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Supporting information

Bio-inspired Cu(II) Amido-Quinoline Complexes as Catalyst for Aromatic C-H Bond Hydroxylation

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Physical methods and materials

All commercially available chemicals (Sigma Aldrich Co, Finar, Chempure(P) Ltd., Rankem, etc.) were used without further purification. HPLC graded anhydrous solvents were used. Ligands were synthesized according to a reported method.^{S0} High-resolution mass spectroscopy (HRMS) was carried out using 6540 UHD Accurate-Mass Q-TOF LC/MS system (Agilent, USA) equipped with 1290 UPLC (Agilent) system. Products were identified from a reaction mixture by Agilent 5977B GC/MSD equipped with an HP-5 MS capillary column ($30 \text{ m} \times 0.32 \text{ mm} \times 0.25 \text{ µm}$) and quantified using Agilent 7890B GC system equipped with an HP-5 capillary column ($30 \text{ m} \times 0.32 \text{ mm} \times 0.25 \text{ µm}$). For each compound calibration curve was obtained with authentic compounds.

Structure determination by X-ray crystallography

Single-crystal X-ray study was carried on a D8 Venture Bruker AXS single-crystal X-ray diffractometer equipped with CMOS PHOTON 100 detector having monochromatized microfocus sources (Mo–K α = 0.71073 Å) at room temperature. Structures were solved using the SHELX program implemented in APEX3.^{S1-S4} The non-H atoms were located in successive difference Fourier syntheses and refined with anisotropic thermal parameters. All the hydrogen atoms were placed at the calculated positions and refined using a riding model with appropriate HFIX commands. The crystallographic data and structure refinement parameters are summarized in (Table S1) and geometrical parameters including bond lengths and bond angles are listed in (Table S2).

Electrochemical measurements

Cyclic voltammetry (CV) experiments were performed in CHI-660 potentiostat, using a glassy carbon (working electrode), a platinum wire (counter electrode), and an Ag/AgNO₃ (0.01 M) as reference electrode in DCM ([Cu(II)L_{1/2}] = 1 mM, scan rate: 0.1 Vs⁻¹). The supporting electrolyte was 0.1 M $^{n}Bu_{4}NPF_{6}$ ($^{n}Bu = n$ -butyl). The potential was referenced to the NHE coupled by the addition of an Fc standard to the solution. The respective plots are shown in Fig. S4.

Synