	-1.941832000
H	3.809076000	-3.719509000	-2.733222000
C	2.639279000	-2.168007000	-1.809476000
H	1.792582000	-2.260210000	-2.482867000
C	1.471015000	-0.833362000	2.320976000
H	1.753806000	-0.658609000	3.369603000
H	1.955594000	-1.767153000	2.012242000

C	-0.032574000	-1.018021000	2.210472000
C	-0.781666000	-1.401693000	3.315123000
H	-0.312625000	-1.510354000	4.287289000
C	-2.141694000	-1.675148000	3.131850000
H	-2.749677000	-2.018229000	3.963600000
C	-2.703966000	-1.533803000	1.874424000
H	-3.738541000	-1.794216000	1.692062000
C	-1.899182000	-1.078237000	0.812919000
C	-3.689772000	-0.802345000	-1.001404000
N	1.061197000	2.130079000	-0.371795000
N	1.972976000	0.231096000	1.435043000
N	2.531547000	-1.234776000	-0.850433000
N	-0.579070000	-0.842145000	0.986381000
N	-2.373738000	-0.912459000	-0.478133000
H	-1.731762000	-1.226348000	-1.210296000
O	-3.907506000	-1.376505000	-2.051079000
C	-4.746430000	0.151653000	-0.390005000
C	-5.237994000	1.015249000	-1.581760000
H	-5.602427000	0.385862000	-2.395441000
H	-6.048436000	1.671009000	-1.246171000
H	-4.430904000	1.646211000	-1.972328000
C	-4.229851000	1.103627000	0.704403000
H	-4.008729000	0.602696000	1.649924000
H	-3.330348000	1.638468000	0.378360000
H	-5.000904000	1.853014000	0.913157000
C	-5.937668000	-0.690477000	0.122226000
H	-6.298422000	-1.362466000	-0.661794000
H	-5.679788000	-1.296087000	0.999127000
H	-6.759375000	-0.027601000	0.414219000
O	0.094618000	0.026841000	-2.314412000
O	-0.450300000	-1.068972000	-2.632059000
<b>4a</b>			
Cu	-0.840914000	0.023094000	0.446976000
C	-0.838693000	2.961445000	1.423434000
H	-0.448518000	2.507817000	2.329759000
C	-1.109940000	4.324870000	1.341120000
H	-0.928413000	4.967219000	2.196006000
C	-1.623585000	4.830232000	0.146893000
H	-1.855843000	5.886349000	0.048482000

C	-1.843005000	3.959904000	-0.922062000
H	-2.245456000	4.322881000	-1.862902000
C	-1.533285000	2.609306000	-0.767938000
C	-1.662728000	1.614002000	-1.908185000
H	-2.411449000	1.956983000	-2.637057000
H	-0.701958000	1.568597000	-2.434744000
C	-3.375185000	0.068507000	-1.046806000
H	-4.008131000	-0.101248000	-1.930317000
H	-3.715818000	1.002625000	-0.583717000
C	-3.547685000	-1.060467000	-0.044662000
C	-4.706286000	-1.834005000	0.003996000
H	-5.501024000	-1.672046000	-0.717883000
C	-4.825260000	-2.811413000	0.993489000
H	-5.719603000	-3.424359000	1.052429000
C	-3.778925000	-2.992664000	1.896866000
H	-3.828892000	-3.743579000	2.677949000
C	-2.647818000	-2.188497000	1.775247000
H	-1.799151000	-2.292308000	2.444520000
C	-1.465318000	-0.804525000	-2.323534000
H	-1.761029000	-0.616292000	-3.365808000
H	-1.945952000	-1.741284000	-2.018282000
C	0.038511000	-0.983326000	-2.227006000
C	0.788151000	-1.324167000	-3.344608000
H	0.318692000	-1.406076000	-4.319166000
C	2.151460000	-1.590372000	-3.171348000
H	2.761896000	-1.899567000	-4.014503000
C	2.712844000	-1.487407000	-1.910215000
H	3.749655000	-1.745846000	-1.737022000
C	1.904533000	-1.077085000	-0.832110000
C	3.699932000	-0.867778000	0.981893000
N	-1.044150000	2.127364000	0.391657000
N	-1.958669000	0.252808000	-1.420161000
N	-2.537157000	-1.243682000	0.828372000
N	0.583492000	-0.842695000	-0.997653000
N	2.379703000	-0.959599000	0.463319000
H	1.744065000	-1.314384000	1.178905000
O	3.934362000	-1.498831000	1.993988000
C	4.738143000	0.133919000	0.417419000
C	5.204238000	0.954888000	1.648982000

H	5.579165000	0.298065000	2.435844000
H	6.001108000	1.642931000	1.347096000
H	4.380963000	1.549284000	2.062423000
C	4.207660000	1.121107000	-0.638079000
H	3.996667000	0.655291000	-1.603783000
H	3.299027000	1.627458000	-0.292531000
H	4.966671000	1.890873000	-0.814608000
C	5.948778000	-0.660154000	-0.124596000
H	6.317088000	-1.361904000	0.629163000
H	5.707464000	-1.227527000	-1.031477000
H	6.759574000	0.031254000	-0.378520000
O	-0.112173000	0.027084000	2.279954000
O	0.314553000	-1.121780000	2.639754000

**<sup>3</sup>5a**

Cu	0.040605000	0.796187000	0.212760000
C	0.726192000	1.950236000	3.021681000
H	0.372613000	0.979711000	3.356664000
C	1.135046000	2.931473000	3.921049000
H	1.105490000	2.736605000	4.987606000
C	1.569701000	4.157066000	3.416401000
H	1.888221000	4.949246000	4.087215000
C	1.585346000	4.356765000	2.035295000
H	1.915133000	5.300630000	1.611960000
C	1.172689000	3.321073000	1.198125000
C	1.233959000	3.429292000	-0.315126000
H	1.169632000	4.481331000	-0.629779000
H	2.208230000	3.053948000	-0.650116000
C	-1.143229000	3.217511000	-0.885741000
H	-1.247543000	4.047990000	-1.599262000
H	-1.250191000	3.641167000	0.120123000
C	-2.242507000	2.196828000	-1.108990000
C	-3.397722000	2.548687000	-1.790473000
H	-3.511519000	3.545123000	-2.203522000
C	-4.394232000	1.577604000	-1.948456000
H	-5.296911000	1.802172000	-2.508639000
C	-4.205891000	0.315735000	-1.418440000
H	-4.931452000	-0.469773000	-1.580774000
C	-3.022678000	0.037369000	-0.700848000



C	0.556901000	2.188603000	-2.330247000
H	0.908241000	3.039469000	-2.931747000
H	-0.356526000	1.814816000	-2.806856000
C	1.594215000	1.082114000	-2.333374000
C	2.540238000	1.009266000	-3.346888000
H	2.582313000	1.774267000	-4.114923000
C	3.406861000	-0.088892000	-3.367119000
H	4.129483000	-0.204814000	-4.169285000
C	3.319848000	-1.042509000	-2.368414000
H	3.939553000	-1.929418000	-2.387634000
C	2.381455000	-0.869361000	-1.332195000
C	3.084893000	-2.816330000	0.179206000
N	0.746089000	2.142597000	1.693169000
N	0.195876000	2.604385000	-0.962403000
N	-2.045455000	0.968182000	-0.573386000
N	1.514713000	0.170953000	-1.336117000
N	2.241470000	-1.773199000	-0.294301000
H	1.275758000	-1.954354000	-0.014083000
O	2.537065000	-3.850894000	0.505657000
C	4.593286000	-2.598484000	0.460209000
C	4.799780000	-3.088010000	1.918261000
H	4.458570000	-4.118016000	2.035425000
H	5.863450000	-3.032201000	2.173560000
H	4.246713000	-2.461913000	2.628178000
C	5.081289000	-1.140907000	0.375631000
H	5.113006000	-0.749314000	-0.643955000
H	4.457966000	-0.473863000	0.982354000
H	6.101615000	-1.086657000	0.770071000
C	5.412028000	-3.516188000	-0.476926000
H	5.052124000	-4.547281000	-0.415343000
H	5.365465000	-3.199704000	-1.525585000
H	6.465954000	-3.499888000	-0.178814000
O	-0.101202000	-0.652794000	1.568192000
O	-0.285212000	-1.806426000	1.066765000
N	-2.763517000	-1.198714000	-0.151414000
H	-1.778045000	-1.456862000	-0.096235000
C	-3.568414000	-2.366519000	0.018856000
C	-4.953039000	-2.323308000	0.709606000
C	-6.035019000	-2.761667000	-0.304730000

H	-5.761142000	-3.711972000	-0.772305000
H	-6.990642000	-2.895199000	0.213585000
H	-6.197378000	-2.024168000	-1.099592000
C	-5.314508000	-0.980602000	1.370021000
H	-4.520519000	-0.640435000	2.044109000
H	-5.522147000	-0.181602000	0.654186000
H	-6.220877000	-1.114456000	1.970088000
C	-4.872956000	-3.400020000	1.824719000
H	-4.121945000	-3.135175000	2.577589000
H	-5.844107000	-3.475331000	2.325267000
H	-4.609779000	-4.374051000	1.408513000
O	-3.040874000	-3.424863000	-0.258548000

**15a**

Cu	0.026617000	0.805494000	0.225622000
C	0.816392000	2.011656000	2.982213000
H	0.443613000	1.058865000	3.345751000
C	1.282042000	3.000116000	3.845594000
H	1.279842000	2.829884000	4.916752000
C	1.737206000	4.200658000	3.300271000
H	2.099831000	4.996944000	3.943266000
C	1.716295000	4.370840000	1.915044000
H	2.060841000	5.294893000	1.460919000
C	1.247242000	3.329920000	1.115351000
C	1.262100000	3.396467000	-0.400489000
H	1.204624000	4.439347000	-0.744547000
H	2.216938000	2.992509000	-0.756962000
C	-1.135927000	3.221224000	-0.886250000
H	-1.236038000	4.043780000	-1.609275000
H	-1.205320000	3.662086000	0.115464000
C	-2.264193000	2.224963000	-1.068340000
C	-3.448392000	2.608554000	-1.679186000
H	-3.569114000	3.615350000	-2.064272000
C	-4.466099000	1.654874000	-1.804396000
H	-5.395350000	1.905723000	-2.306983000
C	-4.265273000	0.375789000	-1.321851000
H	-5.007573000	-0.397218000	-1.467683000
C	-3.047659000	0.062913000	-0.680902000
C	0.495005000	2.120709000	-2.359901000
H	0.834803000	2.954596000	-2.990590000

H	-0.437752000	1.746443000	-2.796056000
C	1.521187000	1.004884000	-2.367254000
C	2.436626000	0.898168000	-3.405061000
H	2.461119000	1.641321000	-4.194989000
C	3.296335000	-0.205895000	-3.418865000
H	3.994641000	-0.349265000	-4.237936000
C	3.233792000	-1.129146000	-2.390730000
H	3.848775000	-2.019564000	-2.401503000
C	2.326403000	-0.921581000	-1.332648000
C	3.077032000	-2.824916000	0.206170000
N	0.801977000	2.176642000	1.650107000
N	0.186222000	2.572985000	-0.989130000
N	-2.057533000	0.982068000	-0.572036000
N	1.463656000	0.122128000	-1.342876000
N	2.216667000	-1.793592000	-0.265705000
H	1.260645000	-1.966877000	0.047033000
O	2.544437000	-3.856098000	0.565239000
C	4.590372000	-2.591640000	0.445758000
C	4.830817000	-3.034409000	1.913609000
H	4.497683000	-4.061954000	2.069340000
H	5.899446000	-2.965708000	2.144132000
H	4.289498000	-2.389247000	2.615440000
C	5.069370000	-1.135770000	0.303634000
H	5.074314000	-0.777664000	-0.728695000
H	4.457816000	-0.452090000	0.903764000
H	6.098800000	-1.065026000	0.671034000
C	5.391918000	-3.534765000	-0.480766000
H	5.035982000	-4.564254000	-0.381524000
H	5.322239000	-3.248823000	-1.536974000
H	6.451870000	-3.507729000	-0.205683000
O	-0.162521000	-0.542211000	1.641692000
O	-0.306791000	-1.750903000	1.244917000
N	-2.765827000	-1.195824000	-0.199122000
H	-1.782817000	-1.456254000	-0.217898000
C	-3.564346000	-2.367632000	-0.023694000
C	-4.906281000	-2.344837000	0.746399000
C	-6.046935000	-2.739742000	-0.220461000
H	-5.808853000	-3.675498000	-0.734654000
H	-6.973464000	-2.883366000	0.345729000

H	-6.245914000	-1.974135000	-0.979771000
C	-5.221035000	-1.025940000	1.475644000
H	-4.387757000	-0.714554000	2.115238000
H	-5.464695000	-0.200052000	0.802692000
H	-6.092545000	-1.178460000	2.121171000
C	-4.768712000	-3.462876000	1.814318000
H	-3.974517000	-3.228292000	2.531885000
H	-5.710338000	-3.553782000	2.365992000
H	-4.534743000	-4.421398000	1.347690000
O	-3.058406000	-3.415317000	-0.371630000

<sup>3</sup>RC<sub>R1</sub>

Cu	2.352820000	0.118999000	-0.323782000
C	3.578308000	2.695883000	-1.594221000
H	2.987092000	2.383199000	-2.449965000
C	4.420440000	3.803423000	-1.657054000
H	4.497942000	4.376415000	-2.574845000
C	5.156764000	4.142509000	-0.522550000
H	5.831187000	4.993469000	-0.533974000
C	5.019280000	3.368539000	0.630331000
H	5.579836000	3.605140000	1.529756000
C	4.144780000	2.281825000	0.618030000
C	3.885882000	1.451001000	1.865252000
H	4.729651000	1.544943000	2.565871000
H	3.005636000	1.863889000	2.372939000
C	4.775945000	-0.740517000	1.186694000
H	5.306603000	-1.116598000	2.074711000
H	5.468607000	-0.067250000	0.666749000
C	4.442926000	-1.892796000	0.250858000
C	5.169352000	-3.082911000	0.277295000
H	5.955517000	-3.223021000	1.013101000
C	4.874131000	-4.080550000	-0.652606000
H	5.429591000	-5.013612000	-0.650492000
C	3.852811000	-3.862177000	-1.575612000
H	3.585852000	-4.611207000	-2.313361000
C	3.162443000	-2.653050000	-1.529374000
C	2.725471000	-0.610075000	2.544285000
H	3.073610000	-0.426994000	3.572198000

H	2.797132000	-1.691193000	2.374209000
C	1.265871000	-0.205471000	2.403117000
C	0.416345000	-0.146174000	3.506754000
H	0.807417000	-0.326819000	4.503685000
C	-0.936177000	0.137291000	3.307805000
H	-1.616453000	0.181167000	4.153130000
C	-1.399552000	0.359412000	2.012289000
H	-2.443186000	0.571000000	1.806356000
C	-0.483566000	0.300133000	0.963543000
N	3.442870000	1.952384000	-0.484631000
N	3.586323000	0.046375000	1.546473000
N	3.450771000	-1.688787000	-0.640339000
N	0.818110000	0.026317000	1.151802000
O	1.262801000	0.435585000	-2.017503000
O	0.876718000	-0.586301000	-2.634884000
H	2.349051000	-2.435661000	-2.215171000
H	-0.796126000	0.465109000	-0.062110000
C	-4.664374000	-1.322812000	0.876449000
C	-3.920401000	-1.397887000	-0.300479000
C	-3.727375000	-0.192495000	-1.025591000
C	-4.281161000	1.037465000	-0.608070000
C	-5.035321000	1.044337000	0.581710000
C	-5.221400000	-0.120311000	1.323098000
H	-4.856238000	-2.202820000	1.476153000
H	-5.484043000	1.966211000	0.920931000
O	-2.937574000	-0.286449000	-2.159316000
H	-3.122623000	0.461279000	-2.742116000
C	-3.371278000	-2.755538000	-0.800645000
C	-3.983450000	-3.092936000	-2.183116000
C	-1.825921000	-2.722053000	-0.900094000
C	-3.739188000	-3.910385000	0.154733000
H	-5.075831000	-3.152479000	-2.116115000
H	-3.723275000	-2.345536000	-2.934052000
H	-3.615904000	-4.067882000	-2.526359000
H	-1.381317000	-2.522117000	0.083195000
H	-1.456662000	-3.697875000	-1.239912000
H	-1.477014000	-1.961963000	-1.601207000
H	-3.333108000	-4.847087000	-0.242658000
H	-3.319499000	-3.769573000	1.157697000

H	-4.822929000	-4.038579000	0.249778000
C	-4.106602000	2.349025000	-1.420481000
C	-2.606858000	2.721759000	-1.566187000
C	-4.783611000	2.225697000	-2.813184000
C	-4.782507000	3.553906000	-0.729614000
H	-2.166336000	2.904166000	-0.578788000
H	-2.006366000	1.948544000	-2.053492000
H	-2.503531000	3.642094000	-2.152939000
H	-5.850860000	2.010044000	-2.699297000
H	-4.681842000	3.166575000	-3.365976000
H	-4.374799000	1.438391000	-3.459115000
H	-4.618478000	4.454166000	-1.331589000
H	-5.864769000	3.419322000	-0.632208000
H	-4.364898000	3.743103000	0.265343000
O	-5.932649000	-0.196771000	2.490370000
C	-6.610813000	0.962830000	2.943370000
H	-7.138961000	0.666727000	3.851466000
H	-5.911782000	1.776680000	3.182554000
H	-7.337722000	1.321745000	2.202726000

<sup>3</sup>RC<sub>R2</sub>

Cu	2.958624000	-0.123877000	-0.391932000
C	3.657788000	2.676290000	-1.633312000
H	3.303286000	2.206172000	-2.545913000
C	4.179408000	3.967573000	-1.633264000
H	4.238044000	4.530484000	-2.558626000
C	4.625439000	4.503238000	-0.425459000
H	5.046746000	5.503264000	-0.385645000
C	4.528213000	3.733884000	0.734484000
H	4.868713000	4.121216000	1.690035000
C	3.980127000	2.453670000	0.654902000
C	3.766859000	1.594577000	1.890478000
H	4.460395000	1.895157000	2.689931000
H	2.752706000	1.776144000	2.265688000
C	5.262268000	-0.306577000	1.459361000
H	5.719138000	-0.502858000	2.441137000
H	5.837676000	0.504826000	0.996716000
C	5.372255000	-1.535428000	0.573017000
C	6.369630000	-2.490102000	0.768316000

H	7.059231000	-2.392480000	1.601347000
C	6.466507000	-3.561731000	-0.119849000
H	7.237220000	-4.315201000	0.012242000
C	5.555400000	-3.651986000	-1.170815000
H	5.590153000	-4.470136000	-1.882152000
C	4.578782000	-2.666082000	-1.291400000
H	3.838273000	-2.688715000	-2.084817000
C	3.054374000	-0.690963000	2.476660000
H	3.248492000	-0.471825000	3.536885000
H	3.361995000	-1.728569000	2.300178000
C	1.572301000	-0.563014000	2.177334000
C	0.640549000	-0.588990000	3.198266000
H	0.957670000	-0.649646000	4.233739000
C	-0.723382000	-0.542102000	2.853211000
H	-1.483807000	-0.561564000	3.628429000
C	-1.092197000	-0.463094000	1.529925000
H	-2.134061000	-0.417796000	1.230970000
C	-0.080036000	-0.423401000	0.532212000
N	3.559708000	1.937355000	-0.516970000
N	3.871032000	0.156861000	1.586147000
N	4.489730000	-1.629597000	-0.442522000
N	1.232604000	-0.473017000	0.865034000
N	-0.415574000	-0.350219000	-0.777038000
H	0.305642000	-0.211282000	-1.470210000
O	2.253799000	-0.123653000	-2.288965000
O	2.303539000	-1.212268000	-2.933649000
H	-1.381979000	-0.179925000	-1.049381000
C	-6.327376000	0.224549000	1.123544000
C	-5.664741000	1.380229000	0.702809000
C	-4.669165000	1.345228000	-0.273652000
C	-4.327041000	0.072497000	-0.796954000
C	-4.999595000	-1.111724000	-0.424473000
C	-6.009566000	-1.003100000	0.548098000
H	-5.975506000	2.312118000	1.155424000
H	-6.547693000	-1.886547000	0.856330000
H	-3.415044000	-0.674021000	-2.341064000
O	-3.255974000	0.035261000	-1.700941000
C	-4.702308000	-2.494252000	-1.068705000
C	-5.031102000	-2.469400000	-2.586461000

C	-3.234337000	-2.930627000	-0.833321000
C	-5.584954000	-3.612280000	-0.469067000
H	-6.078596000	-2.195582000	-2.748196000
H	-4.429272000	-1.769687000	-3.182886000
H	-4.864968000	-3.460469000	-3.023545000
H	-3.020758000	-2.988488000	0.239974000
H	-3.067327000	-3.926124000	-1.261272000
H	-2.499782000	-2.255704000	-1.277648000
H	-5.337035000	-4.563762000	-0.951463000
H	-5.414920000	-3.735594000	0.605873000
H	-6.652035000	-3.430500000	-0.634036000
C	-4.033783000	2.664127000	-0.781436000
C	-2.513895000	2.709105000	-0.495185000
C	-4.288094000	2.817427000	-2.301769000
C	-4.654513000	3.898558000	-0.091595000
H	-2.311183000	2.558632000	0.572271000
H	-1.965423000	1.956301000	-1.062804000
H	-2.114516000	3.691717000	-0.775317000
H	-5.363168000	2.834552000	-2.513816000
H	-3.862087000	3.763349000	-2.658007000
H	-3.836585000	2.004331000	-2.873081000
H	-4.194217000	4.804864000	-0.499832000
H	-5.732913000	3.970947000	-0.267564000
H	-4.480101000	3.901067000	0.990310000
O	-7.276408000	0.409724000	2.087613000
C	-8.027330000	-0.711925000	2.523623000
H	-7.385327000	-1.476268000	2.982258000
H	-8.724563000	-0.332630000	3.272567000
H	-8.593677000	-1.164552000	1.698842000

<sup>3</sup>RC<sub>R3</sub>

Cu	-2.860065000	0.106838000	-0.427402000
C	-2.556980000	-2.050375000	-2.736844000
H	-2.039279000	-1.246635000	-3.249723000
C	-2.771239000	-3.282396000	-3.349721000
H	-2.423088000	-3.452330000	-4.362861000
C	-3.442738000	-4.273534000	-2.634770000
H	-3.636083000	-5.244157000	-3.081542000
C	-3.868052000	-3.999832000	-1.334684000



H	-4.393690000	-4.748987000	-0.750315000
C	-3.604278000	-2.744798000	-0.786518000
C	-3.960730000	-2.407016000	0.649628000
H	-4.804952000	-3.022594000	0.993282000
H	-3.103496000	-2.654650000	1.286436000
C	-5.575767000	-0.587187000	0.332363000
H	-6.363304000	-0.901483000	1.032916000
H	-5.744109000	-1.127383000	-0.607271000
C	-5.671925000	0.902372000	0.070112000
C	-6.851027000	1.587403000	0.303669000
H	-7.712897000	1.076278000	0.718367000
C	-6.897370000	2.955194000	-0.014282000
H	-7.807611000	3.524722000	0.148036000
C	-5.778851000	3.572350000	-0.529649000
H	-5.782060000	4.628322000	-0.780595000
C	-4.598088000	2.812967000	-0.727249000
C	-3.960501000	-0.485707000	2.188529000
H	-4.452866000	-1.114471000	2.944375000
H	-4.396117000	0.516660000	2.269448000
C	-2.471513000	-0.402283000	2.461082000
C	-1.978601000	-0.639417000	3.730625000
H	-2.644107000	-0.935847000	4.534089000
C	-0.598183000	-0.475546000	3.947684000
H	-0.175389000	-0.647633000	4.933194000
C	0.216697000	-0.111796000	2.901108000
H	1.288233000	0.001275000	3.025225000
C	-0.352320000	0.090441000	1.614182000
N	-2.965125000	-1.786193000	-1.485359000
N	-4.237007000	-0.968752000	0.820780000
N	-4.556908000	1.492307000	-0.431455000
N	-1.687114000	-0.041550000	1.411183000
N	0.438245000	0.439944000	0.572817000
H	0.081127000	0.396587000	-0.374204000
O	-1.853366000	1.084334000	-1.833911000
O	-0.720008000	0.610953000	-2.184860000
H	1.449934000	0.409600000	0.685496000
N	-3.464636000	3.410793000	-1.185501000
H	-2.719724000	2.835160000	-1.558234000
H	-3.536732000	4.345046000	-1.560651000

C	5.084617000	-0.883049000	0.396931000
C	6.216626000	-1.098577000	-0.406853000
C	6.796524000	-0.061505000	-1.133138000
C	6.252862000	1.222394000	-1.061235000
C	5.119775000	1.499377000	-0.295443000
C	4.544181000	0.418020000	0.419613000
H	6.653611000	-2.084638000	-0.451563000
H	6.750646000	1.993476000	-1.633022000
O	3.378073000	0.617905000	1.176319000
H	3.387829000	1.531726000	1.496911000
C	4.497477000	-2.052346000	1.226368000
C	4.495416000	-1.695475000	2.733396000
C	3.065382000	-2.391102000	0.747541000
C	5.328669000	-3.345851000	1.078304000
H	5.516912000	-1.512934000	3.086263000
H	3.900317000	-0.805088000	2.942337000
H	4.085459000	-2.530316000	3.315288000
H	3.069354000	-2.668737000	-0.313188000
H	2.671070000	-3.242644000	1.316241000
H	2.376162000	-1.555713000	0.875889000
H	4.882739000	-4.130114000	1.699847000
H	5.341506000	-3.716103000	0.046946000
H	6.363401000	-3.213080000	1.412678000
C	4.564226000	2.948139000	-0.239644000
C	3.099576000	3.012151000	-0.744002000
C	4.678260000	3.529733000	1.196045000
C	5.374278000	3.904860000	-1.143332000
H	3.033004000	2.625401000	-1.766894000
H	2.399318000	2.441119000	-0.129620000
H	2.754525000	4.052924000	-0.754243000
H	5.717187000	3.502550000	1.540030000
H	4.341510000	4.572538000	1.205841000
H	4.080303000	3.013055000	1.960636000
H	4.944061000	4.910204000	-1.080038000
H	6.422239000	3.976178000	-0.834970000
H	5.343049000	3.597400000	-2.193619000
O	7.895419000	-0.188828000	-1.933714000
C	8.513732000	-1.461159000	-2.037346000
H	7.827619000	-2.212020000	-2.451949000

H	9.356402000	-1.329632000	-2.718260000
H	8.885944000	-1.810785000	-1.065088000

<sup>3</sup>RC<sub>R4</sub>

Cu	-2.378488000	-0.139633000	0.499203000
C	-4.522275000	1.760278000	1.707484000
H	-3.816678000	1.799347000	2.532097000
C	-5.752004000	2.410692000	1.769000000
H	-6.023267000	2.977224000	2.653324000
C	-6.614993000	2.304451000	0.678667000
H	-7.586466000	2.789350000	0.692450000
C	-6.216058000	1.559214000	-0.431474000
H	-6.866319000	1.453502000	-1.294649000
C	-4.961789000	0.949206000	-0.424111000
C	-4.431721000	0.195732000	-1.633859000
H	-5.266441000	-0.166101000	-2.253012000
H	-3.861618000	0.899926000	-2.251862000
C	-4.213932000	-2.093154000	-0.760596000
H	-4.600049000	-2.711019000	-1.585781000
H	-5.082695000	-1.752946000	-0.183652000
C	-3.327410000	-2.927027000	0.149694000
C	-3.453141000	-4.313564000	0.223333000
H	-4.165496000	-4.829176000	-0.413691000
C	-2.655316000	-5.019911000	1.124449000
H	-2.738208000	-6.099928000	1.200117000
C	-1.746883000	-4.318847000	1.915531000
H	-1.101231000	-4.827325000	2.623308000
C	-1.671033000	-2.935007000	1.773755000
H	-0.971394000	-2.343648000	2.356313000
C	-2.500841000	-1.191814000	-2.274951000
H	-2.946457000	-1.308291000	-3.274271000
H	-2.050477000	-2.156143000	-2.012076000
C	-1.396189000	-0.150268000	-2.315326000
C	-0.785364000	0.192137000	-3.515705000
H	-1.139754000	-0.228311000	-4.451140000
C	0.312781000	1.056940000	-3.479834000
H	0.841818000	1.308930000	-4.394111000
C	0.745552000	1.565960000	-2.265122000
H	1.646345000	2.161706000	-2.195307000

C	0.030271000	1.236292000	-1.101837000
C	1.028399000	2.852143000	0.649568000
N	-4.135655000	1.048607000	0.636516000
N	-3.517273000	-0.892874000	-1.252703000
N	-2.445558000	-2.253169000	0.915294000
N	-1.010919000	0.377192000	-1.131995000
N	0.387257000	1.695631000	0.164603000
H	0.393762000	0.975720000	0.883688000
O	1.617706000	2.735371000	1.712662000
C	0.891464000	4.244668000	-0.012535000
C	0.585041000	5.224450000	1.149269000
H	1.337551000	5.145833000	1.935175000
H	0.574497000	6.250317000	0.765709000
H	-0.396172000	5.018181000	1.593126000
C	-0.236245000	4.384048000	-1.053244000
H	-0.013253000	3.902655000	-2.007289000
H	-1.184960000	3.982946000	-0.676661000
H	-0.390834000	5.448149000	-1.261685000
C	2.262603000	4.626416000	-0.620640000
H	3.036239000	4.618313000	0.152858000
H	2.583730000	3.945910000	-1.416354000
H	2.207736000	5.636838000	-1.040867000
O	-1.705891000	0.480052000	2.310553000
O	-0.579347000	0.020930000	2.634754000
C	3.573233000	-0.706797000	-1.693447000
C	4.005788000	0.551688000	-1.283269000
C	4.258800000	0.797500000	0.063726000
C	4.082882000	-0.192627000	1.035359000
C	3.628056000	-1.461322000	0.593303000
C	3.368724000	-1.740659000	-0.767841000
H	3.390114000	-0.888530000	-2.743116000
H	4.604291000	1.786911000	0.331787000
H	3.717798000	-2.236004000	2.355199000
O	3.406744000	-2.497016000	1.479292000
C	2.873608000	-3.128889000	-1.237484000
C	3.917378000	-4.220159000	-0.892486000
C	1.515465000	-3.462823000	-0.570366000
C	2.650556000	-3.180070000	-2.763883000
H	4.868254000	-4.014730000	-1.397494000

H	4.104105000	-4.275535000	0.180643000
H	3.562313000	-5.200669000	-1.233613000
H	0.762327000	-2.709151000	-0.838295000
H	1.155431000	-4.439410000	-0.918767000
H	1.598247000	-3.494090000	0.517007000
H	2.300106000	-4.180197000	-3.042285000
H	1.891977000	-2.460527000	-3.096391000
H	3.573463000	-2.991680000	-3.323626000
C	4.398612000	0.107941000	2.523812000
C	3.126633000	-0.052517000	3.400938000
C	5.554599000	-0.797686000	3.031337000
C	4.873656000	1.563057000	2.727777000
H	2.371745000	0.676866000	3.092074000
H	2.664943000	-1.044653000	3.346125000
H	3.372089000	0.135330000	4.452777000
H	6.460682000	-0.622258000	2.441602000
H	5.779394000	-0.563593000	4.078028000
H	5.355780000	-1.875124000	2.981491000
H	5.082824000	1.724717000	3.790933000
H	5.796973000	1.773949000	2.177219000
H	4.106811000	2.283450000	2.428013000
O	4.172631000	1.624754000	-2.139863000
C	4.482746000	1.339948000	-3.496600000
H	3.615851000	0.947002000	-4.047223000
H	4.785256000	2.288354000	-3.946054000
H	5.305836000	0.618807000	-3.574201000

**<sup>3</sup>RC<sub>R5</sub>**

Cu	-4.121520000	-0.402721000	-0.162779000
C	-4.770643000	-1.779815000	-2.882877000
H	-3.988043000	-1.116408000	-3.238620000
C	-5.464394000	-2.630369000	-3.740263000
H	-5.228093000	-2.645028000	-4.798771000
C	-6.463184000	-3.444905000	-3.206308000
H	-7.030508000	-4.114449000	-3.845809000
C	-6.730680000	-3.385991000	-1.837779000
H	-7.504277000	-4.004708000	-1.393115000
C	-5.983659000	-2.518451000	-1.041905000

C	-6.152862000	-2.450150000	0.465551000
H	-7.169691000	-2.754249000	0.755508000
H	-5.461151000	-3.166857000	0.923882000
C	-6.878083000	-0.126717000	0.732625000
H	-7.745787000	-0.278776000	1.391737000
H	-7.226856000	-0.282554000	-0.295352000
C	-6.351385000	1.286611000	0.868262000
C	-7.153791000	2.301691000	1.368212000
H	-8.164015000	2.092429000	1.703486000
C	-6.611467000	3.590593000	1.448655000
H	-7.193142000	4.406402000	1.867298000
C	-5.311320000	3.810430000	1.030267000
H	-4.844245000	4.779900000	1.145781000
C	-4.567889000	2.734730000	0.498140000
C	-5.392423000	-1.144767000	2.400630000
H	-6.086438000	-1.730184000	3.021681000
H	-5.420439000	-0.116992000	2.779439000
C	-3.983808000	-1.685293000	2.534231000
C	-3.602519000	-2.407044000	3.658171000
H	-4.323928000	-2.640155000	4.434333000
C	-2.262687000	-2.793649000	3.770523000
H	-1.913437000	-3.319060000	4.654346000
C	-1.376715000	-2.480277000	2.752099000
H	-0.324628000	-2.721943000	2.830836000
C	-1.853052000	-1.804742000	1.611176000
C	0.230277000	-1.948401000	0.124181000
N	-5.026638000	-1.728668000	-1.566294000
N	-5.816294000	-1.113877000	0.991721000
N	-5.085986000	1.487821000	0.437986000
N	-3.135368000	-1.389564000	1.526986000
N	-1.034047000	-1.461800000	0.547725000
H	-1.200424000	-0.530476000	0.163683000
O	1.017045000	-1.121012000	-0.296596000
C	0.538338000	-3.463593000	0.016612000
C	1.060588000	-3.664169000	-1.430449000
H	1.914775000	-3.016148000	-1.632154000
H	1.366196000	-4.707398000	-1.564597000
H	0.279692000	-3.441494000	-2.166987000
C	-0.666561000	-4.402001000	0.214946000

H	-1.017152000	-4.448751000	1.248522000
H	-1.509197000	-4.112584000	-0.423603000
H	-0.372235000	-5.418132000	-0.069125000
C	1.680790000	-3.811441000	0.998281000
H	2.536062000	-3.147184000	0.844871000
H	1.372800000	-3.734532000	2.047660000
H	2.009548000	-4.842796000	0.829709000
O	-2.827477000	0.194814000	-1.528937000
O	-1.771517000	0.758969000	-1.072813000
N	-3.260652000	2.873450000	0.083364000
H	-2.672416000	2.052396000	0.205121000
C	-2.455822000	4.028097000	-0.146201000
C	-2.915535000	5.173252000	-1.081536000
C	-2.946609000	6.491300000	-0.275617000
H	-2.000032000	6.642474000	0.251113000
H	-3.103798000	7.335983000	-0.955009000
H	-3.756829000	6.511640000	0.463521000
C	-4.247127000	4.939070000	-1.818006000
H	-4.275562000	3.952626000	-2.293822000
H	-5.124422000	5.036724000	-1.173714000
H	-4.348545000	5.688721000	-2.610054000
C	-1.790909000	5.275848000	-2.148005000
H	-1.740053000	4.366389000	-2.757484000
H	-1.998975000	6.120416000	-2.813482000
H	-0.818758000	5.425414000	-1.674546000
O	-1.324244000	3.998922000	0.294569000
C	8.975544000	0.853085000	0.289583000
C	7.587521000	0.819085000	0.018519000
C	6.951794000	-0.316396000	-0.553279000
C	7.753930000	-1.416398000	-0.841844000
C	9.130686000	-1.412325000	-0.593060000
C	9.730300000	-0.286410000	-0.032622000
H	7.338464000	-2.317242000	-1.273916000
H	10.792009000	-0.292907000	0.163579000
O	6.766532000	1.889524000	0.295410000
H	7.287575000	2.604334000	0.680896000
C	9.668826000	2.090929000	0.916011000
C	9.538751000	3.326073000	-0.017403000
C	9.093803000	2.390012000	2.328467000

C	11.184018000	1.868918000	1.116452000
H	10.036554000	3.128706000	-0.972792000
H	8.507986000	3.608420000	-0.257201000
H	10.017768000	4.198483000	0.442195000
H	9.273598000	1.539792000	2.995189000
H	9.588290000	3.269263000	2.757654000
H	8.015412000	2.580828000	2.352355000
H	11.628001000	2.775660000	1.541572000
H	11.389992000	1.045741000	1.809148000
H	11.698047000	1.665529000	0.171064000
C	5.431891000	-0.350793000	-0.832408000
C	4.643224000	-0.201615000	0.492504000
C	5.031163000	0.775657000	-1.818307000
C	4.997805000	-1.684815000	-1.475078000
H	4.908257000	-1.005094000	1.191457000
H	4.852264000	0.753209000	0.978475000
H	3.565924000	-0.261581000	0.294955000
H	5.560789000	0.660058000	-2.771737000
H	3.954732000	0.721968000	-2.021778000
H	5.255615000	1.765331000	-1.419126000
H	3.928654000	-1.629598000	-1.707898000
H	5.530120000	-1.888838000	-2.410902000
H	5.148634000	-2.536890000	-0.801237000
O	9.792542000	-2.559833000	-0.931650000
C	11.193761000	-2.617026000	-0.725718000
H	11.451405000	-2.516425000	0.337439000
H	11.509633000	-3.599875000	-1.080285000
H	11.718882000	-1.840211000	-1.297668000

<sup>3</sup>RC<sub>R6</sub>

Cu	1.482086000	0.008587000	-0.373001000
C	2.827517000	2.312318000	-1.977249000
H	2.141324000	1.986499000	-2.753508000
C	3.749842000	3.331655000	-2.199717000
H	3.796149000	3.821208000	-3.166487000
C	4.604029000	3.693413000	-1.158519000
H	5.342363000	4.477625000	-1.296016000
C	4.500729000	3.031393000	0.065685000
H	5.151302000	3.290691000	0.895435000



C	3.541123000	2.030717000	0.215740000
C	3.309064000	1.336068000	1.548352000
H	4.217457000	1.382184000	2.167292000
H	2.528903000	1.886955000	2.087462000
C	3.896845000	-0.993371000	1.011127000
H	4.467829000	-1.331350000	1.888811000
H	4.598960000	-0.455440000	0.362391000
C	3.356057000	-2.188282000	0.242287000
C	3.952676000	-3.445704000	0.326646000
H	4.794877000	-3.604724000	0.993265000
C	3.453786000	-4.486946000	-0.457411000
H	3.905390000	-5.473264000	-0.409662000
C	2.364636000	-4.243299000	-1.292851000
H	1.941523000	-5.025223000	-1.914217000
C	1.813579000	-2.964087000	-1.310295000
C	1.995685000	-0.514116000	2.504468000
H	2.456637000	-0.283555000	3.476305000
H	1.936524000	-1.606765000	2.432891000
C	0.582564000	0.045261000	2.441995000
C	-0.166630000	0.267645000	3.595979000
H	0.276079000	0.101707000	4.573634000
C	-1.490240000	0.695251000	3.471755000
H	-2.094206000	0.867588000	4.357669000
C	-2.018965000	0.900457000	2.199057000
H	-3.042365000	1.227287000	2.049410000
C	-1.201256000	0.677715000	1.092168000
N	2.726827000	1.676975000	-0.798732000
N	2.829074000	-0.047149000	1.380130000
N	2.300312000	-1.959266000	-0.564970000
N	0.069116000	0.254829000	1.212593000
O	0.342951000	0.211869000	-2.003434000
O	-0.472814000	-0.742073000	-2.179210000
H	0.954288000	-2.721820000	-1.928437000
H	-1.566573000	0.843745000	0.082545000
C	-5.609944000	-1.213387000	-0.909869000
C	-4.388912000	-0.791659000	-1.425093000
C	-4.013066000	0.553806000	-1.329442000
C	-4.868441000	1.465040000	-0.711208000
C	-6.095187000	1.042795000	-0.189293000

C	-6.474186000	-0.302207000	-0.285696000
H	-5.917152000	-2.251701000	-0.984126000
H	-3.730289000	-1.509361000	-1.910455000
H	-4.578937000	2.510488000	-0.658953000
H	-6.746911000	1.773498000	0.275852000
O	-2.808194000	1.025111000	-1.806765000
H	-2.341942000	0.310932000	-2.273673000
O	-7.644722000	-0.821480000	0.187809000
C	-8.582345000	0.064810000	0.777382000
H	-8.908097000	0.837603000	0.068531000
H	-9.439095000	-0.549252000	1.059682000
H	-8.173379000	0.548562000	1.675055000

$^3R_{C_{R7}}$

Cu	1.016931000	-0.034310000	0.222365000
C	-1.394036000	1.897538000	-0.136753000
H	-1.795071000	1.341371000	0.704540000
C	-2.150639000	2.869652000	-0.789348000
H	-3.164197000	3.071854000	-0.458694000
C	-1.580833000	3.536727000	-1.872482000
H	-2.138903000	4.297958000	-2.409598000
C	-0.283737000	3.205689000	-2.271875000
H	0.182253000	3.700918000	-3.118410000
C	0.408739000	2.221919000	-1.568729000
C	1.834949000	1.825890000	-1.908618000
H	2.073044000	2.091408000	-2.949067000
H	2.521127000	2.392207000	-1.267640000
C	1.481120000	-0.488421000	-2.668902000
H	2.142612000	-0.589248000	-3.541879000
H	0.559422000	-0.010150000	-3.021339000
C	1.119436000	-1.855945000	-2.114286000
C	1.133032000	-2.996401000	-2.915963000
H	1.481061000	-2.936354000	-3.942797000
C	0.685788000	-4.205207000	-2.380168000
H	0.685975000	-5.106262000	-2.986236000
C	0.237831000	-4.235316000	-1.060836000
H	-0.129072000	-5.149753000	-0.607337000
C	0.272229000	-3.057093000	-0.317474000
H	-0.077776000	-3.026888000	0.708717000

C	3.485833000	0.075911000	-1.369448000
H	4.149513000	0.492366000	-2.141023000
H	3.583915000	-1.015484000	-1.412475000
C	3.916548000	0.544995000	0.005378000
C	5.172479000	1.090064000	0.206395000
H	5.847611000	1.241484000	-0.628710000
C	5.547638000	1.429298000	1.517508000
H	6.525976000	1.857460000	1.714342000
C	4.668298000	1.207650000	2.554493000
H	4.931722000	1.449366000	3.579326000
C	3.394532000	0.652420000	2.273797000
N	-0.144981000	1.586197000	-0.516443000
N	2.070800000	0.391890000	-1.642573000
N	0.710837000	-1.896243000	-0.830201000
N	3.024287000	0.345433000	1.009458000
N	2.495644000	0.446007000	3.276345000
H	1.737815000	-0.207753000	3.125945000
O	-0.209551000	-0.309743000	1.763955000
O	0.085178000	-1.295802000	2.522439000
H	2.825513000	0.518400000	4.227971000
C	-4.840500000	0.502897000	0.595266000
C	-4.669662000	-0.661983000	-0.164078000
C	-3.850264000	-1.690755000	0.307403000
C	-3.199927000	-1.573856000	1.537670000
C	-3.396582000	-0.420415000	2.311367000
C	-4.208236000	0.608150000	1.842359000
H	-5.163471000	-0.779996000	-1.121879000
H	-3.713373000	-2.595668000	-0.276574000
H	-2.919751000	-0.331134000	3.284485000
H	-4.374269000	1.501067000	2.437385000
O	-2.402998000	-2.610984000	1.948529000
H	-1.844380000	-2.305698000	2.683393000
O	-5.577386000	1.590373000	0.206065000
C	-6.411818000	1.459212000	-0.936883000
H	-6.970218000	2.393966000	-1.009899000
H	-5.825271000	1.316392000	-1.854789000
H	-7.114184000	0.623690000	-0.825086000

<sup>3</sup>RC<sub>RS</sub>

Cu	-1.557478000	-0.022690000	0.313601000
C	-1.628416000	2.916651000	1.509699000
H	-1.006961000	2.482652000	2.285813000
C	-2.037822000	4.246541000	1.565239000
H	-1.742188000	4.870746000	2.401568000
C	-2.831988000	4.742422000	0.532000000
H	-3.177630000	5.771725000	0.544266000
C	-3.180182000	3.895399000	-0.520377000
H	-3.795918000	4.249664000	-1.341540000
C	-2.719639000	2.579146000	-0.509767000
C	-2.982393000	1.629568000	-1.663859000
H	-3.897940000	1.916871000	-2.201310000
H	-2.152749000	1.712897000	-2.375406000
C	-4.318296000	-0.109145000	-0.560950000
H	-5.127498000	-0.224252000	-1.296864000
H	-4.583922000	0.738232000	0.082760000
C	-4.199157000	-1.358445000	0.288001000
C	-5.260716000	-2.237193000	0.408116000
H	-6.182636000	-2.066435000	-0.136883000
C	-5.109452000	-3.347866000	1.255423000
H	-5.923736000	-4.055088000	1.381894000
C	-3.918823000	-3.538909000	1.921015000
H	-3.769537000	-4.390830000	2.576770000
C	-2.864597000	-2.608758000	1.736223000
C	-2.663614000	-0.732082000	-2.275023000
H	-3.216256000	-0.537180000	-3.205445000
H	-2.959940000	-1.728551000	-1.928554000
C	-1.169560000	-0.725963000	-2.538432000
C	-0.681567000	-1.031632000	-3.795985000
H	-1.360214000	-1.223094000	-4.620096000
C	0.712373000	-1.101693000	-3.966438000
H	1.133021000	-1.352577000	-4.935756000
C	1.542845000	-0.834223000	-2.902079000
H	2.622869000	-0.864379000	-3.004479000
C	0.974806000	-0.488447000	-1.647172000
N	-1.963317000	2.100386000	0.497766000
N	-3.038608000	0.225794000	-1.215479000
N	-3.016302000	-1.529301000	0.932357000
N	-0.370088000	-0.462647000	-1.472847000

N	1.774077000	-0.199154000	-0.593806000
H	1.414023000	0.280114000	0.222404000
O	-0.412604000	-0.230898000	1.919072000
O	0.538634000	0.614571000	2.046566000
H	2.767924000	-0.088106000	-0.745431000
N	-1.661037000	-2.806782000	2.337539000
H	-1.001719000	-2.040800000	2.396321000
H	-1.593018000	-3.515297000	3.052864000
C	5.203133000	-0.078524000	1.798850000
C	6.385233000	-0.618827000	1.280421000
C	6.848653000	-0.215317000	0.023071000
C	6.116874000	0.738483000	-0.702470000
C	4.945330000	1.277897000	-0.183728000
C	4.480974000	0.868229000	1.074608000
H	4.853949000	-0.399829000	2.778383000
H	6.929024000	-1.348841000	1.868504000
H	6.495835000	1.054353000	-1.669318000
H	4.395437000	2.040550000	-0.728054000
O	3.304601000	1.425346000	1.524944000
H	3.098419000	1.073479000	2.405179000
O	7.981132000	-0.678276000	-0.578636000
C	8.783339000	-1.613000000	0.127324000
H	9.632588000	-1.829467000	-0.522524000
H	9.148754000	-1.195163000	1.074630000
H	8.235673000	-2.543297000	0.329334000

<sup>3</sup>RC<sub>R9</sub>

Cu	-1.688142000	-0.411434000	-0.174056000
C	-0.043953000	-2.135912000	1.833243000
H	0.634462000	-2.275313000	0.995104000
C	0.182651000	-2.784549000	3.046076000
H	1.046464000	-3.431526000	3.152954000
C	-0.717414000	-2.589343000	4.091267000
H	-0.575925000	-3.086705000	5.046150000
C	-1.812412000	-1.746773000	3.891975000
H	-2.535219000	-1.574496000	4.683691000
C	-1.967716000	-1.119733000	2.657618000
C	-3.087800000	-0.125771000	2.405993000
H	-3.934025000	-0.319617000	3.081212000

H	-2.718078000	0.879470000	2.640493000
C	-4.381970000	-1.259796000	0.649378000
H	-5.419013000	-1.088806000	0.974558000
H	-4.013036000	-2.132297000	1.202130000
C	-4.336421000	-1.570902000	-0.836139000
C	-5.427324000	-2.123716000	-1.505476000
H	-6.358272000	-2.301376000	-0.975621000
C	-5.299744000	-2.444792000	-2.857431000
H	-6.134810000	-2.879430000	-3.398480000
C	-4.089402000	-2.191648000	-3.501433000
H	-3.948202000	-2.420436000	-4.552232000
C	-3.050394000	-1.625391000	-2.766666000
H	-2.092278000	-1.398063000	-3.222890000
C	-4.069873000	1.174459000	0.560959000
H	-4.843792000	1.532025000	1.255925000
H	-4.558890000	1.011711000	-0.406594000
C	-2.994911000	2.231483000	0.387755000
C	-3.258915000	3.564232000	0.678015000
H	-4.220591000	3.858706000	1.084844000
C	-2.267227000	4.511158000	0.404086000
H	-2.451529000	5.566899000	0.578707000
C	-1.053144000	4.095736000	-0.117735000
H	-0.288272000	4.810530000	-0.389108000
C	-0.832194000	2.722945000	-0.328276000
C	1.698692000	2.627951000	-0.898765000
N	-1.096932000	-1.319896000	1.644955000
N	-3.510374000	-0.119949000	0.992356000
N	-3.168974000	-1.325011000	-1.463385000
N	-1.803644000	1.811835000	-0.093392000
N	0.344978000	2.214400000	-0.863235000
H	0.201169000	1.478719000	-1.552262000
O	2.351447000	2.210676000	-1.839965000
C	2.374769000	3.432159000	0.238850000
C	3.779626000	2.803875000	0.417410000
H	4.346156000	2.840501000	-0.514231000
H	4.326760000	3.358308000	1.187268000
H	3.714186000	1.756172000	0.729033000
C	1.649259000	3.368329000	1.596847000
H	0.708945000	3.923398000	1.619478000

H	1.445999000	2.332175000	1.891675000
H	2.296945000	3.805961000	2.363940000
C	2.567019000	4.895238000	-0.228619000
H	3.087453000	4.925217000	-1.190696000
H	1.623945000	5.442424000	-0.334937000
H	3.174731000	5.434743000	0.505911000
O	-0.112531000	-0.982926000	-1.258697000
O	-0.085806000	-0.387218000	-2.386171000
C	5.715662000	-2.523159000	0.162999000
C	6.055155000	-1.316881000	-0.461904000
C	5.061355000	-0.588791000	-1.131586000
C	3.750652000	-1.052655000	-1.175117000
C	3.417083000	-2.260815000	-0.551239000
C	4.399148000	-2.990737000	0.114049000
H	6.462773000	-3.111724000	0.682919000
H	5.333317000	0.341756000	-1.618857000
H	2.996356000	-0.470194000	-1.699886000
H	4.133074000	-3.932668000	0.584336000
O	2.129789000	-2.766319000	-0.562655000
H	1.580765000	-2.211567000	-1.141122000
O	7.306733000	-0.768817000	-0.477729000
C	8.359348000	-1.483437000	0.148341000
H	9.258487000	-0.882095000	0.003066000
H	8.179484000	-1.609592000	1.224789000
H	8.506544000	-2.470638000	-0.309855000

<sup>3</sup>RC<sub>R10</sub>

Cu	-1.582484000	-0.219348000	-0.270971000
C	-4.369936000	-0.148821000	1.222598000
H	-3.749948000	-0.375572000	2.084141000
C	-5.754955000	-0.055465000	1.334718000
H	-6.233234000	-0.208882000	2.296219000
C	-6.496607000	0.229220000	0.189100000
H	-7.579163000	0.302219000	0.232427000
C	-5.824789000	0.412796000	-1.019210000
H	-6.370147000	0.631906000	-1.932329000
C	-4.433068000	0.316389000	-1.045773000
C	-3.647392000	0.588609000	-2.317205000
H	-4.287125000	0.428503000	-3.199191000

H	-3.362388000	1.647740000	-2.322714000
C	-2.643556000	-1.606424000	-2.721834000
H	-2.774254000	-1.752984000	-3.805916000
H	-3.587357000	-1.905683000	-2.249374000
C	-1.547655000	-2.528690000	-2.210995000
C	-1.289737000	-3.739447000	-2.849489000
H	-1.837680000	-4.012569000	-3.745698000
C	-0.309291000	-4.580486000	-2.321471000
H	-0.073109000	-5.522980000	-2.806098000
C	0.397744000	-4.177814000	-1.195320000
H	1.212490000	-4.771144000	-0.799512000
C	0.075859000	-2.951213000	-0.600915000
C	-1.349239000	0.439739000	-3.170087000
H	-1.699529000	0.739448000	-4.169901000
H	-0.557182000	-0.303932000	-3.316969000
C	-0.759853000	1.637393000	-2.445203000
C	-0.443447000	2.807374000	-3.126095000
H	-0.648865000	2.895115000	-4.187998000
C	0.154375000	3.854274000	-2.416725000
H	0.435337000	4.772649000	-2.923553000
C	0.413267000	3.695052000	-1.063999000
H	0.925296000	4.461491000	-0.494633000
C	0.038868000	2.496456000	-0.431648000
C	0.383551000	3.109419000	2.013804000
N	-3.719031000	0.033110000	0.061949000
N	-2.410817000	-0.199990000	-2.379532000
N	-0.888135000	-2.149651000	-1.097116000
N	-0.542957000	1.491004000	-1.117828000
N	0.326176000	2.234571000	0.910705000
H	0.975034000	1.447532000	1.034968000
O	1.230914000	2.892530000	2.861745000
C	-0.690918000	4.203019000	2.247080000
C	-1.215134000	3.953126000	3.684104000
H	-0.392193000	3.946478000	4.400985000
H	-1.923752000	4.742067000	3.959278000
H	-1.735029000	2.989916000	3.752792000
C	-1.894540000	4.177698000	1.286839000
H	-1.647149000	4.513396000	0.276402000
H	-2.337232000	3.176738000	1.220927000



H	-2.666376000	4.855345000	1.668477000
C	0.004975000	5.582596000	2.210679000
H	0.860178000	5.599726000	2.892200000
H	0.361486000	5.840427000	1.206147000
H	-0.699785000	6.362989000	2.518719000
O	-1.413155000	-0.503965000	1.818482000
O	-0.372625000	-0.319485000	2.467607000
N	0.811146000	-2.405769000	0.462121000
H	1.170389000	-1.464895000	0.269724000
C	1.307595000	-2.888998000	1.666784000
C	0.777918000	-4.158930000	2.369933000
C	1.792497000	-5.304149000	2.134834000
H	2.796696000	-5.002319000	2.447668000
H	1.498269000	-6.178555000	2.725299000
H	1.839134000	-5.616940000	1.085832000
C	-0.641683000	-4.585737000	1.947835000
H	-1.345712000	-3.746910000	1.998667000
H	-0.687404000	-5.014411000	0.944599000
H	-0.997711000	-5.355241000	2.640851000
C	0.751921000	-3.831304000	3.883243000
H	0.050618000	-3.017679000	4.098895000
H	0.428812000	-4.718110000	4.438502000
H	1.737732000	-3.529185000	4.239702000
O	2.168378000	-2.203887000	2.225285000
C	3.547722000	0.949088000	-1.152144000
C	3.551898000	0.273682000	0.072212000
C	4.756740000	-0.144671000	0.630938000
C	5.963972000	0.108605000	-0.028876000
C	5.965987000	0.787926000	-1.252347000
C	4.745794000	1.204886000	-1.807195000
H	2.604950000	1.271988000	-1.584232000
H	4.761896000	-0.668267000	1.583211000
H	6.888957000	-0.225169000	0.426506000
H	4.763428000	1.730522000	-2.756702000
O	2.335043000	0.043471000	0.699914000
H	2.463849000	-0.578205000	1.458759000
O	7.080636000	1.090423000	-1.977468000
C	8.345957000	0.718927000	-1.451313000
H	8.433214000	-0.370213000	-1.340990000

H	9.084823000	1.067432000	-2.174661000
H	8.534512000	1.196898000	-0.481043000

<sup>3</sup>RC<sub>R11</sub>

Cu	0.934938000	0.003040000	-0.369306000
C	2.151821000	2.293543000	-2.090867000
H	1.431523000	1.939421000	-2.822564000
C	3.043371000	3.322433000	-2.383475000
H	3.029915000	3.791432000	-3.361387000
C	3.945478000	3.720358000	-1.397283000
H	4.662056000	4.512924000	-1.590555000
C	3.918590000	3.083621000	-0.155648000
H	4.607941000	3.370869000	0.632533000
C	2.985123000	2.071733000	0.066465000
C	2.834962000	1.403140000	1.423945000
H	3.773521000	1.476815000	1.993080000
H	2.075019000	1.953517000	1.991721000
C	3.433778000	-0.929106000	0.909613000
H	4.050979000	-1.239926000	1.765735000
H	4.096108000	-0.394674000	0.217674000
C	2.876076000	-2.148039000	0.192201000
C	3.498163000	-3.393389000	0.271400000
H	4.375174000	-3.524607000	0.897982000
C	2.979210000	-4.458724000	-0.465785000
H	3.449798000	-5.436266000	-0.421137000
C	1.845874000	-4.250268000	-1.250464000
H	1.406301000	-5.051657000	-1.834482000
C	1.272300000	-2.980989000	-1.265707000
C	1.604354000	-0.445628000	2.487409000
H	2.110914000	-0.184338000	3.428253000
H	1.561845000	-1.540518000	2.443957000
C	0.179819000	0.086869000	2.486293000
C	-0.512922000	0.322531000	3.672551000
H	-0.016857000	0.188366000	4.629239000
C	-1.849539000	0.721580000	3.608086000
H	-2.410282000	0.903514000	4.520088000
C	-2.447697000	0.885922000	2.360345000
H	-3.484179000	1.188706000	2.257453000
C	-1.683929000	0.652743000	1.217809000

N	2.124478000	1.682905000	-0.895470000
N	2.369886000	0.008817000	1.310655000
N	1.777532000	-1.953129000	-0.565359000
N	-0.400527000	0.257631000	1.280914000
O	-0.287044000	0.156871000	-1.943832000
O	-1.089009000	-0.817047000	-2.070073000
H	0.379534000	-2.765622000	-1.845147000
H	-2.104184000	0.786712000	0.225134000
C	-6.198059000	-1.356581000	-0.683167000
C	-4.999978000	-0.921622000	-1.253938000
C	-4.610756000	0.413671000	-1.109062000
C	-5.415508000	1.309913000	-0.396276000
C	-6.608378000	0.861390000	0.170299000
C	-7.005640000	-0.471950000	0.033207000
H	-6.498563000	-2.393755000	-0.803869000
H	-4.374416000	-1.613029000	-1.815354000
H	-5.105466000	2.347706000	-0.315695000
H	-7.235795000	1.562104000	0.714593000
H	-7.937743000	-0.814144000	0.472177000
O	-3.436434000	0.900341000	-1.630655000
H	-2.975136000	0.194491000	-2.115944000

<sup>3</sup>RC<sub>R12</sub>

Cu	0.855268000	0.056351000	0.238370000
C	1.303524000	2.701478000	1.823312000
H	0.443394000	2.348296000	2.383789000
C	1.898728000	3.930595000	2.093913000
H	1.508098000	4.560524000	2.885751000
C	2.990970000	4.325083000	1.321496000
H	3.476470000	5.280277000	1.497265000
C	3.449967000	3.478197000	0.312198000
H	4.294855000	3.758822000	-0.309327000
C	2.809700000	2.255882000	0.110686000
C	3.303241000	1.247872000	-0.912132000
H	3.843472000	1.755174000	-1.724543000
H	4.021245000	0.581037000	-0.420112000
C	1.395880000	1.089033000	-2.458536000
H	1.889323000	1.063199000	-3.441478000
H	1.317627000	2.143831000	-2.167855000

C	-0.003793000	0.506633000	-2.550386000
C	-0.733551000	0.533170000	-3.737059000
H	-0.284797000	0.927822000	-4.643687000
C	-2.045294000	0.055022000	-3.734646000
H	-2.635975000	0.074216000	-4.645628000
C	-2.579224000	-0.449879000	-2.550707000
H	-3.594719000	-0.826602000	-2.496056000
C	-1.780258000	-0.462853000	-1.408784000
H	-2.156058000	-0.866373000	-0.473513000
C	2.654210000	-0.935629000	-1.847112000
H	3.515596000	-0.879598000	-2.528043000
H	1.828774000	-1.391772000	-2.405648000
C	2.980595000	-1.812099000	-0.654174000
C	4.049522000	-2.689837000	-0.692512000
H	4.699178000	-2.730503000	-1.559923000
C	4.260887000	-3.528210000	0.415680000
H	5.086425000	-4.233675000	0.419131000
C	3.411624000	-3.452508000	1.497507000
H	3.545271000	-4.089807000	2.365827000
C	2.342869000	-2.521143000	1.473346000
N	1.750718000	1.883255000	0.856886000
N	2.205803000	0.408010000	-1.429434000
N	-0.522629000	0.011083000	-1.408566000
N	2.143187000	-1.708572000	0.409984000
N	1.507891000	-2.393599000	2.540358000
H	0.596189000	-1.968988000	2.398089000
O	-0.573542000	0.191910000	1.625421000
O	-1.020087000	-0.894864000	2.125050000
H	1.549695000	-3.102518000	3.258648000
C	-6.928376000	0.839024000	0.353979000
C	-6.781399000	-0.404006000	-0.268747000
C	-5.681396000	-1.213891000	0.011339000
C	-4.717049000	-0.775648000	0.926073000
C	-4.855442000	0.465314000	1.556111000
C	-5.963333000	1.265326000	1.267690000
H	-7.789519000	1.463086000	0.135802000
H	-7.533291000	-0.751564000	-0.972096000
H	-5.565691000	-2.191231000	-0.448114000
H	-4.107388000	0.797537000	2.273607000

H	-6.069667000	2.225591000	1.764994000
O	-3.644303000	-1.602865000	1.153105000
H	-3.068215000	-1.217188000	1.835970000

<sup>3</sup>RC<sub>R12</sub>

Cu	-1.046625000	-0.012219000	0.311892000
C	-0.886350000	2.866650000	1.639947000
H	-0.292196000	2.352180000	2.387667000
C	-1.192637000	4.219841000	1.759584000
H	-0.841456000	4.781770000	2.618290000
C	-1.957991000	4.820088000	0.760408000
H	-2.224302000	5.870925000	0.822763000
C	-2.381022000	4.049790000	-0.323026000
H	-2.977055000	4.485925000	-1.118925000
C	-2.021634000	2.703419000	-0.376871000
C	-2.368880000	1.829127000	-1.567773000
H	-3.268644000	2.205988000	-2.075455000
H	-1.545611000	1.884949000	-2.289324000
C	-3.815418000	0.142585000	-0.525465000
H	-4.637873000	0.119093000	-1.255194000
H	-4.012969000	0.976812000	0.158703000
C	-3.778298000	-1.149275000	0.265239000
C	-4.898813000	-1.954669000	0.359420000
H	-5.811283000	-1.693686000	-0.165275000
C	-4.819404000	-3.111279000	1.153551000
H	-5.681030000	-3.763821000	1.258375000
C	-3.639388000	-3.416607000	1.794962000
H	-3.545036000	-4.305685000	2.410297000
C	-2.523136000	-2.556183000	1.639058000
C	-2.227649000	-0.520130000	-2.287298000
H	-2.780357000	-0.249541000	-3.198497000
H	-2.583691000	-1.508937000	-1.976958000
C	-0.740764000	-0.599171000	-2.576308000
C	-0.291103000	-0.874660000	-3.854815000
H	-0.991969000	-0.983196000	-4.675402000
C	1.093117000	-1.024900000	-4.051946000
H	1.483038000	-1.256400000	-5.038767000
C	1.953911000	-0.860484000	-2.990938000
H	3.028246000	-0.954016000	-3.112931000

C	1.426735000	-0.539105000	-1.711805000
N	-1.293100000	2.124347000	0.597859000
N	-2.521440000	0.413966000	-1.181502000
N	-2.604415000	-1.433459000	0.885858000
N	0.088726000	-0.438555000	-1.513040000
N	2.256631000	-0.345624000	-0.661289000
H	1.933418000	0.096085000	0.190825000
O	0.093224000	-0.368477000	1.893868000
O	1.123556000	0.378228000	2.030279000
H	3.254700000	-0.301057000	-0.818107000
N	-1.331640000	-2.865622000	2.217106000
H	-0.621229000	-2.149754000	2.305437000
H	-1.308882000	-3.608800000	2.899492000
C	5.656703000	-0.845820000	1.676124000
C	6.754316000	-1.464543000	1.075631000
C	7.265766000	-0.988759000	-0.133554000
C	6.672286000	0.121216000	-0.739672000
C	5.575131000	0.751640000	-0.149908000
C	5.068466000	0.264569000	1.061813000
H	5.262498000	-1.219152000	2.619465000
H	7.210500000	-2.323259000	1.560068000
H	8.121330000	-1.472883000	-0.593904000
H	7.070480000	0.509132000	-1.673307000
H	5.123412000	1.634683000	-0.593130000
O	3.977863000	0.911312000	1.587167000
H	3.723911000	0.493086000	2.425318000

<sup>3</sup>RC<sub>R13</sub>

Cu	-1.320744000	-0.316041000	-0.194424000
C	0.225557000	-2.279958000	1.662732000
H	0.833171000	-2.464889000	0.780412000
C	0.448645000	-2.987212000	2.843010000
H	1.240066000	-3.727717000	2.881613000
C	-0.361651000	-2.726495000	3.945855000
H	-0.220833000	-3.265551000	4.877922000
C	-1.366344000	-1.763556000	3.834582000
H	-2.019017000	-1.538777000	4.672693000
C	-1.522052000	-1.084933000	2.627832000
C	-2.540706000	0.029460000	2.465327000

H	-3.360701000	-0.089828000	3.188557000
H	-2.050789000	0.983458000	2.693046000
C	-4.035645000	-0.931448000	0.765209000
H	-5.033029000	-0.672763000	1.150974000
H	-3.721820000	-1.847694000	1.279870000
C	-4.099726000	-1.210487000	-0.726042000
C	-5.273451000	-1.641354000	-1.342879000
H	-6.187364000	-1.740376000	-0.764942000
C	-5.250403000	-1.943400000	-2.705056000
H	-6.151451000	-2.284211000	-3.206012000
C	-4.057710000	-1.792922000	-3.410996000
H	-3.995960000	-2.011073000	-4.471691000
C	-2.931010000	-1.344189000	-2.725925000
H	-1.981532000	-1.198158000	-3.230932000
C	-3.503053000	1.464161000	0.710079000
H	-4.201462000	1.872453000	1.455433000
H	-4.057518000	1.371983000	-0.231199000
C	-2.346553000	2.423500000	0.498232000
C	-2.472024000	3.768343000	0.825438000
H	-3.381165000	4.139517000	1.286802000
C	-1.412622000	4.627082000	0.518556000
H	-1.490403000	5.691074000	0.720780000
C	-0.267909000	4.113717000	-0.070208000
H	0.546215000	4.760753000	-0.366917000
C	-0.185014000	2.732333000	-0.314626000
C	2.311237000	2.358127000	-0.940480000
N	-0.737805000	-1.346649000	1.560258000
N	-3.043042000	0.113459000	1.080451000
N	-2.949336000	-1.062825000	-1.413215000
N	-1.224311000	1.908961000	-0.050879000
N	0.916431000	2.130494000	-0.914978000
H	0.677312000	1.437347000	-1.620601000
O	2.905951000	1.863459000	-1.883635000
C	3.084494000	3.069100000	0.197562000
C	4.428957000	2.312412000	0.330194000
H	4.975682000	2.317961000	-0.614071000
H	5.041255000	2.797685000	1.097675000
H	4.274684000	1.268537000	0.622840000
C	2.382912000	3.038568000	1.569631000

H	1.500422000	3.679461000	1.626331000
H	2.087546000	2.018823000	1.843488000
H	3.084281000	3.392045000	2.332847000
C	3.400933000	4.520088000	-0.240090000
H	3.904366000	4.527784000	-1.211727000
H	2.510925000	5.154034000	-0.313680000
H	4.069075000	4.982913000	0.494362000
O	0.158445000	-0.966293000	-1.370576000
O	0.131452000	-0.375033000	-2.499276000
C	5.772831000	-3.375808000	0.148357000
C	6.361654000	-2.208038000	-0.344892000
C	5.571083000	-1.272215000	-1.013687000
C	4.202240000	-1.490503000	-1.189134000
C	3.627332000	-2.664422000	-0.692701000
C	4.409212000	-3.609949000	-0.022799000
H	6.379564000	-4.114998000	0.664343000
H	7.425417000	-2.033791000	-0.214652000
H	6.015173000	-0.363058000	-1.409240000
H	3.595575000	-0.752622000	-1.710713000
H	3.942113000	-4.520287000	0.341118000
O	2.284579000	-2.940087000	-0.832483000
H	1.867499000	-2.245294000	-1.368644000

<sup>3</sup>RC<sub>R14</sub>

Cu	-0.971138000	-0.917696000	-0.109414000
C	-3.125378000	-2.230781000	1.759220000
H	-2.408408000	-1.953202000	2.525692000
C	-4.297305000	-2.917470000	2.067173000
H	-4.514061000	-3.187351000	3.095177000
C	-5.166814000	-3.248979000	1.028596000
H	-6.086278000	-3.791241000	1.227715000
C	-4.836125000	-2.878591000	-0.275258000
H	-5.489444000	-3.123271000	-1.107370000
C	-3.650189000	-2.180027000	-0.500534000
C	-3.268731000	-1.672606000	-1.879428000
H	-3.746086000	-2.284578000	-2.659644000
H	-3.659427000	-0.654275000	-1.993065000
C	-1.215341000	-2.930985000	-2.299750000
H	-1.343162000	-3.243749000	-3.347679000



H	-1.765586000	-3.654979000	-1.686271000
C	0.253086000	-3.000220000	-1.916062000
C	1.094518000	-3.938117000	-2.507866000
H	0.720539000	-4.596062000	-3.285742000
C	2.423766000	-4.002459000	-2.085949000
H	3.110752000	-4.711126000	-2.538473000
C	2.874122000	-3.117516000	-1.115114000
H	3.914160000	-3.092661000	-0.815372000
C	1.966883000	-2.205216000	-0.559689000
C	-1.388186000	-0.585641000	-3.027118000
H	-1.928081000	-0.684472000	-3.980524000
H	-0.325155000	-0.750619000	-3.236473000
C	-1.562870000	0.813001000	-2.465763000
C	-2.073510000	1.844779000	-3.243193000
H	-2.389607000	1.657748000	-4.264198000
C	-2.153738000	3.125120000	-2.683266000
H	-2.526038000	3.959754000	-3.269782000
C	-1.720624000	3.324632000	-1.382548000
H	-1.710737000	4.312653000	-0.938254000
C	-1.239630000	2.228016000	-0.642364000
C	-1.025570000	3.299980000	1.654128000
N	-2.809131000	-1.870164000	0.505218000
N	-1.807310000	-1.608053000	-2.051423000
N	0.676061000	-2.160461000	-0.949285000
N	-1.175074000	0.991795000	-1.181778000
N	-0.719831000	2.362844000	0.642647000
H	0.257654000	2.059959000	0.713313000
O	-0.102814000	3.724458000	2.324689000
C	-2.489144000	3.643787000	2.032985000
C	-2.586843000	3.349154000	3.552189000
H	-1.820896000	3.898306000	4.102729000
H	-3.574893000	3.645724000	3.920969000
H	-2.453398000	2.280055000	3.756296000
C	-3.579178000	2.826582000	1.315703000
H	-3.694764000	3.092534000	0.261501000
H	-3.385371000	1.749633000	1.383422000
H	-4.542770000	3.019068000	1.800299000
C	-2.706987000	5.157478000	1.810335000
H	-1.925081000	5.735169000	2.311184000

H	-2.703671000	5.425056000	0.746650000
H	-3.677236000	5.458502000	2.220697000
O	-0.495233000	-0.771358000	1.839707000
O	0.385192000	0.035239000	2.239906000
N	2.351756000	-1.198480000	0.332025000
H	2.036042000	-0.264153000	0.056123000
C	3.178788000	-1.133135000	1.449226000
C	3.571075000	-2.357901000	2.304748000
C	5.030106000	-2.746655000	1.964137000
H	5.696885000	-1.886323000	2.075876000
H	5.366839000	-3.531804000	2.649666000
H	5.136985000	-3.133830000	0.944560000
C	2.630288000	-3.571161000	2.165398000
H	1.580620000	-3.280861000	2.290036000
H	2.733788000	-4.096823000	1.213743000
H	2.867804000	-4.291630000	2.955107000
C	3.522020000	-1.879518000	3.777326000
H	2.506336000	-1.582882000	4.060891000
H	3.837223000	-2.698204000	4.432666000
H	4.179789000	-1.023917000	3.936900000
O	3.539422000	-0.008637000	1.803539000
C	2.429996000	2.905051000	-1.871097000
C	3.001745000	2.412505000	-0.695580000
C	4.356184000	2.624636000	-0.422023000
C	5.135370000	3.336089000	-1.335659000
C	4.575318000	3.834236000	-2.513674000
C	3.220774000	3.615518000	-2.774568000
H	1.374861000	2.735639000	-2.064384000
H	4.790887000	2.237847000	0.495556000
H	6.186863000	3.502783000	-1.119126000
H	5.186322000	4.390047000	-3.218265000
H	2.773322000	4.002236000	-3.686325000
O	2.192889000	1.710294000	0.178219000
H	2.737287000	1.364617000	0.928927000
 <sup>3</sup> TS <sub>R1</sub>			
Cu	2.116733000	0.193939000	-0.229868000
C	0.647485000	-0.012529000	2.515644000
H	-0.137720000	0.499975000	1.969377000

C	0.533042000	-0.279031000	3.879148000
H	-0.353776000	0.034637000	4.419352000
C	1.577282000	-0.944489000	4.518791000
H	1.527717000	-1.162037000	5.581596000
C	2.694489000	-1.325393000	3.773664000
H	3.526226000	-1.843880000	4.241289000
C	2.729794000	-1.034032000	2.410369000
C	3.878222000	-1.489946000	1.524392000
H	4.772099000	-1.694241000	2.133807000
H	3.591113000	-2.438424000	1.054410000
C	4.870978000	0.670432000	0.896008000
H	5.958377000	0.507470000	0.951495000
H	4.531262000	0.886250000	1.916300000
C	4.562732000	1.882351000	0.030485000
C	5.495443000	2.898319000	-0.178133000
H	6.496532000	2.812777000	0.233988000
C	5.118596000	4.020575000	-0.917483000
H	5.827521000	4.824706000	-1.091026000
C	3.824743000	4.090705000	-1.433150000
H	3.493192000	4.944176000	-2.014921000
C	2.956192000	3.027977000	-1.193273000
C	4.760876000	-1.154456000	-0.745960000
H	5.604131000	-1.811566000	-0.482346000
H	5.171253000	-0.345591000	-1.362828000
C	3.743881000	-1.915690000	-1.582739000
C	4.109926000	-3.027781000	-2.340910000
H	5.126034000	-3.408310000	-2.294387000
C	3.155037000	-3.633074000	-3.158951000
H	3.418488000	-4.497895000	-3.760691000
C	1.861564000	-3.113934000	-3.187031000
H	1.088915000	-3.554527000	-3.808094000
C	1.568681000	-2.010395000	-2.387834000
N	1.721386000	-0.381528000	1.799119000
N	4.155004000	-0.532602000	0.441249000
N	3.318367000	1.952537000	-0.477981000
N	2.489486000	-1.425487000	-1.604945000
O	0.447962000	1.054222000	-0.799155000
O	-0.488175000	0.195859000	-1.200167000
H	1.939178000	3.016501000	-1.575084000

H	0.578366000	-1.565975000	-2.354638000
C	-5.565551000	1.090200000	-0.516118000
C	-4.249851000	1.273434000	-0.102636000
C	-3.454317000	0.099808000	0.173018000
C	-4.042570000	-1.222204000	0.133099000
C	-5.355183000	-1.329694000	-0.286034000
C	-6.114212000	-0.195567000	-0.633689000
H	-6.183526000	1.946444000	-0.741423000
H	-5.857039000	-2.285355000	-0.357872000
O	-2.178579000	0.234281000	0.515941000
H	-1.420854000	0.239273000	-0.324373000
C	-3.260752000	-2.480005000	0.571539000
C	-2.038669000	-2.725633000	-0.346531000
C	-2.796171000	-2.316832000	2.040295000
C	-4.136833000	-3.749522000	0.507535000
H	-2.349607000	-2.811801000	-1.394720000
H	-1.298327000	-1.929145000	-0.270924000
H	-1.553073000	-3.667920000	-0.063849000
H	-3.656986000	-2.193061000	2.707700000
H	-2.253366000	-3.215254000	2.358669000
H	-2.139562000	-1.453662000	2.158543000
H	-3.549325000	-4.606166000	0.854677000
H	-5.019906000	-3.676146000	1.151596000
H	-4.469393000	-3.973639000	-0.512344000
C	-3.697874000	2.702395000	0.100051000
C	-3.251097000	2.879634000	1.573494000
C	-2.507457000	2.987841000	-0.848460000
C	-4.769964000	3.777492000	-0.183013000
H	-4.095785000	2.737572000	2.257760000
H	-2.466415000	2.169902000	1.840078000
H	-2.866676000	3.895706000	1.722831000
H	-2.772640000	2.776922000	-1.891019000
H	-2.239081000	4.049269000	-0.781647000
H	-1.624922000	2.404870000	-0.591261000
H	-4.340639000	4.766327000	0.008570000
H	-5.104867000	3.766169000	-1.226830000
H	-5.646338000	3.672910000	0.466533000
O	-7.371483000	-0.454550000	-1.043404000
C	-8.232451000	0.623432000	-1.410174000

H	-7.816795000	1.192932000	-2.249256000
H	-9.170832000	0.158239000	-1.712781000
H	-8.411801000	1.292056000	-0.560389000

<sup>3</sup>TS<sub>R2</sub>

Cu	2.103694000	-0.139071000	-0.156099000
C	2.955775000	-2.576417000	-1.912212000
H	1.878712000	-2.654714000	-2.029716000
C	3.833420000	-3.502125000	-2.472177000
H	3.449545000	-4.336364000	-3.049654000
C	5.201978000	-3.330181000	-2.264757000
H	5.916827000	-4.035373000	-2.678351000
C	5.644122000	-2.240412000	-1.513501000
H	6.702933000	-2.079869000	-1.333269000
C	4.702423000	-1.350008000	-0.997217000
C	5.106187000	-0.092475000	-0.245637000
H	6.099737000	-0.218830000	0.210562000
H	5.190850000	0.726196000	-0.969889000
C	4.160867000	-0.493528000	1.982005000
H	4.950605000	-0.131541000	2.658570000
H	4.431927000	-1.517801000	1.697510000
C	2.826775000	-0.541067000	2.706455000
C	2.752218000	-0.685034000	4.091810000
H	3.660616000	-0.701682000	4.686577000
C	1.499269000	-0.812276000	4.691890000
H	1.416415000	-0.927043000	5.768617000
C	0.360357000	-0.787550000	3.888585000
H	-0.633536000	-0.885332000	4.312108000
C	0.515542000	-0.626679000	2.513121000
H	-0.341886000	-0.600550000	1.849261000
C	4.061050000	1.753785000	1.004303000
H	5.056635000	2.143401000	1.265046000
H	3.414296000	1.911044000	1.875729000
C	3.492818000	2.519925000	-0.174254000
C	4.030284000	3.740626000	-0.545145000
H	4.888264000	4.147653000	-0.021177000
C	3.429889000	4.432606000	-1.611252000
H	3.818481000	5.396382000	-1.927152000
C	2.347332000	3.878266000	-2.256408000

H	1.864468000	4.385430000	-3.085917000
C	1.859330000	2.613496000	-1.833262000
N	3.383170000	-1.528301000	-1.192993000
N	4.092370000	0.303223000	0.747048000
N	1.722298000	-0.501607000	1.936304000
N	2.431107000	1.952276000	-0.798656000
N	0.825912000	2.020918000	-2.482290000
H	0.316128000	1.254495000	-2.040768000
O	0.465471000	-0.967329000	-0.839363000
O	-0.535925000	-0.135741000	-1.156433000
H	0.314863000	2.567383000	-3.159576000
C	-5.492781000	1.123896000	-0.215002000
C	-6.181979000	0.009674000	-0.719421000
C	-5.572022000	-1.259604000	-0.736745000
C	-4.271556000	-1.447002000	-0.306641000
C	-3.538804000	-0.279921000	0.134358000
C	-4.180470000	1.009821000	0.230363000
H	-5.997694000	2.077459000	-0.170802000
H	-6.179937000	-2.080619000	-1.091955000
H	-1.501120000	-0.324912000	-0.305232000
O	-2.266992000	-0.399649000	0.504192000
C	-3.668076000	-2.867977000	-0.251279000
C	-2.437619000	-2.999706000	-1.182358000
C	-3.261365000	-3.199057000	1.206966000
C	-4.690858000	-3.935875000	-0.696075000
H	-2.674134000	-2.668253000	-2.200149000
H	-1.580733000	-2.431278000	-0.823734000
H	-2.137892000	-4.053275000	-1.236888000
H	-4.132735000	-3.170723000	1.871605000
H	-2.839830000	-4.210368000	1.251099000
H	-2.514782000	-2.497633000	1.583529000
H	-4.232267000	-4.926060000	-0.606106000
H	-5.591466000	-3.935195000	-0.072172000
H	-4.992925000	-3.810851000	-1.742202000
C	-3.457231000	2.238117000	0.827272000
C	-3.009231000	1.929782000	2.278483000
C	-2.233496000	2.631421000	-0.035530000
C	-4.379696000	3.474762000	0.893864000
H	-3.874443000	1.699086000	2.910788000

H	-2.319116000	1.086119000	2.315032000
H	-2.509221000	2.808108000	2.704234000
H	-2.536360000	2.836469000	-1.069529000
H	-1.780271000	3.545624000	0.366872000
H	-1.469678000	1.854311000	-0.047228000
H	-3.830433000	4.304470000	1.350896000
H	-4.702693000	3.808572000	-0.099104000
H	-5.269005000	3.295375000	1.508384000
O	-7.444607000	0.041883000	-1.186334000
C	-8.165685000	1.274200000	-1.198726000
H	-7.660092000	2.020862000	-1.821652000
H	-9.139648000	1.038475000	-1.627895000
H	-8.296688000	1.664639000	-0.183069000

<sup>3</sup>TS<sub>R3</sub>

Cu	-2.121603000	-0.074700000	-0.105542000
C	-1.114874000	0.951430000	-2.923815000
H	-0.201983000	0.456591000	-2.608504000
C	-1.214292000	1.635961000	-4.133360000
H	-0.358543000	1.687782000	-4.798041000
C	-2.423458000	2.249366000	-4.456820000
H	-2.535666000	2.799644000	-5.386339000
C	-3.491172000	2.149731000	-3.564656000
H	-4.447063000	2.616336000	-3.783206000
C	-3.318734000	1.432972000	-2.380843000
C	-4.464204000	1.208413000	-1.412013000
H	-5.203692000	2.019191000	-1.494267000
H	-4.975366000	0.280029000	-1.692932000
C	-3.620352000	2.330240000	0.600414000
H	-4.510362000	2.907845000	0.891710000
H	-3.085994000	2.918183000	-0.155685000
C	-2.713712000	2.122733000	1.797630000
C	-2.768931000	2.966842000	2.892904000
H	-3.494606000	3.771848000	2.934604000
C	-1.855256000	2.751802000	3.939420000
H	-1.860103000	3.400639000	4.810414000
C	-0.960896000	1.706341000	3.863447000
H	-0.256124000	1.505846000	4.664039000
C	-0.980482000	0.861940000	2.723859000

C	-4.907798000	0.242147000	0.800486000
H	-5.942837000	0.605581000	0.720329000
H	-4.600450000	0.371743000	1.844187000
C	-4.836717000	-1.231685000	0.448034000
C	-5.955827000	-2.042654000	0.537186000
H	-6.919660000	-1.628453000	0.812734000
C	-5.799179000	-3.414009000	0.272083000
H	-6.650811000	-4.084411000	0.342535000
C	-4.562389000	-3.906561000	-0.085755000
H	-4.415562000	-4.959402000	-0.305370000
C	-3.466855000	-3.011130000	-0.182468000
N	-2.143895000	0.852493000	-2.066638000
N	-3.988069000	1.047055000	-0.027923000
N	-1.837342000	1.093587000	1.701304000
N	-3.615022000	-1.695339000	0.096184000
N	-2.243280000	-3.435747000	-0.589344000
H	-1.449198000	-2.806754000	-0.493910000
O	-0.488442000	-1.182831000	-0.094821000
O	0.486770000	-0.818729000	-0.952156000
H	-2.058760000	-4.425682000	-0.643313000
N	-0.173731000	-0.226979000	2.641759000
H	-0.068469000	-0.681125000	1.736850000
H	0.618071000	-0.288742000	3.264949000
C	4.404707000	-1.530280000	0.048222000
C	5.737527000	-1.380653000	-0.292301000
C	6.323440000	-0.112774000	-0.465588000
C	5.564851000	1.052133000	-0.276277000
C	4.218304000	0.977311000	0.063708000
C	3.620504000	-0.326572000	0.206730000
H	6.390498000	-2.232733000	-0.425138000
H	6.039492000	2.014726000	-0.395175000
O	2.339148000	-0.394024000	0.572585000
H	1.592059000	-0.648123000	-0.163936000
C	3.819215000	-2.945267000	0.259286000
C	3.120081000	-3.057558000	1.637183000
C	2.824546000	-3.282704000	-0.879103000
C	4.920656000	-4.027993000	0.230519000
H	3.823492000	-2.836122000	2.448529000
H	2.272685000	-2.377319000	1.722962000



H	2.758869000	-4.082643000	1.780432000
H	3.326260000	-3.248036000	-1.853148000
H	2.439551000	-4.300418000	-0.739282000
H	1.971437000	-2.603166000	-0.913933000
H	4.464301000	-5.004225000	0.424831000
H	5.417989000	-4.093570000	-0.743368000
H	5.683583000	-3.861858000	0.999321000
C	3.402490000	2.271203000	0.282901000
C	2.246466000	2.359522000	-0.743826000
C	2.840999000	2.309489000	1.726669000
C	4.265115000	3.538483000	0.099104000
H	1.697158000	3.297654000	-0.596794000
H	2.637539000	2.359769000	-1.768433000
H	1.540270000	1.534458000	-0.643485000
H	3.655606000	2.279200000	2.459843000
H	2.287019000	3.243393000	1.881258000
H	2.170207000	1.471119000	1.915802000
H	3.641521000	4.422024000	0.271716000
H	5.096062000	3.583732000	0.812209000
H	4.671381000	3.621991000	-0.915471000
O	7.628228000	-0.128588000	-0.801014000
C	8.326831000	1.102185000	-0.987250000
H	8.335261000	1.694802000	-0.065224000
H	9.346969000	0.822381000	-1.250803000
H	7.884555000	1.688060000	-1.801204000

<sup>3</sup>TS<sub>R4</sub>

Cu	-1.739717000	-0.968326000	-0.145034000
C	-0.286625000	-0.819033000	2.610434000
H	0.486167000	-0.350951000	2.008117000
C	-0.109128000	-1.070541000	3.969617000
H	0.819494000	-0.791349000	4.455839000
C	-1.140502000	-1.691296000	4.673319000
H	-1.034531000	-1.911677000	5.731427000
C	-2.313124000	-2.033039000	3.998080000
H	-3.133662000	-2.520057000	4.516634000
C	-2.421721000	-1.734934000	2.639755000
C	-3.701895000	-1.996562000	1.861114000
H	-4.286409000	-2.794636000	2.343921000

H	-4.314118000	-1.087827000	1.897659000
C	-2.954794000	-3.660467000	0.215045000
H	-3.777243000	-4.392394000	0.206048000
H	-2.304591000	-3.921012000	1.059143000
C	-2.141807000	-3.763596000	-1.064317000
C	-2.130976000	-4.923480000	-1.837863000
H	-2.753401000	-5.768791000	-1.559941000
C	-1.309070000	-4.977386000	-2.964724000
H	-1.284679000	-5.870038000	-3.582775000
C	-0.527414000	-3.868707000	-3.284370000
H	0.124311000	-3.867238000	-4.151597000
C	-0.599791000	-2.742143000	-2.466689000
H	-0.010420000	-1.850099000	-2.655317000
C	-4.552626000	-1.924610000	-0.446824000
H	-5.511441000	-2.333278000	-0.091643000
H	-4.353170000	-2.387927000	-1.420649000
C	-4.675907000	-0.423120000	-0.649108000
C	-5.913031000	0.148251000	-0.924711000
H	-6.812101000	-0.459107000	-0.932556000
C	-5.955308000	1.512107000	-1.229500000
H	-6.894212000	1.985409000	-1.501278000
C	-4.787731000	2.257113000	-1.202907000
H	-4.787324000	3.301844000	-1.482177000
C	-3.583917000	1.627964000	-0.832729000
C	-1.979176000	3.638023000	-0.603835000
N	-1.417895000	-1.143871000	1.964257000
N	-3.439305000	-2.289792000	0.442212000
N	-1.391158000	-2.690582000	-1.383347000
N	-3.536442000	0.296012000	-0.599391000
N	-2.369442000	2.289025000	-0.756313000
H	-1.558976000	1.707383000	-0.986336000
O	-0.914726000	3.952339000	-1.109795000
C	-2.745329000	4.652771000	0.286425000
C	-1.650672000	5.421887000	1.069334000
H	-0.936183000	5.887637000	0.388847000
H	-2.120644000	6.199930000	1.680439000
H	-1.098093000	4.751520000	1.737347000
C	-3.703046000	4.023378000	1.316189000
H	-4.594869000	3.576444000	0.872289000

H	-3.195347000	3.256283000	1.912453000
H	-4.044077000	4.803450000	2.005431000
C	-3.479184000	5.669244000	-0.620215000
H	-2.785295000	6.111106000	-1.341906000
H	-4.311122000	5.225123000	-1.177359000
H	-3.893771000	6.475572000	-0.005141000
O	-0.301094000	0.301883000	-0.566994000
O	0.689550000	-0.126367000	-1.351407000
C	6.083118000	-0.492146000	-0.012843000
C	6.484374000	0.828857000	-0.268323000
C	5.529839000	1.859467000	-0.365365000
C	4.174690000	1.623321000	-0.222466000
C	3.766702000	0.256204000	0.032107000
C	4.739146000	-0.807095000	0.140902000
H	6.832345000	-1.266199000	0.062013000
H	5.915412000	2.853500000	-0.546757000
H	1.754914000	0.010457000	-0.544700000
O	2.496456000	-0.057486000	0.252387000
C	3.175647000	2.795222000	-0.352911000
C	2.438015000	2.689506000	-1.712622000
C	2.157221000	2.821212000	0.814773000
C	3.897826000	4.161697000	-0.333617000
H	3.149165000	2.782876000	-2.541805000
H	1.902110000	1.746107000	-1.829567000
H	1.698501000	3.492994000	-1.796473000
H	2.674803000	2.878896000	1.780264000
H	1.524871000	3.709762000	0.714198000
H	1.507586000	1.947402000	0.823180000
H	3.147166000	4.956916000	-0.383802000
H	4.477791000	4.308164000	0.584995000
H	4.564725000	4.298212000	-1.191611000
C	4.310656000	-2.264879000	0.420337000
C	3.606701000	-2.359821000	1.797656000
C	3.367845000	-2.774884000	-0.698692000
C	5.520288000	-3.223225000	0.463717000
H	4.277598000	-2.028706000	2.599152000
H	2.702344000	-1.751451000	1.828054000
H	3.333586000	-3.402707000	2.000678000
H	3.862052000	-2.724457000	-1.676212000

H	3.109969000	-3.824174000	-0.509612000
H	2.442579000	-2.199728000	-0.747882000
H	5.163540000	-4.240080000	0.658372000
H	6.065908000	-3.246377000	-0.486596000
H	6.223589000	-2.968103000	1.264455000
O	7.762794000	1.218695000	-0.431115000
C	8.813977000	0.255931000	-0.348227000
H	9.735592000	0.814948000	-0.510946000
H	8.839644000	-0.215627000	0.640794000
H	8.707943000	-0.511681000	-1.123304000

<sup>3</sup>TS<sub>R5</sub>

Cu	2.105876000	0.762779000	0.146602000
C	3.349020000	0.564606000	3.032574000
H	2.311046000	0.411249000	3.314814000
C	4.368459000	0.619278000	3.980890000
H	4.138711000	0.507952000	5.035245000
C	5.675074000	0.826503000	3.539031000
H	6.495768000	0.884216000	4.247900000
C	5.916326000	0.964840000	2.171411000
H	6.922218000	1.129792000	1.796740000
C	4.842263000	0.884418000	1.284605000
C	5.036357000	0.942257000	-0.223148000
H	5.974476000	1.464106000	-0.466724000
H	5.134914000	-0.083295000	-0.595205000
C	3.876241000	3.018702000	-0.763529000
H	4.603771000	3.493184000	-1.440127000
H	4.195761000	3.245590000	0.260593000
C	2.501523000	3.620594000	-0.975646000
C	2.371259000	4.831063000	-1.644633000
H	3.240134000	5.317975000	-2.074653000
C	1.093297000	5.388550000	-1.760326000
H	0.941758000	6.311898000	-2.311689000
C	0.017845000	4.737908000	-1.185930000
H	-0.989335000	5.118825000	-1.298575000
C	0.235528000	3.533884000	-0.479579000
C	3.725462000	1.123862000	-2.302415000
H	4.656239000	1.253473000	-2.877568000
H	2.977020000	1.780834000	-2.761639000
C	3.255751000	-0.317965000	-2.411859000

C	3.501966000	-1.060912000	-3.561656000
H	4.059521000	-0.632369000	-4.388028000
C	2.980079000	-2.355457000	-3.628689000
H	3.095638000	-2.947725000	-4.531682000
C	2.312484000	-2.887192000	-2.535457000
H	1.881558000	-3.877787000	-2.574636000
C	2.188442000	-2.110881000	-1.369092000
C	1.417013000	-3.805148000	0.436883000
N	3.582508000	0.694317000	1.718519000
N	3.881236000	1.556422000	-0.904217000
N	1.460668000	2.962107000	-0.419984000
N	2.592218000	-0.818723000	-1.352948000
N	1.609763000	-2.558237000	-0.192820000
H	1.169698000	-1.815553000	0.362377000
O	0.539821000	-3.838729000	1.285555000
C	2.320943000	-5.046467000	0.211895000
C	2.439224000	-5.736270000	1.593842000
H	1.456592000	-5.981281000	1.999066000
H	3.022950000	-6.657153000	1.489316000
H	2.949949000	-5.089297000	2.315759000
C	3.748880000	-4.726564000	-0.272821000
H	3.796992000	-4.375135000	-1.304696000
H	4.224889000	-3.975030000	0.367998000
H	4.354498000	-5.637495000	-0.214667000
C	1.603290000	-6.029430000	-0.744197000
H	2.173838000	-6.962867000	-0.804128000
H	0.601776000	-6.264594000	-0.370534000
H	1.500800000	-5.644361000	-1.764003000
O	0.627010000	-0.140116000	1.085131000
O	-0.534982000	0.083286000	0.453761000
N	-0.795376000	2.849475000	0.128476000
H	-0.706385000	1.822485000	0.136723000
C	-2.119651000	3.251052000	0.414773000
C	-2.431066000	4.535377000	1.227259000
C	-3.341549000	5.454008000	0.382663000
H	-4.204188000	4.897254000	0.005207000
H	-3.706550000	6.282840000	0.999129000
H	-2.814237000	5.891302000	-0.473612000
C	-1.207148000	5.304838000	1.755402000

H	-0.518688000	4.642744000	2.291933000
H	-0.646466000	5.817977000	0.970684000
H	-1.546943000	6.070781000	2.461290000
C	-3.243139000	4.034448000	2.452118000
H	-2.634439000	3.383536000	3.090532000
H	-3.564127000	4.892792000	3.052306000
H	-4.123578000	3.474117000	2.131525000
O	-3.016888000	2.466923000	0.149883000
C	-5.936468000	-0.782606000	0.123285000
C	-5.257940000	-1.341498000	1.227815000
C	-3.938648000	-1.737331000	1.144397000
C	-3.259625000	-1.509383000	-0.115801000
C	-3.970984000	-1.024064000	-1.279288000
C	-5.299219000	-0.659180000	-1.124562000
H	-5.834105000	-1.459224000	2.135681000
H	-5.854674000	-0.266396000	-1.962954000
O	-1.970262000	-1.794228000	-0.242642000
H	-1.303279000	-1.068322000	0.170661000
C	-3.280576000	-0.898037000	-2.652798000
C	-2.133273000	0.141570000	-2.585902000
C	-2.730667000	-2.277239000	-3.098083000
C	-4.263687000	-0.423080000	-3.744404000
H	-2.492590000	1.091110000	-2.175207000
H	-1.307120000	-0.205712000	-1.964820000
H	-1.748847000	0.322568000	-3.597413000
H	-3.542101000	-3.008016000	-3.195816000
H	-2.251193000	-2.178935000	-4.079542000
H	-1.997494000	-2.665621000	-2.390135000
H	-3.738663000	-0.387462000	-4.704631000
H	-5.113178000	-1.105243000	-3.864391000
H	-4.647816000	0.584553000	-3.547608000
C	-3.263709000	-2.467530000	2.324130000
C	-2.858922000	-3.892188000	1.865104000
C	-2.013101000	-1.711517000	2.840246000
C	-4.233091000	-2.618450000	3.516215000
H	-3.737538000	-4.459604000	1.535628000
H	-2.127358000	-3.861065000	1.056756000
H	-2.404050000	-4.430253000	2.704467000
H	-2.220858000	-0.645157000	2.985107000

H	-1.719200000	-2.131012000	3.809356000
H	-1.158399000	-1.821419000	2.175003000
H	-3.726770000	-3.169132000	4.315295000
H	-4.538637000	-1.649627000	3.928974000
H	-5.133828000	-3.183961000	3.252473000
O	-7.208179000	-0.427105000	0.362380000
C	-8.002705000	0.138086000	-0.683646000
H	-8.971839000	0.347873000	-0.231179000
H	-7.557862000	1.068065000	-1.053880000
H	-8.127221000	-0.572078000	-1.508472000

<sup>3</sup>TS<sub>R6</sub>

Cu	1.272990000	0.195013000	0.113785000
C	-0.045224000	-2.643977000	0.151576000
H	-0.911540000	-2.077315000	0.477603000
C	-0.068280000	-4.036036000	0.079594000
H	-0.965659000	-4.577268000	0.359873000
C	1.078255000	-4.702379000	-0.349008000
H	1.100294000	-5.786558000	-0.408210000
C	2.204146000	-3.955402000	-0.699602000
H	3.113868000	-4.442688000	-1.037681000
C	2.145245000	-2.564829000	-0.614898000
C	3.302505000	-1.687531000	-1.064779000
H	4.241250000	-2.262768000	-1.062174000
H	3.118216000	-1.386689000	-2.103237000
C	3.994326000	-0.676997000	1.066690000
H	5.094709000	-0.691448000	1.036341000
H	3.673922000	-1.670857000	1.402445000
C	3.507027000	0.343656000	2.083024000
C	4.299832000	0.761536000	3.151960000
H	5.320430000	0.402967000	3.247257000
C	3.757951000	1.639187000	4.092287000
H	4.355653000	1.976354000	4.933948000
C	2.444453000	2.079829000	3.932370000
H	1.987472000	2.763661000	4.639721000
C	1.722582000	1.628531000	2.829529000
C	4.032441000	0.659389000	-0.995661000
H	4.966146000	0.355213000	-1.493716000
H	4.302579000	1.422299000	-0.255215000
C	3.081474000	1.290178000	-2.000792000

C	3.545267000	1.875537000	-3.178627000
H	4.601922000	1.837643000	-3.426497000
C	2.633186000	2.510192000	-4.023086000
H	2.971877000	2.975246000	-4.944187000
C	1.285068000	2.531675000	-3.668786000
H	0.543083000	3.012051000	-4.297759000
C	0.897041000	1.910561000	-2.482842000
N	1.038476000	-1.926690000	-0.187027000
N	3.408738000	-0.455518000	-0.265693000
N	2.243187000	0.780579000	1.930133000
N	1.776403000	1.305692000	-1.668303000
O	-0.512693000	0.747991000	0.682918000
O	-1.324432000	0.956900000	-0.369989000
H	0.699553000	1.941223000	2.640426000
H	-0.137222000	1.880614000	-2.152553000
C	-5.946955000	1.101321000	0.533424000
C	-4.602436000	0.783507000	0.474987000
C	-4.169307000	-0.481874000	-0.017895000
C	-5.156693000	-1.413998000	-0.456544000
C	-6.493943000	-1.106238000	-0.377400000
C	-6.909924000	0.156454000	0.114834000
H	-6.251751000	2.071857000	0.907251000
H	-7.259116000	-1.808071000	-0.692806000
O	-2.903491000	-0.814624000	-0.059622000
H	-2.176706000	0.082890000	-0.196390000
H	-4.820740000	-2.371758000	-0.840342000
H	-3.852382000	1.499146000	0.797376000
O	-8.239184000	0.354966000	0.139117000
C	-8.759560000	1.597736000	0.615111000
H	-9.842982000	1.511075000	0.534168000
H	-8.480373000	1.765084000	1.661502000
H	-8.409319000	2.432233000	-0.002879000
<b><sup>3</sup>TS<sub>R7</sub></b>			
Cu	1.290192000	0.040484000	-0.151263000
C	1.536997000	0.164992000	-3.248858000
H	0.457259000	0.247362000	-3.165439000
C	2.184362000	0.108163000	-4.480971000
H	1.609602000	0.147047000	-5.400138000
C	3.574435000	-0.007032000	-4.497265000



H	4.113420000	-0.062762000	-5.438395000
C	4.267296000	-0.054550000	-3.286895000
H	5.349247000	-0.144905000	-3.266200000
C	3.547550000	0.021705000	-2.094437000
C	4.229495000	0.066610000	-0.737890000
H	5.218603000	-0.413536000	-0.787012000
H	4.398860000	1.117668000	-0.474812000
C	3.407541000	-1.990773000	0.319118000
H	4.311576000	-2.387261000	0.806312000
H	3.440141000	-2.316603000	-0.727844000
C	2.161702000	-2.575322000	0.962358000
C	2.186398000	-3.798465000	1.631487000
H	3.123196000	-4.333936000	1.753453000
C	0.992614000	-4.318236000	2.133210000
H	0.986726000	-5.270086000	2.655994000
C	-0.186058000	-3.595743000	1.956579000
H	-1.135912000	-3.963071000	2.329993000
C	-0.127264000	-2.373542000	1.289392000
H	-1.016934000	-1.773775000	1.129549000
C	3.659822000	0.056390000	1.652660000
H	4.734849000	0.047376000	1.886227000
H	3.163592000	-0.587608000	2.388029000
C	3.101760000	1.460081000	1.785422000
C	3.806233000	2.446061000	2.455147000
H	4.795051000	2.246192000	2.853665000
C	3.196982000	3.703872000	2.608809000
H	3.715532000	4.503026000	3.130518000
C	1.936063000	3.917533000	2.097197000
H	1.439053000	4.876683000	2.205019000
C	1.277454000	2.861464000	1.413515000
N	2.205842000	0.122273000	-2.087018000
N	3.388102000	-0.517981000	0.320984000
N	1.021140000	-1.875968000	0.804445000
N	1.870468000	1.655662000	1.256212000
N	0.045341000	3.044265000	0.872153000
H	-0.521827000	2.232888000	0.624654000
O	-0.476224000	0.360086000	-0.882947000
O	-1.374521000	0.628264000	0.100687000
H	-0.457159000	3.883847000	1.119496000

C	-6.626430000	-1.166790000	0.330432000
C	-6.995157000	0.118027000	-0.144064000
C	-6.001758000	1.010157000	-0.605924000
C	-4.675005000	0.621282000	-0.604057000
C	-4.289279000	-0.666034000	-0.126972000
C	-5.306463000	-1.546985000	0.349841000
H	-7.414173000	-1.827820000	0.676799000
H	-6.270607000	1.994322000	-0.971613000
H	-2.271475000	-0.214396000	-0.093992000
O	-3.044179000	-1.067950000	-0.137060000
H	-3.903083000	1.293989000	-0.964939000
H	-5.006515000	-2.524314000	0.713316000
O	-8.310798000	0.386683000	-0.111800000
C	-8.786707000	1.654299000	-0.570085000
H	-8.545110000	1.804171000	-1.628290000
H	-9.868476000	1.623748000	-0.441521000
H	-8.366978000	2.470318000	0.028836000

<sup>3</sup>TS<sub>RR</sub>

Cu	-1.300074000	-0.091472000	0.031911000
C	-0.311525000	-1.682494000	-2.522887000
H	0.655002000	-1.522000000	-2.055821000
C	-0.457159000	-2.328184000	-3.749155000
H	0.417959000	-2.692258000	-4.276884000
C	-1.738669000	-2.483207000	-4.275298000
H	-1.890010000	-2.973126000	-5.232646000
C	-2.828730000	-1.993242000	-3.555424000
H	-3.840508000	-2.093134000	-3.936850000
C	-2.602844000	-1.371208000	-2.328028000
C	-3.744972000	-0.886508000	-1.455177000
H	-4.628900000	-0.655962000	-2.068620000
H	-4.030459000	-1.697239000	-0.774673000
C	-3.286729000	1.521931000	-1.396234000
H	-4.292696000	1.925129000	-1.586227000
H	-2.846468000	1.283161000	-2.371863000
C	-2.424256000	2.562994000	-0.709358000
C	-2.692855000	3.913981000	-0.845070000
H	-3.556955000	4.252866000	-1.406226000
C	-1.808147000	4.826241000	-0.244177000

H	-1.977793000	5.894776000	-0.339685000
C	-0.731369000	4.360965000	0.478885000
H	-0.043408000	5.041901000	0.969816000
C	-0.535701000	2.961627000	0.604437000
C	-4.143278000	0.381233000	0.609833000
H	-5.221801000	0.339107000	0.398016000
H	-3.936105000	1.369372000	1.035658000
C	-3.761769000	-0.679925000	1.624423000
C	-4.700176000	-1.216443000	2.490175000
H	-5.742942000	-0.924760000	2.427245000
C	-4.256441000	-2.137405000	3.454700000
H	-4.960250000	-2.571757000	4.158757000
C	-2.925911000	-2.495662000	3.501578000
H	-2.559246000	-3.211893000	4.230162000
C	-2.026549000	-1.925200000	2.565417000
N	-1.361368000	-1.215465000	-1.828192000
N	-3.344923000	0.264292000	-0.626931000
N	-1.367941000	2.086160000	-0.008605000
N	-2.452593000	-1.021231000	1.653445000
N	-0.718935000	-2.289287000	2.527373000
H	-0.077166000	-1.742113000	1.955612000
O	0.509409000	-0.371464000	0.750400000
O	1.441465000	-0.675002000	-0.196590000
H	-0.336065000	-2.818776000	3.295586000
N	0.459754000	2.456746000	1.377119000
H	0.680597000	1.466125000	1.282492000
H	1.233187000	3.060993000	1.613908000
C	4.689916000	-0.669768000	0.465985000
C	6.014945000	-1.067022000	0.456469000
C	7.023023000	-0.139443000	0.112803000
C	6.671421000	1.189624000	-0.234309000
C	5.353185000	1.579128000	-0.245232000
C	4.325203000	0.661137000	0.116519000
H	3.905273000	-1.370648000	0.733479000
H	6.269492000	-2.086281000	0.722590000
H	7.469441000	1.876926000	-0.495388000
H	5.065826000	2.588641000	-0.520209000
O	3.076316000	1.072195000	0.133941000
H	2.345831000	0.241232000	0.005320000

O	8.338097000	-0.412600000	0.083463000
C	8.796496000	-1.725647000	0.413204000
H	8.385550000	-2.469695000	-0.278431000
H	9.881007000	-1.690197000	0.311871000
H	8.530865000	-1.986245000	1.443918000

<sup>3</sup>TS<sub>R9</sub>

Cu	-1.577679000	-0.533003000	0.182460000
C	-2.045693000	-0.177480000	3.231575000
H	-0.996464000	-0.457718000	3.256206000
C	-2.782079000	0.034425000	4.395130000
H	-2.310539000	-0.076782000	5.365738000
C	-4.128299000	0.379730000	4.276018000
H	-4.737246000	0.544045000	5.160053000
C	-4.687585000	0.506503000	3.003778000
H	-5.733292000	0.771252000	2.878121000
C	-3.879982000	0.291714000	1.886738000
C	-4.392228000	0.495113000	0.469432000
H	-5.486886000	0.381133000	0.438346000
H	-4.171821000	1.527585000	0.172396000
C	-4.208888000	-1.776537000	-0.444157000
H	-5.153051000	-1.898908000	-0.997386000
H	-4.422762000	-2.008633000	0.606373000
C	-3.170979000	-2.765938000	-0.948660000
C	-3.532535000	-3.957985000	-1.575694000
H	-4.578805000	-4.179137000	-1.764662000
C	-2.530868000	-4.855341000	-1.948691000
H	-2.788201000	-5.791409000	-2.435446000
C	-1.199532000	-4.528828000	-1.694138000
H	-0.390858000	-5.196709000	-1.971195000
C	-0.917780000	-3.311315000	-1.077631000
H	0.098948000	-2.993454000	-0.866917000
C	-3.683457000	0.156625000	-1.860368000
H	-4.677481000	0.495515000	-2.190891000
H	-3.388347000	-0.661729000	-2.527884000
C	-2.672534000	1.280825000	-2.015475000
C	-2.921452000	2.345835000	-2.874193000
H	-3.870116000	2.424875000	-3.394978000
C	-1.904920000	3.285964000	-3.071815000

H	-2.045168000	4.109137000	-3.766241000
C	-0.703480000	3.145949000	-2.396002000
H	0.119665000	3.825516000	-2.574237000
C	-0.548388000	2.078343000	-1.491288000
C	1.659916000	2.660391000	-0.320470000
N	-2.584322000	-0.050306000	2.009361000
N	-3.717813000	-0.389282000	-0.494304000
N	-1.882787000	-2.453800000	-0.712258000
N	-1.519835000	1.154797000	-1.327778000
N	0.626844000	1.841728000	-0.791102000
H	0.871572000	0.844698000	-0.688003000
O	2.764119000	2.143653000	-0.197685000
C	1.441400000	4.112955000	0.182333000
C	2.241278000	4.214133000	1.506190000
H	3.288481000	3.949059000	1.353028000
H	2.184305000	5.239091000	1.888484000
H	1.828701000	3.543360000	2.268528000
C	-0.020094000	4.491009000	0.489675000
H	-0.636704000	4.617992000	-0.402273000
H	-0.497371000	3.743725000	1.134120000
H	-0.033393000	5.445950000	1.026483000
C	2.069724000	5.095335000	-0.833706000
H	3.108100000	4.820381000	-1.042879000
H	1.527156000	5.126592000	-1.785193000
H	2.059714000	6.109689000	-0.419616000
O	0.196718000	-0.712219000	0.947375000
O	1.046718000	-0.872314000	-0.105925000
C	6.234929000	-2.832000000	0.428567000
C	6.611258000	-1.478847000	0.209725000
C	5.620066000	-0.473835000	0.121895000
C	4.287397000	-0.803761000	0.262493000
C	3.897972000	-2.162105000	0.482803000
C	4.911313000	-3.168993000	0.552642000
H	7.021570000	-3.576808000	0.490250000
H	5.890069000	0.561656000	-0.048921000
H	3.531464000	-0.026828000	0.192071000
H	1.918746000	-1.729155000	0.333326000
H	4.600389000	-4.195296000	0.717314000
O	2.651169000	-2.518161000	0.639767000

O	7.929737000	-1.263958000	0.100364000
C	8.418475000	0.063275000	-0.118906000
H	9.502952000	-0.031068000	-0.168587000
H	8.038026000	0.468019000	-1.062951000
H	8.141317000	0.722528000	0.710686000

<sup>3</sup>TS<sub>R10</sub>

Cu	1.786850000	0.168909000	0.278727000
C	2.264744000	-0.225892000	3.328990000
H	1.198745000	-0.019648000	3.357140000
C	3.011435000	-0.447735000	4.484015000
H	2.532368000	-0.414979000	5.456730000
C	4.377120000	-0.702175000	4.354814000
H	4.992834000	-0.871358000	5.233230000
C	4.947202000	-0.733030000	3.081283000
H	6.007306000	-0.927539000	2.948606000
C	4.129418000	-0.513104000	1.972890000
C	4.645242000	-0.610935000	0.547296000
H	5.724757000	-0.398488000	0.511986000
H	4.510484000	-1.643142000	0.202576000
C	4.257061000	1.680623000	-0.222525000
H	5.230233000	1.896807000	-0.688676000
H	4.361197000	1.881399000	0.850330000
C	3.191108000	2.598210000	-0.788765000
C	3.544220000	3.749668000	-1.477989000
H	4.587696000	3.987890000	-1.654230000
C	2.517951000	4.572746000	-1.957407000
H	2.750439000	5.459226000	-2.540100000
C	1.201688000	4.231302000	-1.712295000
H	0.389169000	4.817985000	-2.120512000
C	0.916300000	3.072499000	-0.956348000
C	3.954066000	-0.189133000	-1.770951000
H	4.989738000	-0.393508000	-2.082580000
H	3.592037000	0.637647000	-2.393286000
C	3.082221000	-1.403466000	-2.028957000
C	3.455256000	-2.350583000	-2.976137000
H	4.402556000	-2.264373000	-3.498233000
C	2.561229000	-3.387736000	-3.259514000
H	2.793542000	-4.120511000	-4.026698000

C	1.363747000	-3.460976000	-2.567971000
H	0.629556000	-4.222077000	-2.799833000
C	1.089307000	-2.507744000	-1.567174000
C	-0.964857000	-3.549315000	-0.487166000
N	2.816210000	-0.257293000	2.106858000
N	3.888636000	0.261392000	-0.369808000
N	1.908018000	2.250574000	-0.538221000
N	1.929833000	-1.475952000	-1.333160000
N	-0.084498000	-2.518643000	-0.832573000
H	-0.481136000	-1.585859000	-0.618873000
O	-2.151487000	-3.263314000	-0.377898000
C	-0.492068000	-4.970503000	-0.073136000
C	-1.215748000	-5.256809000	1.268992000
H	-2.296522000	-5.153941000	1.159512000
H	-0.984346000	-6.275918000	1.597215000
H	-0.884128000	-4.564288000	2.051480000
C	1.020656000	-5.129289000	0.169441000
H	1.611220000	-5.125269000	-0.748857000
H	1.404398000	-4.343234000	0.829935000
H	1.200116000	-6.091107000	0.662358000
C	-0.995029000	-5.989918000	-1.120730000
H	-2.070151000	-5.872051000	-1.285932000
H	-0.487008000	-5.885580000	-2.086367000
H	-0.810892000	-7.009146000	-0.763390000
O	0.069639000	-0.092801000	1.083796000
O	-0.892887000	-0.010770000	0.103007000
N	-0.369756000	2.678716000	-0.665600000
H	-0.521325000	1.663526000	-0.574326000
C	-1.605265000	3.365697000	-0.746964000
C	-1.813242000	4.775164000	-0.131455000
C	-2.178897000	5.770689000	-1.255545000
H	-2.999533000	5.379057000	-1.863932000
H	-2.498310000	6.722040000	-0.815973000
H	-1.334260000	5.987670000	-1.919821000
C	-0.647746000	5.303574000	0.724396000
H	-0.348260000	4.573570000	1.484550000
H	0.235181000	5.572193000	0.140469000
H	-0.974401000	6.209645000	1.246406000
C	-3.047368000	4.619962000	0.796796000

H	-2.843061000	3.906849000	1.603121000
H	-3.289359000	5.589464000	1.245631000
H	-3.911388000	4.261714000	0.233494000
O	-2.558349000	2.739459000	-1.176580000
C	-6.532558000	-0.540395000	0.369012000
C	-5.382290000	-1.272386000	-0.009553000
C	-4.127249000	-0.796577000	0.307114000
C	-3.982914000	0.438410000	1.009172000
C	-5.151605000	1.167414000	1.388488000
C	-6.396500000	0.685196000	1.078094000
H	-5.470507000	-2.214119000	-0.538162000
H	-3.248247000	-1.372981000	0.033516000
H	-5.022158000	2.103659000	1.920109000
H	-7.300407000	1.217908000	1.354176000
O	-2.813811000	0.922526000	1.344911000
H	-1.997139000	0.469613000	0.821983000
O	-7.792554000	-0.914047000	0.114910000
C	-8.046607000	-2.128253000	-0.601074000
H	-9.131102000	-2.195236000	-0.682409000
H	-7.600566000	-2.090580000	-1.600481000
H	-7.661680000	-2.992453000	-0.049415000

<sup>3</sup>TS<sub>R11</sub>

Cu	0.781906000	-0.034568000	-0.230654000
C	-0.884105000	1.657604000	1.821681000
H	-1.677770000	1.519362000	1.093910000
C	-1.067740000	2.453628000	2.951377000
H	-2.016203000	2.955754000	3.109415000
C	-0.014169000	2.590844000	3.853156000
H	-0.118783000	3.211356000	4.738216000
C	1.183413000	1.919171000	3.601943000
H	2.023572000	2.001942000	4.284936000
C	1.286838000	1.129703000	2.457463000
C	2.525751000	0.296382000	2.172827000
H	3.396689000	0.708737000	2.703837000
H	2.358499000	-0.711245000	2.571816000
C	3.396490000	1.360637000	0.134211000
H	4.486381000	1.379916000	0.283867000
H	2.987163000	2.229246000	0.664197000
C	3.059251000	1.504232000	-1.340839000



C	3.922211000	2.123644000	-2.244273000
H	4.898081000	2.470080000	-1.917629000
C	3.506875000	2.293400000	-3.566162000
H	4.160850000	2.775020000	-4.286962000
C	2.246906000	1.832851000	-3.947807000
H	1.888375000	1.944653000	-4.965432000
C	1.448921000	1.210715000	-2.990257000
C	3.506096000	-1.082826000	0.387902000
H	4.386070000	-1.230891000	1.031844000
H	3.876946000	-0.972400000	-0.638355000
C	2.599165000	-2.301607000	0.440658000
C	3.083574000	-3.565895000	0.774224000
H	4.123480000	-3.694362000	1.059435000
C	2.212212000	-4.655483000	0.730105000
H	2.566964000	-5.650223000	0.982941000
C	0.883107000	-4.446129000	0.364826000
H	0.173340000	-5.265378000	0.321893000
C	0.471287000	-3.149951000	0.060011000
N	0.270064000	1.013326000	1.580553000
N	2.783133000	0.157160000	0.727103000
N	1.848642000	1.053439000	-1.719446000
N	1.312508000	-2.104459000	0.095502000
O	-0.867454000	-0.070375000	-1.246181000
O	-1.756504000	-0.925762000	-0.697368000
H	0.462503000	0.820909000	-3.224504000
H	-0.551969000	-2.916525000	-0.218584000
C	-6.426677000	-0.854984000	-1.688776000
C	-5.101820000	-0.529375000	-1.459567000
C	-4.740252000	0.230216000	-0.304042000
C	-5.766764000	0.638544000	0.600094000
C	-7.088341000	0.321503000	0.341919000
C	-7.427683000	-0.429356000	-0.797558000
H	-6.697837000	-1.434935000	-2.566159000
H	-7.867935000	0.646794000	1.024553000
O	-3.502335000	0.574991000	-0.074725000
H	-2.652357000	-0.224913000	-0.466509000
H	-5.476040000	1.210214000	1.475655000
H	-4.316612000	-0.840894000	-2.142023000
H	-8.466038000	-0.681645000	-0.989888000

${}^3\text{TS}_{\text{R12}}$ 

Cu	0.791683000	-0.005378000	-0.174040000
C	1.372790000	-0.259227000	-3.214297000
H	0.302487000	-0.084081000	-3.270939000
C	2.144448000	-0.512064000	-4.345947000
H	1.680442000	-0.537382000	-5.326060000
C	3.511379000	-0.736987000	-4.182649000
H	4.143170000	-0.946095000	-5.040752000
C	4.060233000	-0.694731000	-2.900113000
H	5.120535000	-0.866317000	-2.740841000
C	3.224034000	-0.420894000	-1.818146000
C	3.751507000	-0.264943000	-0.402647000
H	4.685932000	-0.830400000	-0.272340000
H	3.992964000	0.792241000	-0.240371000
C	2.635662000	-2.103098000	0.784088000
H	3.440539000	-2.491052000	1.426232000
H	2.763622000	-2.564224000	-0.203020000
C	1.277900000	-2.508552000	1.329367000
C	1.114057000	-3.637773000	2.130073000
H	1.978094000	-4.222188000	2.431589000
C	-0.173085000	-4.001953000	2.527802000
H	-0.326334000	-4.879156000	3.149319000
C	-1.253276000	-3.222415000	2.118096000
H	-2.270043000	-3.471046000	2.402352000
C	-1.008047000	-2.098812000	1.330980000
H	-1.817420000	-1.462717000	0.988901000
C	2.912569000	0.075875000	1.884729000
H	3.947504000	0.006848000	2.250027000
H	2.274007000	-0.424719000	2.621756000
C	2.484706000	1.525608000	1.773794000
C	3.199613000	2.529680000	2.403244000
H	4.108649000	2.303250000	2.949747000
C	2.705784000	3.843667000	2.319632000
H	3.235793000	4.659188000	2.802935000
C	1.543374000	4.091749000	1.623917000
H	1.135983000	5.094965000	1.546446000
C	0.868052000	3.012800000	0.994602000
N	1.904081000	-0.216118000	-1.983153000

N	2.741412000	-0.642607000	0.605264000
N	0.230918000	-1.750488000	0.948169000
N	1.350049000	1.750414000	1.067317000
N	-0.263981000	3.226689000	0.275437000
H	-0.879809000	2.442963000	0.066510000
O	-0.852372000	0.331907000	-1.133114000
O	-1.815634000	0.829414000	-0.311014000
H	-0.702797000	4.133063000	0.344779000
C	-7.185656000	-0.351034000	0.204954000
C	-7.449107000	0.869368000	-0.443149000
C	-6.411243000	1.569906000	-1.083343000
C	-5.124461000	1.062205000	-1.089416000
C	-4.839088000	-0.173368000	-0.428742000
C	-5.902467000	-0.865720000	0.226699000
H	-7.993934000	-0.886606000	0.694110000
H	-6.625262000	2.509398000	-1.584511000
H	-2.733126000	0.120371000	-0.475081000
O	-3.641284000	-0.691589000	-0.431676000
H	-8.457804000	1.270871000	-0.451373000
H	-4.313953000	1.582117000	-1.591380000
H	-5.669129000	-1.802130000	0.723160000

<sup>3</sup>TS<sub>R13</sub>

Cu	-0.806818000	-0.074502000	0.045129000
C	0.114566000	-2.142964000	-2.178674000
H	1.073998000	-2.020948000	-1.687140000
C	-0.055905000	-2.956234000	-3.297135000
H	0.790388000	-3.497411000	-3.706582000
C	-1.322620000	-3.047059000	-3.871845000
H	-1.490780000	-3.664417000	-4.749271000
C	-2.374966000	-2.326341000	-3.306353000
H	-3.373600000	-2.370042000	-3.730420000
C	-2.128298000	-1.545599000	-2.177995000
C	-3.236982000	-0.798044000	-1.463285000
H	-4.053692000	-0.555561000	-2.158794000
H	-3.656586000	-1.451506000	-0.689660000
C	-2.467942000	1.517824000	-1.734932000
H	-3.404062000	1.999830000	-2.052474000
H	-2.011541000	1.077033000	-2.629234000

C	-1.517025000	2.542337000	-1.149229000
C	-1.590396000	3.875710000	-1.509987000
H	-2.364859000	4.225301000	-2.184022000
C	-0.625948000	4.754628000	-0.985827000
H	-0.641287000	5.806096000	-1.257288000
C	0.330951000	4.281433000	-0.114943000
H	1.074500000	4.941110000	0.320677000
C	0.325623000	2.907787000	0.239991000
C	-3.566169000	0.820246000	0.357527000
H	-4.626476000	0.882643000	0.073871000
H	-3.247235000	1.827525000	0.647502000
C	-3.384679000	-0.113496000	1.538136000
C	-4.427081000	-0.388140000	2.406338000
H	-5.415927000	0.022435000	2.233456000
C	-4.159218000	-1.203591000	3.519920000
H	-4.948012000	-1.432674000	4.230457000
C	-2.894699000	-1.719590000	3.705442000
H	-2.664543000	-2.359319000	4.551539000
C	-1.881354000	-1.417298000	2.760271000
N	-0.900264000	-1.454675000	-1.630325000
N	-2.726786000	0.411658000	-0.789673000
N	-0.579053000	2.056200000	-0.300483000
N	-2.136510000	-0.612558000	1.702577000
N	-0.637161000	-1.949357000	2.864175000
H	0.103819000	-1.582917000	2.269775000
O	0.897104000	-0.466916000	0.919679000
O	1.851253000	-0.954112000	0.071298000
H	-0.371059000	-2.409503000	3.721386000
N	1.190751000	2.416548000	1.162816000
H	1.282093000	1.405286000	1.238625000
H	2.027940000	2.945341000	1.361314000
C	5.111399000	-1.246658000	0.828826000
C	6.402510000	-1.744705000	0.814380000
C	7.465208000	-0.951850000	0.346602000
C	7.222936000	0.351509000	-0.122387000
C	5.936346000	0.859863000	-0.135798000
C	4.851515000	0.073609000	0.351769000
H	4.280079000	-1.840117000	1.197214000
H	6.598977000	-2.749917000	1.175666000

H	8.476400000	-1.347096000	0.348509000
H	8.049295000	0.957064000	-0.482644000
H	5.718018000	1.857525000	-0.502969000
O	3.646398000	0.587829000	0.370264000
H	2.790368000	-0.214608000	0.273350000

<sup>3</sup>TS<sub>R14</sub>

Cu	-1.180003000	-0.509169000	0.187720000
C	-1.735864000	-0.011674000	3.200175000
H	-0.694012000	-0.308781000	3.278365000
C	-2.512663000	0.265493000	4.322751000
H	-2.081167000	0.189651000	5.315067000
C	-3.846219000	0.629508000	4.135547000
H	-4.485012000	0.844233000	4.987048000
C	-4.354385000	0.710080000	2.838085000
H	-5.388751000	0.988789000	2.660256000
C	-3.509027000	0.430772000	1.764530000
C	-3.956984000	0.580982000	0.319926000
H	-5.048790000	0.469855000	0.241120000
H	-3.716143000	1.598958000	-0.008810000
C	-3.776974000	-1.723615000	-0.511575000
H	-4.692811000	-1.835430000	-1.111286000
H	-4.052682000	-1.916468000	0.532385000
C	-2.739963000	-2.752296000	-0.929926000
C	-3.097196000	-3.960705000	-1.526370000
H	-4.137689000	-4.168714000	-1.757095000
C	-2.098265000	-4.892092000	-1.814091000
H	-2.352273000	-5.841674000	-2.275628000
C	-0.773982000	-4.582821000	-1.506810000
H	0.032008000	-5.277906000	-1.716114000
C	-0.494400000	-3.347490000	-0.925989000
H	0.518039000	-3.045332000	-0.676744000
C	-3.140740000	0.152963000	-1.961004000
H	-4.116097000	0.485920000	-2.346430000
H	-2.820017000	-0.689133000	-2.585488000
C	-2.116036000	1.265721000	-2.096027000
C	-2.318343000	2.316060000	-2.983034000
H	-3.241666000	2.392520000	-3.547703000
C	-1.286058000	3.245891000	-3.149879000

H	-1.388313000	4.057867000	-3.863751000
C	-0.117672000	3.109396000	-2.418863000
H	0.717594000	3.779836000	-2.572093000
C	-0.009336000	2.055405000	-1.490653000
C	2.181413000	2.625044000	-0.266718000
N	-2.226075000	0.070717000	1.953794000
N	-3.246026000	-0.348592000	-0.577946000
N	-1.457443000	-2.456562000	-0.643781000
N	-0.996107000	1.142364000	-1.354133000
N	1.129410000	1.821127000	-0.735446000
H	1.351486000	0.826671000	-0.599398000
O	3.260035000	2.072393000	-0.101157000
C	1.997528000	4.098007000	0.183401000
C	2.775092000	4.219758000	1.518885000
H	3.816908000	3.920311000	1.395327000
H	2.740428000	5.258019000	1.866134000
H	2.329163000	3.586557000	2.294427000
C	0.541313000	4.525445000	0.447675000
H	-0.056408000	4.631742000	-0.459911000
H	0.033415000	3.817600000	1.113049000
H	0.543686000	5.501383000	0.945193000
C	2.674961000	5.027499000	-0.851051000
H	3.708502000	4.715521000	-1.029641000
H	2.153206000	5.044897000	-1.814542000
H	2.687569000	6.054320000	-0.469257000
O	0.542348000	-0.689727000	1.033996000
O	1.443960000	-0.903023000	0.031701000
C	6.471527000	-3.244461000	0.367195000
C	6.956046000	-1.947598000	0.104705000
C	6.074697000	-0.850950000	0.077497000
C	4.724685000	-1.025027000	0.319703000
C	4.219272000	-2.340443000	0.584285000
C	5.125285000	-3.448849000	0.593299000
H	7.160480000	-4.083645000	0.387227000
H	8.015566000	-1.794443000	-0.077060000
H	6.456845000	0.144609000	-0.127181000
H	4.044674000	-0.177864000	0.300771000
H	2.231673000	-1.693807000	0.495718000
H	4.717804000	-4.434159000	0.795197000

O 2.961193000 -2.562068000 0.837400000

<sup>3</sup>TS<sub>R15</sub>

Cu 1.024463000 0.996323000 0.287261000  
C 1.607104000 0.844169000 3.344865000  
H 0.657531000 0.317213000 3.339492000  
C 2.312736000 1.095446000 4.519321000  
H 1.916155000 0.765389000 5.473474000  
C 3.524783000 1.781365000 4.434171000  
H 4.097957000 2.002607000 5.329589000  
C 3.993600000 2.184919000 3.183005000  
H 4.933316000 2.720027000 3.084539000  
C 3.235102000 1.883641000 2.052130000  
C 3.707928000 2.201599000 0.644480000  
H 4.392285000 3.063112000 0.650034000  
H 4.276576000 1.342535000 0.269549000  
C 1.949141000 3.739067000 -0.088632000  
H 2.568236000 4.542464000 -0.514450000  
H 1.883843000 3.917205000 0.991230000  
C 0.553552000 3.783156000 -0.676486000  
C 0.095388000 4.919012000 -1.326895000  
H 0.744692000 5.777791000 -1.458679000  
C -1.212840000 4.911012000 -1.826863000  
H -1.595037000 5.762785000 -2.381556000  
C -2.006040000 3.796095000 -1.637524000  
H -3.000040000 3.740979000 -2.061247000  
C -1.492338000 2.693294000 -0.919022000  
C 2.931110000 2.165608000 -1.687232000  
H 3.854449000 2.693462000 -1.968536000  
H 2.125293000 2.581722000 -2.302897000  
C 3.060059000 0.685605000 -1.990828000  
C 3.974158000 0.235902000 -2.936478000  
H 4.645502000 0.931424000 -3.429285000  
C 3.975406000 -1.125440000 -3.256687000  
H 4.640141000 -1.509782000 -4.024643000  
C 3.105251000 -1.979322000 -2.600317000  
H 3.048669000 -3.028371000 -2.860781000  
C 2.259291000 -1.462402000 -1.599176000  
C 1.353652000 -3.619106000 -0.575825000

N	2.061397000	1.233694000	2.144316000
N	2.574804000	2.416854000	-0.277569000
N	-0.209877000	2.681930000	-0.482411000
N	2.220365000	-0.138026000	-1.330774000
N	1.366136000	-2.254087000	-0.896909000
H	0.456764000	-1.813632000	-0.692771000
O	0.258788000	-4.156456000	-0.475229000
C	2.628048000	-4.415386000	-0.184624000
C	2.251258000	-5.162611000	1.121459000
H	1.362949000	-5.779429000	0.977077000
H	3.085576000	-5.802963000	1.427216000
H	2.048292000	-4.456922000	1.935434000
C	3.879827000	-3.566348000	0.107214000
H	4.335580000	-3.138544000	-0.788024000
H	3.655626000	-2.750139000	0.803889000
H	4.636349000	-4.203173000	0.578513000
C	2.913761000	-5.470801000	-1.277823000
H	2.020530000	-6.070953000	-1.475241000
H	3.239539000	-5.022290000	-2.223229000
H	3.712419000	-6.141970000	-0.943023000
O	-0.124556000	-0.339635000	1.026750000
O	-0.920935000	-0.879875000	0.039589000
N	-2.231464000	1.557421000	-0.684856000
H	-1.700779000	0.678944000	-0.624515000
C	-3.620829000	1.293112000	-0.790596000
C	-4.694964000	2.222396000	-0.166021000
C	-5.587607000	2.791270000	-1.292293000
H	-5.954125000	1.985829000	-1.935604000
H	-6.451153000	3.304056000	-0.854446000
H	-5.062704000	3.519524000	-1.921520000
C	-4.155125000	3.345143000	0.738769000
H	-3.472345000	2.952160000	1.500295000
H	-3.639285000	4.136338000	0.190402000
H	-4.996496000	3.813965000	1.260440000
C	-5.563444000	1.282809000	0.712079000
H	-4.964668000	0.833759000	1.512224000
H	-6.375527000	1.858839000	1.168732000
H	-5.990681000	0.478125000	0.110491000
O	-3.938791000	0.213410000	-1.255554000



C	-4.958773000	-4.860519000	0.247456000
C	-3.604617000	-4.732098000	-0.115959000
C	-2.896304000	-3.588938000	0.199697000
C	-3.556446000	-2.523258000	0.894457000
C	-4.935502000	-2.663668000	1.254956000
C	-5.615250000	-3.820620000	0.937740000
H	-5.501650000	-5.767088000	-0.002628000
H	-3.106518000	-5.541689000	-0.640577000
H	-1.845868000	-3.496866000	-0.060724000
H	-5.410611000	-1.840430000	1.777260000
H	-6.659401000	-3.932287000	1.213811000
O	-2.936347000	-1.431815000	1.239239000
H	-1.962061000	-1.231249000	0.684072000

<sup>3</sup>PC<sub>R11</sub>

Cu	2.264984000	0.237999000	-0.190776000
C	0.442419000	0.108918000	2.321042000
H	-0.225284000	0.664420000	1.670022000
C	0.134298000	-0.142737000	3.657148000
H	-0.796546000	0.222999000	4.077005000
C	1.046457000	-0.861751000	4.427877000
H	0.844695000	-1.068694000	5.474692000
C	2.229544000	-1.311124000	3.837958000
H	2.960953000	-1.872473000	4.411657000
C	2.459982000	-1.030589000	2.491876000
C	3.682383000	-1.550482000	1.753807000
H	4.484794000	-1.799052000	2.464643000
H	3.405234000	-2.482482000	1.246658000
C	4.879738000	0.542837000	1.267772000
H	5.936956000	0.298848000	1.451683000
H	4.434890000	0.780181000	2.241748000
C	4.762606000	1.770617000	0.379062000
C	5.769270000	2.731680000	0.293461000
H	6.704689000	2.593915000	0.827633000
C	5.548161000	3.869895000	-0.484639000
H	6.316284000	4.633310000	-0.565690000
C	4.334825000	4.010057000	-1.158169000
H	4.127677000	4.879039000	-1.773600000
C	3.384421000	2.998253000	-1.033815000

C	4.859401000	-1.271841000	-0.385956000
H	5.620598000	-1.974000000	-0.013062000
H	5.393659000	-0.491545000	-0.941759000
C	3.916393000	-1.974937000	-1.347819000
C	4.306984000	-3.112712000	-2.053249000
H	5.281094000	-3.557978000	-1.873719000
C	3.431282000	-3.658598000	-2.992926000
H	3.714834000	-4.542418000	-3.556747000
C	2.191391000	-3.054174000	-3.192782000
H	1.482135000	-3.444571000	-3.914847000
C	1.866859000	-1.929147000	-2.436489000
N	1.578861000	-0.325898000	1.756277000
N	4.139782000	-0.608296000	0.715511000
N	3.599581000	1.909360000	-0.281913000
N	2.710623000	-1.403806000	-1.533345000
O	0.777375000	1.240469000	-0.857679000
O	-0.079021000	0.439800000	-1.632968000
H	2.420840000	3.031492000	-1.534695000
H	0.917658000	-1.412640000	-2.538069000
C	-5.797038000	1.142247000	-0.240373000
C	-4.420860000	1.280233000	-0.264452000
C	-3.588363000	0.072690000	-0.117265000
C	-4.241923000	-1.241796000	0.033026000
C	-5.614274000	-1.290546000	0.040788000
C	-6.400604000	-0.121133000	-0.090252000
H	-6.428353000	2.013427000	-0.340112000
H	-6.155812000	-2.222084000	0.146412000
O	-2.324542000	0.156726000	-0.105820000
H	-0.875389000	0.345787000	-1.053236000
C	-3.398877000	-2.521617000	0.176299000
C	-2.501781000	-2.712946000	-1.072585000
C	-2.520681000	-2.434885000	1.449242000
C	-4.282469000	-3.779420000	0.306889000
H	-3.109130000	-2.782345000	-1.982596000
H	-1.795922000	-1.889542000	-1.188958000
H	-1.934571000	-3.647078000	-0.977464000
H	-3.144300000	-2.329325000	2.345129000
H	-1.934396000	-3.355768000	1.557586000
H	-1.835359000	-1.587951000	1.399607000

H	-3.640148000	-4.660966000	0.407011000
H	-4.926752000	-3.742758000	1.192599000
H	-4.914851000	-3.933742000	-0.574689000
C	-3.773341000	2.662959000	-0.460536000
C	-2.807901000	2.989147000	0.707325000
C	-3.005764000	2.688542000	-1.807099000
C	-4.825820000	3.791307000	-0.508666000
H	-3.332615000	2.953420000	1.669852000
H	-1.969577000	2.293189000	0.737136000
H	-2.411839000	4.003516000	0.580502000
H	-3.685335000	2.495581000	-2.645444000
H	-2.561970000	3.679879000	-1.957682000
H	-2.202381000	1.952179000	-1.837258000
H	-4.314477000	4.751061000	-0.636042000
H	-5.517907000	3.681078000	-1.351548000
H	-5.410226000	3.852615000	0.417039000
O	-7.728304000	-0.329355000	-0.060553000
C	-8.627126000	0.774001000	-0.194589000
H	-8.491454000	1.276393000	-1.158660000
H	-9.626955000	0.342825000	-0.143410000
H	-8.493524000	1.491949000	0.622200000

<sup>3</sup>PC<sub>R1</sub>

Cu	3.016533000	-0.095109000	-0.450017000
C	3.398357000	2.572999000	-2.024000000
H	2.834317000	2.023973000	-2.771798000
C	3.874859000	3.863573000	-2.241551000
H	3.692150000	4.358843000	-3.189239000
C	4.588727000	4.490486000	-1.220015000
H	4.983039000	5.493007000	-1.356841000
C	4.792823000	3.814228000	-0.016177000
H	5.341608000	4.277414000	0.798199000
C	4.270901000	2.529350000	0.130144000
C	4.355429000	1.756458000	1.432963000
H	5.225966000	2.077204000	2.023298000
H	3.462622000	1.983362000	2.027380000
C	5.692220000	-0.197584000	0.782442000
H	6.381784000	-0.279992000	1.635398000
H	6.116162000	0.544714000	0.095205000

C	5.577027000	-1.525543000	0.059164000
C	6.572320000	-2.498761000	0.131602000
H	7.452971000	-2.332799000	0.744662000
C	6.413531000	-3.682184000	-0.591001000
H	7.175462000	-4.454854000	-0.550681000
C	5.258751000	-3.860256000	-1.351169000
H	5.089400000	-4.769951000	-1.917309000
C	4.305628000	-2.843820000	-1.365877000
H	3.379899000	-2.922038000	-1.926662000
C	3.812320000	-0.459293000	2.353330000
H	4.271831000	-0.137254000	3.298571000
H	4.081312000	-1.511255000	2.204210000
C	2.302566000	-0.339692000	2.420153000
C	1.635414000	-0.311923000	3.629174000
H	2.180787000	-0.318519000	4.566727000
C	0.224746000	-0.292590000	3.599465000
H	-0.337269000	-0.282386000	4.529009000
C	-0.439485000	-0.281802000	2.396294000
H	-1.522423000	-0.262860000	2.339654000
C	0.312096000	-0.280282000	1.183971000
N	3.597963000	1.925036000	-0.866418000
N	4.366096000	0.296369000	1.203726000
N	4.465101000	-1.698879000	-0.683265000
N	1.670893000	-0.319591000	1.221249000
N	-0.291864000	-0.236470000	-0.013138000
H	0.282575000	-0.230061000	-0.857673000
O	1.830369000	-0.150315000	-1.956050000
O	1.815132000	-1.427648000	-2.602840000
H	-1.305391000	-0.190251000	-0.079219000
C	-7.283482000	0.175415000	-0.154385000
C	-6.512317000	1.359500000	-0.078836000
C	-5.139087000	1.328306000	-0.063204000
C	-4.468414000	0.014504000	-0.120363000
C	-5.286484000	-1.207568000	-0.222715000
C	-6.664193000	-1.087267000	-0.231126000
H	-7.065964000	2.289026000	-0.036595000
H	-7.283056000	-1.970692000	-0.300141000
O	-3.208125000	-0.061228000	-0.088007000
H	2.279473000	-1.225863000	-3.436144000

C	-4.609791000	-2.585815000	-0.323696000
C	-3.716544000	-2.641859000	-1.589369000
C	-3.753804000	-2.853067000	0.940484000
C	-5.638511000	-3.730543000	-0.432271000
H	-4.315680000	-2.491035000	-2.495199000
H	-2.935517000	-1.881330000	-1.559678000
H	-3.241711000	-3.627640000	-1.662463000
H	-4.372420000	-2.819672000	1.845356000
H	-3.306109000	-3.852135000	0.878147000
H	-2.952201000	-2.120838000	1.039334000
H	-5.106199000	-4.684485000	-0.509498000
H	-6.287055000	-3.790585000	0.449536000
H	-6.269783000	-3.637612000	-1.323654000
C	-4.310654000	2.623086000	0.006600000
C	-3.448088000	2.633473000	1.293807000
C	-3.399096000	2.736172000	-1.241347000
C	-5.209199000	3.876656000	0.041426000
H	-4.079259000	2.555356000	2.186968000
H	-2.732343000	1.810667000	1.299521000
H	-2.892407000	3.576982000	1.359137000
H	-3.997519000	2.759935000	-2.159616000
H	-2.823205000	3.668388000	-1.193663000
H	-2.702178000	1.899298000	-1.303375000
H	-4.577718000	4.770628000	0.082964000
H	-5.836550000	3.959691000	-0.853136000
H	-5.860133000	3.894587000	0.923031000
O	-8.615827000	0.369744000	-0.154080000
C	-9.496617000	-0.751186000	-0.240093000
H	-9.343122000	-1.302266000	-1.174652000
H	-9.363622000	-1.424041000	0.614350000
H	-10.503378000	-0.333173000	-0.223111000

<sup>3</sup>PC<sub>R2</sub>

Cu	-3.006164000	0.033126000	-0.410397000
C	-3.288490000	-2.487023000	-2.276872000
H	-2.793433000	-1.827481000	-2.982079000
C	-3.709216000	-3.770769000	-2.619130000
H	-3.545498000	-4.146731000	-3.623394000
C	-4.346791000	-4.545236000	-1.649785000

H	-4.696105000	-5.546262000	-1.884840000
C	-4.538793000	-4.017338000	-0.371706000
H	-5.036796000	-4.593592000	0.402245000
C	-4.075071000	-2.730432000	-0.103118000
C	-4.166629000	-2.092937000	1.269893000
H	-5.007037000	-2.509401000	1.843157000
H	-3.250161000	-2.321910000	1.825547000
C	-5.627238000	-0.170283000	0.805560000
H	-6.318507000	-0.265283000	1.655008000
H	-5.985840000	-0.840337000	0.015115000
C	-5.611492000	1.251512000	0.284311000
C	-6.671131000	2.115762000	0.492379000
H	-7.532020000	1.808499000	1.075911000
C	-6.595157000	3.398178000	-0.080385000
H	-7.409829000	4.103777000	0.053620000
C	-5.482885000	3.761578000	-0.808174000
H	-5.398498000	4.746978000	-1.255216000
C	-4.424417000	2.830152000	-0.967556000
C	-3.756845000	0.062363000	2.387093000
H	-4.199801000	-0.366588000	3.296869000
H	-4.083111000	1.106498000	2.328470000
C	-2.245206000	0.015582000	2.453807000
C	-1.593699000	-0.009725000	3.671395000
H	-2.154926000	-0.052297000	4.598533000
C	-0.185615000	0.039764000	3.667346000
H	0.362809000	0.037095000	4.604945000
C	0.492715000	0.077536000	2.473037000
H	1.576084000	0.101588000	2.428429000
C	-0.241181000	0.061145000	1.251858000
N	-3.467348000	-1.987687000	-1.045196000
N	-4.265568000	-0.618827000	1.174800000
N	-4.508340000	1.592865000	-0.422899000
N	-1.599934000	0.053819000	1.258813000
N	0.404615000	0.053507000	0.072638000
H	-0.107453000	-0.066403000	-0.799424000
O	-2.280811000	0.587312000	-2.091621000
O	-1.036852000	-0.067275000	-2.446652000
H	1.421614000	0.026006000	0.059307000
N	-3.286711000	3.151341000	-1.632434000

H	-2.677037000	2.381351000	-1.921857000
H	-3.283707000	3.989161000	-2.195429000
C	5.428418000	-1.037860000	0.046999000
C	6.789628000	-0.882058000	-0.141214000
C	7.350022000	0.390001000	-0.366978000
C	6.533935000	1.545098000	-0.414403000
C	5.173263000	1.477981000	-0.238797000
C	4.564890000	0.156748000	0.011826000
H	7.440964000	-1.744003000	-0.116906000
H	7.043153000	2.482841000	-0.597491000
O	3.319466000	0.046622000	0.197746000
H	-0.541215000	0.676919000	-2.835202000
C	4.816807000	-2.428946000	0.288672000
C	4.120799000	-2.469313000	1.672825000
C	3.793113000	-2.758929000	-0.827733000
C	5.884774000	-3.542669000	0.277189000
H	4.835820000	-2.254540000	2.475825000
H	3.307751000	-1.744732000	1.728409000
H	3.709502000	-3.470414000	1.849746000
H	4.275738000	-2.755694000	-1.812258000
H	3.378108000	-3.760466000	-0.662303000
H	2.972144000	-2.041050000	-0.840960000
H	5.397481000	-4.508339000	0.448373000
H	6.406145000	-3.607819000	-0.685010000
H	6.631417000	-3.411245000	1.069190000
C	4.298803000	2.742508000	-0.301200000
C	3.265765000	2.613792000	-1.449192000
C	3.567839000	2.952486000	1.048539000
C	5.137701000	4.008103000	-0.574942000
H	3.769991000	2.488029000	-2.414675000
H	2.599607000	1.764463000	-1.291026000
H	2.659992000	3.526576000	-1.503295000
H	4.288244000	3.068988000	1.866712000
H	2.962990000	3.866181000	1.003168000
H	2.911190000	2.113482000	1.281204000
H	4.473243000	4.877930000	-0.614235000
H	5.873946000	4.194716000	0.215011000
H	5.665496000	3.955497000	-1.534042000
O	8.661946000	0.619988000	-0.555939000

C	9.587388000	-0.468115000	-0.532963000
H	9.364947000	-1.191316000	-1.325506000
H	10.566275000	-0.021887000	-0.709195000
H	9.582057000	-0.969668000	0.441239000

**<sup>3</sup>PC<sub>R3</sub>**

Cu	-3.006164000	0.033126000	-0.410397000
C	-3.288490000	-2.487023000	-2.276872000
H	-2.793433000	-1.827481000	-2.982079000
C	-3.709216000	-3.770769000	-2.619130000
H	-3.545498000	-4.146731000	-3.623394000
C	-4.346791000	-4.545236000	-1.649785000
H	-4.696105000	-5.546262000	-1.884840000
C	-4.538793000	-4.017338000	-0.371706000
H	-5.036796000	-4.593592000	0.402245000
C	-4.075071000	-2.730432000	-0.103118000
C	-4.166629000	-2.092937000	1.269893000
H	-5.007037000	-2.509401000	1.843157000
H	-3.250161000	-2.321910000	1.825547000
C	-5.627238000	-0.170283000	0.805560000
H	-6.318507000	-0.265283000	1.655008000
H	-5.985840000	-0.840337000	0.015115000
C	-5.611492000	1.251512000	0.284311000
C	-6.671131000	2.115762000	0.492379000
H	-7.532020000	1.808499000	1.075911000
C	-6.595157000	3.398178000	-0.080385000
H	-7.409829000	4.103777000	0.053620000
C	-5.482885000	3.761578000	-0.808174000
H	-5.398498000	4.746978000	-1.255216000
C	-4.424417000	2.830152000	-0.967556000
C	-3.756845000	0.062363000	2.387093000
H	-4.199801000	-0.366588000	3.296869000
H	-4.083111000	1.106498000	2.328470000
C	-2.245206000	0.015582000	2.453807000
C	-1.593699000	-0.009725000	3.671395000
H	-2.154926000	-0.052297000	4.598533000
C	-0.185615000	0.039764000	3.667346000
H	0.362809000	0.037095000	4.604945000
C	0.492715000	0.077536000	2.473037000



H	1.576084000	0.101588000	2.428429000
C	-0.241181000	0.061145000	1.251858000
N	-3.467348000	-1.987687000	-1.045196000
N	-4.265568000	-0.618827000	1.174800000
N	-4.508340000	1.592865000	-0.422899000
N	-1.599934000	0.053819000	1.258813000
N	0.404615000	0.053507000	0.072638000
H	-0.107453000	-0.066403000	-0.799424000
O	-2.280811000	0.587312000	-2.091621000
O	-1.036852000	-0.067275000	-2.446652000
H	1.421614000	0.026006000	0.059307000
N	-3.286711000	3.151341000	-1.632434000
H	-2.677037000	2.381351000	-1.921857000
H	-3.283707000	3.989161000	-2.195429000
C	5.428418000	-1.037860000	0.046999000
C	6.789628000	-0.882058000	-0.141214000
C	7.350022000	0.390001000	-0.366978000
C	6.533935000	1.545098000	-0.414403000
C	5.173263000	1.477981000	-0.238797000
C	4.564890000	0.156748000	0.011826000
H	7.440964000	-1.744003000	-0.116906000
H	7.043153000	2.482841000	-0.597491000
O	3.319466000	0.046622000	0.197746000
H	-0.541215000	0.676919000	-2.835202000
C	4.816807000	-2.428946000	0.288672000
C	4.120799000	-2.469313000	1.672825000
C	3.793113000	-2.758929000	-0.827733000
C	5.884774000	-3.542669000	0.277189000
H	4.835820000	-2.254540000	2.475825000
H	3.307751000	-1.744732000	1.728409000
H	3.709502000	-3.470414000	1.849746000
H	4.275738000	-2.755694000	-1.812258000
H	3.378108000	-3.760466000	-0.662303000
H	2.972144000	-2.041050000	-0.840960000
H	5.397481000	-4.508339000	0.448373000
H	6.406145000	-3.607819000	-0.685010000
H	6.631417000	-3.411245000	1.069190000
C	4.298803000	2.742508000	-0.301200000
C	3.265765000	2.613792000	-1.449192000

C	3.567839000	2.952486000	1.048539000
C	5.137701000	4.008103000	-0.574942000
H	3.769991000	2.488029000	-2.414675000
H	2.599607000	1.764463000	-1.291026000
H	2.659992000	3.526576000	-1.503295000
H	4.288244000	3.068988000	1.866712000
H	2.962990000	3.866181000	1.003168000
H	2.911190000	2.113482000	1.281204000
H	4.473243000	4.877930000	-0.614235000
H	5.873946000	4.194716000	0.215011000
H	5.665496000	3.955497000	-1.534042000
O	8.661946000	0.619988000	-0.555939000
C	9.587388000	-0.468115000	-0.532963000
H	9.364947000	-1.191316000	-1.325506000
H	10.566275000	-0.021887000	-0.709195000
H	9.582057000	-0.969668000	0.441239000

**<sup>3</sup>PC<sub>R4</sub>**

Cu	2.057647000	-0.857705000	-0.302309000
C	2.229746000	-0.022566000	-3.282337000
H	1.197899000	0.259549000	-3.093783000
C	2.817262000	0.091634000	-4.540396000
H	2.242169000	0.473780000	-5.376963000
C	4.146874000	-0.302507000	-4.692665000
H	4.634867000	-0.235958000	-5.660508000
C	4.845821000	-0.788629000	-3.586497000
H	5.881607000	-1.102551000	-3.674510000
C	4.191981000	-0.859845000	-2.356861000
C	4.898012000	-1.286239000	-1.080890000
H	5.748104000	-1.946201000	-1.308292000
H	5.308487000	-0.389900000	-0.601312000
C	3.656579000	-3.312836000	-0.455313000
H	4.463483000	-3.992485000	-0.143015000
H	3.586716000	-3.379438000	-1.547941000
C	2.330171000	-3.749570000	0.141438000
C	2.072118000	-5.072749000	0.495471000
H	2.848018000	-5.825888000	0.396417000
C	0.803570000	-5.406826000	0.972920000
H	0.577500000	-6.431624000	1.252182000

C	-0.162081000	-4.408275000	1.093087000
H	-1.158912000	-4.624119000	1.461647000
C	0.176420000	-3.105413000	0.733659000
H	-0.522354000	-2.279755000	0.819564000
C	4.405171000	-1.751564000	1.284708000
H	5.454418000	-2.055599000	1.413117000
H	3.796621000	-2.433969000	1.889426000
C	4.198590000	-0.337567000	1.797015000
C	5.095801000	0.233506000	2.689850000
H	5.993025000	-0.297367000	2.990355000
C	4.786176000	1.494078000	3.215449000
H	5.437751000	1.957171000	3.950649000
C	3.628896000	2.137032000	2.814037000
H	3.338436000	3.085218000	3.247949000
C	2.797576000	1.524416000	1.851675000
C	1.150850000	3.428554000	1.412126000
N	2.906124000	-0.488698000	-2.221782000
N	3.966890000	-1.908397000	-0.118011000
N	1.393688000	-2.789614000	0.266356000
N	3.081883000	0.291235000	1.375038000
N	1.622367000	2.097337000	1.406472000
H	0.851422000	1.442065000	1.232428000
O	-0.041705000	3.590787000	1.604375000
C	2.039348000	4.635852000	1.007877000
C	1.218764000	5.389076000	-0.071668000
H	0.230127000	5.654068000	0.306678000
H	1.749169000	6.302546000	-0.362073000
H	1.087483000	4.772021000	-0.968321000
C	3.408705000	4.284265000	0.397392000
H	4.124577000	3.897430000	1.126170000
H	3.309525000	3.550630000	-0.411000000
H	3.848138000	5.191320000	-0.032269000
C	2.198424000	5.568448000	2.230179000
H	1.220356000	5.811374000	2.655815000
H	2.814536000	5.125203000	3.021374000
H	2.683562000	6.501869000	1.923523000
O	0.471205000	0.099912000	-0.664447000
O	-0.264278000	0.117293000	0.555677000
C	-6.443041000	-0.457829000	0.416694000

C	-6.784245000	0.507331000	-0.550654000
C	-5.783426000	1.166358000	-1.302634000
C	-4.446750000	0.901122000	-1.127017000
C	-4.067337000	-0.113581000	-0.125688000
C	-5.121987000	-0.789234000	0.652116000
H	-7.231285000	-0.938957000	0.978079000
H	-6.131530000	1.894599000	-2.023843000
O	-2.855970000	-0.423653000	0.072830000
H	-1.200353000	-0.032422000	0.260677000
C	-4.747161000	-1.841689000	1.711155000
C	-4.017076000	-3.029643000	1.034137000
C	-3.841820000	-1.204253000	2.796642000
C	-5.988745000	-2.413643000	2.426190000
H	-4.669600000	-3.523797000	0.304711000
H	-3.114729000	-2.697308000	0.518847000
H	-3.745307000	-3.773118000	1.794747000
H	-4.359941000	-0.379678000	3.299816000
H	-3.594316000	-1.954609000	3.557520000
H	-2.915331000	-0.817511000	2.371021000
H	-5.666947000	-3.152032000	3.168394000
H	-6.551139000	-1.639655000	2.960720000
H	-6.668680000	-2.923705000	1.733855000
C	-3.376976000	1.647068000	-1.943030000
C	-2.506536000	2.507985000	-0.992913000
C	-2.499406000	0.640518000	-2.730829000
C	-4.009614000	2.603292000	-2.976216000
H	-3.116676000	3.268663000	-0.492993000
H	-2.009692000	1.917469000	-0.224162000
H	-1.732998000	3.028336000	-1.570274000
H	-3.117529000	0.030481000	-3.400864000
H	-1.782659000	1.193740000	-3.350785000
H	-1.941363000	-0.023670000	-2.071286000
H	-3.210817000	3.105696000	-3.532156000
H	-4.634629000	2.073001000	-3.704018000
H	-4.614929000	3.384288000	-2.502712000
O	-8.043094000	0.880958000	-0.839567000
C	-9.140643000	0.293066000	-0.138392000
H	-9.181180000	-0.788968000	-0.306262000
H	-9.078494000	0.501719000	0.935421000

H -10.034360000 0.761217000 -0.551174000

<sup>3</sup>PC<sub>R6</sub>

Cu -1.291144000 -0.195133000 -0.112224000  
C -1.588673000 -3.255307000 0.218243000  
H -0.635940000 -3.223918000 -0.303061000  
C -2.224854000 -4.449188000 0.553319000  
H -1.768353000 -5.399681000 0.298474000  
C -3.454848000 -4.386901000 1.207852000  
H -3.984580000 -5.296390000 1.475418000  
C -4.004659000 -3.139659000 1.510482000  
H -4.962767000 -3.060256000 2.015378000  
C -3.299431000 -1.990300000 1.155499000  
C -3.779688000 -0.592851000 1.511947000  
H -4.869024000 -0.586951000 1.668703000  
H -3.319031000 -0.304777000 2.464712000  
C -4.180802000 0.352443000 -0.720270000  
H -5.131104000 0.894870000 -0.601117000  
H -4.434958000 -0.699593000 -0.898190000  
C -3.422779000 0.870209000 -1.931777000  
C -4.075706000 1.489504000 -2.997287000  
H -5.145918000 1.668624000 -2.952044000  
C -3.332436000 1.866197000 -4.117102000  
H -3.819177000 2.347407000 -4.960290000  
C -1.960394000 1.620230000 -4.132885000  
H -1.346512000 1.898449000 -4.982992000  
C -1.378212000 1.010627000 -3.022482000  
C -3.244002000 1.763466000 1.058217000  
H -4.118917000 2.039616000 1.666463000  
H -3.216350000 2.455760000 0.208305000  
C -1.963509000 1.945767000 1.855685000  
C -1.896580000 2.803846000 2.952157000  
H -2.789273000 3.315218000 3.299805000  
C -0.666630000 2.996588000 3.584154000  
H -0.588905000 3.662267000 4.438743000  
C 0.453752000 2.322309000 3.102466000  
H 1.429343000 2.447309000 3.559822000  
C 0.303792000 1.467489000 2.010937000  
N -2.117236000 -2.060044000 0.517450000

N	-3.364638000	0.402517000	0.505849000
N	-2.095609000	0.644760000	-1.948292000
N	-0.880044000	1.283927000	1.405026000
O	0.406660000	-0.963898000	-0.516141000
O	1.105904000	-0.131491000	-1.409141000
H	-0.315183000	0.797646000	-2.963826000
H	1.146322000	0.924189000	1.595206000
C	5.746693000	-1.001316000	-1.212729000
C	4.474114000	-0.542686000	-1.010608000
C	4.193246000	0.448954000	0.009885000
C	5.312709000	0.921499000	0.795847000
C	6.590244000	0.456277000	0.585706000
C	6.825431000	-0.511469000	-0.422893000
H	5.973423000	-1.743124000	-1.972097000
H	3.640655000	-0.906863000	-1.603314000
H	5.105890000	1.665844000	1.558290000
H	7.409167000	0.831658000	1.188504000
O	3.024121000	0.896481000	0.213960000
H	1.781452000	0.299322000	-0.813868000
O	8.024934000	-1.031312000	-0.714024000
C	9.183069000	-0.610175000	0.015071000
H	10.014038000	-1.172784000	-0.409891000
H	9.357648000	0.463142000	-0.116270000
H	9.081861000	-0.847791000	1.079575000

<sup>3</sup>PC<sub>R7</sub>

Cu	-1.296300000	-0.017347000	-0.189134000
C	-1.843947000	-0.286205000	-3.230722000
H	-0.778359000	-0.497587000	-3.217604000
C	-2.587473000	-0.215376000	-4.407016000
H	-2.105992000	-0.374754000	-5.365961000
C	-3.950127000	0.069675000	-4.317317000
H	-4.559583000	0.140904000	-5.213388000
C	-4.524502000	0.267298000	-3.060486000
H	-5.582145000	0.491710000	-2.958961000
C	-3.715719000	0.166958000	-1.928691000
C	-4.267985000	0.278211000	-0.518160000
H	-5.187777000	0.881677000	-0.507202000
H	-4.542424000	-0.726693000	-0.176908000

C	-3.126935000	2.268222000	0.348069000
H	-3.935459000	2.777704000	0.894448000
H	-3.225550000	2.552743000	-0.706842000
C	-1.771974000	2.737260000	0.845198000
C	-1.593704000	3.993273000	1.423654000
H	-2.446623000	4.646152000	1.583176000
C	-0.306192000	4.391525000	1.785395000
H	-0.141039000	5.365108000	2.237427000
C	0.758546000	3.520490000	1.561300000
H	1.774916000	3.789205000	1.828488000
C	0.499547000	2.276696000	0.987797000
H	1.296984000	1.565977000	0.798510000
C	-3.455393000	0.323001000	1.805426000
H	-4.481379000	0.507657000	2.156752000
H	-2.783137000	0.906371000	2.445459000
C	-3.109899000	-1.146023000	1.936144000
C	-3.871401000	-1.981708000	2.734301000
H	-4.748097000	-1.605414000	3.250128000
C	-3.470819000	-3.323929000	2.857885000
H	-4.037797000	-4.009738000	3.480703000
C	-2.357023000	-3.765180000	2.180772000
H	-2.024718000	-4.796125000	2.252595000
C	-1.632005000	-2.854829000	1.364846000
N	-2.400895000	-0.097780000	-2.025942000
N	-3.259929000	0.802697000	0.423340000
N	-0.740900000	1.895181000	0.643043000
N	-2.012441000	-1.558636000	1.254617000
N	-0.559339000	-3.270848000	0.651538000
H	0.092153000	-2.588736000	0.256606000
O	0.361568000	-0.374342000	-1.075742000
O	1.192636000	-1.303673000	-0.409973000
H	-0.202472000	-4.199079000	0.822217000
C	6.940262000	-0.462823000	-0.487670000
C	6.690557000	0.445413000	0.571924000
C	5.398023000	0.662455000	0.989710000
C	4.277405000	-0.016711000	0.375984000
C	4.572668000	-0.934536000	-0.707134000
C	5.860049000	-1.144221000	-1.117987000
H	7.510071000	0.966033000	1.054010000

H	5.179344000	1.348241000	1.802101000
H	3.738840000	-1.444037000	-1.180457000
H	6.098080000	-1.827326000	-1.927269000
O	3.093579000	0.189853000	0.783386000
H	1.858527000	-0.726360000	0.060211000
O	8.153698000	-0.752226000	-0.972640000
C	9.316670000	-0.128521000	-0.415671000
H	9.424521000	-0.381252000	0.644447000
H	10.158739000	-0.531485000	-0.977608000
H	9.273992000	0.958496000	-0.541919000

<sup>3</sup>PC<sub>R8</sub>

Cu	1.356129000	0.031186000	-0.171026000
C	1.300127000	2.239781000	-2.382816000
H	0.236103000	2.034785000	-2.312627000
C	1.838236000	3.140203000	-3.299646000
H	1.187397000	3.681274000	-3.978164000
C	3.222134000	3.316190000	-3.327492000
H	3.677058000	4.003000000	-4.035135000
C	4.020662000	2.592322000	-2.440458000
H	5.101116000	2.701097000	-2.444378000
C	3.404124000	1.722289000	-1.542051000
C	4.175260000	0.947353000	-0.489511000
H	5.208270000	0.762563000	-0.819072000
H	4.232584000	1.557713000	0.418761000
C	3.716923000	-1.382744000	-1.126895000
H	4.733896000	-1.794393000	-1.048265000
H	3.625778000	-0.925924000	-2.119800000
C	2.685194000	-2.484026000	-0.990397000
C	2.999648000	-3.810097000	-1.227760000
H	4.011601000	-4.103022000	-1.484873000
C	1.965812000	-4.759362000	-1.126345000
H	2.171290000	-5.809951000	-1.310558000
C	0.692608000	-4.356435000	-0.789183000
H	-0.121034000	-5.069796000	-0.702925000
C	0.441430000	-2.979671000	-0.546295000
C	3.793039000	-0.751230000	1.247294000
H	4.876846000	-0.770074000	1.431792000
H	3.429566000	-1.779966000	1.346803000



C	3.097172000	0.121551000	2.271475000
C	3.690640000	0.378032000	3.494905000
H	4.679920000	-0.005114000	3.720069000
C	2.969168000	1.137385000	4.432870000
H	3.395109000	1.350900000	5.408904000
C	1.723678000	1.620230000	4.103504000
H	1.148164000	2.220086000	4.801543000
C	1.188124000	1.344145000	2.816350000
N	2.070561000	1.557133000	-1.524463000
N	3.491924000	-0.313179000	-0.131377000
N	1.441861000	-2.069325000	-0.650542000
N	1.870102000	0.583313000	1.923929000
N	-0.005124000	1.852564000	2.444909000
H	-0.432564000	1.626738000	1.542243000
O	-0.477314000	0.213447000	-0.719422000
O	-1.272261000	1.193847000	-0.039230000
H	-0.551086000	2.372488000	3.114098000
N	-0.778972000	-2.530205000	-0.176576000
H	-0.959825000	-1.525003000	-0.263184000
H	-1.565964000	-3.160093000	-0.215949000
C	-5.547188000	-0.847930000	1.057970000
C	-6.841252000	-0.594483000	0.666866000
C	-7.094053000	0.391932000	-0.318724000
C	-6.015207000	1.117829000	-0.901084000
C	-4.725429000	0.872296000	-0.515815000
C	-4.425794000	-0.131322000	0.488984000
H	-7.659615000	-1.146890000	1.114340000
H	-6.255885000	1.862194000	-1.653487000
O	-3.243344000	-0.381210000	0.872637000
H	-2.008154000	0.605808000	0.301211000
O	-8.310401000	0.717699000	-0.773808000
C	-9.469160000	0.052393000	-0.256813000
H	-9.571457000	0.226454000	0.819389000
H	-10.315516000	0.492239000	-0.783504000
H	-9.424829000	-1.022920000	-0.462042000
H	-3.892991000	1.415182000	-0.954464000
H	-5.324796000	-1.595921000	1.812854000
<sup>3</sup> PC <sub>R9</sub>			
Cu	-1.574784000	-0.357911000	-0.153634000

C	-0.286506000	-1.951826000	2.190814000
H	0.444754000	-2.202583000	1.426960000
C	-0.224764000	-2.484651000	3.477766000
H	0.573985000	-3.169302000	3.742087000
C	-1.209145000	-2.127113000	4.398152000
H	-1.195602000	-2.530006000	5.406570000
C	-2.222200000	-1.249073000	4.006921000
H	-3.005545000	-0.956205000	4.699604000
C	-2.211519000	-0.749684000	2.705675000
C	-3.229765000	0.265431000	2.213675000
H	-4.153638000	0.207658000	2.807973000
H	-2.816752000	1.270403000	2.358564000
C	-4.380629000	-1.042811000	0.480014000
H	-5.438953000	-0.798312000	0.654309000
H	-4.115913000	-1.841495000	1.183149000
C	-4.174411000	-1.559005000	-0.932416000
C	-5.205473000	-2.144677000	-1.664522000
H	-6.208713000	-2.193174000	-1.251842000
C	-4.921756000	-2.669324000	-2.926794000
H	-5.707791000	-3.131595000	-3.516511000
C	-3.619250000	-2.588876000	-3.416161000
H	-3.356298000	-2.986284000	-4.390638000
C	-2.644077000	-1.978861000	-2.628461000
H	-1.608593000	-1.895463000	-2.941569000
C	-3.982661000	1.348182000	0.132952000
H	-4.803303000	1.803768000	0.707269000
H	-4.396079000	1.068841000	-0.843575000
C	-2.877146000	2.365311000	-0.093207000
C	-3.173099000	3.721841000	-0.163466000
H	-4.181641000	4.078475000	0.018030000
C	-2.144448000	4.599668000	-0.517491000
H	-2.344889000	5.660372000	-0.636321000
C	-0.867439000	4.109003000	-0.738587000
H	-0.070408000	4.762944000	-1.063325000
C	-0.620544000	2.734558000	-0.562938000
C	1.961022000	2.527073000	-0.627761000
N	-1.259484000	-1.103928000	1.821864000
N	-3.501894000	0.107951000	0.769665000
N	-2.919611000	-1.471818000	-1.415940000

N	-1.634024000	1.880641000	-0.280343000
N	0.615887000	2.137790000	-0.746093000
H	0.556899000	1.157362000	-1.063754000
O	2.774338000	1.820734000	-1.208415000
C	2.457096000	3.690425000	0.272078000
C	3.820296000	3.231811000	0.845908000
H	4.524132000	2.994751000	0.046484000
H	4.241044000	4.032846000	1.463103000
H	3.706000000	2.340978000	1.473432000
C	1.536423000	4.016625000	1.464990000
H	0.598517000	4.495789000	1.179568000
H	1.298646000	3.113885000	2.039760000
H	2.057654000	4.706605000	2.137465000
C	2.715252000	4.940016000	-0.604300000
H	3.386896000	4.695812000	-1.433450000
H	1.801616000	5.369184000	-1.027627000
H	3.190060000	5.719411000	0.002095000
O	0.177120000	-0.580585000	-0.854763000
O	0.298917000	-1.637715000	-1.777256000
C	5.485126000	-3.203128000	0.177765000
C	5.811365000	-1.892984000	-0.276415000
C	4.791816000	-1.017689000	-0.723962000
C	3.483098000	-1.441316000	-0.731519000
C	3.115489000	-2.767346000	-0.281112000
C	4.185025000	-3.628996000	0.181533000
H	6.298259000	-3.840220000	0.511439000
H	5.019010000	-0.011545000	-1.056877000
H	2.702427000	-0.769194000	-1.068631000
H	3.915521000	-4.625431000	0.517184000
O	1.909708000	-3.172039000	-0.277186000
H	0.842266000	-2.288541000	-1.241187000
O	7.115678000	-1.586291000	-0.236276000
C	7.556536000	-0.303042000	-0.691620000
H	8.639673000	-0.308174000	-0.571116000
H	7.301050000	-0.154465000	-1.746099000
H	7.119979000	0.497779000	-0.085103000

<sup>3</sup>PC<sub>R10</sub>

Cu	-1.535603000	-0.210926000	-0.151613000
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C	-3.960615000	-0.358543000	1.818769000
H	-3.144712000	-0.529300000	2.515158000
C	-5.298256000	-0.392318000	2.208692000
H	-5.557779000	-0.592493000	3.242818000
C	-6.279866000	-0.173858000	1.242321000
H	-7.332770000	-0.201117000	1.507002000
C	-5.892349000	0.072334000	-0.075850000
H	-6.631766000	0.240092000	-0.853319000
C	-4.532283000	0.101625000	-0.383219000
C	-4.021427000	0.428157000	-1.774484000
H	-4.790453000	0.202652000	-2.529603000
H	-3.829008000	1.506362000	-1.829921000
C	-2.954739000	-1.690172000	-2.349863000
H	-3.316819000	-1.849352000	-3.377814000
H	-3.745289000	-2.048599000	-1.679442000
C	-1.713437000	-2.529919000	-2.102521000
C	-1.557343000	-3.737481000	-2.775572000
H	-2.276086000	-4.040723000	-3.530172000
C	-0.461141000	-4.541492000	-2.454162000
H	-0.297607000	-5.483393000	-2.969424000
C	0.436990000	-4.103593000	-1.494883000
H	1.329347000	-4.671225000	-1.258892000
C	0.212956000	-2.872040000	-0.849670000
C	-1.955896000	0.418232000	-3.089196000
H	-2.550036000	0.646698000	-3.987706000
H	-1.158499000	-0.268791000	-3.395933000
C	-1.313870000	1.679884000	-2.546961000
C	-1.186797000	2.828017000	-3.326429000
H	-1.597642000	2.854676000	-4.330698000
C	-0.508257000	3.926021000	-2.795881000
H	-0.373525000	4.828114000	-3.385140000
C	0.016284000	3.840651000	-1.510610000
H	0.588755000	4.652222000	-1.078852000
C	-0.184045000	2.666511000	-0.775441000
C	0.052004000	2.832266000	1.774980000
N	-3.591057000	-0.114276000	0.552740000
N	-2.753197000	-0.264446000	-2.060524000
N	-0.851362000	-2.098541000	-1.157621000
N	-0.837271000	1.608627000	-1.288372000

N	0.406919000	2.460561000	0.489764000
H	1.044372000	1.652305000	0.465859000
O	0.607617000	2.232899000	2.699694000
C	-0.945491000	3.971724000	2.078645000
C	-1.316095000	3.872909000	3.572760000
H	-0.432457000	3.953643000	4.208922000
H	-2.008932000	4.682309000	3.827663000
H	-1.800953000	2.918004000	3.798640000
C	-2.243091000	3.867037000	1.246887000
H	-2.091659000	4.078452000	0.185456000
H	-2.696582000	2.873887000	1.342702000
H	-2.964540000	4.601094000	1.622409000
C	-0.250356000	5.332271000	1.833530000
H	0.679418000	5.406711000	2.407316000
H	-0.018787000	5.501766000	0.778345000
H	-0.912501000	6.142105000	2.159457000
O	-1.030665000	-0.248039000	1.719241000
O	0.299142000	-0.388105000	2.078478000
N	1.117809000	-2.389680000	0.084508000
H	1.451537000	-1.423300000	-0.026339000
C	1.842654000	-3.111824000	1.044974000
C	1.174353000	-4.210598000	1.912239000
C	1.881775000	-5.557535000	1.645745000
H	2.965884000	-5.450606000	1.747436000
H	1.540528000	-6.306346000	2.369267000
H	1.663824000	-5.945881000	0.643611000
C	-0.350319000	-4.349481000	1.748369000
H	-0.850186000	-3.379171000	1.841469000
H	-0.640656000	-4.804542000	0.797315000
H	-0.732120000	-5.000173000	2.543099000
C	1.457813000	-3.777856000	3.375469000
H	0.981747000	-2.816008000	3.594706000
H	1.053233000	-4.530252000	4.061610000
H	2.530803000	-3.677710000	3.550376000
O	2.991094000	-2.769330000	1.288232000
C	3.937065000	1.977622000	-0.750795000
C	3.491160000	0.649082000	-0.379781000
C	4.511568000	-0.350619000	-0.146951000
C	5.848125000	-0.052471000	-0.284305000

C	6.246339000	1.252731000	-0.663091000
C	5.267464000	2.261755000	-0.892114000
H	3.181239000	2.737831000	-0.921745000
H	4.179258000	-1.331404000	0.181099000
H	6.590363000	-0.818599000	-0.090707000
H	5.617147000	3.249490000	-1.175838000
O	2.254768000	0.374508000	-0.262657000
H	0.535460000	0.521755000	2.409958000
O	7.515783000	1.647011000	-0.828366000
C	8.584335000	0.717860000	-0.613228000
H	8.509804000	-0.128754000	-1.303968000
H	9.498791000	1.276318000	-0.811653000
H	8.586300000	0.359496000	0.421572000

<sup>3</sup>PC<sub>R11</sub>

Cu	-0.758620000	0.011960000	-0.228732000
C	-1.289940000	-1.509812000	-2.863626000
H	-0.335885000	-1.052945000	-3.111391000
C	-2.014182000	-2.280776000	-3.770770000
H	-1.629505000	-2.449453000	-4.770925000
C	-3.236919000	-2.814385000	-3.363640000
H	-3.833122000	-3.412328000	-4.046540000
C	-3.692196000	-2.566501000	-2.067181000
H	-4.641495000	-2.966161000	-1.723329000
C	-2.902622000	-1.797160000	-1.213347000
C	-3.276422000	-1.542607000	0.237874000
H	-4.363452000	-1.638918000	0.379515000
H	-2.805292000	-2.317009000	0.855394000
C	-3.590329000	0.893221000	0.232466000
H	-4.494441000	1.032376000	0.844355000
H	-3.927668000	0.645089000	-0.781181000
C	-2.790520000	2.183561000	0.165722000
C	-3.389915000	3.428811000	0.352038000
H	-4.442607000	3.494685000	0.610574000
C	-2.616396000	4.579944000	0.194817000
H	-3.061232000	5.561144000	0.331818000
C	-1.268150000	4.449442000	-0.134421000
H	-0.632099000	5.318526000	-0.264871000
C	-0.738745000	3.169066000	-0.287735000

C	-2.549893000	-0.203933000	2.168639000
H	-3.401399000	-0.625469000	2.723711000
H	-2.471090000	0.850284000	2.459993000
C	-1.259336000	-0.901697000	2.564221000
C	-1.122125000	-1.561181000	3.784871000
H	-1.968709000	-1.641328000	4.460234000
C	0.117956000	-2.107227000	4.121038000
H	0.249938000	-2.623634000	5.067235000
C	1.178129000	-1.982351000	3.224979000
H	2.158386000	-2.389489000	3.448349000
C	0.958316000	-1.323085000	2.016550000
N	-1.728611000	-1.279546000	-1.617651000
N	-2.774817000	-0.238095000	0.711335000
N	-1.485054000	2.062701000	-0.140938000
N	-0.234113000	-0.796213000	1.696790000
O	0.886631000	0.000223000	-1.193447000
O	1.633939000	1.153530000	-0.878726000
H	0.303634000	2.993675000	-0.534803000
H	1.748195000	-1.197688000	1.283362000
C	6.226873000	0.633522000	-1.893618000
C	4.982963000	0.627462000	-1.303250000
C	4.810624000	0.095370000	0.035925000
C	5.981176000	-0.423290000	0.716924000
C	7.212963000	-0.403479000	0.102829000
C	7.346431000	0.122471000	-1.201208000
H	6.354066000	1.031401000	-2.896122000
H	4.101751000	1.008738000	-1.810471000
H	5.841568000	-0.815979000	1.719099000
H	8.088436000	-0.789797000	0.616345000
H	8.322464000	0.133964000	-1.677149000
O	3.678515000	0.081207000	0.605034000
H	2.338591000	0.789553000	-0.280209000

<sup>3</sup>PC<sub>R12</sub>

Cu	-0.755021000	-0.009198000	-0.179501000
C	-1.372206000	-0.133247000	-3.215695000
H	-0.317265000	-0.392021000	-3.233898000
C	-2.135274000	0.017879000	-4.371667000
H	-1.681041000	-0.124451000	-5.346438000

C	-3.481340000	0.360160000	-4.241057000
H	-4.104792000	0.494577000	-5.120059000
C	-4.020723000	0.533163000	-2.965231000
H	-5.064668000	0.800772000	-2.831910000
C	-3.194859000	0.351712000	-1.856232000
C	-3.712663000	0.432832000	-0.430766000
H	-4.600226000	1.080304000	-0.375289000
H	-4.030480000	-0.570003000	-0.122641000
C	-2.461838000	2.329482000	0.494011000
H	-3.235874000	2.849569000	1.078702000
H	-2.567138000	2.664440000	-0.545279000
C	-1.077584000	2.712883000	0.983406000
C	-0.827643000	3.932382000	1.611360000
H	-1.644577000	4.617763000	1.816124000
C	0.484154000	4.252448000	1.963311000
H	0.704683000	5.196226000	2.453220000
C	1.501606000	3.342585000	1.680147000
H	2.534450000	3.551115000	1.937654000
C	1.171218000	2.139653000	1.058936000
H	1.927987000	1.400309000	0.820299000
C	-2.851579000	0.339466000	1.873833000
H	-3.861061000	0.555888000	2.253215000
H	-2.140988000	0.863267000	2.523807000
C	-2.572757000	-1.147896000	1.934199000
C	-3.357332000	-1.981749000	2.711237000
H	-4.205269000	-1.588412000	3.261271000
C	-3.018193000	-3.345301000	2.768380000
H	-3.604862000	-4.030928000	3.372828000
C	-1.939651000	-3.807108000	2.049345000
H	-1.654974000	-4.854467000	2.069244000
C	-1.188356000	-2.896132000	1.258227000
N	-1.895687000	0.031810000	-1.992513000
N	-2.660657000	0.868928000	0.508611000
N	-0.092100000	1.832689000	0.724144000
N	-1.508644000	-1.579963000	1.212324000
N	-0.150533000	-3.330513000	0.505494000
H	0.522682000	-2.664545000	0.121169000
O	0.869731000	-0.393258000	-1.114264000
O	1.669518000	-1.403513000	-0.526686000



H	0.162272000	-4.282394000	0.624164000
C	7.423330000	-0.662505000	-0.967633000
C	7.285015000	0.162048000	0.170856000
C	6.041983000	0.375941000	0.722028000
C	4.864687000	-0.242121000	0.143589000
C	5.042051000	-1.083588000	-1.025170000
C	6.297084000	-1.278403000	-1.556563000
H	8.408237000	-0.825122000	-1.395121000
H	8.165651000	0.623420000	0.607799000
H	5.898242000	0.999082000	1.599006000
H	4.156165000	-1.540035000	-1.456500000
H	6.428276000	-1.907040000	-2.432357000
O	3.721387000	-0.046963000	0.655051000
H	2.373675000	-0.888859000	-0.049798000

<sup>3</sup>PC<sub>R14</sub>

Cu	-1.233922000	-0.298038000	-0.116247000
C	-0.041356000	-1.901275000	2.263321000
H	0.661029000	-2.219399000	1.498294000
C	-0.001379000	-2.397259000	3.565165000
H	0.751604000	-3.125945000	3.845598000
C	-0.949554000	-1.943743000	4.481976000
H	-0.952651000	-2.314833000	5.502559000
C	-1.903363000	-1.009993000	4.072052000
H	-2.656427000	-0.641679000	4.762234000
C	-1.872386000	-0.552659000	2.755504000
C	-2.819970000	0.517985000	2.240726000
H	-3.744305000	0.537805000	2.836506000
H	-2.338328000	1.495012000	2.362974000
C	-4.074877000	-0.736099000	0.538533000
H	-5.109703000	-0.404291000	0.709122000
H	-3.872477000	-1.537446000	1.259282000
C	-3.915654000	-1.296166000	-0.863073000
C	-4.992078000	-1.816214000	-1.579103000
H	-5.993285000	-1.782407000	-1.160149000
C	-4.757379000	-2.381367000	-2.833999000
H	-5.579902000	-2.793751000	-3.410758000
C	-3.456576000	-2.403881000	-3.333545000
H	-3.231182000	-2.833268000	-4.303838000
C	-2.433160000	-1.855336000	-2.562293000

H	-1.397156000	-1.847981000	-2.884958000
C	-3.487701000	1.608925000	0.135845000
H	-4.264329000	2.142950000	0.703524000
H	-3.930176000	1.342511000	-0.831420000
C	-2.302583000	2.525780000	-0.117169000
C	-2.486601000	3.899160000	-0.224960000
H	-3.462036000	4.342836000	-0.055027000
C	-1.388327000	4.678175000	-0.601444000
H	-1.500177000	5.748100000	-0.750325000
C	-0.155667000	4.079219000	-0.804774000
H	0.691215000	4.658410000	-1.143560000
C	-0.021061000	2.694074000	-0.590734000
C	2.537047000	2.259532000	-0.679570000
N	-0.957149000	-1.000403000	1.875819000
N	-3.106007000	0.347716000	0.800406000
N	-2.660754000	-1.311895000	-1.355454000
N	-1.103904000	1.935357000	-0.289132000
N	1.157649000	1.987337000	-0.746812000
H	1.008375000	0.995640000	-0.997050000
O	3.265056000	1.440565000	-1.223238000
C	3.159633000	3.429484000	0.127250000
C	4.509325000	2.901826000	0.672242000
H	5.161657000	2.573382000	-0.138383000
H	5.011068000	3.700254000	1.229351000
H	4.359011000	2.054393000	1.350021000
C	2.314893000	3.885164000	1.333776000
H	1.389428000	4.393424000	1.058376000
H	2.059067000	3.036577000	1.979109000
H	2.901973000	4.588831000	1.933903000
C	3.472757000	4.605959000	-0.829097000
H	4.085325000	4.264041000	-1.669315000
H	2.578443000	5.085772000	-1.238839000
H	4.034845000	5.375040000	-0.287860000
O	0.509303000	-0.700962000	-0.766561000
O	0.549994000	-1.637693000	-1.821432000
C	5.594053000	-3.860568000	-0.009085000
C	6.037223000	-2.570918000	-0.381708000
C	5.119828000	-1.586361000	-0.805382000
C	3.773124000	-1.870003000	-0.869453000

C	3.284357000	-3.182717000	-0.489928000
C	4.253873000	-4.170037000	-0.053949000
H	6.318192000	-4.604077000	0.311246000
H	7.097211000	-2.337336000	-0.340971000
H	5.468983000	-0.596120000	-1.081419000
H	3.062329000	-1.117027000	-1.190939000
H	3.876565000	-5.149898000	0.221557000
O	2.049703000	-3.477112000	-0.522794000
H	1.019608000	-2.395697000	-1.372025000

<sup>3</sup>PC<sub>R15</sub>

Cu	-0.996582000	-0.678384000	-0.099404000
C	-2.967544000	-1.757932000	2.076728000
H	-2.118620000	-1.506008000	2.705694000
C	-4.120856000	-2.357447000	2.579618000
H	-4.196552000	-2.587868000	3.636979000
C	-5.156206000	-2.657458000	1.694670000
H	-6.066126000	-3.132993000	2.048601000
C	-5.005362000	-2.347055000	0.342079000
H	-5.789733000	-2.573883000	-0.373893000
C	-3.825309000	-1.735453000	-0.080071000
C	-3.602906000	-1.301128000	-1.516877000
H	-4.237666000	-1.886633000	-2.199851000
H	-3.911927000	-0.253498000	-1.615196000
C	-1.746579000	-2.765509000	-2.121251000
H	-2.070634000	-3.133496000	-3.107397000
H	-2.246911000	-3.390831000	-1.371965000
C	-0.248031000	-2.954639000	-1.964152000
C	0.383355000	-4.004624000	-2.622891000
H	-0.173845000	-4.635851000	-3.307689000
C	1.741474000	-4.222905000	-2.379175000
H	2.272146000	-5.022184000	-2.887980000
C	2.412688000	-3.381975000	-1.506930000
H	3.477612000	-3.483494000	-1.334383000
C	1.707292000	-2.342989000	-0.869818000
C	-1.836663000	-0.484989000	-3.004081000
H	-2.528294000	-0.600107000	-3.852976000
H	-0.839731000	-0.770412000	-3.359686000
C	-1.788994000	0.962366000	-2.556400000

C	-2.239952000	1.994520000	-3.376843000
H	-2.681157000	1.771089000	-4.342998000
C	-2.096564000	3.311243000	-2.937805000
H	-2.418856000	4.138970000	-3.562368000
C	-1.512257000	3.550817000	-1.698753000
H	-1.341952000	4.558039000	-1.339508000
C	-1.115641000	2.460507000	-0.916078000
C	-0.826994000	2.873862000	1.603545000
N	-2.828930000	-1.453353000	0.777845000
N	-2.179517000	-1.381024000	-1.890193000
N	0.393057000	-2.134704000	-1.103949000
N	-1.251441000	1.191362000	-1.341397000
N	-0.420429000	2.624898000	0.302235000
H	0.509445000	2.189070000	0.257530000
O	-0.004610000	2.642249000	2.493468000
C	-2.208424000	3.465805000	1.956495000
C	-2.404486000	3.301522000	3.477724000
H	-1.609332000	3.797017000	4.038259000
H	-3.365697000	3.739273000	3.768213000
H	-2.403951000	2.245382000	3.765154000
C	-3.368080000	2.744222000	1.234607000
H	-3.392346000	2.937914000	0.159447000
H	-3.318645000	1.660697000	1.392374000
H	-4.318540000	3.099288000	1.647882000
C	-2.210997000	4.975973000	1.619104000
H	-1.384446000	5.491411000	2.119559000
H	-2.135534000	5.166541000	0.544940000
H	-3.147565000	5.424389000	1.968563000
O	-0.409207000	-0.357064000	1.716249000
O	0.867002000	0.131122000	1.947848000
N	2.362622000	-1.463258000	-0.020537000
H	2.220719000	-0.458816000	-0.169144000
C	3.411119000	-1.733735000	0.874523000
C	3.379605000	-2.965173000	1.815910000
C	4.603964000	-3.856865000	1.514023000
H	5.523533000	-3.264275000	1.516258000
H	4.694507000	-4.635897000	2.279166000
H	4.518007000	-4.359359000	0.543003000
C	2.079840000	-3.790413000	1.789944000

H	1.199674000	-3.150067000	1.914523000
H	1.960555000	-4.377740000	0.875261000
H	2.097405000	-4.500333000	2.624442000
C	3.534385000	-2.367350000	3.240123000
H	2.688233000	-1.714926000	3.481909000
H	3.566222000	-3.180262000	3.973888000
H	4.452655000	-1.782051000	3.318457000
O	4.295760000	-0.899933000	1.001243000
C	2.952152000	3.761497000	-0.956713000
C	3.168344000	2.360986000	-0.644372000
C	4.535870000	1.889961000	-0.537832000
C	5.585297000	2.759052000	-0.747599000
C	5.341734000	4.110416000	-1.067142000
C	4.020017000	4.602674000	-1.166468000
H	1.927040000	4.111950000	-1.025497000
H	4.682764000	0.854559000	-0.245327000
H	6.608694000	2.406543000	-0.658289000
H	6.177371000	4.784551000	-1.230807000
H	3.855808000	5.649153000	-1.406736000
O	2.187942000	1.572335000	-0.472638000
H	0.692184000	1.064454000	2.249864000

**<sup>21</sup>b**

Cu	0.035422000	-0.041972000	-0.706418000
C	2.818103000	-1.280622000	-1.252755000
H	2.427452000	-1.298350000	-2.265450000
C	4.067386000	-1.800784000	-0.923181000
H	4.689201000	-2.250228000	-1.689945000
C	4.487045000	-1.733011000	0.405394000
H	5.450485000	-2.136906000	0.701621000
C	3.652843000	-1.138969000	1.354152000
H	3.954141000	-1.067684000	2.394885000
C	2.422874000	-0.626902000	0.942888000
C	1.502055000	0.128786000	1.885256000
H	1.676433000	-0.177214000	2.927193000
H	1.749804000	1.194979000	1.819735000
C	-0.489700000	-1.311013000	1.919933000
H	-0.759789000	-1.316904000	2.986247000
H	0.291792000	-2.068365000	1.783320000

C	-1.685996000	-1.689111000	1.065315000
C	-2.759799000	-2.415354000	1.577701000
H	-2.777620000	-2.694139000	2.626937000
C	-3.803079000	-2.774905000	0.722679000
H	-4.648997000	-3.341981000	1.099449000
C	-3.746207000	-2.385403000	-0.614422000
H	-4.540017000	-2.634864000	-1.310344000
C	-2.644740000	-1.650495000	-1.048675000
C	-0.738956000	1.139328000	1.938861000
H	-0.520974000	1.422714000	2.978747000
H	-1.788024000	0.822371000	1.907885000
C	-0.573356000	2.330618000	1.009257000
C	-0.702719000	3.647657000	1.447850000
H	-0.870716000	3.862400000	2.498993000
C	-0.617362000	4.678777000	0.509574000
H	-0.717382000	5.713057000	0.825022000
C	-0.396935000	4.364937000	-0.831539000
H	-0.322761000	5.139224000	-1.587638000
C	-0.263133000	3.024018000	-1.187417000
N	2.017309000	-0.712792000	-0.338016000
N	0.081215000	-0.013510000	1.506670000
N	-1.634729000	-1.316038000	-0.229731000
N	-0.352596000	2.037230000	-0.284465000
O	0.268592000	0.103203000	-2.593864000
O	-0.898127000	-0.263378000	-3.315458000
H	-2.546120000	-1.300915000	-2.071497000
H	-0.077117000	2.703144000	-2.208495000
H	-0.609089000	-1.081310000	-3.762408000

**2b**

Cu	-0.040435000	0.011175000	0.609439000
C	-0.925520000	2.877017000	1.393286000
H	-0.899206000	2.447203000	2.390552000
C	-1.338099000	4.186125000	1.154491000
H	-1.645799000	4.818519000	1.980251000
C	-1.352727000	4.650320000	-0.160901000
H	-1.677094000	5.662030000	-0.385295000
C	-0.951078000	3.797628000	-1.191319000
H	-0.955139000	4.130740000	-2.224713000

C	-0.538256000	2.505303000	-0.871438000
C	-0.009403000	1.531722000	-1.910934000
H	-0.399654000	1.776614000	-2.909129000
H	1.081245000	1.632426000	-1.959128000
C	-1.709263000	-0.241435000	-1.816841000
H	-1.855936000	-0.499174000	-2.875815000
H	-2.326524000	0.642247000	-1.614845000
C	-2.180335000	-1.371888000	-0.919238000
C	-3.171894000	-2.266037000	-1.319598000
H	-3.590355000	-2.206104000	-2.319806000
C	-3.616384000	-3.229318000	-0.412450000
H	-4.390254000	-3.935044000	-0.699239000
C	-3.048970000	-3.274433000	0.860155000
H	-3.364600000	-4.008433000	1.593813000
C	-2.049826000	-2.357055000	1.179681000
H	-1.555864000	-2.347049000	2.145562000
C	0.658384000	-0.833576000	-2.118478000
H	0.800469000	-0.662754000	-3.195143000
H	0.218660000	-1.831555000	-2.006235000
C	1.993318000	-0.811036000	-1.395628000
C	3.180420000	-1.085141000	-2.055301000
H	3.192070000	-1.266160000	-3.124681000
C	4.361034000	-1.131875000	-1.295968000
H	5.309695000	-1.351393000	-1.776728000
C	4.317693000	-0.887711000	0.063090000
H	5.217677000	-0.911598000	0.669206000
C	3.073468000	-0.588670000	0.663917000
N	-0.535507000	2.063084000	0.400676000
N	-0.305369000	0.129951000	-1.541126000
N	-1.627900000	-1.426115000	0.308201000
N	1.937407000	-0.567440000	-0.066552000
N	2.955735000	-0.347092000	2.008365000
H	2.113614000	0.161074000	2.303234000
O	0.248668000	0.119103000	2.497025000
O	0.225654000	-1.213736000	3.003327000
H	3.805593000	-0.137584000	2.514665000
H	1.173498000	-1.467377000	2.970811000

Cu	-0.037427000	0.098489000	0.556051000
C	1.040325000	2.972959000	1.198619000
H	0.666129000	2.722027000	2.186554000
C	1.593520000	4.216581000	0.906395000
H	1.685688000	4.968689000	1.682578000
C	2.006926000	4.468294000	-0.402566000
H	2.436737000	5.428816000	-0.670280000
C	1.846219000	3.476426000	-1.371021000
H	2.141799000	3.649397000	-2.401298000
C	1.293612000	2.252319000	-0.995258000
C	1.112343000	1.099688000	-1.963119000
H	1.005161000	1.467862000	-2.993395000
H	2.008139000	0.468708000	-1.936528000
C	-1.338712000	0.872774000	-1.913140000
H	-1.536166000	0.809849000	-2.992579000
H	-1.271173000	1.935899000	-1.654090000
C	-2.464636000	0.237399000	-1.124020000
C	-3.731367000	0.085352000	-1.656006000
H	-3.944310000	0.382207000	-2.677035000
C	-4.730298000	-0.461282000	-0.828578000
H	-5.739921000	-0.591222000	-1.206994000
C	-4.425969000	-0.834994000	0.461654000
H	-5.178175000	-1.260535000	1.118199000
C	-3.099791000	-0.665109000	0.940000000
C	0.074230000	-1.125900000	-2.091851000
H	0.275286000	-1.128317000	-3.172384000
H	-0.900156000	-1.603678000	-1.941928000
C	1.130967000	-1.916580000	-1.353298000
C	1.863203000	-2.884985000	-2.015431000
H	1.728244000	-3.047371000	-3.079176000
C	2.767927000	-3.658327000	-1.267294000
H	3.352635000	-4.437019000	-1.747996000
C	2.911753000	-3.416660000	0.079034000
H	3.606465000	-3.989999000	0.684624000
C	2.148214000	-2.384748000	0.688445000
N	0.908416000	2.012659000	0.271815000
N	-0.036456000	0.253247000	-1.573317000
N	-2.143637000	-0.132653000	0.139291000
N	1.259430000	-1.650476000	-0.027174000



N	2.317558000	-2.098615000	1.998817000
H	1.701853000	-1.443208000	2.479793000
O	-0.316358000	0.333401000	2.443091000
O	0.725489000	-0.143896000	3.308272000
H	2.874137000	-2.720312000	2.565472000
N	-2.734679000	-1.051327000	2.185054000
H	-1.851532000	-0.683663000	2.552237000
H	-3.457159000	-1.299577000	2.844637000
H	1.223440000	0.670116000	3.506403000

**<sup>24</sup>b**

Cu	-0.746806000	0.042495000	0.415925000
C	-0.754836000	2.980130000	1.317826000
H	-0.287772000	2.534497000	2.191443000
C	-1.089230000	4.331062000	1.252118000
H	-0.876886000	4.984419000	2.091487000
C	-1.707151000	4.809864000	0.096900000
H	-1.990630000	5.854920000	0.015158000
C	-1.966915000	3.927981000	-0.954083000
H	-2.452466000	4.270146000	-1.863009000
C	-1.589509000	2.592912000	-0.819342000
C	-1.757951000	1.578088000	-1.935591000
H	-2.560972000	1.884064000	-2.621961000
H	-0.830375000	1.552999000	-2.520307000
C	-3.370308000	-0.003137000	-0.956774000
H	-4.045244000	-0.195993000	-1.803870000
H	-3.707993000	0.927492000	-0.484708000
C	-3.461962000	-1.122601000	0.066895000
C	-4.605479000	-1.907932000	0.204914000
H	-5.446362000	-1.774153000	-0.469109000
C	-4.648949000	-2.858292000	1.226778000
H	-5.529249000	-3.480653000	1.356982000
C	-3.549490000	-2.997496000	2.072975000
H	-3.546316000	-3.722487000	2.879856000
C	-2.437133000	-2.184457000	1.862025000
H	-1.549551000	-2.243878000	2.484306000
C	-1.526692000	-0.830610000	-2.348842000
H	-1.882112000	-0.637578000	-3.371466000
H	-1.976947000	-1.776421000	-2.025776000

C	-0.018886000	-0.996953000	-2.334378000
C	0.695630000	-1.285776000	-3.491682000
H	0.194019000	-1.331995000	-4.452644000
C	2.065042000	-1.542338000	-3.377005000
H	2.649698000	-1.801152000	-4.254604000
C	2.672363000	-1.499903000	-2.129401000
H	3.716213000	-1.754660000	-2.011628000
C	1.896008000	-1.156321000	-1.012619000
C	3.376100000	-0.585386000	1.068020000
N	-0.997668000	2.139183000	0.301011000
N	-1.980057000	0.214456000	-1.410041000
N	-2.398085000	-1.272311000	0.877867000
N	0.574168000	-0.908759000	-1.126607000
N	2.347186000	-1.162845000	0.311727000
H	1.589714000	-1.414129000	0.948353000
O	3.225785000	-0.652946000	2.287502000
C	4.633589000	0.077548000	0.475428000
C	5.301764000	0.886704000	1.608364000
H	5.552210000	0.251842000	2.460284000
H	6.221164000	1.343835000	1.227571000
H	4.644812000	1.684487000	1.968802000
C	4.305415000	1.050901000	-0.677986000
H	3.933943000	0.559902000	-1.579135000
H	3.565524000	1.796688000	-0.364105000
H	5.217422000	1.589857000	-0.955715000
C	5.622345000	-1.027848000	0.028968000
H	5.893213000	-1.667337000	0.875365000
H	5.228233000	-1.672523000	-0.761629000
H	6.538798000	-0.561909000	-0.348725000
O	0.085182000	0.200773000	2.123831000
O	0.512750000	-1.050628000	2.640000000
H	1.484158000	-0.895145000	2.777525000

**<sup>25</sup>b**

Cu	0.506083000	0.759341000	0.307845000
C	3.007924000	2.092814000	1.579268000
H	2.676148000	1.497609000	2.425099000
C	4.111456000	2.941339000	1.642727000
H	4.680303000	3.023532000	2.562667000

C	4.452768000	3.678722000	0.509177000
H	5.301494000	4.355948000	0.525152000
C	3.683082000	3.544265000	-0.647942000
H	3.918160000	4.110312000	-1.544308000
C	2.601467000	2.665126000	-0.636234000
C	1.744932000	2.405616000	-1.861108000
H	1.781382000	3.263774000	-2.549108000
H	2.157548000	1.545024000	-2.401842000
C	-0.407965000	3.241007000	-1.036290000
H	-0.742923000	3.854918000	-1.887029000
H	0.270124000	3.866631000	-0.444211000
C	-1.603518000	2.859360000	-0.174281000
C	-2.661765000	3.745458000	0.033012000
H	-2.665187000	4.721021000	-0.443589000
C	-3.694733000	3.357002000	0.885260000
H	-4.509230000	4.040058000	1.106743000
C	-3.680875000	2.078458000	1.442392000
H	-4.464207000	1.743233000	2.110331000
C	-2.626673000	1.220755000	1.124188000
C	-0.328722000	1.281985000	-2.529454000
H	-0.134557000	1.687470000	-3.533125000
H	-1.405935000	1.372240000	-2.352938000
C	0.020486000	-0.198142000	-2.483988000
C	0.027515000	-0.973968000	-3.642438000
H	-0.127832000	-0.510757000	-4.611816000
C	0.210141000	-2.352663000	-3.526417000
H	0.195083000	-2.985220000	-4.408827000
C	0.384082000	-2.911999000	-2.263531000
H	0.477398000	-3.981896000	-2.124514000
C	0.413094000	-2.067771000	-1.149667000
C	1.572538000	-2.868688000	0.990679000
N	2.277335000	1.958919000	0.462046000
N	0.359673000	2.063073000	-1.485620000
N	-1.581037000	1.637037000	0.381351000
N	0.233212000	-0.737169000	-1.266569000
N	0.498296000	-2.571101000	0.169377000
H	-0.373390000	-2.444733000	0.699795000
O	1.341381000	-2.952350000	2.199996000
C	2.986161000	-3.157250000	0.443971000

C	3.949946000	-3.195888000	1.646794000
H	3.650358000	-3.954356000	2.372756000
H	4.961074000	-3.426211000	1.294038000
H	3.974981000	-2.232479000	2.165727000
C	3.476801000	-2.073266000	-0.542270000
H	2.944585000	-2.087662000	-1.496953000
H	3.388427000	-1.070730000	-0.107803000
H	4.535590000	-2.249112000	-0.761894000
C	2.984294000	-4.546447000	-0.237973000
H	2.624942000	-5.320339000	0.448323000
H	2.363360000	-4.570391000	-1.138068000
H	4.006292000	-4.807512000	-0.534290000
O	0.955384000	0.085290000	2.045849000
O	0.020298000	-0.676020000	2.750357000
N	-2.556458000	-0.117796000	1.588751000
H	-1.674721000	-0.319114000	2.079702000
C	-2.959681000	-1.272560000	0.909073000
C	-4.268209000	-1.332304000	0.088708000
C	-4.237061000	-0.364525000	-1.118437000
H	-3.360642000	-0.551594000	-1.751276000
H	-5.128153000	-0.534945000	-1.732368000
H	-4.239855000	0.688781000	-0.827664000
C	-5.474196000	-1.020268000	1.004295000
H	-5.494613000	-1.690555000	1.870149000
H	-5.469147000	0.008217000	1.371538000
H	-6.403982000	-1.168076000	0.443833000
C	-4.418684000	-2.769117000	-0.449828000
H	-4.440596000	-3.499326000	0.362577000
H	-5.353301000	-2.847863000	-1.015601000
H	-3.590733000	-3.037896000	-1.112664000
O	-2.269030000	-2.279932000	1.050132000
H	0.406285000	-1.597830000	2.699840000

**<sup>1</sup>Hc**

Cu	0.001600000	-0.000685000	-0.897309000
C	2.871925000	-1.014340000	-1.476456000
H	2.530360000	-1.057751000	-2.506126000
C	4.139061000	-1.470107000	-1.123489000
H	4.801834000	-1.872884000	-1.881932000

C	4.519664000	-1.401899000	0.215713000
H	5.495568000	-1.755436000	0.534378000
C	3.621452000	-0.875568000	1.143951000
H	3.884302000	-0.810007000	2.195506000
C	2.373794000	-0.424487000	0.711807000
C	1.406282000	0.241466000	1.685803000
H	1.654426000	-0.061329000	2.715301000
H	1.570855000	1.324846000	1.631058000
C	-0.493907000	-1.339455000	1.685813000
H	-0.880909000	-1.402036000	2.715078000
H	0.361172000	-2.024732000	1.631853000
C	-1.554595000	-1.842918000	0.711109000
C	-2.570859000	-2.695672000	1.143112000
H	-2.646043000	-2.956192000	2.194613000
C	-3.477234000	-3.208070000	0.214966000
H	-4.272892000	-3.874550000	0.533838000
C	-3.345401000	-2.844481000	-1.124169000
H	-4.026780000	-3.215052000	-1.882528000
C	-2.314922000	-1.977407000	-1.477087000
C	-0.913402000	1.095308000	1.685339000
H	-0.775877000	1.461722000	2.714899000
H	-1.933500000	0.695179000	1.630296000
C	-0.820614000	2.265946000	0.711211000
C	-1.052203000	3.572062000	1.143757000
H	-1.240159000	3.766888000	2.195371000
C	-1.043985000	4.613489000	0.215984000
H	-1.224727000	5.635444000	0.535171000
C	-0.794247000	4.318296000	-1.123159000
H	-0.775190000	5.094009000	-1.881187000
C	-0.556835000	2.992798000	-1.476578000
N	2.003652000	-0.502050000	-0.586090000
N	0.000196000	-0.000824000	1.353191000
N	-1.435782000	-1.483768000	-0.586906000
N	-0.568632000	1.984155000	-0.586850000
H	-2.181164000	-1.659786000	-2.506648000
H	-0.347552000	2.719165000	-2.506180000

'2c

Cu	0.035980000	-0.029753000	-0.778407000
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C	0.434955000	2.972735000	-1.499481000
H	0.452870000	2.612485000	-2.523534000
C	0.663005000	4.315272000	-1.210467000
H	0.858831000	5.018110000	-2.013210000
C	0.641126000	4.719405000	0.123450000
H	0.823201000	5.755334000	0.393030000
C	0.386730000	3.767294000	1.110122000
H	0.365570000	4.046910000	2.159211000
C	0.152274000	2.442104000	0.741027000
C	-0.217299000	1.396005000	1.788064000
H	0.134040000	1.726057000	2.778349000
H	-1.311958000	1.350923000	1.844854000
C	1.685562000	-0.173442000	1.660468000
H	1.908147000	-0.515725000	2.683471000
H	2.190392000	0.792996000	1.537822000
C	2.295577000	-1.144411000	0.654216000
C	3.364746000	-1.965116000	1.015656000
H	3.726137000	-1.960062000	2.039608000
C	3.960080000	-2.780436000	0.053621000
H	4.794208000	-3.423469000	0.317590000
C	3.461303000	-2.757685000	-1.247841000
H	3.889596000	-3.374478000	-2.030700000
C	2.382209000	-1.924593000	-1.528742000
C	-0.617700000	-1.042677000	1.883515000
H	-0.874357000	-0.973722000	2.951961000
H	-0.053600000	-1.974494000	1.753004000
C	-1.894503000	-1.144519000	1.058157000
C	-3.095486000	-1.503622000	1.649266000
H	-3.153795000	-1.663992000	2.720380000
C	-4.224091000	-1.662411000	0.829673000
H	-5.178157000	-1.948678000	1.262119000
C	-4.117898000	-1.450941000	-0.530747000
H	-4.974164000	-1.561341000	-1.188321000
C	-2.865471000	-1.070335000	-1.062558000
N	0.183808000	2.051530000	-0.552575000
N	0.254984000	0.052438000	1.444162000
N	1.806226000	-1.133334000	-0.606098000
N	-1.780290000	-0.922679000	-0.276428000
H	1.956461000	-1.882982000	-2.526663000

N	-2.716713000	-0.790639000	-2.396530000
H	-1.773926000	-0.800868000	-2.763479000
H	-3.429741000	-1.117139000	-3.033784000

**3c**

Cu	-0.008538000	0.048828000	0.658563000
C	1.295786000	-2.729337000	1.070025000
C	2.070629000	-3.818698000	0.615927000
H	2.522163000	-4.498748000	1.331135000
C	2.239469000	-3.989872000	-0.744747000
H	2.835282000	-4.817390000	-1.118255000
C	1.632992000	-3.095169000	-1.639826000
H	1.742219000	-3.214999000	-2.712302000
C	0.878561000	-2.053016000	-1.123093000
C	0.118161000	-1.103547000	-2.039727000
H	0.501770000	-1.193657000	-3.067574000
H	-0.930034000	-1.425957000	-2.064596000
C	1.397012000	0.990859000	-1.762137000
H	1.435919000	1.508619000	-2.733388000
H	2.193698000	0.236625000	-1.779267000
C	1.721188000	1.977615000	-0.644911000
C	2.465101000	3.128808000	-0.908357000
H	2.757656000	3.359642000	-1.928302000
C	2.829548000	3.966724000	0.144712000
H	3.410166000	4.864925000	-0.042627000
C	2.432154000	3.631299000	1.438168000
H	2.691785000	4.250431000	2.290236000
C	1.678220000	2.475725000	1.619962000
C	-1.070669000	1.059893000	-1.880803000
H	-1.334485000	0.999790000	-2.948088000
H	-0.842477000	2.111946000	-1.669155000
C	-2.271639000	0.659198000	-1.033701000
C	-3.546543000	0.600633000	-1.576445000
H	-3.702835000	0.792170000	-2.632541000
C	-4.621761000	0.293835000	-0.729157000
H	-5.631919000	0.241917000	-1.124211000
C	-4.391903000	0.061753000	0.614309000
H	-5.204977000	-0.172784000	1.293909000
C	-3.067426000	0.131651000	1.094375000

N	0.728083000	-1.860592000	0.211270000
N	0.131736000	0.282744000	-1.556266000
N	1.324638000	1.662696000	0.608412000
N	-2.034211000	0.413071000	0.278858000
H	1.341536000	2.181522000	2.609386000
N	-2.764028000	-0.130865000	2.414439000
H	-1.923978000	0.319110000	2.758408000
H	-3.535051000	-0.100310000	3.069323000
N	1.122491000	-2.481660000	2.411471000
H	0.296465000	-1.948689000	2.655074000
H	1.330457000	-3.238062000	3.049788000
<b><sup>14</sup>c</b>			
Cu	0.742636000	0.005456000	-0.426652000
C	1.282364000	-2.741066000	-1.757019000
H	0.443934000	-2.474795000	-2.393353000
C	1.892327000	-3.988118000	-1.861333000
H	1.533193000	-4.709033000	-2.587983000
C	2.956829000	-4.279501000	-1.009965000
H	3.454006000	-5.243840000	-1.052647000
C	3.371790000	-3.311178000	-0.095778000
H	4.196377000	-3.505898000	0.583403000
C	2.720652000	-2.077654000	-0.060559000
C	3.209599000	-0.964319000	0.861343000
H	3.791108000	-1.400167000	1.688876000
H	3.904797000	-0.337684000	0.288754000
C	1.293548000	-0.669637000	2.393210000
H	1.695165000	-0.473361000	3.399497000
H	1.304751000	-1.758444000	2.259211000
C	-0.160063000	-0.209335000	2.328111000
C	-0.926490000	-0.104139000	3.483669000
H	-0.482860000	-0.293131000	4.455654000
C	-2.269718000	0.262933000	3.361898000
H	-2.888353000	0.380284000	4.246522000
C	-2.804123000	0.517347000	2.106820000
H	-3.822530000	0.862798000	1.994864000
C	-1.979989000	0.370024000	0.980531000
C	2.506152000	1.307114000	1.536477000
H	3.432134000	1.413358000	2.123057000
H	1.708623000	1.776692000	2.125595000



C	2.639783000	2.084228000	0.229715000
C	3.558683000	3.127445000	0.112879000
H	4.227727000	3.351894000	0.938157000
C	3.603006000	3.874534000	-1.064230000
H	4.310296000	4.691496000	-1.170245000
C	2.728795000	3.549710000	-2.099999000
H	2.726402000	4.100056000	-3.034737000
C	1.849849000	2.485889000	-1.916417000
N	1.681039000	-1.802744000	-0.879830000
N	2.128570000	-0.094645000	1.334493000
N	-0.681861000	0.020072000	1.102899000
N	1.799552000	1.765591000	-0.781126000
N	-2.371112000	0.655898000	-0.326746000
H	-1.634783000	1.097753000	-0.872288000
C	-3.569555000	0.685576000	-1.077526000
C	-4.805526000	-0.183552000	-0.748727000
C	-5.856760000	0.696561000	-0.028951000
H	-6.086858000	1.585983000	-0.623706000
H	-6.781511000	0.124271000	0.102053000
H	-5.535114000	1.028235000	0.964182000
C	-4.490960000	-1.458257000	0.058149000
H	-3.696548000	-2.044461000	-0.418239000
H	-4.198677000	-1.264220000	1.091958000
H	-5.387323000	-2.086697000	0.091550000
C	-5.397017000	-0.612704000	-2.113455000
H	-4.697721000	-1.251612000	-2.664205000
H	-6.317358000	-1.181885000	-1.945376000
H	-5.623054000	0.254282000	-2.735984000
O	-3.535397000	1.378353000	-2.080253000
H	1.158536000	2.192448000	-2.700511000

**15c**

Cu	-0.016123000	0.685634000	0.041464000
C	0.493340000	1.099084000	3.079988000
H	0.177085000	0.063378000	3.159240000
C	0.779264000	1.849206000	4.217618000
H	0.690634000	1.399623000	5.200862000
C	1.167630000	3.178214000	4.055961000
H	1.390280000	3.800442000	4.917508000

C	1.259855000	3.699808000	2.765702000
H	1.556101000	4.731879000	2.603507000
C	0.971642000	2.881200000	1.673080000
C	1.148103000	3.393796000	0.246712000
H	1.114721000	4.494592000	0.243888000
H	2.153528000	3.111786000	-0.089474000
C	-1.166727000	3.342743000	-0.601016000
H	-1.313824000	4.218992000	-1.251715000
H	-1.308674000	3.693223000	0.428817000
C	-2.251753000	2.309775000	-0.889833000
C	-3.488128000	2.706765000	-1.388365000
H	-3.671294000	3.747952000	-1.632904000
C	-4.475739000	1.736723000	-1.576872000
H	-5.443062000	2.010754000	-1.987022000
C	-4.202276000	0.409524000	-1.277237000
H	-4.926844000	-0.368342000	-1.476619000
C	-2.940179000	0.082362000	-0.759745000
C	0.691992000	2.609145000	-2.055994000
H	1.128655000	3.527431000	-2.479505000
H	-0.170609000	2.351837000	-2.683337000
C	1.706466000	1.475196000	-2.154418000
C	2.777631000	1.548759000	-3.038121000
H	2.930997000	2.439465000	-3.638468000
C	3.630065000	0.446662000	-3.151413000
H	4.451700000	0.458382000	-3.861174000
C	3.407374000	-0.674655000	-2.364921000
H	4.022469000	-1.559508000	-2.463449000
C	2.343950000	-0.657908000	-1.449452000
C	2.755875000	-2.758982000	0.030682000
N	0.585649000	1.595878000	1.833726000
N	0.190648000	2.801579000	-0.691349000
N	-1.988352000	1.022244000	-0.575121000
N	1.499965000	0.391455000	-1.370833000
N	2.026849000	-1.734202000	-0.617976000
H	1.038328000	-1.970876000	-0.600260000
O	2.125518000	-3.764651000	0.302706000
C	4.221059000	-2.588471000	0.500445000
C	4.288516000	-3.248238000	1.900318000
H	3.939884000	-4.281368000	1.864844000

H	5.322984000	-3.231819000	2.259533000
H	3.668874000	-2.705459000	2.623444000
C	4.697743000	-1.129470000	0.636524000
H	4.851627000	-0.628922000	-0.321724000
H	3.994662000	-0.531856000	1.228857000
H	5.659539000	-1.119810000	1.160472000
C	5.140041000	-3.389508000	-0.452819000
H	4.803631000	-4.427837000	-0.529263000
H	5.176121000	-2.967732000	-1.463266000
H	6.163240000	-3.387878000	-0.061582000
N	-2.519654000	-1.218173000	-0.483467000
H	-1.565378000	-1.392958000	-0.787797000
C	-3.151383000	-2.461359000	-0.233041000
C	-4.452611000	-2.593293000	0.591390000
C	-5.612561000	-2.950829000	-0.368930000
H	-5.359997000	-3.832442000	-0.965769000
H	-6.512206000	-3.176498000	0.213731000
H	-5.865594000	-2.136186000	-1.056949000
C	-4.798404000	-1.364812000	1.454118000
H	-3.949953000	-1.064807000	2.079873000
H	-5.119846000	-0.496949000	0.874108000
H	-5.624578000	-1.625306000	2.124116000
C	-4.223554000	-3.798010000	1.538530000
H	-3.418691000	-3.591529000	2.253023000
H	-5.140070000	-3.991548000	2.105737000
H	-3.955749000	-4.694432000	0.977067000
O	-2.536799000	-3.445486000	-0.603832000

**<sup>31</sup>d**

Cu	-2.268902000	-0.008160000	-0.208528000
C	-2.790644000	-1.948208000	-2.619720000
H	-1.737781000	-1.753957000	-2.804011000
C	-3.559684000	-2.716715000	-3.490404000
H	-3.111804000	-3.145059000	-4.380763000
C	-4.909309000	-2.906724000	-3.193560000
H	-5.543947000	-3.491821000	-3.852233000
C	-5.438289000	-2.325806000	-2.039791000
H	-6.486275000	-2.450348000	-1.784434000
C	-4.598738000	-1.580110000	-1.212725000

C	-5.084010000	-0.977050000	0.094487000
H	-6.176217000	-0.849343000	0.077708000
H	-4.859565000	-1.680783000	0.905203000
C	-4.892175000	1.423182000	-0.393105000
H	-5.803235000	1.857561000	0.044204000
H	-5.170479000	1.032055000	-1.379170000
C	-3.837653000	2.498286000	-0.593761000
C	-4.190248000	3.837773000	-0.761924000
H	-5.230076000	4.140829000	-0.684287000
C	-3.192657000	4.772790000	-1.038075000
H	-3.445770000	5.819536000	-1.176781000
C	-1.869877000	4.340496000	-1.131512000
H	-1.064029000	5.033734000	-1.348444000
C	-1.596442000	2.988910000	-0.936107000
H	-0.587310000	2.591821000	-0.995683000
C	-4.338585000	0.578421000	1.847198000
H	-5.321093000	0.456058000	2.326547000
H	-4.059735000	1.633220000	1.960255000
C	-3.297424000	-0.271226000	2.555502000
C	-3.475375000	-0.707452000	3.868774000
H	-4.396050000	-0.479575000	4.397239000
C	-2.459656000	-1.438302000	4.485802000
H	-2.579632000	-1.789849000	5.506092000
C	-1.296796000	-1.717741000	3.767906000
H	-0.486948000	-2.290773000	4.206961000
C	-1.197774000	-1.255066000	2.458292000
N	-3.296415000	-1.396154000	-1.505991000
N	-4.390036000	0.288863000	0.402920000
N	-2.555950000	2.086662000	-0.670477000
N	-2.171885000	-0.546660000	1.863816000
O	-0.467614000	-0.491192000	-0.903940000
O	0.459134000	0.452514000	-0.923209000
Cu	2.263748000	-0.001942000	-0.211381000
C	1.479565000	-3.051931000	-0.440341000
H	0.483733000	-2.633861000	-0.554531000
C	1.704115000	-4.426153000	-0.420376000
H	0.871831000	-5.115661000	-0.514967000
C	3.012921000	-4.885440000	-0.273726000
H	3.228382000	-5.949306000	-0.246173000

C	4.045547000	-3.954487000	-0.162562000
H	5.076086000	-4.277701000	-0.050444000
C	3.741030000	-2.593368000	-0.206393000
C	4.835881000	-1.540413000	-0.195674000
H	5.739251000	-1.933081000	0.294167000
H	5.108913000	-1.325607000	-1.235871000
C	4.355696000	-0.322642000	1.883806000
H	5.351632000	-0.164507000	2.323322000
H	4.038815000	-1.332548000	2.171212000
C	3.363056000	0.674767000	2.456172000
C	3.584374000	1.315564000	3.675528000
H	4.504841000	1.138914000	4.223653000
C	2.612545000	2.184409000	4.173037000
H	2.767068000	2.696060000	5.118187000
C	1.449435000	2.392995000	3.431918000
H	0.673890000	3.068378000	3.777420000
C	1.305555000	1.722660000	2.219829000
H	0.426322000	1.856279000	1.596942000
C	5.122470000	0.896795000	-0.109673000
H	6.208605000	0.724374000	-0.123349000
H	4.943088000	1.730517000	0.579897000
C	4.630466000	1.300429000	-1.489092000
C	5.476851000	1.876058000	-2.436445000
H	6.533246000	2.002831000	-2.219650000
C	4.943689000	2.285728000	-3.659633000
H	5.583470000	2.736842000	-4.412041000
C	3.582769000	2.099364000	-3.902231000
H	3.130841000	2.398105000	-4.842083000
C	2.807232000	1.505541000	-2.909258000
N	2.472634000	-2.153074000	-0.332366000
N	4.389784000	-0.274446000	0.411210000
N	2.236498000	0.880490000	1.742343000
N	3.317476000	1.118110000	-1.730095000
H	1.744722000	1.323481000	-3.043465000
H	-0.319373000	-1.452969000	1.851426000

<sup>1</sup>**d<sub>CSS</sub>**

Cu	2.286929000	-0.047392000	-0.012095000
C	2.236268000	-3.130864000	-0.112127000

H	1.177193000	-2.968382000	0.067270000
C	2.783867000	-4.409326000	-0.177425000
H	2.151141000	-5.280971000	-0.048581000
C	4.155202000	-4.534468000	-0.401797000
H	4.620891000	-5.514094000	-0.450393000
C	4.925235000	-3.381325000	-0.558506000
H	5.994993000	-3.446082000	-0.732467000
C	4.301305000	-2.135624000	-0.493197000
C	5.056610000	-0.841683000	-0.740101000
H	6.127557000	-0.973991000	-0.527134000
H	4.972822000	-0.594907000	-1.805595000
C	4.855134000	0.272532000	1.445890000
H	5.856984000	0.696109000	1.609336000
H	4.898569000	-0.776441000	1.763418000
C	3.827932000	0.992474000	2.304131000
C	4.182738000	1.662557000	3.475138000
H	5.224496000	1.723843000	3.775149000
C	3.179995000	2.247450000	4.249819000
H	3.432860000	2.772509000	5.165993000
C	1.854305000	2.155691000	3.825034000
H	1.047790000	2.603482000	4.396097000
C	1.582081000	1.480161000	2.637462000
H	0.573454000	1.387198000	2.243419000
C	4.722847000	1.590644000	-0.627500000
H	5.764480000	1.690658000	-0.965503000
H	4.560980000	2.365927000	0.130768000
C	3.762810000	1.849502000	-1.776469000
C	4.130911000	2.619348000	-2.880350000
H	5.146050000	2.994174000	-2.970109000
C	3.175635000	2.902232000	-3.857233000
H	3.439917000	3.498819000	-4.725126000
C	1.880679000	2.407751000	-3.700699000
H	1.107964000	2.609167000	-4.435154000
C	1.595641000	1.636448000	-2.576473000
N	2.976812000	-2.022583000	-0.266301000
N	4.481679000	0.285906000	0.017497000
N	2.545573000	0.908893000	1.898658000
N	2.515417000	1.357958000	-1.639353000
O	0.401044000	-0.533383000	-0.003693000

O	-0.401148000	0.534490000	-0.004707000
Cu	-2.286981000	0.047836000	-0.012487000
C	-1.594662000	-1.639714000	-2.573890000
H	-0.603404000	-1.234467000	-2.392635000
C	-1.879202000	-2.412587000	-3.697152000
H	-1.106236000	-2.614834000	-4.431114000
C	-3.174010000	-2.907562000	-3.853408000
H	-3.437894000	-3.505365000	-4.720586000
C	-4.129647000	-2.623552000	-2.877215000
H	-5.144684000	-2.998697000	-2.966774000
C	-3.762037000	-1.852142000	-1.774258000
C	-4.722479000	-1.591912000	-0.625934000
H	-5.763993000	-1.692632000	-0.964101000
H	-4.560641000	-2.366139000	0.133415000
C	-5.056809000	0.840210000	-0.741793000
H	-6.127845000	0.972517000	-0.529266000
H	-4.972672000	0.592088000	-1.806949000
C	-4.301894000	2.134656000	-0.496323000
C	-4.926096000	3.380134000	-0.563279000
H	-5.995830000	3.444429000	-0.737551000
C	-4.156364000	4.533639000	-0.407778000
H	-4.622266000	5.513099000	-0.457656000
C	-2.785048000	4.409096000	-0.182930000
H	-2.152574000	5.281056000	-0.054979000
C	-2.237150000	3.130856000	-0.115983000
H	-1.178094000	2.968800000	0.063882000
C	-4.855403000	-0.271115000	1.445692000
H	-5.857154000	-0.694765000	1.609578000
H	-4.899213000	0.778269000	1.761825000
C	-3.828109000	-0.989615000	2.305035000
C	-4.182926000	-1.658204000	3.476904000
H	-5.224715000	-1.719356000	3.776832000
C	-3.180157000	-2.241777000	4.252529000
H	-3.433016000	-2.765649000	5.169385000
C	-1.854424000	-2.150269000	3.827810000
H	-1.047887000	-2.597090000	4.399601000
C	-1.582207000	-1.476297000	2.639354000
N	-2.514800000	-1.360158000	-1.637416000
N	-4.481782000	-0.286270000	0.017377000

N	-2.977425000	2.022214000	-0.269009000
N	-2.545729000	-0.906266000	1.899630000
H	-0.573555000	-1.383614000	2.245307000
H	0.604233000	1.231672000	-2.394979000

**<sup>1</sup>d<sub>oss</sub>**

Cu	-2.226001000	-0.003675000	-0.217584000
C	-2.753546000	-1.734876000	-2.761162000
H	-1.694607000	-1.544966000	-2.911067000
C	-3.525838000	-2.420252000	-3.696224000
H	-3.074736000	-2.788617000	-4.611432000
C	-4.882545000	-2.606436000	-3.430411000
H	-5.518611000	-3.127572000	-4.139500000
C	-5.417589000	-2.106184000	-2.241784000
H	-6.470799000	-2.231261000	-2.009302000
C	-4.575546000	-1.441540000	-1.351105000
C	-5.057946000	-0.929806000	-0.005400000
H	-6.145764000	-0.770311000	-0.017593000
H	-4.857302000	-1.698511000	0.750508000
C	-4.807797000	1.495304000	-0.306471000
H	-5.715275000	1.909498000	0.156569000
H	-5.082929000	1.187218000	-1.322369000
C	-3.730904000	2.560262000	-0.412571000
C	-4.050985000	3.916309000	-0.481804000
H	-5.084188000	4.237634000	-0.390831000
C	-3.028341000	4.844727000	-0.678130000
H	-3.255236000	5.904824000	-0.739202000
C	-1.715381000	4.388769000	-0.794468000
H	-0.891875000	5.077026000	-0.953134000
C	-1.474503000	3.020098000	-0.699538000
H	-0.476632000	2.599395000	-0.783352000
C	-4.298572000	0.470572000	1.868456000
H	-5.292378000	0.335649000	2.319535000
H	-3.997659000	1.506768000	2.064867000
C	-3.288567000	-0.456662000	2.521353000
C	-3.488050000	-0.990453000	3.794642000
H	-4.406468000	-0.782754000	4.335261000
C	-2.494574000	-1.793991000	4.355750000
H	-2.630557000	-2.222521000	5.344126000
C	-1.334019000	-2.046182000	3.623965000



H	-0.542944000	-2.673718000	4.020706000
C	-1.213395000	-1.483668000	2.355565000
N	-3.267223000	-1.260577000	-1.615970000
N	-4.332815000	0.292265000	0.403764000
N	-2.458339000	2.125524000	-0.508918000
N	-2.165342000	-0.705126000	1.817504000
O	-0.465118000	-0.493807000	-0.900331000
O	0.464379000	0.486243000	-0.904683000
Cu	2.225319000	0.002035000	-0.217581000
C	1.466710000	-3.028060000	-0.648076000
H	0.469686000	-2.606591000	-0.737924000
C	1.704406000	-4.398617000	-0.720939000
H	0.879170000	-5.087497000	-0.867459000
C	3.016465000	-4.855613000	-0.598592000
H	3.240911000	-5.917077000	-0.642603000
C	4.041372000	-3.926405000	-0.418616000
H	5.073987000	-4.248456000	-0.323649000
C	3.724402000	-2.568666000	-0.371122000
C	4.804048000	-1.504790000	-0.283919000
H	5.710831000	-1.913428000	0.185407000
H	5.079241000	-1.214908000	-1.305141000
C	4.300142000	-0.441751000	1.873620000
H	5.294964000	-0.301655000	2.320867000
H	3.996946000	-1.473659000	2.088193000
C	3.293560000	0.499276000	2.511906000
C	3.496100000	1.054010000	3.775715000
H	4.414445000	0.852653000	4.318859000
C	2.505840000	1.870243000	4.324044000
H	2.644291000	2.315162000	5.304807000
C	1.345363000	2.113776000	3.589222000
H	0.556801000	2.750663000	3.975938000
C	1.221546000	1.530101000	2.330720000
H	0.347074000	1.692080000	1.707804000
C	5.060219000	0.924483000	-0.025065000
H	6.147651000	0.762238000	-0.035880000
H	4.862408000	1.706602000	0.717714000
C	4.577207000	1.413966000	-1.378768000
C	5.419489000	2.061340000	-2.281864000
H	6.473265000	2.188185000	-2.052923000

C	4.883952000	2.542144000	-3.478269000
H	5.520205000	3.049590000	-4.197051000
C	3.526504000	2.354346000	-3.739098000
H	3.074980000	2.707886000	-4.659927000
C	2.753991000	1.686865000	-2.791356000
N	2.452712000	-2.132627000	-0.473088000
N	4.332774000	-0.288689000	0.406063000
N	2.170333000	0.739276000	1.805136000
N	3.268185000	1.231266000	-1.638836000
H	1.694419000	1.496787000	-2.936439000
H	-0.338926000	-1.653303000	1.734681000

**3d**

Cu	-2.246746000	-0.174148000	0.158335000
C	-2.743903000	-0.739478000	3.228617000
H	-1.660227000	-0.813865000	3.229591000
C	-3.503770000	-0.988743000	4.369011000
H	-3.019015000	-1.265833000	5.299120000
C	-4.892055000	-0.882632000	4.278843000
H	-5.519143000	-1.077445000	5.143578000
C	-5.468089000	-0.528993000	3.057737000
H	-6.545496000	-0.442136000	2.954660000
C	-4.635833000	-0.284223000	1.965652000
C	-5.173531000	0.176001000	0.623562000
H	-6.222892000	-0.126771000	0.499313000
H	-5.152284000	1.271599000	0.596013000
C	-4.602298000	-1.728566000	-0.808914000
H	-5.497604000	-1.837805000	-1.438019000
H	-4.813108000	-2.242559000	0.136678000
C	-3.409115000	-2.403297000	-1.456697000
C	-3.568668000	-3.467951000	-2.343677000
H	-4.564289000	-3.784833000	-2.638952000
C	-2.435895000	-4.117994000	-2.833654000
H	-2.536699000	-4.950779000	-3.523109000
C	-1.177649000	-3.681198000	-2.420780000
H	-0.270162000	-4.162821000	-2.769182000
C	-1.100488000	-2.601794000	-1.544058000
H	-0.151500000	-2.223436000	-1.178893000
C	-4.406997000	0.557330000	-1.684227000
H	-5.447397000	0.741500000	-1.987397000

H	-3.920378000	0.018759000	-2.506232000
C	-3.683524000	1.866743000	-1.447227000
C	-4.180869000	3.066625000	-1.923159000
H	-5.122877000	3.101380000	-2.459314000
C	-3.434658000	4.234825000	-1.686523000
H	-3.795398000	5.194637000	-2.044012000
C	-2.246698000	4.158857000	-0.990717000
H	-1.652619000	5.044999000	-0.790832000
C	-1.802414000	2.897101000	-0.523375000
N	-3.296766000	-0.393875000	2.056428000
N	-4.334091000	-0.313644000	-0.491580000
N	-2.190049000	-1.969423000	-1.075569000
N	-2.517188000	1.773631000	-0.757629000
N	-0.625438000	2.767865000	0.149403000
O	-0.477447000	-0.026323000	1.016849000
O	0.503349000	-0.811069000	0.478238000
Cu	2.238401000	-0.005287000	0.078916000
C	1.789074000	1.426076000	2.878386000
H	0.777692000	1.054869000	2.741543000
C	2.152013000	2.188454000	3.985395000
H	1.417954000	2.426556000	4.747946000
C	3.470462000	2.635024000	4.084295000
H	3.789693000	3.238110000	4.928903000
C	4.376324000	2.294873000	3.080111000
H	5.410131000	2.623501000	3.128068000
C	3.939058000	1.513065000	2.009895000
C	4.899810000	1.017452000	0.944966000
H	5.739993000	1.715736000	0.824006000
H	5.325262000	0.065904000	1.284137000
C	4.019410000	1.998583000	-1.126445000
H	4.942667000	2.307612000	-1.637447000
H	3.760889000	2.797519000	-0.420764000
C	2.884639000	1.841721000	-2.120003000
C	2.866752000	2.516043000	-3.340322000
H	3.702978000	3.146439000	-3.626653000
C	1.764285000	2.362768000	-4.181640000
H	1.730560000	2.874717000	-5.138560000
C	0.715276000	1.536037000	-3.779023000
H	-0.155821000	1.384523000	-4.407433000

C	0.810245000	0.892401000	-2.548299000
H	0.026116000	0.236350000	-2.186201000
C	4.885563000	-0.301982000	-1.130260000
H	5.962346000	-0.108614000	-1.233436000
H	4.453358000	-0.276601000	-2.137393000
C	4.644812000	-1.667739000	-0.521426000
C	5.634356000	-2.633677000	-0.513604000
H	6.621375000	-2.419696000	-0.908757000
C	5.320548000	-3.898066000	0.016951000
H	6.070421000	-4.683106000	0.038066000
C	4.058366000	-4.134816000	0.516009000
H	3.788761000	-5.100388000	0.932136000
C	3.097409000	-3.092202000	0.487784000
N	2.661022000	1.098290000	1.909433000
N	4.221642000	0.763263000	-0.342609000
N	1.869597000	1.040586000	-1.737795000
N	3.397653000	-1.877470000	-0.027545000
N	1.834053000	-3.294237000	0.948789000
H	1.209861000	-2.496641000	1.045790000
H	1.644121000	-4.114059000	1.505392000
H	-0.200515000	3.593289000	0.544492000
H	-0.406714000	1.867460000	0.573794000

**'2d<sub>CSS</sub>**

Cu	2.354341000	0.067683000	0.023539000
C	2.008522000	2.042906000	2.413527000
H	0.957906000	1.915203000	2.170086000
C	2.436950000	2.915415000	3.410771000
H	1.714336000	3.492959000	3.977489000
C	3.806656000	3.032121000	3.649728000
H	4.179696000	3.707276000	4.413889000
C	4.695766000	2.275255000	2.885451000
H	5.767561000	2.348960000	3.042465000
C	4.188355000	1.415497000	1.911420000
C	5.081350000	0.512309000	1.082053000
H	6.100998000	0.920241000	1.025546000
H	5.154766000	-0.461630000	1.580574000
C	4.702056000	1.423607000	-1.170189000
H	5.716391000	1.441059000	-1.594856000

H	4.588482000	2.338534000	-0.576324000
C	3.663177000	1.429558000	-2.276241000
C	3.946860000	1.916339000	-3.552182000
H	4.946146000	2.267160000	-3.791223000
C	2.931771000	1.942443000	-4.509489000
H	3.131150000	2.315559000	-5.509494000
C	1.664846000	1.473277000	-4.163449000
H	0.849779000	1.467930000	-4.879438000
C	1.464236000	0.994412000	-2.870557000
H	0.500775000	0.611515000	-2.544291000
C	4.965664000	-0.999360000	-0.855527000
H	6.056852000	-1.111200000	-0.784519000
H	4.714663000	-0.965464000	-1.922100000
C	4.266707000	-2.191183000	-0.234023000
C	4.928517000	-3.391550000	-0.045467000
H	5.982893000	-3.485222000	-0.281483000
C	4.193726000	-4.484363000	0.446801000
H	4.680247000	-5.441950000	0.606253000
C	2.851595000	-4.336165000	0.725824000
H	2.258448000	-5.164509000	1.100301000
C	2.242084000	-3.073730000	0.521041000
N	2.863524000	1.308220000	1.685659000
N	4.514643000	0.276660000	-0.261267000
N	2.436274000	0.975275000	-1.946766000
N	2.952041000	-2.020417000	0.057409000
N	0.912593000	-2.882471000	0.747185000
O	0.442758000	-0.021214000	0.523100000
O	-0.436614000	0.138838000	-0.485540000
Cu	-2.353104000	-0.040038000	-0.038845000
C	-1.568635000	-0.309687000	3.009491000
H	-0.561793000	-0.343973000	2.600854000
C	-1.813460000	-0.450953000	4.373359000
H	-0.989728000	-0.601030000	5.063281000
C	-3.134195000	-0.403118000	4.819635000
H	-3.368028000	-0.517010000	5.873827000
C	-4.155369000	-0.212663000	3.888579000
H	-5.193969000	-0.173917000	4.202756000
C	-3.827096000	-0.067623000	2.540259000
C	-4.881931000	0.221862000	1.488445000

H	-5.866661000	-0.137085000	1.820893000
H	-4.962538000	1.308696000	1.370168000
C	-4.759642000	-1.791513000	0.082745000
H	-5.812807000	-2.007109000	-0.149140000
H	-4.555602000	-2.223484000	1.069928000
C	-3.842348000	-2.454667000	-0.927935000
C	-4.221781000	-3.591534000	-1.640772000
H	-5.221970000	-3.998514000	-1.527146000
C	-3.296934000	-4.193013000	-2.495831000
H	-3.570551000	-5.078419000	-3.061694000
C	-2.022628000	-3.638263000	-2.615068000
H	-1.275729000	-4.075869000	-3.268867000
C	-1.724244000	-2.494296000	-1.878586000
H	-0.752378000	-2.013536000	-1.927873000
C	-5.094959000	0.410852000	-0.957985000
H	-6.182258000	0.529230000	-0.845510000
H	-4.927075000	-0.187882000	-1.861201000
C	-4.429238000	1.760771000	-1.128101000
C	-5.143370000	2.872768000	-1.538041000
H	-6.212571000	2.811964000	-1.709058000
C	-4.443190000	4.076660000	-1.729587000
H	-4.969865000	4.967497000	-2.058387000
C	-3.085613000	4.125581000	-1.491105000
H	-2.522797000	5.044390000	-1.622212000
C	-2.421634000	2.953446000	-1.053965000
N	-2.548610000	-0.121755000	2.113245000
N	-4.512646000	-0.339770000	0.175258000
N	-2.613332000	-1.916263000	-1.057167000
N	-3.094092000	1.791992000	-0.888365000
N	-1.093441000	2.955777000	-0.750654000
H	-0.633684000	2.050323000	-0.662715000
H	-0.535923000	3.743945000	-1.044425000
H	0.410974000	-3.572406000	1.286097000
H	0.564739000	-1.924093000	0.749030000
<b>'2d<sub>oss</sub></b>			
Cu	-2.280318000	-0.155398000	0.058828000
C	-2.398501000	-1.599915000	2.844645000
H	-1.324298000	-1.637592000	2.689415000

C	-3.013712000	-2.177126000	3.952860000
H	-2.419657000	-2.688574000	4.702803000
C	-4.401838000	-2.088342000	4.065109000
H	-4.917639000	-2.532291000	4.911179000
C	-5.123977000	-1.427446000	3.070032000
H	-6.205208000	-1.346431000	3.126736000
C	-4.432421000	-0.867248000	1.996453000
C	-5.123151000	-0.073874000	0.904167000
H	-6.177916000	-0.368821000	0.812102000
H	-5.109244000	0.987427000	1.178577000
C	-4.688028000	-1.496329000	-1.048254000
H	-5.658386000	-1.482258000	-1.564772000
H	-4.753215000	-2.260319000	-0.264390000
C	-3.577117000	-1.882190000	-2.004845000
C	-3.821912000	-2.646830000	-3.145198000
H	-4.836823000	-2.937008000	-3.399322000
C	-2.745668000	-3.031459000	-3.945433000
H	-2.911888000	-3.627327000	-4.837818000
C	-1.458936000	-2.634836000	-3.582137000
H	-0.594856000	-2.911737000	-4.176929000
C	-1.297677000	-1.862719000	-2.433988000
H	-0.324460000	-1.524357000	-2.092471000
C	-4.650564000	0.949046000	-1.283136000
H	-5.723774000	1.163173000	-1.381962000
H	-4.282604000	0.667310000	-2.276694000
C	-3.901088000	2.175641000	-0.807905000
C	-4.441002000	3.444627000	-0.911834000
H	-5.440792000	3.591423000	-1.305355000
C	-3.655547000	4.534151000	-0.493256000
H	-4.046645000	5.545019000	-0.559528000

C	-2.389619000	4.315635000	0.007079000
H	-1.764154000	5.138766000	0.337782000
C	-1.903733000	2.986763000	0.094472000
N	-3.092951000	-0.958994000	1.892706000
N	-4.410893000	-0.205083000	-0.386857000
N	-2.332526000	-1.492506000	-1.661783000
N	-2.660655000	1.940842000	-0.309699000
N	-0.656808000	2.711223000	0.557788000
O	-0.455128000	-0.157921000	0.743650000
O	0.471294000	-0.693752000	-0.157750000
Cu	2.280187000	-0.022386000	0.009857000
C	1.601331000	0.698115000	3.026900000
H	0.588800000	0.480461000	2.700019000
C	1.891002000	1.119441000	4.322322000
H	1.092600000	1.242447000	5.046500000
C	3.219718000	1.380268000	4.658163000
H	3.483652000	1.718122000	5.655762000
C	4.209178000	1.201324000	3.691321000
H	5.253008000	1.392894000	3.920727000
C	3.840664000	0.762432000	2.419442000
C	4.872738000	0.449752000	1.353419000
H	5.786782000	1.039466000	1.509444000
H	5.153648000	-0.605652000	1.444905000
C	4.323574000	2.069307000	-0.410160000
H	5.318921000	2.396995000	-0.741592000
H	4.070760000	2.659674000	0.478849000
C	3.283279000	2.334788000	-1.480450000
C	3.438354000	3.328221000	-2.446325000
H	4.350702000	3.915452000	-2.485574000
C	2.404412000	3.548734000	-3.357737000



H	2.503171000	4.313989000	-4.121709000
C	1.250529000	2.768740000	-3.277870000
H	0.427728000	2.907751000	-3.970999000
C	1.175307000	1.790971000	-2.289279000
H	0.308101000	1.148748000	-2.177546000
C	5.003954000	-0.215693000	-1.011987000
H	6.096103000	-0.107868000	-0.959558000
H	4.689190000	0.136579000	-2.001379000
C	4.598893000	-1.664942000	-0.844650000
C	5.487470000	-2.698588000	-1.073939000
H	6.517988000	-2.495956000	-1.344148000
C	5.010621000	-4.017247000	-0.950859000
H	5.676251000	-4.856116000	-1.130751000
C	3.699340000	-4.242684000	-0.593236000
H	3.310448000	-5.250016000	-0.483018000
C	2.847591000	-3.133561000	-0.351917000
N	2.553278000	0.527357000	2.094459000
N	4.331728000	0.645832000	-0.008907000
N	2.169367000	1.579393000	-1.413610000
N	3.304801000	-1.865810000	-0.490496000
N	1.561549000	-3.295450000	0.040675000
H	0.952114000	-2.475021000	0.086053000
H	1.161910000	-4.220352000	0.072775000
H	-0.145508000	3.430269000	1.046218000
H	-0.399361000	1.731637000	0.704729000
<b><sup>3</sup>d</b>			
Cu	2.281556000	0.009788000	0.058493000
C	1.077399000	0.545315000	2.929037000
H	0.134378000	0.550446000	2.396215000
C	1.144535000	0.775016000	4.301100000
H	0.236899000	0.966012000	4.863470000
C	2.393142000	0.759008000	4.921971000

H	2.483836000	0.938924000	5.988933000
C	3.531046000	0.517054000	4.150844000
H	4.518625000	0.505221000	4.601529000
C	3.381909000	0.290138000	2.783869000
C	4.553501000	-0.032725000	1.881422000
H	5.486612000	0.385729000	2.283572000
H	4.681677000	-1.120644000	1.834478000
C	4.463935000	1.917870000	0.390747000
H	5.524984000	2.200155000	0.419560000
H	3.981211000	2.363638000	1.267768000
C	3.801524000	2.433961000	-0.865967000
C	4.392161000	3.413523000	-1.643235000
H	5.365410000	3.815631000	-1.384043000
C	3.692051000	3.869315000	-2.774323000
H	4.121746000	4.636094000	-3.411887000
C	2.455605000	3.336918000	-3.067948000
H	1.891565000	3.670929000	-3.933280000
C	1.911620000	2.334006000	-2.224878000
C	5.144396000	-0.268887000	-0.489949000
H	6.193814000	-0.300487000	-0.167114000
H	5.108106000	0.310026000	-1.419596000
C	4.620731000	-1.660664000	-0.760586000
C	5.479012000	-2.702523000	-1.063063000
H	6.553515000	-2.556515000	-1.047089000
C	4.917491000	-3.943735000	-1.406728000
H	5.558375000	-4.783451000	-1.657954000
C	3.546482000	-4.089148000	-1.426871000
H	3.084364000	-5.034686000	-1.692657000
C	2.729122000	-2.983811000	-1.087078000
N	2.171732000	0.307318000	2.188038000
N	4.307666000	0.446490000	0.501696000
N	2.591710000	1.885290000	-1.144388000
N	3.269684000	-1.789603000	-0.751151000
N	1.370468000	-3.102755000	-1.048459000
O	0.476329000	-0.550299000	-0.339344000
O	-0.447822000	0.537529000	-0.238814000
Cu	-2.309619000	0.018568000	-0.106740000
C	-1.777756000	-2.283293000	2.110208000
C	-2.232560000	-3.235019000	3.060874000

H	-1.516615000	-3.903300000	3.528902000
C	-3.573423000	-3.297424000	3.366535000
H	-3.935668000	-4.025710000	4.085887000
C	-4.472330000	-2.419902000	2.733303000
H	-5.535233000	-2.453991000	2.945619000
C	-3.961774000	-1.506733000	1.830452000
C	-4.857180000	-0.501884000	1.141520000
H	-5.902959000	-0.836822000	1.155002000
H	-4.813177000	0.455809000	1.671504000
C	-4.668581000	-1.410019000	-1.137312000
H	-5.709412000	-1.396389000	-1.488181000
H	-4.541259000	-2.321649000	-0.542820000
C	-3.701725000	-1.448564000	-2.302328000
C	-4.044608000	-1.997289000	-3.538020000
H	-5.049693000	-2.369508000	-3.711374000
C	-3.075120000	-2.057410000	-4.539626000
H	-3.317001000	-2.478771000	-5.510691000
C	-1.797311000	-1.562038000	-4.276792000
H	-1.017905000	-1.585796000	-5.031143000
C	-1.536231000	-1.018870000	-3.020886000
H	-0.563356000	-0.611963000	-2.764711000
C	-4.938061000	1.007500000	-0.803580000
H	-6.031774000	1.041538000	-0.706299000
H	-4.705897000	1.015522000	-1.875259000
C	-4.302494000	2.210466000	-0.143791000
C	-5.006171000	3.383235000	0.056605000
H	-6.052522000	3.456063000	-0.218762000
C	-4.323111000	4.474609000	0.621630000
H	-4.839886000	5.414879000	0.788387000
C	-2.995358000	4.345117000	0.968831000
H	-2.446570000	5.169744000	1.412536000
C	-2.339904000	3.107788000	0.751113000
N	-2.641680000	-1.426577000	1.513868000
N	-4.397649000	-0.255788000	-0.247346000
N	-2.469061000	-0.965261000	-2.055296000
N	-2.996555000	2.062023000	0.195522000
N	-1.044430000	2.919915000	1.126192000
H	-0.547717000	2.119615000	0.732271000
H	-0.497533000	3.738194000	1.352093000

H	0.960918000	-3.913226000	-1.490552000
H	0.817610000	-2.247522000	-1.060850000
N	-0.461724000	-2.192298000	1.798259000
H	-0.139056000	-1.617934000	1.011334000
H	0.146898000	-2.946380000	2.081051000
N	0.698335000	1.773706000	-2.496957000
H	0.187076000	1.337623000	-1.719802000
H	0.130113000	2.250168000	-3.184069000

**<sup>13</sup>d<sub>CSS</sub>**

Cu	2.320936000	0.026411000	0.056927000
C	1.340460000	0.483191000	3.044857000
H	0.356480000	0.492010000	2.589339000
C	1.509183000	0.694924000	4.411348000
H	0.646475000	0.880515000	5.042301000
C	2.800763000	0.665440000	4.936478000
H	2.972771000	0.831997000	5.995558000
C	3.874527000	0.424678000	4.078329000
H	4.893187000	0.400238000	4.453125000
C	3.622755000	0.213555000	2.723026000
C	4.727389000	-0.114068000	1.739465000
H	5.694503000	0.265187000	2.100207000
H	4.819544000	-1.203752000	1.660225000
C	4.601224000	1.867885000	0.297457000
H	5.667424000	2.128833000	0.237565000
H	4.211119000	2.307381000	1.222904000
C	3.846536000	2.442061000	-0.881244000
C	4.393140000	3.448794000	-1.659136000
H	5.392937000	3.819193000	-1.460527000
C	3.618409000	3.972220000	-2.706608000
H	4.013025000	4.761797000	-3.338933000
C	2.348578000	3.478323000	-2.923545000
H	1.722107000	3.868750000	-3.719570000
C	1.857108000	2.447059000	-2.088099000
C	5.134613000	-0.320494000	-0.675336000
H	6.208602000	-0.394851000	-0.453546000
H	5.034058000	0.271034000	-1.592483000
C	4.544859000	-1.692608000	-0.913017000
C	5.351471000	-2.762396000	-1.259684000

H	6.428507000	-2.646104000	-1.310820000
C	4.738359000	-3.990956000	-1.553716000
H	5.339638000	-4.849991000	-1.835549000
C	3.365479000	-4.098877000	-1.482664000
H	2.861354000	-5.034391000	-1.704077000
C	2.603468000	-2.967745000	-1.105462000
N	2.371974000	0.247056000	2.219323000
N	4.415952000	0.404898000	0.391990000
N	2.608367000	1.928914000	-1.092247000
N	3.192047000	-1.783884000	-0.820713000
N	1.245027000	-3.056015000	-0.977686000
O	0.433596000	-0.460243000	-0.117507000
O	-0.448029000	0.564828000	0.047730000
Cu	-2.332378000	0.055080000	-0.090550000
C	-1.943826000	-2.275058000	2.203579000
C	-2.452296000	-3.260907000	3.086438000
H	-1.762847000	-3.905822000	3.622357000
C	-3.815788000	-3.386562000	3.241546000
H	-4.222639000	-4.141564000	3.907490000
C	-4.674402000	-2.536302000	2.524841000
H	-5.751745000	-2.613271000	2.623347000
C	-4.108613000	-1.585649000	1.693254000
C	-4.978733000	-0.595202000	0.948469000
H	-6.010720000	-0.966726000	0.876993000
H	-5.012096000	0.347095000	1.506039000
C	-4.579854000	-1.422484000	-1.329138000
H	-5.585751000	-1.437514000	-1.772948000
H	-4.472021000	-2.348529000	-0.752719000
C	-3.518956000	-1.399130000	-2.410830000
C	-3.750910000	-1.938706000	-3.676676000
H	-4.728142000	-2.341564000	-3.924922000
C	-2.713597000	-1.951725000	-4.608676000
H	-2.872150000	-2.365258000	-5.600080000
C	-1.476484000	-1.417462000	-4.247825000
H	-0.644404000	-1.399065000	-4.943861000
C	-1.326114000	-0.886316000	-2.969021000
H	-0.387386000	-0.444253000	-2.650518000
C	-4.932351000	0.975438000	-0.949780000
H	-6.031592000	1.000586000	-0.948019000

H	-4.610737000	1.021543000	-1.997345000
C	-4.376890000	2.168378000	-0.201778000
C	-5.119098000	3.324831000	-0.044507000
H	-6.132265000	3.386601000	-0.426244000
C	-4.525720000	4.409340000	0.623543000
H	-5.075182000	5.336356000	0.756357000
C	-3.246298000	4.286343000	1.122050000
H	-2.767904000	5.102166000	1.654683000
C	-2.551922000	3.064633000	0.947825000
N	-2.768283000	-1.447944000	1.521872000
N	-4.425744000	-0.295029000	-0.390224000
N	-2.323435000	-0.877495000	-2.067591000
N	-3.111585000	2.032395000	0.274757000
N	-1.314840000	2.881686000	1.489322000
H	-0.760902000	2.090945000	1.178066000
H	-0.815258000	3.692192000	1.824485000
H	0.790930000	-3.857705000	-1.391514000
H	0.713300000	-2.192990000	-0.978640000
N	-0.597833000	-2.118566000	2.051413000
H	-0.227151000	-1.571106000	1.276034000
H	-0.002825000	-2.867289000	2.376042000
N	0.607765000	1.918591000	-2.287300000
H	0.143998000	1.497813000	-1.480029000
H	-0.003636000	2.450692000	-2.892489000

**<sup>13</sup>d<sub>oss</sub>**

Cu	2.294402000	0.030376000	0.059106000
C	1.247357000	0.801199000	2.953153000
H	0.279092000	0.790530000	2.466721000
C	1.388063000	1.124999000	4.300678000
H	0.514589000	1.379822000	4.891279000
C	2.665395000	1.117610000	4.860647000
H	2.813349000	1.370183000	5.906269000
C	3.757256000	0.788265000	4.055899000
H	4.765235000	0.779312000	4.459059000
C	3.533975000	0.469127000	2.717549000
C	4.649190000	0.047224000	1.784296000
H	5.613696000	0.459229000	2.112094000
H	4.741070000	-1.045110000	1.804291000
C	4.538665000	1.898166000	0.174148000

H	5.606668000	2.146643000	0.112181000
H	4.133213000	2.413898000	1.052019000
C	3.804425000	2.360869000	-1.063201000
C	4.353536000	3.297166000	-1.920378000
H	5.346169000	3.696396000	-1.743178000
C	3.586204000	3.713426000	-3.022264000
H	3.982117000	4.445469000	-3.719722000
C	2.325734000	3.188591000	-3.210096000
H	1.708506000	3.495824000	-4.048608000
C	1.827105000	2.231610000	-2.290484000
C	5.113138000	-0.358814000	-0.594878000
H	6.177170000	-0.399970000	-0.325687000
H	5.041426000	0.159992000	-1.557565000
C	4.540903000	-1.749571000	-0.743547000
C	5.356101000	-2.831945000	-1.019037000
H	6.432891000	-2.714075000	-1.070855000
C	4.747916000	-4.078695000	-1.244742000
H	5.354532000	-4.950231000	-1.471466000
C	3.375908000	-4.189216000	-1.177413000
H	2.878198000	-5.138735000	-1.347467000
C	2.602679000	-3.042277000	-0.869681000
N	2.297345000	0.479937000	2.180144000
N	4.348696000	0.443097000	0.388754000
N	2.573465000	1.817104000	-1.240604000
N	3.188572000	-1.840634000	-0.652697000
N	1.249711000	-3.125619000	-0.746888000
O	0.459314000	-0.525024000	-0.133725000
O	-0.460389000	0.569874000	-0.078459000
Cu	-2.309320000	0.022189000	-0.105088000
C	-1.850081000	-2.048672000	2.373985000
C	-2.334670000	-2.922485000	3.382715000
H	-1.629672000	-3.510487000	3.962013000
C	-3.690798000	-3.013163000	3.603931000
H	-4.075566000	-3.683245000	4.366846000
C	-4.574046000	-2.239319000	2.829979000
H	-5.647072000	-2.294126000	2.977251000
C	-4.034070000	-1.397015000	1.876149000
C	-4.916225000	-0.487961000	1.049397000
H	-5.948421000	-0.862306000	1.024281000

H	-4.940764000	0.508584000	1.503317000
C	-4.566039000	-1.555829000	-1.136042000
H	-5.584224000	-1.601830000	-1.546068000
H	-4.449720000	-2.415555000	-0.466420000
C	-3.531858000	-1.652816000	-2.237676000
C	-3.786301000	-2.310992000	-3.440629000
H	-4.768185000	-2.731135000	-3.635900000
C	-2.760825000	-2.418032000	-4.380578000
H	-2.934882000	-2.924476000	-5.325178000
C	-1.516003000	-1.858444000	-4.090889000
H	-0.694658000	-1.914056000	-4.797525000
C	-1.342347000	-1.207394000	-2.871644000
H	-0.398775000	-0.745922000	-2.600237000
C	-4.913657000	0.872126000	-1.004038000
H	-6.011783000	0.882385000	-0.975147000
H	-4.616174000	0.809673000	-2.057682000
C	-4.349899000	2.136089000	-0.393681000
C	-5.092582000	3.299271000	-0.320841000
H	-6.118893000	3.324364000	-0.670168000
C	-4.476558000	4.443612000	0.216572000
H	-5.025110000	5.378275000	0.283278000
C	-3.176270000	4.372439000	0.667738000
H	-2.681234000	5.237629000	1.097189000
C	-2.478826000	3.141472000	0.581766000
N	-2.700417000	-1.294869000	1.637142000
N	-4.377743000	-0.331488000	-0.323818000
N	-2.329660000	-1.107915000	-1.964737000
N	-3.067101000	2.046570000	0.043536000
N	-1.215431000	3.013042000	1.068419000
H	-0.674887000	2.191595000	0.797629000
H	-0.707033000	3.853383000	1.301403000
H	0.793058000	-3.962520000	-1.078133000
H	0.707278000	-2.263795000	-0.745523000
N	-0.517593000	-1.929237000	2.146094000
H	-0.160510000	-1.435214000	1.320475000
H	0.093289000	-2.622877000	2.552030000
N	0.590771000	1.677785000	-2.452237000
H	0.123664000	1.298883000	-1.617441000
H	-0.015672000	2.132289000	-3.121633000



**34d**

Cu	2.385804000	1.207742000	0.167863000
C	2.758082000	0.735735000	3.275167000
H	1.701750000	0.492705000	3.203774000
C	3.424548000	0.769665000	4.497673000
H	2.892650000	0.550055000	5.417308000
C	4.779359000	1.101864000	4.506001000
H	5.332293000	1.149175000	5.439292000
C	5.415612000	1.381688000	3.295938000
H	6.467772000	1.648793000	3.269310000
C	4.679027000	1.313595000	2.112976000
C	5.322559000	1.533542000	0.753767000
H	6.236763000	2.136358000	0.854722000
H	5.627368000	0.559457000	0.354613000
C	4.206126000	3.583656000	0.002091000
H	5.016839000	4.160770000	-0.467074000
H	4.268993000	3.768453000	1.081331000
C	2.854369000	4.067701000	-0.484610000
C	2.662522000	5.380301000	-0.909425000
H	3.507154000	6.059950000	-0.972819000
C	1.372731000	5.805903000	-1.232471000
H	1.199413000	6.827809000	-1.556525000
C	0.316747000	4.904234000	-1.122242000
H	-0.709746000	5.183612000	-1.324109000
C	0.593810000	3.599877000	-0.716635000
H	-0.197601000	2.868029000	-0.611100000
C	4.667958000	1.797325000	-1.608058000
H	5.715637000	2.005135000	-1.873547000
H	4.046307000	2.447670000	-2.235439000
C	4.334632000	0.349655000	-1.918656000
C	5.005550000	-0.347932000	-2.917799000
H	5.809170000	0.122711000	-3.474225000
C	4.597311000	-1.653626000	-3.200318000
H	5.064204000	-2.212317000	-4.005860000
C	3.588816000	-2.238037000	-2.446096000
H	3.241388000	-3.238940000	-2.663273000
C	3.016296000	-1.500365000	-1.397941000
N	3.369280000	0.999207000	2.110811000
N	4.377009000	2.135639000	-0.204960000

N	1.834429000	3.186001000	-0.410301000
N	3.347378000	-0.209722000	-1.188558000
N	2.021869000	-1.985767000	-0.554401000
O	0.686746000	0.309113000	0.711978000
O	-0.497218000	0.521119000	0.066498000
Cu	-1.571023000	-1.135276000	-0.137620000
C	-1.509538000	-0.736273000	2.907096000
H	-1.033119000	0.198840000	2.632787000
C	-1.824759000	-1.047020000	4.226566000
H	-1.596919000	-0.344432000	5.021098000
C	-2.448259000	-2.266776000	4.493237000
H	-2.717045000	-2.540552000	5.509087000
C	-2.732180000	-3.128761000	3.434550000
H	-3.221028000	-4.082494000	3.608559000
C	-2.378669000	-2.750929000	2.138833000
C	-2.574196000	-3.678437000	0.953284000
H	-1.657187000	-4.264324000	0.849195000
H	-3.400088000	-4.376142000	1.146719000
C	-2.215157000	-3.620560000	-1.503859000
H	-2.895992000	-4.387112000	-1.898557000
H	-1.292144000	-4.115600000	-1.191298000
C	-1.867233000	-2.612644000	-2.584501000
C	-1.963960000	-2.904713000	-3.944266000
H	-2.345637000	-3.868601000	-4.266560000
C	-1.570436000	-1.942613000	-4.875906000
H	-1.643498000	-2.149587000	-5.939339000
C	-1.095587000	-0.711185000	-4.423282000
H	-0.789296000	0.065380000	-5.115881000
C	-1.033482000	-0.486713000	-3.050867000
H	-0.683148000	0.451918000	-2.633728000
C	-4.205821000	-2.581579000	-0.545939000
H	-4.853043000	-3.436480000	-0.307624000
H	-4.317614000	-2.380779000	-1.616992000
C	-4.667502000	-1.344007000	0.195144000
C	-5.865132000	-1.319710000	0.901828000
H	-6.472657000	-2.213720000	0.997586000
C	-6.256168000	-0.113453000	1.492191000
H	-7.165393000	-0.059721000	2.083356000
C	-5.463475000	1.014389000	1.332595000

H	-5.723963000	1.949982000	1.808088000
C	-4.293494000	0.913852000	0.561188000
N	-1.777343000	-1.571741000	1.890615000
N	-2.781573000	-2.938668000	-0.314794000
N	-1.408719000	-1.416298000	-2.157338000
N	-3.891659000	-0.255630000	0.037907000
N	-3.409673000	1.983248000	0.347931000
H	-2.432434000	1.692431000	0.321556000
H	1.408491000	-1.255577000	-0.169506000
C	-3.511224000	3.299779000	-0.124524000
O	-2.443139000	3.886524000	-0.259781000
C	-4.840136000	4.002962000	-0.489638000
C	-4.483199000	5.154035000	-1.457688000
H	-5.395810000	5.698879000	-1.719487000
H	-3.778316000	5.853548000	-1.004713000
H	-4.037389000	4.773181000	-2.382742000
C	-5.447373000	4.633618000	0.788385000
H	-6.338056000	5.211036000	0.518579000
H	-5.751252000	3.894368000	1.534790000
H	-4.733020000	5.315702000	1.260823000
C	-5.855045000	3.084308000	-1.203805000
H	-6.309856000	2.337892000	-0.551202000
H	-6.668285000	3.699654000	-1.602404000
H	-5.393578000	2.563666000	-2.051417000
C	1.608670000	-3.257220000	-0.159089000
O	0.422613000	-3.357517000	0.162469000
C	2.560253000	-4.464615000	0.031944000
C	2.119058000	-5.141984000	1.355940000
H	1.072934000	-5.450566000	1.318082000
H	2.738659000	-6.027379000	1.528846000
H	2.247134000	-4.467037000	2.209431000
C	4.050221000	-4.095902000	0.173453000
H	4.600891000	-4.980994000	0.507815000
H	4.512446000	-3.766859000	-0.758431000
H	4.197407000	-3.313813000	0.926920000
C	2.340264000	-5.477693000	-1.117619000
H	2.652596000	-5.094150000	-2.094635000
H	2.925744000	-6.381914000	-0.921788000
H	1.286449000	-5.766994000	-1.185810000

**<sup>14</sup>d<sub>CSS</sub>**

Cu	2.403223000	1.257222000	0.205844000
C	2.700926000	0.529890000	3.239398000
H	1.646948000	0.292375000	3.131882000
C	3.346195000	0.459572000	4.471104000
H	2.798299000	0.162379000	5.358967000
C	4.700542000	0.788412000	4.531340000
H	5.237294000	0.756695000	5.474645000
C	5.357428000	1.164930000	3.359840000
H	6.410619000	1.428787000	3.372974000
C	4.643615000	1.196420000	2.161230000
C	5.324173000	1.509975000	0.839248000
H	6.226974000	2.115189000	1.007915000
H	5.655275000	0.564579000	0.394899000
C	4.212765000	3.590416000	0.152123000
H	5.035102000	4.198099000	-0.253835000
H	4.226169000	3.723087000	1.240863000
C	2.878380000	4.079594000	-0.375729000
C	2.690250000	5.394491000	-0.793356000
H	3.528369000	6.084775000	-0.806473000
C	1.414029000	5.807313000	-1.182377000
H	1.246287000	6.830181000	-1.506253000
C	0.365456000	4.891171000	-1.145951000
H	-0.649564000	5.154150000	-1.415980000
C	0.635947000	3.586616000	-0.735365000
H	-0.153183000	2.843902000	-0.690964000
C	4.745496000	1.882607000	-1.524928000
H	5.802042000	2.103340000	-1.740599000
H	4.147489000	2.564242000	-2.141718000
C	4.424095000	0.452742000	-1.923808000
C	5.114407000	-0.178180000	-2.955069000
H	5.928049000	0.326218000	-3.465850000
C	4.709887000	-1.460972000	-3.329912000
H	5.191600000	-1.966919000	-4.161185000
C	3.682983000	-2.090151000	-2.637470000
H	3.335979000	-3.071286000	-2.930458000
C	3.092686000	-1.420605000	-1.555238000
N	3.331906000	0.889318000	2.110669000

N	4.407677000	2.154956000	-0.117576000
N	1.861265000	3.189118000	-0.362546000
N	3.427933000	-0.151007000	-1.248698000
N	2.065586000	-1.939726000	-0.765930000
O	0.700858000	0.285273000	0.549859000
O	-0.403116000	0.428274000	-0.203244000
Cu	-1.614487000	-1.132896000	-0.054258000
C	-1.358436000	-0.453536000	2.906842000
H	-0.903539000	0.452903000	2.520235000
C	-1.597561000	-0.639418000	4.265807000
H	-1.343896000	0.141187000	4.975272000
C	-2.181497000	-1.836834000	4.681434000
H	-2.390707000	-2.015251000	5.731935000
C	-2.501560000	-2.802332000	3.727152000
H	-2.955771000	-3.744300000	4.018832000
C	-2.230164000	-2.545827000	2.382951000
C	-2.466720000	-3.582915000	1.299995000
H	-1.524844000	-4.121590000	1.160354000
H	-3.226116000	-4.307441000	1.625397000
C	-2.351205000	-3.725805000	-1.177600000
H	-3.050747000	-4.525457000	-1.457900000
H	-1.396197000	-4.186835000	-0.912369000
C	-2.107552000	-2.797104000	-2.354045000
C	-2.311674000	-3.189100000	-3.676379000
H	-2.714373000	-4.173394000	-3.895006000
C	-1.992962000	-2.301275000	-4.705691000
H	-2.149742000	-2.586667000	-5.741584000
C	-1.480143000	-1.044116000	-4.385530000
H	-1.224419000	-0.324708000	-5.156045000
C	-1.310241000	-0.719396000	-3.041943000
H	-0.916576000	0.241224000	-2.722952000
C	-4.267898000	-2.643438000	-0.112158000
H	-4.874188000	-3.461445000	0.300977000
H	-4.499083000	-2.581914000	-1.181281000
C	-4.674308000	-1.320849000	0.508328000
C	-5.826764000	-1.201709000	1.278786000
H	-6.428158000	-2.072813000	1.517597000
C	-6.181224000	0.069604000	1.741131000
H	-7.053998000	0.200618000	2.373739000

C	-5.399197000	1.165423000	1.401518000
H	-5.632360000	2.152286000	1.776729000
C	-4.278139000	0.962684000	0.580645000
N	-1.667390000	-1.384854000	1.991398000
N	-2.823930000	-2.966845000	0.003535000
N	-1.619438000	-1.574103000	-2.056946000
N	-3.910663000	-0.263825000	0.176938000
N	-3.397126000	1.985638000	0.189745000
H	-2.434153000	1.659662000	0.111473000
H	1.467344000	-1.207320000	-0.363277000
C	-3.504786000	3.230030000	-0.448229000
O	-2.435661000	3.746546000	-0.756413000
C	-4.839030000	3.937888000	-0.776704000
C	-4.534209000	4.981526000	-1.875469000
H	-5.453600000	5.522941000	-2.120697000
H	-3.783964000	5.702973000	-1.546218000
H	-4.166100000	4.503258000	-2.788921000
C	-5.331142000	4.704315000	0.476196000
H	-6.230556000	5.274239000	0.219912000
H	-5.585650000	4.051008000	1.315087000
H	-4.570429000	5.412496000	0.820924000
C	-5.924146000	2.983679000	-1.320837000
H	-6.326873000	2.300607000	-0.571817000
H	-6.762012000	3.580407000	-1.695782000
H	-5.545191000	2.388810000	-2.160317000
C	1.649430000	-3.201417000	-0.355665000
O	0.490863000	-3.268824000	0.066230000
C	2.561734000	-4.451891000	-0.289097000
C	2.108468000	-5.255878000	0.955240000
H	1.059694000	-5.549636000	0.883600000
H	2.717772000	-6.161264000	1.037906000
H	2.238353000	-4.674093000	1.874192000
C	4.060437000	-4.131839000	-0.114081000
H	4.595446000	-5.059375000	0.113727000
H	4.526632000	-3.704600000	-1.002772000
H	4.223832000	-3.444799000	0.724296000
C	2.315703000	-5.336405000	-1.536123000
H	2.636525000	-4.867088000	-2.471119000
H	2.875286000	-6.272016000	-1.433084000

H	1.254115000	-5.588527000	-1.630781000
<b><sup>14</sup>d<sub>oss</sub></b>			
Cu	2.356283000	1.239104000	0.166418000
C	2.671209000	0.686176000	3.250049000
H	1.617548000	0.443068000	3.151066000
C	3.318311000	0.686970000	4.483194000
H	2.772389000	0.440538000	5.387652000
C	4.672279000	1.020952000	4.523174000
H	5.209345000	1.043361000	5.466591000
C	5.329084000	1.333668000	3.332301000
H	6.381457000	1.601053000	3.330538000
C	4.612320000	1.296840000	2.136074000
C	5.275931000	1.545170000	0.792677000
H	6.179359000	2.159476000	0.915223000
H	5.599574000	0.580889000	0.385066000
C	4.160715000	3.597771000	0.040422000
H	4.984921000	4.177951000	-0.399505000
H	4.189929000	3.772005000	1.122821000
C	2.823848000	4.075968000	-0.487632000
C	2.633207000	5.382518000	-0.928231000
H	3.471883000	6.071129000	-0.968226000
C	1.350074000	5.790164000	-1.299707000
H	1.176832000	6.807484000	-1.637851000
C	0.300763000	4.878048000	-1.220464000
H	-0.720519000	5.146075000	-1.459290000
C	0.575505000	3.579379000	-0.794140000
H	-0.207318000	2.835463000	-0.710324000
C	4.668571000	1.829075000	-1.577682000
H	5.723624000	2.041073000	-1.806319000
H	4.066292000	2.488978000	-2.213503000
C	4.341430000	0.386102000	-1.914794000
C	5.011804000	-0.295463000	-2.925243000
H	5.817268000	0.180911000	-3.474169000
C	4.597609000	-1.594946000	-3.228910000
H	5.063387000	-2.141973000	-4.043091000
C	3.584819000	-2.188476000	-2.487098000
H	3.233497000	-3.183615000	-2.723493000
C	3.013608000	-1.466965000	-1.426643000
N	3.302864000	0.983078000	2.104711000

N	4.338577000	2.149375000	-0.175921000
N	1.809094000	3.185116000	-0.441296000
N	3.354397000	-0.182804000	-1.195253000
N	2.010391000	-1.948340000	-0.592703000
O	0.704083000	0.290320000	0.632335000
O	-0.470723000	0.484410000	-0.099550000
Cu	-1.541386000	-1.160789000	-0.121866000
C	-1.420856000	-0.566826000	2.864876000
H	-0.955041000	0.348315000	2.515380000
C	-1.701066000	-0.796741000	4.208705000
H	-1.462225000	-0.042919000	4.951412000
C	-2.305467000	-2.002580000	4.567695000
H	-2.545920000	-2.213388000	5.605445000
C	-2.607717000	-2.933155000	3.573902000
H	-3.081897000	-3.878019000	3.821043000
C	-2.292711000	-2.634804000	2.248013000
C	-2.511957000	-3.630946000	1.124109000
H	-1.593776000	-4.216390000	1.027977000
H	-3.328440000	-4.320368000	1.376853000
C	-2.230284000	-3.710246000	-1.346046000
H	-2.927898000	-4.491507000	-1.676815000
H	-1.299514000	-4.192337000	-1.037197000
C	-1.914029000	-2.759207000	-2.485940000
C	-2.035780000	-3.118631000	-3.827302000
H	-2.418469000	-4.098600000	-4.095352000
C	-1.663596000	-2.201022000	-4.811543000
H	-1.756134000	-2.459750000	-5.862067000
C	-1.183001000	-0.948066000	-4.429160000
H	-0.890908000	-0.206864000	-5.165275000
C	-1.095255000	-0.655992000	-3.070755000
H	-0.735301000	0.298337000	-2.699485000
C	-4.189435000	-2.619830000	-0.386465000
H	-4.824180000	-3.464620000	-0.087055000
H	-4.330289000	-2.474262000	-1.462906000
C	-4.633423000	-1.347493000	0.302883000
C	-5.808783000	-1.284458000	1.043403000
H	-6.415360000	-2.170154000	1.201777000
C	-6.177904000	-0.048119000	1.584650000
H	-7.068711000	0.038972000	2.199435000



C	-5.386130000	1.066434000	1.347198000
H	-5.627731000	2.025150000	1.785433000
C	-4.240473000	0.922856000	0.545684000
N	-1.708359000	-1.468493000	1.912650000
N	-2.756212000	-2.961393000	-0.177329000
N	-1.453712000	-1.541742000	-2.128877000
N	-3.860797000	-0.271973000	0.066964000
N	-3.358403000	1.972807000	0.256625000
H	-2.380291000	1.678539000	0.221462000
H	1.414030000	-1.201806000	-0.192629000
C	-3.479349000	3.288667000	-0.206945000
O	-2.422365000	3.898037000	-0.330775000
C	-4.815645000	3.965207000	-0.600348000
C	-4.464326000	5.065106000	-1.629849000
H	-5.379146000	5.593561000	-1.916700000
H	-3.759321000	5.788570000	-1.216705000
H	-4.021805000	4.636433000	-2.535575000
C	-5.416436000	4.663762000	0.644881000
H	-6.300514000	5.237026000	0.345987000
H	-5.730100000	3.964381000	1.425216000
H	-4.694831000	5.359867000	1.084611000
C	-5.835575000	3.013990000	-1.261229000
H	-6.289599000	2.302833000	-0.569687000
H	-6.649416000	3.610880000	-1.685778000
H	-5.379961000	2.450298000	-2.084031000
C	1.598593000	-3.210261000	-0.181319000
O	0.420089000	-3.298538000	0.176994000
C	2.538162000	-4.432158000	-0.019699000
C	2.103283000	-5.134145000	1.292744000
H	1.055909000	-5.438820000	1.256567000
H	2.720395000	-6.025292000	1.443706000
H	2.239206000	-4.477089000	2.158813000
C	4.032502000	-4.078443000	0.117617000
H	4.578944000	-4.974098000	0.430136000
H	4.490236000	-3.734001000	-0.810773000
H	4.191324000	-3.312711000	0.885501000
C	2.301677000	-5.420092000	-1.187882000
H	2.606683000	-5.019006000	-2.159928000
H	2.882913000	-6.331927000	-1.015863000

H	1.245471000	-5.702012000	-1.252477000
<b>35d</b>			
Cu	0.686663000	-2.181443000	0.040066000
C	0.880698000	-1.449666000	-2.992399000
H	0.432149000	-0.522961000	-2.654325000
C	1.150781000	-1.698942000	-4.336513000
H	0.900822000	-0.957625000	-5.087773000
C	1.735107000	-2.914747000	-4.689193000
H	1.953566000	-3.143113000	-5.727989000
C	2.030265000	-3.842698000	-3.688819000
H	2.480332000	-4.800886000	-3.929122000
C	1.726989000	-3.518535000	-2.368988000
C	2.012758000	-4.437994000	-1.202246000
H	2.070435000	-5.486485000	-1.525478000
H	2.979758000	-4.175620000	-0.758525000
C	-0.319896000	-4.837591000	-0.583978000
H	-0.288113000	-5.935686000	-0.548445000
H	-0.483445000	-4.546786000	-1.627375000
C	-1.469857000	-4.313568000	0.244639000
C	-2.605106000	-5.092416000	0.432365000
H	-2.650408000	-6.103050000	0.040741000
C	-3.690254000	-4.523412000	1.101456000
H	-4.613402000	-5.080587000	1.229597000
C	-3.585095000	-3.229519000	1.585103000
H	-4.427005000	-2.746246000	2.061237000
C	-2.375648000	-2.529921000	1.425661000
C	1.407101000	-4.780051000	1.159387000
H	1.834191000	-5.787840000	1.062581000
H	0.512802000	-4.868572000	1.785719000
C	2.391118000	-3.851327000	1.838669000
C	3.312881000	-4.346264000	2.750108000
H	3.386131000	-5.411589000	2.940952000
C	4.111144000	-3.426601000	3.436774000
H	4.810927000	-3.764997000	4.194942000
C	3.999405000	-2.075668000	3.156234000
H	4.582916000	-1.352385000	3.704758000
C	3.103915000	-1.647340000	2.157202000
N	1.161437000	-2.342895000	-2.036594000
N	0.974482000	-4.261918000	-0.156654000

N	-1.340620000	-3.061452000	0.734060000
N	2.279952000	-2.536467000	1.545616000
N	2.916313000	-0.330166000	1.786682000
O	0.614592000	-0.257532000	0.073300000
O	-0.754874000	0.151149000	-0.054415000
Cu	-1.120502000	2.006665000	0.257680000
C	1.549951000	3.122209000	-1.617927000
C	2.346432000	4.228322000	-1.977710000
H	3.397228000	4.093133000	-2.178756000
C	1.779711000	5.488601000	-2.031316000
H	2.384978000	6.344696000	-2.313685000
C	0.435246000	5.652399000	-1.682906000
H	-0.039512000	6.627493000	-1.705525000
C	-0.264439000	4.531546000	-1.257446000
C	-1.696262000	4.649961000	-0.779414000
H	-1.985111000	5.704973000	-0.682493000
H	-2.372790000	4.183037000	-1.500723000
C	-1.121003000	4.620096000	1.608261000
H	-1.750971000	5.377324000	2.093134000
H	-0.274450000	5.150220000	1.158729000
C	-0.580882000	3.632548000	2.616393000
C	-0.270059000	4.006111000	3.922893000
H	-0.473658000	5.016484000	4.263964000
C	0.308121000	3.064337000	4.772433000
H	0.563703000	3.332076000	5.793198000
C	0.545730000	1.776773000	4.292804000
H	0.993766000	1.014846000	4.921494000
C	0.191653000	1.477053000	2.981652000
H	0.335022000	0.490578000	2.560065000
C	-3.283064000	3.721079000	0.879086000
H	-3.834545000	4.671714000	0.891748000
H	-3.297574000	3.305802000	1.893459000
C	-3.951231000	2.729750000	-0.047931000
C	-5.324856000	2.754050000	-0.246578000
H	-5.936075000	3.525764000	0.208882000
C	-5.892608000	1.732814000	-1.012799000
H	-6.968453000	1.683370000	-1.151424000
C	-5.077225000	0.769545000	-1.585047000
H	-5.501911000	-0.053801000	-2.141122000

C	-3.683669000	0.856928000	-1.414730000
N	0.269594000	3.289570000	-1.218401000
N	-1.862966000	3.941970000	0.516251000
N	-0.354126000	2.386271000	2.162584000
N	-3.143604000	1.811518000	-0.619419000
N	-2.779090000	-0.042840000	-1.955604000
H	-1.932118000	-0.157192000	-1.378116000
H	2.026372000	-0.166948000	1.304046000
N	2.029720000	1.818406000	-1.593410000
H	1.559735000	1.199090000	-0.920894000
N	-2.188969000	-1.226550000	1.868639000
H	-1.650059000	-0.651290000	1.189314000
C	3.652669000	0.878080000	1.793712000
O	2.981553000	1.882474000	1.599799000
C	3.229868000	1.214909000	-2.029454000
O	3.622186000	0.265651000	-1.361844000
C	-2.857723000	-1.046329000	-2.938662000
O	-2.147093000	-2.028968000	-2.758622000
C	-2.888726000	-0.428813000	2.781012000
O	-2.972858000	0.768488000	2.511720000
C	3.958104000	1.568641000	-3.358571000
C	3.063284000	2.244998000	-4.416657000
C	5.233017000	2.399458000	-3.065641000
C	4.442296000	0.218561000	-3.947396000
H	2.148202000	1.666309000	-4.587906000
H	2.771950000	3.266480000	-4.167486000
H	3.607184000	2.289444000	-5.366073000
H	5.871022000	1.879344000	-2.344450000
H	5.802702000	2.521207000	-3.993132000
H	5.036439000	3.402577000	-2.676794000
H	5.003359000	0.410225000	-4.867834000
H	5.088248000	-0.309444000	-3.244299000
H	3.599732000	-0.434900000	-4.192002000
C	5.188947000	0.979714000	1.947916000
C	5.548264000	1.183825000	3.441479000
C	5.953190000	-0.201228000	1.313816000
C	5.615210000	2.265736000	1.200069000
H	5.034111000	2.063739000	3.842219000
H	5.299584000	0.332837000	4.082378000

H	6.626531000	1.351975000	3.532733000
H	5.638110000	-0.347221000	0.275553000
H	7.023890000	0.029545000	1.313748000
H	5.832714000	-1.146937000	1.844718000
H	6.696142000	2.402468000	1.308644000
H	5.384613000	2.189211000	0.133500000
H	5.107664000	3.146899000	1.596561000
C	-3.395135000	-0.939358000	4.155841000
C	-4.942917000	-0.949483000	4.155411000
C	-2.827560000	-2.301819000	4.598754000
C	-2.932550000	0.119402000	5.190421000
H	-5.335309000	0.025276000	3.849859000
H	-5.367827000	-1.710956000	3.492585000
H	-5.306487000	-1.162788000	5.166166000
H	-1.733603000	-2.319643000	4.531408000
H	-3.094965000	-2.472313000	5.646825000
H	-3.218728000	-3.146600000	4.029074000
H	-3.311547000	-0.153226000	6.180553000
H	-1.839433000	0.165937000	5.248184000
H	-3.303986000	1.112501000	4.931712000
C	-3.643626000	-0.890246000	-4.266999000
C	-4.900447000	-1.793541000	-4.225366000
C	-4.000481000	0.561638000	-4.641552000
C	-2.709338000	-1.441873000	-5.374085000
H	-4.625357000	-2.824565000	-3.982216000
H	-5.648805000	-1.462496000	-3.497656000
H	-5.382409000	-1.791115000	-5.208613000
H	-3.116226000	1.208601000	-4.610652000
H	-4.383623000	0.578470000	-5.667224000
H	-4.769575000	1.006154000	-4.007782000
H	-3.233052000	-1.416174000	-6.335003000
H	-1.805167000	-0.829328000	-5.467971000
H	-2.408071000	-2.468904000	-5.161872000

**<sup>15</sup>d<sub>CSS</sub>**

Cu	-0.399770000	-2.324896000	-0.123665000
C	0.990565000	-1.438906000	-2.759538000
H	0.894136000	-0.451249000	-2.318612000
C	1.486056000	-1.624502000	-4.048563000

H	1.783323000	-0.768912000	-4.645455000
C	1.577305000	-2.922494000	-4.547992000
H	1.950745000	-3.106729000	-5.550837000
C	1.171820000	-3.986376000	-3.741574000
H	1.223780000	-5.009866000	-4.099832000
C	0.689083000	-3.717111000	-2.462528000
C	0.270992000	-4.816788000	-1.509424000
H	-0.006668000	-5.726473000	-2.060913000
H	1.123623000	-5.073373000	-0.871039000
C	-2.123324000	-4.331302000	-1.331428000
H	-2.525173000	-5.344973000	-1.478156000
H	-1.948277000	-3.899194000	-2.323748000
C	-3.135117000	-3.463707000	-0.613453000
C	-4.496495000	-3.711441000	-0.746718000
H	-4.847926000	-4.569486000	-1.309844000
C	-5.389907000	-2.806759000	-0.169537000
H	-6.461051000	-2.939270000	-0.288811000
C	-4.901107000	-1.723882000	0.545309000
H	-5.572537000	-0.984550000	0.958722000
C	-3.512212000	-1.585216000	0.706663000
C	-0.876307000	-5.103134000	0.647164000
H	-0.864254000	-6.190270000	0.480844000
H	-1.830472000	-4.863496000	1.128622000
C	0.259018000	-4.705118000	1.571498000
C	0.773138000	-5.609052000	2.492166000
H	0.401768000	-6.627371000	2.536006000
C	1.760567000	-5.156241000	3.371175000
H	2.158702000	-5.815634000	4.136529000
C	2.233386000	-3.857643000	3.268709000
H	2.977299000	-3.492252000	3.959134000
C	1.721491000	-3.017139000	2.262920000
N	0.600227000	-2.457939000	-1.988910000
N	-0.826467000	-4.365429000	-0.630413000
N	-2.646875000	-2.432073000	0.105741000
N	0.709305000	-3.436730000	1.464566000
N	2.112587000	-1.706057000	2.038546000
O	-0.135075000	-0.486330000	0.533417000
O	0.206199000	0.495673000	-0.335651000
Cu	0.020781000	2.353494000	0.264567000

C	3.000877000	2.736491000	-1.150509000
C	4.102890000	3.558724000	-1.453219000
H	5.072527000	3.127162000	-1.635971000
C	3.940451000	4.933262000	-1.479396000
H	4.786742000	5.572060000	-1.713114000
C	2.696570000	5.488754000	-1.170491000
H	2.541867000	6.562247000	-1.167684000
C	1.666344000	4.624550000	-0.826083000
C	0.306064000	5.160900000	-0.431873000
H	0.365400000	6.240014000	-0.230290000
H	-0.397493000	5.019307000	-1.258864000
C	0.538067000	4.692341000	1.970272000
H	0.206101000	5.623322000	2.451521000
H	1.587955000	4.832621000	1.689896000
C	0.443737000	3.526313000	2.929732000
C	0.555129000	3.692169000	4.308908000
H	0.667141000	4.686533000	4.730101000
C	0.521365000	2.564519000	5.129206000
H	0.609732000	2.668182000	6.206496000
C	0.363408000	1.309474000	4.544596000
H	0.327750000	0.406898000	5.145230000
C	0.246148000	1.230772000	3.159227000
H	0.107365000	0.283817000	2.649737000
C	-1.674915000	4.618414000	0.931539000
H	-1.928243000	5.687358000	0.991506000
H	-1.938104000	4.159810000	1.891770000
C	-2.496084000	3.942463000	-0.144186000
C	-3.763233000	4.416826000	-0.463024000
H	-4.145050000	5.321274000	-0.001581000
C	-4.537983000	3.673627000	-1.355360000
H	-5.550931000	3.983234000	-1.594663000
C	-4.013182000	2.522691000	-1.923284000
H	-4.612892000	1.904109000	-2.575785000
C	-2.691588000	2.155103000	-1.618868000
N	1.804604000	3.278859000	-0.816475000
N	-0.226176000	4.426295000	0.734164000
N	0.291085000	2.309425000	2.372163000
N	-1.960673000	2.844746000	-0.715894000
N	-2.063666000	1.028932000	-2.135704000

H	-1.349595000	0.652878000	-1.505018000
H	1.421236000	-1.180365000	1.497674000
N	3.032047000	1.347422000	-1.106878000
H	2.262366000	0.954640000	-0.561267000
N	-2.914295000	-0.542545000	1.403785000
H	-1.985640000	-0.308829000	1.040469000
C	3.224509000	-0.868542000	2.280331000
O	3.012736000	0.323180000	2.095697000
C	3.900412000	0.295571000	-1.469557000
O	3.645966000	-0.780614000	-0.941130000
C	-2.389555000	0.113468000	-3.153428000
O	-2.101868000	-1.058840000	-2.938451000
C	-3.377641000	0.441786000	2.295240000
O	-2.827957000	1.535610000	2.223775000
C	5.025839000	0.393646000	-2.530507000
C	4.640450000	1.274979000	-3.739048000
C	6.353436000	0.841146000	-1.864815000
C	5.262880000	-1.039410000	-3.063946000
H	3.726097000	0.899863000	-4.213313000
H	4.482485000	2.327868000	-3.504207000
H	5.439665000	1.225517000	-4.485859000
H	6.658690000	0.115141000	-1.104555000
H	7.140910000	0.880542000	-2.624965000
H	6.315853000	1.819463000	-1.379748000
H	6.069895000	-1.016300000	-3.803754000
H	5.543613000	-1.723643000	-2.261578000
H	4.366252000	-1.439026000	-3.547153000
C	4.634934000	-1.365140000	2.669892000
C	4.753327000	-1.458148000	4.212334000
C	5.024592000	-2.680261000	1.962061000
C	5.629211000	-0.274998000	2.206715000
H	4.547041000	-0.484681000	4.669666000
H	4.081499000	-2.187461000	4.673030000
H	5.776023000	-1.745462000	4.478360000
H	4.902618000	-2.578301000	0.878368000
H	6.079460000	-2.894503000	2.164524000
H	4.453155000	-3.550437000	2.289277000
H	6.644867000	-0.572960000	2.487261000
H	5.592243000	-0.153719000	1.120651000



H	5.407846000	0.690641000	2.665253000
C	-4.391179000	0.154713000	3.431979000
C	-5.744955000	0.824418000	3.092706000
C	-4.569564000	-1.336840000	3.775124000
C	-3.818248000	0.862498000	4.687161000
H	-5.603246000	1.884897000	2.861924000
H	-6.257306000	0.357802000	2.244776000
H	-6.414933000	0.749611000	3.955700000
H	-3.603860000	-1.819087000	3.965158000
H	-5.164534000	-1.420741000	4.690459000
H	-5.089207000	-1.907625000	3.003565000
H	-4.509178000	0.726569000	5.525271000
H	-2.849578000	0.437913000	4.974140000
H	-3.682665000	1.930876000	4.510827000
C	-2.911493000	0.541918000	-4.548716000
C	-4.389919000	0.109892000	-4.699801000
C	-2.721622000	2.034939000	-4.879795000
C	-2.077463000	-0.275268000	-5.570031000
H	-4.506099000	-0.953568000	-4.468746000
H	-5.072829000	0.674496000	-4.056184000
H	-4.712385000	0.272193000	-5.733581000
H	-1.682851000	2.347513000	-4.723800000
H	-2.958169000	2.195551000	-5.936665000
H	-3.367026000	2.700589000	-4.303989000
H	-2.423851000	-0.046893000	-6.583009000
H	-1.014058000	-0.016831000	-5.510580000
H	-2.178697000	-1.347793000	-5.395161000

**15d<sub>oss</sub>**

Cu	0.666935000	-2.155694000	0.045328000
C	0.839437000	-1.407785000	-2.977433000
H	0.413176000	-0.473221000	-2.632028000
C	1.095921000	-1.653403000	-4.324544000
H	0.860391000	-0.900386000	-5.068835000
C	1.648949000	-2.880586000	-4.689192000
H	1.855679000	-3.107050000	-5.730803000
C	1.927251000	-3.821659000	-3.696844000
H	2.351528000	-4.789218000	-3.946242000
C	1.641424000	-3.499756000	-2.372221000
C	1.914085000	-4.436313000	-1.215871000

H	1.943315000	-5.482510000	-1.550465000
H	2.892090000	-4.202037000	-0.780086000
C	-0.421547000	-4.783305000	-0.575065000
H	-0.413510000	-5.882356000	-0.561520000
H	-0.596898000	-4.466405000	-1.608842000
C	-1.546612000	-4.251092000	0.282482000
C	-2.685729000	-5.018797000	0.492476000
H	-2.750536000	-6.027691000	0.099096000
C	-3.749971000	-4.440229000	1.186648000
H	-4.675584000	-4.988439000	1.334437000
C	-3.621774000	-3.148058000	1.669281000
H	-4.448582000	-2.657241000	2.163778000
C	-2.408487000	-2.460886000	1.484442000
C	1.327182000	-4.785479000	1.147044000
H	1.738715000	-5.798159000	1.034634000
H	0.436686000	-4.869501000	1.779285000
C	2.328885000	-3.881380000	1.834084000
C	3.241104000	-4.404616000	2.739765000
H	3.294938000	-5.473661000	2.915911000
C	4.053899000	-3.509407000	3.440876000
H	4.746485000	-3.870826000	4.195008000
C	3.963749000	-2.152465000	3.181242000
H	4.556150000	-1.446811000	3.743109000
C	3.077236000	-1.695177000	2.187774000
N	1.106720000	-2.312896000	-2.028378000
N	0.892095000	-4.244197000	-0.158152000
N	-1.393095000	-3.002617000	0.772670000
N	2.241913000	-2.561039000	1.558568000
N	2.907164000	-0.367869000	1.841373000
O	0.611052000	-0.241259000	0.128800000
O	-0.744252000	0.178807000	-0.021994000
Cu	-1.085239000	2.046943000	0.184196000
C	1.604530000	3.066131000	-1.691925000
C	2.408924000	4.149522000	-2.099284000
H	3.459092000	3.999034000	-2.291151000
C	1.851023000	5.409912000	-2.211925000
H	2.463185000	6.247952000	-2.531156000
C	0.507417000	5.599144000	-1.874161000
H	0.040476000	6.575977000	-1.940359000

C	-0.201771000	4.504145000	-1.400406000
C	-1.631875000	4.657409000	-0.925770000
H	-1.906967000	5.718896000	-0.866999000
H	-2.315813000	4.173429000	-1.628971000
C	-1.047189000	4.699299000	1.460203000
H	-1.659359000	5.490135000	1.913437000
H	-0.186955000	5.190692000	0.993136000
C	-0.535315000	3.736864000	2.506927000
C	-0.231726000	4.149366000	3.803086000
H	-0.420177000	5.174380000	4.107232000
C	0.319453000	3.226569000	4.690767000
H	0.568975000	3.524197000	5.704731000
C	0.537861000	1.919604000	4.257582000
H	0.965056000	1.171396000	4.916506000
C	0.192257000	1.581883000	2.953086000
H	0.321894000	0.578889000	2.567741000
C	-3.222687000	3.805354000	0.770518000
H	-3.765540000	4.760784000	0.748552000
H	-3.236481000	3.431206000	1.800975000
C	-3.905883000	2.784190000	-0.111803000
C	-5.281112000	2.811602000	-0.298455000
H	-5.881410000	3.605934000	0.131909000
C	-5.864835000	1.765118000	-1.016633000
H	-6.942439000	1.718662000	-1.141869000
C	-5.062711000	0.772856000	-1.557345000
H	-5.499337000	-0.069539000	-2.074146000
C	-3.667165000	0.855952000	-1.405490000
N	0.323090000	3.260457000	-1.305883000
N	-1.802627000	3.997068000	0.393322000
N	-0.327484000	2.471936000	2.096960000
N	-3.111027000	1.837156000	-0.654404000
N	-2.776090000	-0.072335000	-1.921374000
H	-1.928210000	-0.176969000	-1.344733000
H	2.016843000	-0.186068000	1.368026000
N	2.074112000	1.761187000	-1.603346000
H	1.590469000	1.176081000	-0.910288000
N	-2.200372000	-1.158394000	1.922208000
H	-1.657136000	-0.594199000	1.239820000
C	3.668576000	0.823994000	1.833618000

O	3.018563000	1.839670000	1.625889000
C	3.267754000	1.118852000	-2.002091000
O	3.624689000	0.181084000	-1.299520000
C	-2.878708000	-1.112295000	-2.864191000
O	-2.179340000	-2.097023000	-2.654306000
C	-2.891938000	-0.342306000	2.826536000
O	-2.972637000	0.850531000	2.539098000
C	4.033325000	1.418789000	-3.323268000
C	3.171148000	2.058541000	-4.430283000
C	5.304622000	2.253648000	-3.024780000
C	4.526335000	0.046372000	-3.849972000
H	2.262288000	1.472628000	-4.609549000
H	2.871418000	3.087403000	-4.226216000
H	3.743657000	2.070552000	-5.363720000
H	5.923871000	1.751182000	-2.275289000
H	5.895430000	2.347675000	-3.942193000
H	5.104830000	3.267455000	-2.666711000
H	5.115754000	0.203106000	-4.759233000
H	5.148044000	-0.460518000	-3.110554000
H	3.687156000	-0.610410000	-4.097424000
C	5.205107000	0.897357000	1.998521000
C	5.556644000	1.084206000	3.496169000
C	5.952192000	-0.293731000	1.362500000
C	5.660670000	2.179919000	1.262655000
H	5.059866000	1.973534000	3.898089000
H	5.281897000	0.235706000	4.129486000
H	6.637731000	1.226619000	3.597458000
H	5.637400000	-0.431903000	0.323095000
H	7.026413000	-0.079983000	1.365965000
H	5.815166000	-1.238975000	1.889999000
H	6.742995000	2.296350000	1.381000000
H	5.437414000	2.115271000	0.193625000
H	5.165966000	3.067793000	1.660395000
C	-3.388498000	-0.830216000	4.212915000
C	-4.936162000	-0.826299000	4.229628000
C	-2.827748000	-2.191583000	4.667272000
C	-2.904989000	0.238359000	5.227727000
H	-5.323022000	0.147502000	3.914135000
H	-5.375239000	-1.593402000	3.582587000

H	-5.290529000	-1.021610000	5.247288000
H	-1.734575000	-2.218348000	4.591423000
H	-3.088241000	-2.348063000	5.719281000
H	-3.229324000	-3.039946000	4.110235000
H	-3.273454000	-0.018407000	6.226050000
H	-1.810871000	0.277078000	5.271166000
H	-3.271924000	1.230827000	4.960255000
C	-3.676793000	-0.995561000	-4.189476000
C	-4.942770000	-1.882754000	-4.102795000
C	-4.021664000	0.445648000	-4.613222000
C	-2.760561000	-1.598612000	-5.284836000
H	-4.676297000	-2.906922000	-3.823815000
H	-5.680967000	-1.516781000	-3.381623000
H	-5.433670000	-1.911777000	-5.081205000
H	-3.131138000	1.084742000	-4.610349000
H	-4.410955000	0.430163000	-5.636585000
H	-4.782675000	0.919666000	-3.991095000
H	-3.293776000	-1.600328000	-6.240819000
H	-1.849126000	-1.002776000	-5.409215000
H	-2.470750000	-2.621446000	-5.038906000

${}_3TS_{1d}^{1a}$

Cu	2.701616000	0.018595000	-0.034958000
C	1.965921000	-2.108177000	-2.225610000
H	0.957636000	-1.931861000	-1.862948000
C	2.237896000	-3.059998000	-3.204990000
H	1.431980000	-3.647894000	-3.631185000
C	3.560257000	-3.240675000	-3.609219000
H	3.813927000	-3.979136000	-4.363680000
C	4.558260000	-2.461504000	-3.022924000
H	5.598175000	-2.580379000	-3.311423000
C	4.204672000	-1.519037000	-2.057893000
C	5.234436000	-0.588568000	-1.440763000
H	6.239457000	-1.029432000	-1.508770000
H	5.254913000	0.340014000	-2.023805000
C	5.177772000	-1.308368000	0.912479000
H	6.234539000	-1.309318000	1.216109000
H	4.993318000	-2.261771000	0.402905000
C	4.275576000	-1.236855000	2.132868000

C	4.705815000	-1.669127000	3.387381000
H	5.724970000	-2.018128000	3.522792000
C	3.809856000	-1.647846000	4.456721000
H	4.123863000	-1.980444000	5.441408000
C	2.511080000	-1.186638000	4.241731000
H	1.784580000	-1.149193000	5.046404000
C	2.161885000	-0.760568000	2.963260000
H	1.167617000	-0.382850000	2.744138000
C	5.442434000	1.075703000	0.359780000
H	6.504290000	1.169313000	0.090321000
H	5.386737000	1.124417000	1.453967000
C	4.645390000	2.236271000	-0.210990000
C	5.243838000	3.457983000	-0.517960000
H	6.316193000	3.583311000	-0.403219000
C	4.445655000	4.510166000	-0.968642000
H	4.891004000	5.469864000	-1.212545000
C	3.072456000	4.307420000	-1.106200000
H	2.417078000	5.097556000	-1.456632000
C	2.552113000	3.055057000	-0.791150000
N	2.924064000	-1.351883000	-1.665105000
N	4.888032000	-0.229151000	-0.052257000
N	3.020475000	-0.785464000	1.930596000
N	3.317904000	2.042428000	-0.353126000
O	0.725426000	0.451679000	0.093965000
O	-0.104458000	-0.413702000	-0.344442000
Cu	-2.753629000	0.001749000	-0.029332000
C	-2.488765000	0.385718000	-3.102337000
H	-1.425932000	0.395195000	-2.878494000
C	-2.956226000	0.624262000	-4.391606000
H	-2.257434000	0.822994000	-5.197368000
C	-4.333264000	0.609351000	-4.611118000
H	-4.740588000	0.799110000	-5.599535000
C	-5.182349000	0.351554000	-3.535370000
H	-6.259651000	0.335331000	-3.670541000
C	-4.636469000	0.108275000	-2.274016000
C	-5.528924000	-0.262299000	-1.095421000
H	-6.557169000	0.082162000	-1.286141000
H	-5.572076000	-1.357059000	-1.038554000
C	-5.194573000	1.656128000	0.416950000

H	-6.170119000	1.884234000	0.873921000
H	-5.186512000	2.149084000	-0.563256000
C	-4.080323000	2.272179000	1.254661000
C	-4.339232000	3.346768000	2.107138000
H	-5.355543000	3.710727000	2.224288000
C	-3.284556000	3.944140000	2.796390000
H	-3.467879000	4.781502000	3.462838000
C	-1.995645000	3.443158000	2.616325000
H	-1.144680000	3.875474000	3.132353000
C	-1.818331000	2.360289000	1.759525000
H	-0.834884000	1.931850000	1.587970000
C	-5.326921000	-0.628805000	1.335524000
H	-6.394861000	-0.894187000	1.377569000
H	-5.113975000	-0.047788000	2.241648000
C	-4.481937000	-1.896178000	1.382675000
C	-5.000206000	-3.082840000	1.903570000
H	-6.035089000	-3.123315000	2.229873000
C	-4.178241000	-4.205221000	2.000305000
H	-4.564743000	-5.136427000	2.403275000
C	-2.857398000	-4.110039000	1.563476000
H	-2.182611000	-4.958062000	1.614405000
C	-2.417151000	-2.895697000	1.044406000
N	-3.302400000	0.132914000	-2.062643000
N	-5.006129000	0.221660000	0.185747000
N	-2.831899000	1.781638000	1.092177000
N	-3.203808000	-1.809180000	0.953394000
H	-1.400270000	-2.775406000	0.682099000
H	1.491878000	2.840063000	-0.887176000

${}_3T_{2d}^{2a}$

Cu	2.832922000	0.124483000	0.143866000
C	3.160191000	0.364604000	3.254307000
H	2.078297000	0.455023000	3.228468000
C	3.874399000	0.477721000	4.443672000
H	3.353192000	0.658871000	5.377509000
C	5.264097000	0.362429000	4.398169000
H	5.856752000	0.453180000	5.303336000
C	5.886068000	0.135486000	3.169893000
H	6.965852000	0.045656000	3.101291000
C	5.100032000	0.021433000	2.023712000

C	5.697226000	-0.301738000	0.666509000
H	6.747660000	0.017515000	0.618308000
H	5.687745000	-1.389674000	0.531898000
C	5.168019000	1.728207000	-0.617993000
H	6.092251000	1.895650000	-1.189060000
H	5.322582000	2.164435000	0.376301000
C	3.996999000	2.430063000	-1.279219000
C	4.176604000	3.550216000	-2.089148000
H	5.177601000	3.912107000	-2.302980000
C	3.055141000	4.194126000	-2.613606000
H	3.171842000	5.069176000	-3.245768000
C	1.788723000	3.691591000	-2.317869000
H	0.889386000	4.157532000	-2.705890000
C	1.690733000	2.559408000	-1.512728000
H	0.729212000	2.125819000	-1.258327000
C	5.012207000	-0.478176000	-1.694586000
H	6.062392000	-0.657788000	-1.963460000
H	4.577197000	0.142176000	-2.486965000
C	4.252886000	-1.787586000	-1.621825000
C	4.729996000	-2.922694000	-2.252835000
H	5.681753000	-2.906796000	-2.772487000
C	3.948223000	-4.089135000	-2.203354000
H	4.290680000	-4.998237000	-2.688294000
C	2.746045000	-4.075540000	-1.528025000
H	2.121823000	-4.961584000	-1.470225000
C	2.328290000	-2.881975000	-0.891736000
N	3.757067000	0.139530000	2.072501000
N	4.902282000	0.286838000	-0.432924000
N	2.769133000	1.941978000	-1.001659000
N	3.075627000	-1.757434000	-0.943867000
N	1.129978000	-2.828999000	-0.237763000
O	0.979381000	0.005737000	0.907171000
O	0.031714000	0.416297000	0.137568000
Cu	-2.887893000	-0.005066000	0.108369000
C	-2.326841000	-1.137593000	2.948745000
H	-1.290866000	-0.932937000	2.692646000
C	-2.663101000	-1.760933000	4.146662000
H	-1.887800000	-2.051783000	4.847733000
C	-4.010583000	-2.004091000	4.412542000



H	-4.316053000	-2.495136000	5.331482000
C	-4.962061000	-1.609532000	3.473179000
H	-6.019255000	-1.786328000	3.646805000
C	-4.548084000	-0.976600000	2.299472000
C	-5.569598000	-0.455986000	1.293962000
H	-6.519013000	-0.999772000	1.418171000
H	-5.776920000	0.592804000	1.540251000
C	-5.088768000	-1.817272000	-0.707178000
H	-6.058559000	-2.059807000	-1.169473000
H	-4.928852000	-2.554289000	0.089969000
C	-3.975313000	-1.988608000	-1.734035000
C	-4.160956000	-2.784036000	-2.865467000
H	-5.126425000	-3.246125000	-3.048072000
C	-3.100276000	-2.974359000	-3.750929000
H	-3.228468000	-3.587191000	-4.638083000
C	-1.880015000	-2.357487000	-3.478609000
H	-1.028166000	-2.472299000	-4.140673000
C	-1.773877000	-1.570877000	-2.334510000
H	-0.845444000	-1.068716000	-2.082197000
C	-5.578389000	0.587168000	-0.945994000
H	-6.674498000	0.682022000	-0.906981000
H	-5.322601000	0.319986000	-1.978859000
C	-4.939151000	1.934063000	-0.637117000
C	-5.671384000	3.105330000	-0.760785000
H	-6.723337000	3.069527000	-1.022742000
C	-5.021355000	4.328849000	-0.544315000
H	-5.567073000	5.263028000	-0.636785000
C	-3.681514000	4.338798000	-0.205515000
H	-3.150717000	5.269524000	-0.031810000
C	-3.005418000	3.107261000	-0.077247000
N	-3.240733000	-0.751143000	2.041180000
N	-5.079369000	-0.491268000	-0.085525000
N	-2.793618000	-1.383757000	-1.478432000
N	-3.625976000	1.930893000	-0.293130000
N	-1.661923000	3.066836000	0.231655000
H	-1.309644000	2.175058000	0.561732000
H	-1.290813000	3.868332000	0.724877000
H	0.682363000	-3.699029000	0.010989000
H	0.938867000	-2.038795000	0.363200000

$3TS_{3d}^{3a}$

Cu	-2.747152000	0.048742000	0.085068000
C	-1.043358000	0.809713000	-2.418545000
H	-0.205625000	0.700717000	-1.740065000
C	-0.850576000	1.250608000	-3.724786000
H	0.147686000	1.494468000	-4.072460000
C	-1.962897000	1.377557000	-4.555389000
H	-1.857670000	1.724250000	-5.579017000
C	-3.220222000	1.058647000	-4.044223000
H	-4.109916000	1.151033000	-4.659736000
C	-3.332826000	0.616386000	-2.725334000
C	-4.679132000	0.194327000	-2.156276000
H	-5.491225000	0.664048000	-2.732894000
H	-4.782060000	-0.889259000	-2.294281000
C	-4.992408000	1.881903000	-0.390912000
H	-6.045688000	2.183552000	-0.497644000
H	-4.417907000	2.471409000	-1.116215000
C	-4.500078000	2.218896000	1.006744000
C	-5.189181000	3.121139000	1.800651000
H	-6.113544000	3.567414000	1.450459000
C	-4.662426000	3.440684000	3.062100000
H	-5.176226000	4.147155000	3.707119000
C	-3.491073000	2.844208000	3.482346000
H	-3.065943000	3.061008000	4.457278000
C	-2.850188000	1.919886000	2.625256000
C	-5.661909000	-0.457835000	0.004749000
H	-6.640912000	-0.574503000	-0.484218000
H	-5.851550000	-0.018699000	0.991570000
C	-5.023877000	-1.821965000	0.209802000
C	-5.795863000	-2.974596000	0.170229000
H	-6.853284000	-2.916892000	-0.064517000
C	-5.184318000	-4.203295000	0.450329000
H	-5.763448000	-5.121586000	0.433343000
C	-3.834980000	-4.237309000	0.752920000
H	-3.331728000	-5.172150000	0.979148000
C	-3.114096000	-3.027344000	0.762334000
N	-2.252365000	0.498121000	-1.920899000
N	-4.783428000	0.466069000	-0.721073000
N	-3.346164000	1.623207000	1.405575000

N	-3.695279000	-1.845182000	0.487270000
N	-1.748001000	-3.017433000	1.007500000
O	-0.060883000	-0.274260000	0.980684000
O	0.884131000	0.599263000	0.721942000
Cu	2.720511000	0.042774000	0.199485000
C	1.688562000	-2.280088000	-1.793146000
C	1.899562000	-3.222592000	-2.832219000
H	1.087338000	-3.878673000	-3.128206000
C	3.135031000	-3.294450000	-3.435812000
H	3.315051000	-4.017297000	-4.225787000
C	4.166809000	-2.437681000	-3.011608000
H	5.155340000	-2.486140000	-3.454776000
C	3.887816000	-1.526059000	-2.011435000
C	4.937237000	-0.546165000	-1.534238000
H	5.945626000	-0.914539000	-1.766530000
H	4.812309000	0.410200000	-2.054182000
C	5.193552000	-1.427743000	0.754116000
H	6.282851000	-1.447027000	0.895076000
H	4.922736000	-2.342857000	0.215581000
C	4.476464000	-1.418011000	2.089498000
C	5.043835000	-1.967940000	3.238693000
H	6.050127000	-2.374362000	3.209217000
C	4.298491000	-1.987187000	4.417774000
H	4.719463000	-2.409657000	5.325029000
C	3.010538000	-1.450517000	4.413920000
H	2.400062000	-1.443000000	5.310547000
C	2.520065000	-0.909627000	3.228888000
H	1.527226000	-0.475502000	3.172374000
C	5.456570000	0.975872000	0.331914000
H	6.506164000	0.987288000	0.007580000
H	5.454914000	0.996876000	1.428286000
C	4.724247000	2.190663000	-0.191674000
C	5.412465000	3.330619000	-0.563858000
H	6.495963000	3.357617000	-0.527784000
C	4.670108000	4.447917000	-0.981007000
H	5.175309000	5.363163000	-1.274060000
C	3.294181000	4.374009000	-1.015617000
H	2.692838000	5.220624000	-1.331303000
C	2.654692000	3.170316000	-0.633292000

N	2.671362000	-1.429547000	-1.408806000
N	4.788387000	-0.277229000	-0.084717000
N	3.234306000	-0.893112000	2.091737000
N	3.368643000	2.092616000	-0.230600000
N	1.294736000	3.055462000	-0.704024000
H	0.855282000	2.338607000	-0.136602000
H	0.767205000	3.911127000	-0.808323000
H	-1.403456000	-3.821676000	1.519064000
H	-1.398606000	-2.143636000	1.385838000
N	0.486594000	-2.193532000	-1.173020000
H	0.372529000	-1.634718000	-0.333953000
H	-0.198574000	-2.924573000	-1.295765000
N	-1.718424000	1.260203000	3.021620000
H	-1.161440000	0.802900000	2.306995000
H	-1.218095000	1.624140000	3.819481000

${}_3T_{4d}^{4a}$

Cu	2.976525000	0.858451000	0.165459000
C	3.534185000	0.439314000	3.216649000
H	2.454160000	0.337811000	3.271754000
C	4.313725000	0.445558000	4.370187000
H	3.847211000	0.345453000	5.344524000
C	5.693568000	0.594619000	4.236860000
H	6.337527000	0.614936000	5.110829000
C	6.234144000	0.726127000	2.958053000
H	7.303844000	0.849632000	2.817949000
C	5.387054000	0.697542000	1.849105000
C	5.951191000	0.763466000	0.434362000
H	6.961343000	1.200955000	0.458970000
H	6.065868000	-0.264086000	0.067911000
C	5.069074000	2.925503000	-0.356100000
H	5.842805000	3.396940000	-0.981978000
H	5.331272000	3.153374000	0.684488000
C	3.715421000	3.564201000	-0.643131000
C	3.638098000	4.873694000	-1.117099000
H	4.547948000	5.415301000	-1.358955000
C	2.388025000	5.476275000	-1.261807000
H	2.311178000	6.497591000	-1.622977000
C	1.247324000	4.746045000	-0.933886000
H	0.247906000	5.157752000	-1.011724000

C	1.403627000	3.435540000	-0.489152000
H	0.538739000	2.835984000	-0.232115000
C	5.101300000	0.988039000	-1.873032000
H	6.124228000	0.957451000	-2.281582000
H	4.541780000	1.708834000	-2.482858000
C	4.452352000	-0.378940000	-2.048368000
C	4.923078000	-1.258427000	-3.020130000
H	5.791628000	-0.998438000	-3.616064000
C	4.238788000	-2.456197000	-3.229898000
H	4.555070000	-3.142521000	-4.009518000
C	3.137070000	-2.758141000	-2.440286000
H	2.562275000	-3.659668000	-2.606583000
C	2.768563000	-1.860905000	-1.428395000
N	4.049599000	0.559854000	1.981244000
N	5.059049000	1.465972000	-0.491759000
N	2.606990000	2.850062000	-0.347393000
N	3.390777000	-0.676460000	-1.264195000
N	1.672062000	-2.074691000	-0.582835000
O	0.349521000	0.348146000	0.523840000
O	-0.759716000	0.494967000	-0.143449000
Cu	-2.011830000	-1.051918000	-0.074678000
C	-1.734936000	-0.421544000	2.936489000
H	-1.132784000	0.411331000	2.589596000
C	-2.040339000	-0.590257000	4.284174000
H	-1.677324000	0.122550000	5.016772000
C	-2.825908000	-1.680585000	4.658420000
H	-3.092115000	-1.840037000	5.698947000
C	-3.272079000	-2.563495000	3.674868000
H	-3.885108000	-3.421522000	3.932971000
C	-2.917773000	-2.332792000	2.346417000
C	-3.277516000	-3.303841000	1.237913000
H	-2.435228000	-3.993693000	1.126982000
H	-4.161765000	-3.894353000	1.512446000
C	-3.087070000	-3.457350000	-1.231862000
H	-3.890704000	-4.150058000	-1.515539000
H	-2.214734000	-4.049989000	-0.942076000
C	-2.693030000	-2.581809000	-2.407508000
C	-2.932973000	-2.944758000	-3.731541000
H	-3.463670000	-3.864907000	-3.955680000

C	-2.485646000	-2.108037000	-4.755830000
H	-2.665365000	-2.370729000	-5.793930000
C	-1.817915000	-0.928077000	-4.427600000
H	-1.462697000	-0.247620000	-5.193928000
C	-1.624010000	-0.626154000	-3.082202000
H	-1.123330000	0.283456000	-2.764809000
C	-4.829910000	-2.049197000	-0.235400000
H	-5.579779000	-2.748290000	0.157241000
H	-5.006441000	-1.962002000	-1.312878000
C	-5.031287000	-0.669239000	0.364207000
C	-6.185590000	-0.355353000	1.072489000
H	-6.934787000	-1.111524000	1.282588000
C	-6.346530000	0.963694000	1.510422000
H	-7.217182000	1.245241000	2.095070000
C	-5.379286000	1.911841000	1.212495000
H	-5.468962000	2.925009000	1.577257000
C	-4.259144000	1.521106000	0.456594000
N	-2.162893000	-1.273375000	1.991168000
N	-3.464591000	-2.621508000	-0.064190000
N	-2.048287000	-1.436057000	-2.099977000
N	-4.084988000	0.242392000	0.072534000
N	-3.200834000	2.367216000	0.115695000
H	-2.312575000	1.876551000	0.028139000
H	1.171015000	-1.221893000	-0.325279000
C	-2.994487000	3.723534000	-0.193447000
O	-1.818231000	4.062760000	-0.253459000
C	-4.120791000	4.728453000	-0.528024000
C	-3.499775000	5.786850000	-1.470663000
H	-4.258554000	6.536529000	-1.716952000
H	-2.651972000	6.290212000	-1.002599000
H	-3.153609000	5.333330000	-2.405475000
C	-4.556183000	5.458217000	0.767384000
H	-5.278612000	6.241372000	0.514425000
H	-5.031354000	4.802556000	1.503066000
H	-3.695819000	5.934143000	1.248953000
C	-5.320961000	4.094011000	-1.260683000
H	-5.912336000	3.416955000	-0.642358000
H	-5.992597000	4.891372000	-1.595119000
H	-4.994027000	3.545431000	-2.151628000

C	0.995451000	-3.206007000	-0.144954000
O	-0.206254000	-3.066093000	0.111906000
C	1.689260000	-4.554421000	0.171838000
C	1.123469000	-5.003387000	1.545132000
H	0.036652000	-5.101771000	1.516735000
H	1.554569000	-5.973691000	1.810174000
H	1.384339000	-4.290245000	2.335069000
C	3.223135000	-4.481628000	0.305395000
H	3.583078000	-5.422382000	0.734165000
H	3.738875000	-4.346908000	-0.646358000
H	3.527960000	-3.674247000	0.980582000
C	1.273124000	-5.603865000	-0.886165000
H	1.665223000	-5.380485000	-1.883981000
H	1.659868000	-6.586624000	-0.597355000
H	0.182869000	-5.677234000	-0.956433000

${}_3TS_{5d}^{5a}$

Cu	2.891342000	-0.204948000	0.703268000
C	1.750046000	-1.886763000	3.086855000
H	0.814020000	-1.394565000	2.848535000
C	1.838988000	-2.783091000	4.150800000
H	0.954511000	-3.001353000	4.738303000
C	3.070587000	-3.367932000	4.436621000
H	3.174734000	-4.068076000	5.260055000
C	4.179929000	-3.030197000	3.657701000
H	5.157030000	-3.457292000	3.862129000
C	4.014802000	-2.128124000	2.610582000
C	5.156512000	-1.729712000	1.695563000
H	6.122483000	-1.822397000	2.211696000
H	5.183217000	-2.406044000	0.834308000
C	5.206418000	0.662951000	2.214858000
H	6.284139000	0.824842000	2.361775000
H	4.810753000	0.273046000	3.159618000
C	4.523016000	1.979747000	1.905839000
C	5.037831000	3.158671000	2.431849000
H	5.952902000	3.144603000	3.014523000
C	4.330372000	4.343383000	2.222106000
H	4.670933000	5.275665000	2.662222000
C	3.177062000	4.314321000	1.454655000
H	2.584072000	5.206417000	1.306367000

C	2.761151000	3.101750000	0.880153000
C	5.687527000	-0.093008000	-0.073862000
H	6.748469000	-0.367153000	0.017394000
H	5.649874000	0.987331000	-0.254173000
C	5.065126000	-0.815424000	-1.254259000
C	5.841528000	-1.155035000	-2.354229000
H	6.906694000	-0.949919000	-2.362501000
C	5.204662000	-1.734924000	-3.454906000
H	5.765451000	-1.967484000	-4.355120000
C	3.849053000	-2.012822000	-3.394663000
H	3.333753000	-2.438575000	-4.243209000
C	3.142281000	-1.724708000	-2.212644000
N	2.816538000	-1.571664000	2.333392000
N	4.956186000	-0.355875000	1.179807000
N	3.403649000	1.937743000	1.145198000
N	3.739209000	-1.073595000	-1.183673000
N	1.799890000	-2.009806000	-2.034015000
O	0.942669000	-0.419713000	0.292719000
O	0.101842000	0.559780000	0.341721000
Cu	-2.380549000	0.653801000	-0.837853000
C	-3.594104000	-2.257907000	-0.831385000
C	-4.564904000	-3.218041000	-1.145606000
H	-4.316121000	-4.271205000	-1.100114000
C	-5.825669000	-2.790749000	-1.544566000
H	-6.594652000	-3.514819000	-1.796400000
C	-6.080111000	-1.421934000	-1.652005000
H	-7.050624000	-1.057440000	-1.973258000
C	-5.056607000	-0.524743000	-1.357214000
C	-5.285529000	0.980337000	-1.426477000
H	-6.172995000	1.192882000	-2.042682000
H	-5.509175000	1.338854000	-0.415161000
C	-3.834224000	1.534218000	-3.325338000
H	-4.341434000	2.304071000	-3.928569000
H	-4.257124000	0.570769000	-3.636003000
C	-2.350747000	1.516271000	-3.662022000
C	-1.919564000	1.885186000	-4.938350000
H	-2.639298000	2.248992000	-5.665626000
C	-0.570511000	1.772408000	-5.264000000
H	-0.217812000	2.046179000	-6.253863000



C	0.313419000	1.307733000	-4.290484000
H	1.374317000	1.202910000	-4.493738000
C	-0.191566000	0.981884000	-3.035835000
H	0.462285000	0.632442000	-2.247247000
C	-3.944592000	3.064906000	-1.411217000
H	-4.817780000	3.692660000	-1.652617000
H	-3.080596000	3.501194000	-1.927900000
C	-3.673512000	3.133503000	0.082614000
C	-4.110815000	4.229071000	0.822370000
H	-4.686230000	5.015627000	0.345494000
C	-3.767229000	4.302637000	2.171726000
H	-4.050155000	5.165279000	2.767425000
C	-3.052723000	3.261767000	2.749940000
H	-2.746490000	3.305590000	3.785297000
C	-2.719742000	2.151688000	1.962927000
N	-3.836430000	-0.939794000	-0.951674000
N	-4.092770000	1.690492000	-1.895457000
N	-1.493303000	1.074546000	-2.719115000
N	-2.982061000	2.116240000	0.639695000
N	-2.024269000	1.037759000	2.450177000
H	-1.377577000	0.641735000	1.770732000
H	1.343170000	-1.447437000	-1.318788000
N	-2.276322000	-2.596879000	-0.467495000
H	-1.566865000	-2.267438000	-1.126348000
N	1.636475000	3.010125000	0.068103000
H	1.047507000	2.192842000	0.251728000
C	0.824645000	-2.765922000	-2.724019000
O	-0.313065000	-2.313451000	-2.672581000
C	-1.727439000	-3.513442000	0.426749000
O	-0.539268000	-3.787407000	0.277778000
C	-1.953536000	0.310993000	3.643003000
O	-1.022542000	-0.488608000	3.716522000
C	0.923730000	3.961340000	-0.693274000
O	-0.282658000	3.783766000	-0.787288000
C	-2.517298000	-4.126586000	1.611433000
C	-3.790973000	-3.368078000	2.032513000
C	-2.851464000	-5.593237000	1.245993000
C	-1.548565000	-4.131694000	2.818328000
H	-3.603570000	-2.293202000	2.138542000

H	-4.627511000	-3.504265000	1.344922000
H	-4.118332000	-3.744202000	3.008084000
H	-1.942337000	-6.142574000	0.983261000
H	-3.317496000	-6.089889000	2.104066000
H	-3.550176000	-5.666728000	0.405106000
H	-2.009624000	-4.674867000	3.650572000
H	-0.605390000	-4.615186000	2.558034000
H	-1.339674000	-3.109195000	3.153052000
C	1.095145000	-4.140724000	-3.375054000
C	1.149371000	-3.984491000	-4.914881000
C	2.340933000	-4.862249000	-2.824717000
C	-0.141474000	-5.012675000	-3.032633000
H	0.253863000	-3.473994000	-5.283069000
H	2.025355000	-3.431468000	-5.270337000
H	1.187876000	-4.977230000	-5.375128000
H	2.300097000	-4.933831000	-1.732488000
H	2.361060000	-5.882308000	-3.221901000
H	3.286321000	-4.393476000	-3.105254000
H	-0.010693000	-6.004208000	-3.477880000
H	-0.250243000	-5.124590000	-1.949913000
H	-1.057593000	-4.569572000	-3.428411000
C	1.613226000	5.080861000	-1.517595000
C	1.291276000	6.452385000	-0.876696000
C	3.129421000	4.905702000	-1.728699000
C	0.934929000	5.043597000	-2.911660000
H	0.212628000	6.567276000	-0.733511000
H	1.781558000	6.600781000	0.091347000
H	1.635903000	7.253636000	-1.538872000
H	3.369000000	3.903182000	-2.102382000
H	3.466573000	5.625369000	-2.481897000
H	3.721052000	5.087118000	-0.829404000
H	1.342566000	5.847518000	-3.533042000
H	1.122385000	4.091597000	-3.420262000
H	-0.144776000	5.177271000	-2.826217000
C	-2.988988000	0.399808000	4.790851000
C	-2.486991000	1.411898000	5.851208000
C	-4.421936000	0.729084000	4.323960000
C	-3.020795000	-0.993979000	5.463171000
H	-1.482287000	1.143915000	6.193880000

H	-2.457297000	2.444441000	5.491494000
H	-3.157285000	1.388870000	6.716977000
H	-4.744792000	0.049048000	3.526822000
H	-5.107471000	0.593622000	5.166845000
H	-4.546780000	1.753293000	3.970141000
H	-3.715824000	-0.967688000	6.308554000
H	-3.362997000	-1.764970000	4.765479000
H	-2.034119000	-1.282371000	5.829453000

**AI**

C	-1.133646000	-0.309382000	0.000019000
C	-1.361808000	1.075129000	0.000066000
C	-0.304977000	1.982242000	0.000004000
C	1.008135000	1.514335000	-0.000054000
C	1.300668000	0.148584000	-0.000027000
C	0.205841000	-0.753052000	-0.000031000
H	-2.377797000	1.441639000	0.000117000
H	1.794149000	2.258066000	-0.000077000
O	0.393830000	-2.123927000	-0.000023000
C	-2.322450000	-1.300500000	0.000008000
C	-2.281499000	-2.186486000	-1.269891000
C	-2.281462000	-2.186603000	1.269822000
C	-3.683916000	-0.573615000	0.000060000
H	-2.355126000	-1.568648000	-2.172928000
H	-1.361701000	-2.769894000	-1.326584000
H	-3.131293000	-2.880757000	-1.268055000
H	-2.354995000	-1.568848000	2.172921000
H	-3.131285000	-2.880838000	1.267972000
H	-1.361692000	-2.770066000	1.326413000
H	-4.487164000	-1.318949000	0.000015000
H	-3.819626000	0.052825000	0.889330000
H	-3.819619000	0.052943000	-0.889126000
C	2.774526000	-0.332164000	0.000027000
C	3.085355000	-1.152881000	1.281958000
C	3.085570000	-1.152692000	-1.281994000
C	3.767723000	0.849090000	0.000168000
H	2.952301000	-0.525384000	2.169796000
H	2.447370000	-2.031399000	1.424926000
H	4.124479000	-1.502609000	1.264822000
H	2.952876000	-0.524996000	-2.169743000

H	4.124618000	-1.502630000	-1.264637000
H	2.447485000	-2.031082000	-1.425382000
H	4.792145000	0.460192000	0.000149000
H	3.652543000	1.479341000	-0.887692000
H	3.652505000	1.479140000	0.888168000
O	-0.445803000	3.348458000	-0.000027000
C	-1.755768000	3.883933000	-0.000015000
H	-2.319719000	3.583388000	0.894071000
H	-1.637325000	4.969597000	-0.000103000
H	-2.319806000	3.583257000	-0.894000000
H	1.338711000	-2.316170000	-0.000701000

### A2

C	-0.408104000	1.016795000	0.000237000
C	-0.929223000	-0.282265000	0.000141000
C	-0.050185000	-1.372241000	-0.000029000
C	1.325759000	-1.168421000	-0.000258000
C	1.847038000	0.131055000	-0.000083000
C	0.973943000	1.218268000	0.000158000
H	-1.062958000	1.880664000	0.000538000
H	-0.464564000	-2.375532000	-0.000187000
H	1.997387000	-2.025464000	-0.000683000
H	1.385004000	2.222943000	0.000372000
O	3.195014000	0.392576000	-0.000334000
H	3.675324000	-0.449378000	0.001965000
O	-2.264788000	-0.592212000	0.000740000
C	-3.194053000	0.476279000	-0.000571000
H	-4.183625000	0.014777000	-0.001603000
H	-3.090807000	1.106378000	0.893806000
H	-3.088622000	1.105889000	-0.895024000

### A3

C	-0.264007000	-1.199595000	-0.000018000
C	1.131786000	-1.219279000	-0.000031000
C	1.857370000	-0.027885000	0.000044000
C	1.171539000	1.190467000	0.000025000
C	-0.220784000	1.224212000	-0.000067000
C	-0.940944000	0.024414000	-0.000025000
H	-0.826644000	-2.131920000	-0.000037000
H	1.649839000	-2.174735000	-0.000035000

H	2.943167000	-0.046880000	0.000084000
H	1.725672000	2.125510000	0.000060000
H	-0.766192000	2.162767000	-0.000109000
O	-2.307115000	0.111885000	0.000040000
H	-2.678683000	-0.783828000	0.000144000

**A1'**

C	-1.160780000	-0.302409000	0.000142000
C	-1.366844000	1.066311000	0.000128000
C	-0.280887000	1.960588000	0.000094000
C	1.051830000	1.490362000	0.000085000
C	1.342064000	0.146720000	0.000069000
C	0.221503000	-0.815159000	0.000182000
H	-2.373660000	1.460452000	0.000145000
H	1.829326000	2.244958000	0.000095000
O	0.442428000	-2.053957000	0.000088000
C	-2.338088000	-1.291207000	0.000001000
C	-2.276227000	-2.181264000	-1.267669000
C	-2.276391000	-2.181931000	1.267176000
C	-3.701886000	-0.571433000	0.000172000
H	-2.344033000	-1.570598000	-2.176316000
H	-1.348818000	-2.753793000	-1.298971000
H	-3.122010000	-2.879850000	-1.269254000
H	-2.344352000	-1.571746000	2.176150000
H	-3.122216000	-2.880440000	1.268223000
H	-1.348977000	-2.754450000	1.298424000
H	-4.502490000	-1.319163000	0.000300000
H	-3.840421000	0.054476000	0.889945000
H	-3.840707000	0.054477000	-0.889568000
C	2.789545000	-0.369319000	-0.000024000
C	3.043496000	-1.224402000	1.267451000
C	3.043284000	-1.224529000	-1.267464000
C	3.810680000	0.785288000	-0.000169000
H	2.894350000	-0.627823000	2.175777000
H	2.376231000	-2.086487000	1.301883000
H	4.080363000	-1.582809000	1.268938000
H	2.893662000	-0.628125000	-2.175826000
H	4.080243000	-1.582659000	-1.269264000
H	2.376208000	-2.086776000	-1.301531000

H	4.824123000	0.369283000	-0.000285000
H	3.716078000	1.419933000	-0.889089000
H	3.716325000	1.419957000	0.888768000
O	-0.404978000	3.309013000	0.000222000
C	-1.704223000	3.891786000	-0.000187000
H	-2.269358000	3.607286000	0.895464000
H	-1.542702000	4.970670000	-0.000765000
H	-2.269222000	3.606364000	-0.895631000

**A2'**

C	0.352070000	-1.042652000	0.000136000
C	0.862601000	0.275381000	0.000055000
C	-0.020515000	1.387171000	0.000044000
C	-1.376450000	1.194408000	0.000000000
C	-1.952907000	-0.141235000	-0.000027000
C	-1.011372000	-1.245908000	0.000106000
H	1.025319000	-1.892915000	0.000237000
H	0.417791000	2.380841000	0.000079000
H	-2.067856000	2.031438000	-0.000013000
H	-1.428871000	-2.248149000	0.000139000
O	-3.194483000	-0.330295000	-0.000152000
O	2.177464000	0.588222000	0.000106000
C	3.142478000	-0.460199000	-0.000194000
H	4.114569000	0.034411000	-0.000488000
H	3.050166000	-1.085411000	0.895837000
H	3.049606000	-1.085420000	-0.896143000

**A3'**

C	-0.290153000	-1.239653000	-0.000054000
C	1.088009000	-1.225740000	0.000027000
C	1.785416000	0.000001000	0.000019000
C	1.088013000	1.225736000	-0.000008000
C	-0.290151000	1.239656000	-0.000029000
C	-1.048087000	-0.000002000	0.000149000
H	-0.858167000	-2.165050000	-0.000184000
H	1.646010000	-2.158266000	-0.000061000
H	2.871853000	0.000002000	0.000000000
H	1.646013000	2.158264000	-0.000066000
H	-0.858175000	2.165047000	-0.000146000
O	-2.305727000	0.000002000	-0.000021000

**<sup>3</sup>6a**

Cu	1.087730000	-0.026309000	-0.457559000
C	0.893803000	3.002854000	-1.281604000
H	0.622912000	2.585080000	-2.246751000
C	1.035763000	4.375736000	-1.095518000
H	0.874983000	5.056515000	-1.924549000
C	1.394176000	4.840749000	0.169464000
H	1.523160000	5.903301000	0.352309000
C	1.590906000	3.920494000	1.199823000
H	1.872344000	4.250361000	2.195287000
C	1.416177000	2.561860000	0.937202000
C	1.530607000	1.511364000	2.029394000
H	2.159457000	1.880019000	2.853141000
H	0.531188000	1.336133000	2.444846000
C	3.471595000	0.207965000	1.268099000
H	4.033526000	0.017097000	2.194647000
H	3.758381000	1.208300000	0.921205000
C	3.859547000	-0.798253000	0.198729000
C	5.095358000	-1.443276000	0.215305000
H	5.786254000	-1.271674000	1.035148000
C	5.426462000	-2.302564000	-0.833130000
H	6.384389000	-2.813831000	-0.841078000
C	4.507065000	-2.496858000	-1.862505000
H	4.720694000	-3.157513000	-2.695829000
C	3.287475000	-1.826579000	-1.801410000
H	2.532046000	-1.941631000	-2.572273000
C	1.545341000	-0.941264000	2.278392000
H	1.742550000	-0.819427000	3.353501000
H	2.127171000	-1.807297000	1.940901000
C	0.072370000	-1.223273000	2.043966000
C	-0.721818000	-1.716743000	3.065200000
H	-0.317727000	-1.856671000	4.061886000
C	-2.056792000	-2.034394000	2.766795000
H	-2.710956000	-2.423637000	3.541476000

C	-2.545360000	-1.839590000	1.492018000
H	-3.580473000	-2.046971000	1.254153000
C	-1.679858000	-1.316237000	0.496446000
C	-3.404618000	-1.467513000	-1.307439000
N	1.079140000	2.117239000	-0.289921000
N	2.017793000	0.223029000	1.503603000
N	2.969622000	-0.995219000	-0.795956000
N	-0.385198000	-1.020503000	0.785092000
N	-2.100420000	-1.086217000	-0.774113000
H	-1.405049000	-0.740752000	-1.424288000
O	0.191193000	-0.024281000	-2.269232000
O	0.626107000	-0.825799000	-3.151329000
H	-3.313407000	-1.391357000	-2.396895000
H	-3.600824000	-2.526304000	-1.090991000
C	-4.578143000	-0.623275000	-0.829052000
C	-5.812524000	-1.232614000	-0.575455000
C	-4.464542000	0.764806000	-0.685123000
C	-6.916826000	-0.470083000	-0.188472000
H	-5.914263000	-2.310553000	-0.685825000
C	-5.565034000	1.527870000	-0.294472000
H	-3.509748000	1.248147000	-0.877619000
C	-6.794710000	0.912644000	-0.045825000
H	-7.868316000	-0.957391000	0.004708000
H	-5.464791000	2.604541000	-0.186883000
H	-7.651166000	1.507857000	0.257589000
<b>'6c</b>			
Cu	1.042419000	-0.043405000	-0.521801000
C	0.963910000	2.965507000	-1.348841000
H	0.590528000	2.586447000	-2.295417000
C	1.219301000	4.322880000	-1.174084000
H	1.043382000	5.018120000	-1.988019000
C	1.709461000	4.751872000	0.058304000
H	1.930242000	5.800432000	0.233750000
C	1.918890000	3.808323000	1.063656000
H	2.303387000	4.107138000	2.034227000
C	1.626245000	2.466204000	0.817510000
C	1.764713000	1.422083000	1.920540000
H	2.454338000	1.792983000	2.695135000
H	0.785232000	1.308882000	2.401534000



C	3.557527000	-0.020296000	1.023736000
H	4.197390000	-0.333988000	1.863630000
H	3.904079000	0.976258000	0.722770000
C	3.772523000	-0.959331000	-0.159338000
C	4.956100000	-1.688409000	-0.282193000
H	5.704117000	-1.638425000	0.503377000
C	5.166039000	-2.470448000	-1.417407000
H	6.082258000	-3.042220000	-1.529566000
C	4.177368000	-2.507886000	-2.399417000
H	4.293411000	-3.102340000	-3.299366000
C	3.016546000	-1.766648000	-2.198345000
H	2.216482000	-1.775950000	-2.932293000
C	1.611827000	-1.035388000	2.160327000
H	1.810449000	-0.956484000	3.240424000
H	2.139469000	-1.929772000	1.806256000
C	0.120096000	-1.243366000	1.930041000
C	-0.698397000	-1.688089000	2.957082000
H	-0.297570000	-1.839096000	3.953574000
C	-2.048219000	-1.939278000	2.670101000
H	-2.716713000	-2.286726000	3.452359000
C	-2.534449000	-1.736630000	1.392728000
H	-3.578890000	-1.898395000	1.159418000
C	-1.645497000	-1.271925000	0.395038000
C	-3.340138000	-1.427141000	-1.442651000
N	1.158653000	2.052118000	-0.381561000
N	2.150396000	0.104679000	1.408235000
N	2.809927000	-1.007525000	-1.107410000
N	-0.342349000	-1.031410000	0.673762000
N	-2.048390000	-1.028624000	-0.887818000
H	-1.294584000	-0.849699000	-1.538346000
H	-3.230358000	-1.363643000	-2.531430000
H	-3.542668000	-2.483323000	-1.214983000
C	-4.519475000	-0.574622000	-0.996438000
C	-5.763589000	-1.176802000	-0.774849000
C	-4.400655000	0.812734000	-0.850413000
C	-6.873081000	-0.407048000	-0.418450000
H	-5.868588000	-2.254370000	-0.885351000
C	-5.506642000	1.582604000	-0.489626000
H	-3.436886000	1.288267000	-1.013889000

C	-6.746286000	0.975128000	-0.273867000
H	-7.832182000	-0.888368000	-0.249602000
H	-5.402189000	2.658445000	-0.378186000
H	-7.606675000	1.575742000	0.006896000

**<sup>3</sup>6d**

Cu	-0.832316000	2.177795000	0.080846000
C	-1.111711000	2.533147000	-3.068549000
H	-0.540207000	1.609244000	-3.067876000
C	-1.456123000	3.187481000	-4.248973000
H	-1.157991000	2.777935000	-5.208347000
C	-2.177741000	4.378588000	-4.161962000
H	-2.458049000	4.922588000	-5.058905000
C	-2.527161000	4.869689000	-2.903222000
H	-3.082036000	5.797453000	-2.801403000
C	-2.151607000	4.148339000	-1.769758000
C	-2.540363000	4.581046000	-0.368107000
H	-2.735111000	5.662498000	-0.335165000
H	-3.474426000	4.079465000	-0.090739000
C	-0.339386000	5.079158000	0.583662000
H	-0.520726000	6.003858000	1.150763000
H	-0.179710000	5.372522000	-0.460906000
C	0.915828000	4.387803000	1.076874000
C	1.962117000	5.109403000	1.650997000
H	1.857899000	6.177179000	1.818290000
C	3.138512000	4.442373000	1.990465000
H	3.970112000	4.985094000	2.429573000
C	3.228281000	3.071360000	1.752704000
H	4.132818000	2.518030000	1.977340000
C	2.131534000	2.417856000	1.196651000
H	2.142504000	1.353126000	0.986979000
C	-2.056162000	4.017634000	1.981323000
H	-2.610183000	4.908856000	2.309093000
H	-1.200334000	3.901601000	2.657122000
C	-2.937594000	2.788826000	2.062643000
C	-4.091414000	2.780923000	2.826892000
H	-4.399144000	3.665300000	3.373900000
C	-4.854446000	1.602153000	2.856053000
H	-5.770879000	1.560452000	3.437297000

C	-4.454944000	0.502341000	2.125086000
H	-5.057376000	-0.396375000	2.101576000
C	-3.261532000	0.579507000	1.361404000
N	-1.454456000	2.999817000	-1.858876000
N	-1.511495000	4.186543000	0.617554000
N	0.996844000	3.058108000	0.865794000
N	-2.515986000	1.714608000	1.350168000
N	-2.807331000	-0.461848000	0.617047000
O	-0.297103000	0.444190000	-0.700284000
O	0.860653000	-0.118536000	-0.237042000
Cu	0.831626000	-2.038578000	0.148937000
C	-1.053783000	-2.180245000	-2.411394000
H	-1.048433000	-1.101481000	-2.290226000
C	-1.795270000	-2.809368000	-3.407564000
H	-2.390048000	-2.221145000	-4.097877000
C	-1.762104000	-4.202012000	-3.484651000
H	-2.334429000	-4.729323000	-4.241781000
C	-0.983786000	-4.910477000	-2.570029000
H	-0.934828000	-5.994748000	-2.602694000
C	-0.257030000	-4.206019000	-1.609125000
C	0.686783000	-4.914224000	-0.656137000
H	0.343566000	-5.940174000	-0.461276000
H	1.665947000	-4.996378000	-1.142143000
C	-0.208975000	-4.394644000	1.571028000
H	-0.093836000	-5.359881000	2.085049000
H	-1.148132000	-4.442055000	1.006180000
C	-0.301255000	-3.261956000	2.575735000
C	-0.722675000	-3.463073000	3.889835000
H	-0.958594000	-4.463474000	4.239472000
C	-0.828297000	-2.362925000	4.741882000
H	-1.149539000	-2.496172000	5.770482000
C	-0.504840000	-1.095697000	4.256105000
H	-0.566135000	-0.216955000	4.889159000
C	-0.085619000	-0.976914000	2.933799000
H	0.184763000	-0.018166000	2.503809000
C	2.219145000	-4.394899000	1.190439000
H	2.432824000	-5.468731000	1.284262000
H	2.204494000	-3.976827000	2.203641000
C	3.297588000	-3.704681000	0.382653000

C	4.524086000	-4.307657000	0.166906000
H	4.724090000	-5.306794000	0.538205000
C	5.499639000	-3.580357000	-0.535788000
H	6.477437000	-4.015164000	-0.720348000
C	5.216807000	-2.309415000	-0.989624000
H	5.965792000	-1.726959000	-1.510602000
C	3.931074000	-1.758669000	-0.744409000
N	-0.303378000	-2.861509000	-1.527772000
N	0.879947000	-4.163556000	0.601031000
N	0.013107000	-2.034810000	2.113071000
N	2.988227000	-2.464138000	-0.067547000
N	3.590658000	-0.509295000	-1.156530000
H	2.631287000	-0.220292000	-0.982245000
H	-1.940392000	-0.308658000	0.105950000
C	4.432931000	0.358675000	-1.965219000
C	-3.486336000	-1.742925000	0.485205000
H	3.769909000	1.126596000	-2.379349000
H	4.818462000	-0.199879000	-2.829995000
C	5.595589000	1.033104000	-1.239849000
C	6.487405000	1.811104000	-1.991306000
C	5.806403000	0.906482000	0.136604000
C	7.561621000	2.455452000	-1.378946000
H	6.342847000	1.912229000	-3.065316000
C	6.888871000	1.544874000	0.751502000
H	5.134219000	0.293291000	0.730166000
C	7.766763000	2.323350000	-0.002646000
H	8.243511000	3.053497000	-1.976586000
H	7.052277000	1.420858000	1.819053000
H	8.609947000	2.815127000	0.473422000
H	-2.758709000	-2.413535000	0.014298000
H	-3.689001000	-2.161555000	1.480667000
C	-4.774770000	-1.729193000	-0.328697000
C	-5.822239000	-2.590279000	0.019424000
C	-4.917839000	-0.907347000	-1.453339000
C	-6.990635000	-2.635677000	-0.744192000
H	-5.727515000	-3.230177000	0.894991000
C	-6.086763000	-0.947319000	-2.215006000
H	-4.116385000	-0.224621000	-1.725486000
C	-7.125498000	-1.812965000	-1.863690000

H	-7.796519000	-3.305827000	-0.459317000
H	-6.189956000	-0.300294000	-3.081922000
H	-8.035902000	-1.841503000	-2.455032000

**26b**

Cu	-1.068744000	-0.024117000	-0.467236000
C	-0.828814000	-3.019210000	-1.301053000
H	-0.552351000	-2.568698000	-2.249285000
C	-0.928603000	-4.397392000	-1.126645000
H	-0.730944000	-5.066857000	-1.956919000
C	-1.291344000	-4.884941000	0.129221000
H	-1.387593000	-5.952982000	0.299991000
C	-1.532206000	-3.983547000	1.167492000
H	-1.814084000	-4.333102000	2.156035000
C	-1.397304000	-2.618449000	0.917512000
C	-1.545561000	-1.569286000	2.003131000
H	-2.202072000	-1.927965000	2.808689000
H	-0.559862000	-1.389086000	2.447884000
C	-3.475143000	-0.279921000	1.197454000
H	-4.047318000	-0.143215000	2.126538000
H	-3.738576000	-1.267064000	0.798520000
C	-3.850863000	0.777568000	0.177653000
C	-5.080018000	1.434002000	0.207583000
H	-5.792717000	1.220211000	0.998271000
C	-5.372620000	2.365303000	-0.790019000
H	-6.323917000	2.888878000	-0.788200000
C	-4.421927000	2.620160000	-1.777088000
H	-4.604075000	3.344635000	-2.563626000
C	-3.212290000	1.930073000	-1.733267000
H	-2.424689000	2.089662000	-2.462387000
C	-1.587251000	0.876578000	2.274167000
H	-1.809925000	0.713847000	3.338002000
H	-2.178737000	1.739446000	1.947443000
C	-0.116847000	1.187716000	2.073820000
C	0.656299000	1.691529000	3.104928000
H	0.244090000	1.817850000	4.100128000
C	1.986536000	2.041793000	2.811988000
H	2.627955000	2.439760000	3.593038000
C	2.486359000	1.870842000	1.538926000

H	3.517351000	2.106880000	1.309324000
C	1.640558000	1.333434000	0.529526000
C	3.356671000	1.517400000	-1.264834000
N	-1.061293000	-2.155600000	-0.301108000
N	-2.019822000	-0.279942000	1.454253000
N	-2.936156000	1.023388000	-0.781953000
N	0.352320000	1.002745000	0.819231000
N	2.054415000	1.127389000	-0.740440000
H	1.363518000	0.726954000	-1.381134000
O	-0.130132000	-0.068936000	-2.139155000
O	-0.544968000	0.963435000	-3.043706000
H	-0.999407000	0.442847000	-3.731541000
H	3.266647000	1.458099000	-2.355355000
H	3.552335000	2.572899000	-1.032217000
C	4.532756000	0.668396000	-0.799099000
C	5.765695000	1.274190000	-0.530555000
C	4.421379000	-0.722366000	-0.679870000
C	6.869890000	0.506727000	-0.152854000
H	5.866149000	2.354114000	-0.621585000
C	5.521668000	-1.490743000	-0.299110000
H	3.467708000	-1.202784000	-0.885109000
C	6.749626000	-0.878475000	-0.034979000
H	7.819948000	0.992048000	0.052499000
H	5.422811000	-2.569455000	-0.211334000
H	7.605978000	-1.477694000	0.261001000

**<sup>3</sup>TS<sub>R16</sub>**

Cu	-1.628553000	-1.193679000	-0.157251000
C	-0.229440000	-0.760280000	2.606947000
H	0.502952000	-0.250984000	1.988464000
C	-0.047882000	-0.924472000	3.978808000
H	0.842832000	-0.532620000	4.458168000
C	-1.024729000	-1.605001000	4.704673000
H	-0.913414000	-1.758884000	5.773944000
C	-2.148556000	-2.094018000	4.037322000
H	-2.925821000	-2.631266000	4.572517000
C	-2.265140000	-1.878574000	2.664208000
C	-3.494617000	-2.307939000	1.882629000
H	-4.007150000	-3.136070000	2.395150000

H	-4.197256000	-1.466497000	1.855839000
C	-2.549232000	-3.975439000	0.345499000
H	-3.300910000	-4.779341000	0.355795000
H	-1.902502000	-4.131048000	1.217802000
C	-1.692428000	-4.066625000	-0.905352000
C	-1.544585000	-5.258734000	-1.613105000
H	-2.091985000	-6.145146000	-1.306924000
C	-0.684524000	-5.290638000	-2.711919000
H	-0.554386000	-6.207737000	-3.278835000
C	-0.001981000	-4.129450000	-3.070437000
H	0.675130000	-4.110241000	-3.917737000
C	-0.210180000	-2.974037000	-2.319081000
H	0.294944000	-2.038912000	-2.540421000
C	-4.303201000	-2.444435000	-0.434605000
H	-5.214117000	-2.941038000	-0.068615000
H	-4.033879000	-2.921698000	-1.384310000
C	-4.569898000	-0.973752000	-0.692012000
C	-5.865028000	-0.497627000	-0.814215000
H	-6.713996000	-1.157526000	-0.671917000
C	-6.037545000	0.860525000	-1.128645000
H	-7.036840000	1.276136000	-1.221543000
C	-4.938333000	1.672287000	-1.313049000
H	-5.055238000	2.725911000	-1.531336000
C	-3.638785000	1.113819000	-1.178144000
C	-2.477423000	3.246952000	-1.754423000
N	-1.314531000	-1.226256000	1.968200000
N	-3.167989000	-2.646554000	0.485969000
N	-1.038224000	-2.944035000	-1.263195000
N	-3.475903000	-0.194908000	-0.848699000
N	-2.512772000	1.840048000	-1.381179000
H	-1.630396000	1.353717000	-1.239379000
O	-0.303122000	0.201363000	-0.535209000
O	0.743235000	-0.143910000	-1.302050000
C	6.105366000	-0.143249000	-0.071964000
C	6.428547000	1.186939000	-0.379297000
C	5.422428000	2.169235000	-0.438892000
C	4.089674000	1.869473000	-0.219068000
C	3.758231000	0.489375000	0.064757000
C	4.786729000	-0.519398000	0.156719000

H	6.894945000	-0.877627000	-0.013407000
H	5.750355000	3.177220000	-0.653563000
H	1.766621000	0.077773000	-0.488077000
O	2.507050000	0.123221000	0.322427000
C	3.032659000	2.997143000	-0.289310000
C	2.221510000	2.863348000	-1.603115000
C	2.082224000	2.970649000	0.933497000
C	3.694508000	4.393884000	-0.304600000
H	2.881572000	2.943937000	-2.474504000
H	1.682600000	1.916533000	-1.671508000
H	1.487471000	3.677000000	-1.664550000
H	2.649725000	3.042130000	1.869032000
H	1.408367000	3.834229000	0.886292000
H	1.477844000	2.065184000	0.966718000
H	2.910567000	5.158324000	-0.297595000
H	4.326729000	4.558716000	0.575123000
H	4.297878000	4.563643000	-1.202635000
C	4.449067000	-1.986497000	0.503992000
C	3.788195000	-2.063520000	1.903712000
C	3.507318000	-2.591870000	-0.566451000
C	5.710956000	-2.874886000	0.550937000
H	4.461926000	-1.666736000	2.672277000
H	2.854506000	-1.501424000	1.936892000
H	3.576008000	-3.110285000	2.154110000
H	3.975586000	-2.561595000	-1.557556000
H	3.305062000	-3.642720000	-0.325155000
H	2.554031000	-2.064899000	-0.617661000
H	5.417130000	-3.898861000	0.804371000
H	6.227552000	-2.914814000	-0.414938000
H	6.423698000	-2.543401000	1.314560000
O	7.676659000	1.633096000	-0.622483000
C	8.774133000	0.721428000	-0.580777000
H	9.657275000	1.315813000	-0.815852000
H	8.883352000	0.280324000	0.416680000
H	8.656398000	-0.072748000	-1.326993000
H	-1.452980000	3.438848000	-2.093554000
H	-3.122812000	3.416730000	-2.626192000
C	-2.844254000	4.226949000	-0.646940000
C	-3.619531000	5.354917000	-0.937748000



C	-2.375885000	4.044652000	0.660543000
C	-3.922070000	6.287483000	0.057410000
C	-2.679429000	4.972776000	1.656724000
C	-3.453286000	6.097476000	1.357748000
H	-1.773600000	3.170640000	0.896691000
H	-2.309900000	4.820526000	2.667358000
H	-3.689647000	6.819631000	2.134118000
H	-4.526708000	7.157435000	-0.183478000
H	-3.987618000	5.508979000	-1.950388000

${}^3T_{6d}^{6a}$

Cu	-2.044504000	1.891711000	0.101897000
C	-2.289165000	1.806584000	-3.030525000
H	-1.411593000	1.170453000	-2.954433000
C	-2.794414000	2.196632000	-4.268090000
H	-2.316577000	1.862394000	-5.183030000
C	-3.912587000	3.029580000	-4.294796000
H	-4.333372000	3.364237000	-5.238175000
C	-4.478041000	3.436328000	-3.086335000
H	-5.344535000	4.090598000	-3.071279000
C	-3.919727000	2.993246000	-1.886226000
C	-4.543050000	3.358037000	-0.544958000
H	-5.171929000	4.254452000	-0.656274000
H	-5.210479000	2.541224000	-0.244877000
C	-2.783798000	4.766763000	0.449300000
H	-3.265617000	5.567888000	1.030867000
H	-2.782857000	5.100977000	-0.595706000
C	-1.329338000	4.622222000	0.880564000
C	-0.629038000	5.723213000	1.377799000
H	-1.146794000	6.664103000	1.539002000
C	0.733098000	5.603803000	1.645869000
H	1.295738000	6.452901000	2.021980000
C	1.358502000	4.377705000	1.418445000
H	2.421299000	4.243806000	1.589027000
C	0.587090000	3.318719000	0.949670000
H	1.024871000	2.341924000	0.764213000
C	-3.996243000	3.149239000	1.857618000
H	-4.909443000	3.692055000	2.145951000
H	-3.208656000	3.453505000	2.558516000

C	-4.224033000	1.652960000	2.000488000
C	-5.305876000	1.168092000	2.718488000
H	-6.021934000	1.850949000	3.162465000
C	-5.454645000	-0.221117000	2.840287000
H	-6.298678000	-0.634465000	3.384443000
C	-4.535139000	-1.066617000	2.250892000
H	-4.654906000	-2.141000000	2.307107000
C	-3.449278000	-0.503976000	1.538188000
N	-2.835204000	2.188631000	-1.864200000
N	-3.534254000	3.510685000	0.510336000
N	-0.727409000	3.429500000	0.685504000
N	-3.309807000	0.838086000	1.415162000
N	-2.482872000	-1.276834000	0.959726000
O	-0.213318000	0.041853000	-0.687788000
O	1.020833000	0.030137000	-0.285928000
Cu	1.873857000	-1.739491000	0.080667000
C	-0.060720000	-2.818664000	-2.191027000
H	-0.520404000	-1.841419000	-2.083916000
C	-0.575687000	-3.777445000	-3.059379000
H	-1.460784000	-3.558368000	-3.646253000
C	0.057721000	-5.017528000	-3.133002000
H	-0.317711000	-5.793655000	-3.792899000
C	1.178645000	-5.252263000	-2.336252000
H	1.691487000	-6.208832000	-2.364378000
C	1.637729000	-4.238509000	-1.496012000
C	2.887287000	-4.404327000	-0.653374000
H	3.073273000	-5.466159000	-0.438984000
H	3.747763000	-4.037651000	-1.225083000
C	1.964270000	-4.235094000	1.621307000
H	2.503321000	-5.030535000	2.155211000
H	1.118447000	-4.709058000	1.108899000
C	1.424248000	-3.206608000	2.597479000
C	1.172771000	-3.513414000	3.934122000
H	1.410524000	-4.499518000	4.321137000
C	0.615819000	-2.535581000	4.759788000
H	0.414820000	-2.751197000	5.804803000
C	0.331122000	-1.279201000	4.225183000
H	-0.097859000	-0.490369000	4.833689000
C	0.620078000	-1.046792000	2.883111000

H	0.425011000	-0.084860000	2.420203000
C	4.149988000	-3.236513000	1.105122000
H	4.803683000	-4.116146000	1.183576000
H	4.007600000	-2.847697000	2.120288000
C	4.798385000	-2.165956000	0.253572000
C	6.160788000	-2.182634000	0.017018000
H	6.777191000	-2.993039000	0.390239000
C	6.719057000	-1.112748000	-0.702047000
H	7.786477000	-1.084580000	-0.899145000
C	5.909997000	-0.091670000	-1.151781000
H	6.328529000	0.753236000	-1.682945000
C	4.515686000	-0.148840000	-0.892754000
N	1.021556000	-3.039749000	-1.426072000
N	2.813759000	-3.607061000	0.588474000
N	1.154522000	-1.987105000	2.086889000
N	3.974841000	-1.185727000	-0.199865000
N	3.668917000	0.822591000	-1.325690000
H	2.702344000	0.743109000	-1.038344000
H	-1.782295000	-0.788838000	0.413847000
C	4.074473000	2.044033000	-2.006840000
C	-2.536308000	-2.725460000	0.844753000
H	3.152782000	2.490073000	-2.398312000
H	4.676515000	1.789016000	-2.888403000
C	4.820099000	3.067477000	-1.153976000
C	5.523849000	4.095936000	-1.794379000
C	4.803000000	3.029453000	0.244412000
C	6.188676000	5.072708000	-1.052517000
H	5.554980000	4.133915000	-2.881516000
C	5.476666000	4.001940000	0.989728000
H	4.278649000	2.226155000	0.755643000
C	6.167596000	5.028273000	0.343690000
H	6.731512000	5.861875000	-1.564597000
H	5.473145000	3.948471000	2.075428000
H	6.695397000	5.780977000	0.921821000
H	-1.530545000	-3.033194000	0.533698000
H	-2.690890000	-3.167320000	1.837542000
C	-3.570144000	-3.283568000	-0.127858000
C	-4.120627000	-4.550210000	0.102671000
C	-3.949590000	-2.579663000	-1.277383000

C	-5.028135000	-5.108188000	-0.799841000
H	-3.843780000	-5.104606000	0.997622000
C	-4.860785000	-3.133734000	-2.179212000
H	-3.547244000	-1.585604000	-1.458388000
C	-5.400609000	-4.400377000	-1.944388000
H	-5.452246000	-6.088596000	-0.602881000
H	-5.157663000	-2.572355000	-3.061173000
H	-6.114256000	-4.828146000	-2.642364000

**<sup>37</sup>a**

Cu	1.796097000	0.041229000	-0.408957000
C	0.979020000	3.055481000	-0.653725000
H	0.771785000	2.775990000	-1.682367000
C	0.854451000	4.371778000	-0.216584000
H	0.542719000	5.146985000	-0.908231000
C	1.146286000	4.659474000	1.116387000
H	1.070183000	5.675203000	1.492617000
C	1.542670000	3.623299000	1.963037000
H	1.777485000	3.814790000	3.005723000
C	1.629142000	2.327844000	1.453672000
C	1.962705000	1.138464000	2.339508000
H	2.530589000	1.464550000	3.223160000
H	1.022203000	0.710939000	2.706548000
C	4.100047000	0.358534000	1.405595000
H	4.690816000	0.102328000	2.297856000
H	4.203715000	1.440203000	1.254616000
C	4.655548000	-0.351624000	0.183267000
C	5.984880000	-0.766450000	0.119575000
H	6.637166000	-0.632373000	0.977151000
C	6.458537000	-1.348580000	-1.056911000
H	7.491027000	-1.677009000	-1.128785000
C	5.584790000	-1.506546000	-2.131300000
H	5.908596000	-1.956740000	-3.063496000
C	4.266900000	-1.079329000	-1.986254000
H	3.541054000	-1.181326000	-2.786883000
C	2.411860000	-1.276589000	2.132509000
H	2.587189000	-1.324502000	3.217191000
H	3.135950000	-1.950689000	1.659662000
C	1.011171000	-1.762562000	1.805895000

C	0.304465000	-2.544288000	2.705355000
H	0.720726000	-2.782363000	3.678119000
C	-0.959119000	-3.015116000	2.317355000
H	-1.545131000	-3.627748000	2.996165000
C	-1.467783000	-2.691632000	1.075312000
H	-2.450201000	-3.034511000	0.777621000
C	-0.690571000	-1.884299000	0.206885000
C	-2.445006000	-1.773998000	-1.574271000
N	1.357631000	2.057905000	0.161206000
N	2.667257000	0.075759000	1.598771000
N	3.811421000	-0.513410000	-0.856832000
N	0.530395000	-1.428025000	0.585619000
N	-1.108840000	-1.542012000	-1.043888000
H	-0.538427000	-0.863631000	-1.536855000
O	0.908528000	0.219659000	-2.215672000
O	1.444573000	-0.366584000	-3.203175000
H	-2.381135000	-1.613016000	-2.654052000
H	-2.730070000	-2.818039000	-1.428844000
C	-3.518260000	-0.869569000	-0.989905000
C	-4.600674000	-1.367481000	-0.266305000
C	-3.455891000	0.513338000	-1.166477000
C	-5.583720000	-0.534790000	0.266117000
C	-4.418254000	1.372847000	-0.648456000
C	-5.491003000	0.841790000	0.069455000
F	-4.322972000	2.692299000	-0.831194000
F	-6.418628000	1.652021000	0.574248000
F	-6.601335000	-1.044470000	0.960783000
F	-4.707583000	-2.692876000	-0.050474000
F	-2.424599000	1.039606000	-1.855466000

**<sup>27</sup>b**

Cu	-1.797876000	-0.099416000	-0.409659000
C	-1.012078000	-3.095717000	-0.673710000
H	-0.791817000	-2.784425000	-1.690009000
C	-0.878253000	-4.415126000	-0.248551000
H	-0.544519000	-5.178866000	-0.942684000
C	-1.187285000	-4.722638000	1.076660000
H	-1.103960000	-5.742292000	1.440609000
C	-1.607228000	-3.703570000	1.933385000
H	-1.851871000	-3.911773000	2.970542000

C	-1.700340000	-2.403902000	1.437258000
C	-2.047002000	-1.217281000	2.316936000
H	-2.658403000	-1.530340000	3.175140000
H	-1.115458000	-0.804332000	2.721188000
C	-4.143555000	-0.406112000	1.324246000
H	-4.738659000	-0.192451000	2.223976000
H	-4.249176000	-1.477720000	1.115189000
C	-4.666551000	0.380839000	0.138034000
C	-5.980834000	0.839756000	0.072380000
H	-6.660496000	0.666575000	0.901144000
C	-6.401392000	1.522806000	-1.069910000
H	-7.420853000	1.889188000	-1.144363000
C	-5.490945000	1.737472000	-2.103427000
H	-5.773071000	2.274265000	-3.002820000
C	-4.191426000	1.256086000	-1.959223000
H	-3.429563000	1.399654000	-2.718316000
C	-2.465125000	1.201545000	2.136796000
H	-2.670661000	1.204604000	3.216375000
H	-3.177158000	1.891152000	1.669341000
C	-1.056189000	1.688118000	1.856973000
C	-0.364586000	2.460294000	2.774711000
H	-0.793925000	2.694342000	3.742767000
C	0.906142000	2.931868000	2.403310000
H	1.483070000	3.540159000	3.093908000
C	1.432859000	2.617905000	1.167247000
H	2.418866000	2.964573000	0.886230000
C	0.670073000	1.813738000	0.277793000
C	2.410142000	1.753862000	-1.508870000
N	-1.416538000	-2.118865000	0.152553000
N	-2.707519000	-0.137998000	1.549671000
N	-3.790740000	0.585995000	-0.866655000
N	-0.558937000	1.361519000	0.643983000
N	1.095717000	1.462976000	-0.959794000
H	0.496323000	0.809803000	-1.476167000
O	-0.849042000	-0.295574000	-2.063575000
O	-1.389657000	0.503590000	-3.123022000
H	-1.747712000	-0.183713000	-3.714831000
H	2.334430000	1.598868000	-2.588614000
H	2.662790000	2.806051000	-1.356826000

C	3.528197000	0.883909000	-0.953921000
C	4.591155000	1.410692000	-0.221896000
C	3.529080000	-0.495621000	-1.167277000
C	5.612892000	0.610638000	0.287051000
C	4.532282000	-1.322728000	-0.673541000
C	5.581978000	-0.763018000	0.055806000
F	4.498004000	-2.640346000	-0.892200000
F	6.547874000	-1.543316000	0.537252000
F	6.609950000	1.148692000	0.991464000
F	4.642330000	2.734410000	0.026805000
F	2.525604000	-1.051956000	-1.869629000

'7c

Cu	1.515701000	0.001859000	-0.418016000
C	0.057664000	2.739650000	-0.417292000
H	-0.273803000	2.444276000	-1.406382000
C	-0.237121000	4.002771000	0.088612000
H	-0.797991000	4.709237000	-0.513636000
C	0.206800000	4.325891000	1.369603000
H	0.008423000	5.304548000	1.796141000
C	0.910271000	3.367242000	2.098820000
H	1.264747000	3.582464000	3.102444000
C	1.150942000	2.114758000	1.532850000
C	1.811926000	1.008147000	2.349516000
H	2.395322000	1.453020000	3.170517000
H	1.012599000	0.421855000	2.819420000
C	3.935402000	0.581074000	1.166882000
H	4.699073000	0.340009000	1.923022000
H	3.872424000	1.675781000	1.124090000
C	4.400173000	0.092105000	-0.201088000
C	5.755704000	-0.114562000	-0.459390000
H	6.481764000	0.011175000	0.338193000
C	6.162384000	-0.476062000	-1.743439000
H	7.213423000	-0.638930000	-1.961911000
C	5.195713000	-0.628337000	-2.736030000
H	5.462058000	-0.909199000	-3.749388000
C	3.861422000	-0.420108000	-2.398634000
H	3.075464000	-0.537730000	-3.138368000
C	2.567912000	-1.316628000	1.978457000
H	2.794909000	-1.425168000	3.050169000

H	3.353654000	-1.849967000	1.429698000
C	1.234987000	-1.983728000	1.664746000
C	0.610973000	-2.821124000	2.577559000
H	1.047633000	-2.993408000	3.555346000
C	-0.599911000	-3.424484000	2.206866000
H	-1.123036000	-4.071207000	2.905037000
C	-1.131337000	-3.199263000	0.949640000
H	-2.068489000	-3.655819000	0.655122000
C	-0.428790000	-2.353958000	0.062840000
C	-2.206961000	-2.202257000	-1.693336000
N	0.740661000	1.813587000	0.280109000
N	2.607173000	0.084543000	1.536138000
N	3.463660000	-0.068448000	-1.162824000
N	0.710463000	-1.734688000	0.440790000
N	-0.822285000	-2.138391000	-1.238235000
H	-0.261944000	-1.433533000	-1.704606000
H	-2.182510000	-2.185802000	-2.786768000
H	-2.649944000	-3.156707000	-1.407132000
C	-3.067797000	-1.060268000	-1.178274000
C	-4.182630000	-1.267781000	-0.367508000
C	-2.743111000	0.261954000	-1.480209000
C	-4.949813000	-0.208940000	0.119422000
C	-3.477221000	1.339973000	-1.004015000
C	-4.593105000	1.100064000	-0.200765000
F	-3.116779000	2.594316000	-1.301235000
F	-5.306790000	2.121436000	0.266702000
F	-6.008935000	-0.439875000	0.894131000
F	-4.537854000	-2.518375000	-0.029796000
F	-1.656717000	0.512297000	-2.250398000
<b><sup>37</sup>d</b>			
Cu	0.164018000	1.804275000	-0.612738000
C	0.280275000	2.544335000	2.435766000
H	0.139193000	1.472735000	2.536986000
C	0.326698000	3.395219000	3.537115000
H	0.226820000	2.995860000	4.540802000
C	0.496372000	4.762172000	3.315075000
H	0.528505000	5.458090000	4.147950000
C	0.620695000	5.227416000	2.005111000
H	0.751798000	6.285466000	1.799419000



C	0.580292000	4.307539000	0.957715000
C	0.800923000	4.715678000	-0.486817000
H	0.525483000	5.768364000	-0.642020000
H	1.870513000	4.629730000	-0.711161000
C	-1.349527000	4.174968000	-1.534004000
H	-1.501834000	5.057026000	-2.172844000
H	-1.709350000	4.433363000	-0.531438000
C	-2.167395000	3.002814000	-2.034575000
C	-3.317218000	3.184859000	-2.803260000
H	-3.614675000	4.183711000	-3.107067000
C	-4.074078000	2.070760000	-3.165058000
H	-4.971015000	2.188475000	-3.765759000
C	-3.658785000	0.808300000	-2.740976000
H	-4.220818000	-0.084902000	-2.993153000
C	-2.495776000	0.709483000	-1.981240000
H	-2.133647000	-0.240402000	-1.603017000
C	0.740557000	3.735609000	-2.742389000
H	0.953846000	4.731959000	-3.154773000
H	0.034738000	3.249178000	-3.425969000
C	2.010739000	2.912289000	-2.670257000
C	3.126762000	3.254627000	-3.415964000
H	3.123947000	4.139758000	-4.042610000
C	4.256517000	2.427538000	-3.327686000
H	5.151652000	2.663972000	-3.895381000
C	4.239331000	1.317929000	-2.505260000
H	5.115637000	0.689328000	-2.415693000
C	3.065453000	1.031663000	-1.764217000
N	0.406192000	2.991087000	1.177844000
N	0.079142000	3.826784000	-1.422741000
N	-1.757542000	1.779322000	-1.643076000
N	1.968919000	1.825719000	-1.861617000
N	2.961700000	-0.051119000	-0.941347000
O	0.320586000	0.090713000	0.344552000
O	-0.742734000	-0.744270000	0.157144000
Cu	-0.478848000	-2.632508000	-0.232957000
C	1.572398000	-2.538629000	2.170668000
H	1.519121000	-1.470830000	1.987924000
C	2.404128000	-3.075469000	3.150236000
H	3.020114000	-2.419255000	3.755487000

C	2.422983000	-4.460436000	3.320681000
H	3.060531000	-4.917708000	4.071367000
C	1.613510000	-5.255645000	2.508063000
H	1.608287000	-6.336218000	2.615231000
C	0.802515000	-4.640844000	1.553406000
C	-0.165853000	-5.432130000	0.690381000
H	0.194257000	-6.460393000	0.545094000
H	-1.123176000	-5.502019000	1.218657000
C	0.663683000	-4.991739000	-1.577186000
H	0.563060000	-5.969083000	-2.070702000
H	1.608313000	-5.011296000	-1.020257000
C	0.739484000	-3.879536000	-2.605457000
C	1.211265000	-4.102871000	-3.898856000
H	1.481106000	-5.106274000	-4.213598000
C	1.329869000	-3.022119000	-4.772783000
H	1.692766000	-3.173234000	-5.784917000
C	0.970665000	-1.750010000	-4.327172000
H	1.048067000	-0.882894000	-4.974318000
C	0.498160000	-1.609261000	-3.025455000
H	0.204536000	-0.642229000	-2.632323000
C	-1.754976000	-5.070861000	-1.164348000
H	-1.919587000	-6.155684000	-1.231114000
H	-1.770633000	-4.679301000	-2.188765000
C	-2.862335000	-4.420230000	-0.358422000
C	-4.089103000	-5.044118000	-0.206244000
H	-4.271031000	-6.024453000	-0.632952000
C	-5.088585000	-4.358768000	0.501429000
H	-6.076412000	-4.796216000	0.612019000
C	-4.817892000	-3.127673000	1.064676000
H	-5.591114000	-2.585093000	1.592688000
C	-3.518310000	-2.576635000	0.923700000
N	0.792485000	-3.303971000	1.390366000
N	-0.420421000	-4.761841000	-0.603101000
N	0.379817000	-2.649400000	-2.183646000
N	-2.575424000	-3.208512000	0.173574000
N	-3.134998000	-1.421798000	1.534521000
H	-2.234329000	-1.037110000	1.252733000
H	2.101952000	-0.119805000	-0.398910000
C	-3.926704000	-0.647039000	2.477716000

C	4.077315000	-0.895630000	-0.537069000
H	-3.232870000	-0.230005000	3.213897000
H	-4.602535000	-1.307246000	3.022714000
C	-4.717077000	0.493436000	1.855712000
C	-6.105126000	0.468067000	1.723824000
C	-4.061241000	1.638220000	1.402691000
C	-6.818100000	1.524256000	1.155581000
C	-4.740293000	2.707084000	0.832660000
C	-6.128166000	2.649673000	0.706398000
H	3.637496000	-1.761335000	-0.033532000
H	4.601934000	-1.275636000	-1.417285000
C	5.086385000	-0.233848000	0.389335000
C	6.415793000	-0.036066000	0.014617000
C	4.727135000	0.189083000	1.669234000
C	7.348811000	0.561948000	0.860679000
C	5.629361000	0.787786000	2.540545000
C	6.951552000	0.972987000	2.132351000
F	6.826418000	-0.417425000	-1.210207000
F	8.605707000	0.740963000	0.462273000
F	7.825044000	1.545811000	2.952548000
F	5.240670000	1.178721000	3.756105000
F	3.452722000	0.017796000	2.090395000
F	-2.718159000	1.716339000	1.518453000
F	-6.797970000	-0.601036000	2.153301000
F	-8.142053000	1.462504000	1.037894000
F	-6.786654000	3.664120000	0.152350000
F	-4.072500000	3.788631000	0.398965000

<sup>3</sup>TS<sub>R17</sub>

Cu	-0.699980000	-1.928510000	-0.046500000
C	0.254019000	-0.503606000	2.545947000
H	0.702879000	0.164343000	1.817859000
C	0.447609000	-0.345744000	3.916981000
H	1.057900000	0.470964000	4.287639000
C	-0.150644000	-1.257918000	4.785728000
H	-0.014499000	-1.171130000	5.859705000
C	-0.926142000	-2.290428000	4.256649000
H	-1.404821000	-3.018081000	4.905290000

C	-1.086398000	-2.372796000	2.873427000
C	-1.992439000	-3.407632000	2.228208000
H	-2.099107000	-4.286899000	2.881752000
H	-2.991453000	-2.967207000	2.123848000
C	-0.420707000	-4.737141000	0.886132000
H	-0.760686000	-5.766473000	1.078637000
H	0.242223000	-4.457376000	1.714208000
C	0.371547000	-4.674252000	-0.408320000
C	0.953314000	-5.805544000	-0.978818000
H	0.815340000	-6.779670000	-0.519276000
C	1.708526000	-5.662097000	-2.144210000
H	2.168397000	-6.529530000	-2.608526000
C	1.855263000	-4.394084000	-2.703896000
H	2.429545000	-4.239968000	-3.611277000
C	1.238278000	-3.312121000	-2.077106000
H	1.319867000	-2.296642000	-2.453006000
C	-2.649041000	-4.202200000	0.001415000
H	-3.295648000	-4.942782000	0.495305000
H	-2.203510000	-4.696323000	-0.869976000
C	-3.472516000	-3.024436000	-0.487634000
C	-4.848221000	-3.126939000	-0.627131000
H	-5.370576000	-4.030460000	-0.331548000
C	-5.534900000	-2.027327000	-1.164459000
H	-6.614514000	-2.061822000	-1.279803000
C	-4.842824000	-0.894952000	-1.545527000
H	-5.369875000	-0.039748000	-1.948169000
C	-3.432905000	-0.865284000	-1.381012000
C	-3.160765000	1.448162000	-2.282663000
N	-0.496788000	-1.495252000	2.040782000
N	-1.539787000	-3.780175000	0.877329000
N	0.513653000	-3.451490000	-0.956640000
N	-2.776744000	-1.919573000	-0.830870000
N	-2.661192000	0.182415000	-1.774723000
H	-1.671747000	0.136014000	-1.513054000
O	-0.068982000	-0.190800000	-0.659248000
O	1.059029000	-0.207632000	-1.440827000
C	6.260060000	1.320010000	-0.281750000
C	6.206527000	2.708493000	-0.510673000
C	4.975571000	3.400641000	-0.465483000

C	3.786621000	2.749175000	-0.225387000
C	3.830595000	1.302259000	-0.032054000
C	5.106496000	0.595708000	-0.031666000
H	7.218568000	0.822281000	-0.296783000
H	5.019670000	4.471011000	-0.618117000
H	1.944339000	0.252552000	-0.650750000
O	2.738613000	0.639018000	0.210952000
C	2.458529000	3.526025000	-0.168721000
C	1.615427000	3.177748000	-1.423779000
C	1.667375000	3.199486000	1.144400000
C	2.694316000	5.052479000	-0.202227000
H	2.146794000	3.469632000	-2.337302000
H	1.373941000	2.116702000	-1.490882000
H	0.670182000	3.731253000	-1.389590000
H	1.553181000	4.102016000	1.754050000
H	0.664790000	2.827327000	0.916986000
H	2.167863000	2.450715000	1.760551000
H	1.727381000	5.560209000	-0.123848000
H	3.314572000	5.391885000	0.635228000
H	3.157896000	5.385292000	-1.137535000
C	5.178829000	-0.918616000	0.247465000
C	4.595073000	-1.226606000	1.650445000
C	4.399495000	-1.701319000	-0.838006000
C	6.631470000	-1.440337000	0.232647000
H	5.159219000	-0.701342000	2.430157000
H	3.546976000	-0.933822000	1.722704000
H	4.673263000	-2.302017000	1.851145000
H	4.807996000	-1.497148000	-1.834956000
H	4.495927000	-2.777803000	-0.651739000
H	3.338688000	-1.451277000	-0.839948000
H	6.626376000	-2.513565000	0.449256000
H	7.111386000	-1.309728000	-0.744281000
H	7.253970000	-0.958431000	0.995203000
O	7.276612000	3.475879000	-0.764945000
C	8.581338000	2.892298000	-0.830444000
H	9.256618000	3.716687000	-1.058565000
H	8.858139000	2.443547000	0.129678000
H	8.634224000	2.140542000	-1.625282000
H	-2.321204000	1.933705000	-2.787839000

H	-3.929824000	1.276460000	-3.039424000
C	-3.707957000	2.385252000	-1.214763000
C	-5.050624000	2.754287000	-1.153693000
C	-2.862533000	2.919620000	-0.241494000
C	-5.544161000	3.604644000	-0.165174000
C	-3.320325000	3.769974000	0.758513000
C	-4.671919000	4.114689000	0.794100000
F	-2.480032000	4.256932000	1.676858000
F	-5.127033000	4.926421000	1.747671000
F	-6.838197000	3.929114000	-0.132872000
F	-5.920187000	2.277221000	-2.066004000
F	-1.553987000	2.602788000	-0.267171000

${}_3TS_{7d}^{7a}$

Cu	0.241580000	2.993306000	0.228506000
C	-0.531226000	1.580457000	2.934700000
H	-0.674089000	0.712365000	2.298153000
C	-0.835868000	1.534321000	4.293025000
H	-1.214949000	0.618455000	4.734803000
C	-0.653132000	2.687417000	5.055570000
H	-0.884395000	2.696435000	6.116478000
C	-0.181727000	3.838477000	4.425686000
H	-0.042546000	4.759522000	4.983623000
C	0.108801000	3.804182000	3.060485000
C	0.654920000	5.029652000	2.343122000
H	0.430541000	5.934572000	2.929492000
H	1.748169000	4.948092000	2.296906000
C	-1.240831000	5.519155000	0.847225000
H	-1.360469000	6.613666000	0.841722000
H	-1.766027000	5.151952000	1.737625000
C	-1.919214000	4.918127000	-0.376743000
C	-2.958112000	5.589567000	-1.022639000
H	-3.245373000	6.584867000	-0.696867000
C	-3.621662000	4.964923000	-2.078832000
H	-4.436225000	5.469135000	-2.590134000
C	-3.219783000	3.687129000	-2.465081000
H	-3.717155000	3.153646000	-3.267296000
C	-2.157289000	3.095174000	-1.787088000
H	-1.802253000	2.105591000	-2.053829000

C	1.062028000	5.817124000	0.045105000
H	1.372840000	6.799304000	0.433100000
H	0.496105000	6.005949000	-0.875471000
C	2.290308000	5.002727000	-0.326367000
C	3.502972000	5.644048000	-0.529886000
H	3.597403000	6.708796000	-0.346630000
C	4.589062000	4.886357000	-0.983339000
H	5.556719000	5.353086000	-1.141519000
C	4.428430000	3.535152000	-1.224844000
H	5.265167000	2.935164000	-1.556901000
C	3.161675000	2.947246000	-1.002328000
N	-0.059205000	2.682310000	2.325829000
N	0.163553000	5.115085000	0.965496000
N	-1.518578000	3.688868000	-0.765741000
N	2.117593000	3.671842000	-0.533385000
N	2.933059000	1.615455000	-1.246363000
O	-0.008795000	0.436413000	-0.604649000
O	-0.565638000	-0.413452000	0.193792000
Cu	-0.064920000	-2.354095000	0.140034000
C	1.899624000	-1.284363000	2.339624000
H	1.586830000	-0.314224000	1.968458000
C	2.867494000	-1.401798000	3.332439000
H	3.319127000	-0.512752000	3.759642000
C	3.242463000	-2.679377000	3.749950000
H	3.999478000	-2.812578000	4.516828000
C	2.636473000	-3.787381000	3.159608000
H	2.914021000	-4.795514000	3.451520000
C	1.664152000	-3.586595000	2.179865000
C	0.920292000	-4.745247000	1.544708000
H	1.528999000	-5.659839000	1.577198000
H	0.015709000	-4.942374000	2.132126000
C	1.580733000	-4.549993000	-0.822518000
H	1.780547000	-5.600423000	-1.078346000
H	2.490715000	-4.145410000	-0.364423000
C	1.266647000	-3.745816000	-2.070379000
C	1.707798000	-4.133987000	-3.335048000
H	2.260251000	-5.060412000	-3.458483000
C	1.425196000	-3.317969000	-4.431175000
H	1.754641000	-3.603163000	-5.425731000

C	0.705262000	-2.139790000	-4.230689000
H	0.455938000	-1.482894000	-5.057234000
C	0.292853000	-1.824762000	-2.938068000
H	-0.267989000	-0.920692000	-2.724176000
C	-0.720013000	-5.184685000	-0.230837000
H	-0.609496000	-6.257026000	-0.017526000
H	-0.824177000	-5.082794000	-1.317081000
C	-1.970971000	-4.640612000	0.429873000
C	-3.007385000	-5.492310000	0.776761000
H	-2.911819000	-6.564077000	0.640940000
C	-4.185303000	-4.924774000	1.281755000
H	-5.027582000	-5.557056000	1.546167000
C	-4.277713000	-3.555305000	1.439468000
H	-5.191831000	-3.108533000	1.808363000
C	-3.163972000	-2.750100000	1.101032000
N	1.301727000	-2.350421000	1.783037000
N	0.488970000	-4.432309000	0.166920000
N	0.565952000	-2.608480000	-1.883256000
N	-2.031546000	-3.296800000	0.592147000
N	-3.154457000	-1.393911000	1.296855000
H	-2.416144000	-0.893860000	0.815298000
H	1.987686000	1.290632000	-1.082880000
C	-4.346196000	-0.604358000	1.587677000
C	3.761153000	0.794541000	-2.123128000
H	-3.993099000	0.380794000	1.907145000
H	-4.879660000	-1.034876000	2.436679000
C	-5.301164000	-0.441261000	0.415785000
C	-6.619164000	-0.894913000	0.449306000
C	-4.882386000	0.192652000	-0.753191000
C	-7.489091000	-0.727280000	-0.628535000
C	-5.720128000	0.378085000	-1.844983000
C	-7.036047000	-0.083318000	-1.779788000
H	3.087599000	0.154403000	-2.701115000
H	4.288513000	1.427834000	-2.840181000
C	4.766284000	-0.091633000	-1.403619000
C	6.144400000	0.119280000	-1.448085000
C	4.331998000	-1.203872000	-0.686622000
C	7.049592000	-0.722027000	-0.798494000
C	5.201462000	-2.067603000	-0.036071000



C	6.574016000	-1.825711000	-0.090608000
F	6.639761000	1.163829000	-2.133149000
F	8.356099000	-0.481796000	-0.857408000
F	7.419710000	-2.641177000	0.531079000
F	4.724066000	-3.135091000	0.626995000
F	3.007067000	-1.470636000	-0.629053000
F	-3.608139000	0.639758000	-0.831536000
F	-7.078317000	-1.525793000	1.544520000
F	-8.739211000	-1.177569000	-0.564543000
F	-7.849698000	0.084453000	-2.816663000
F	-5.275242000	0.991605000	-2.949211000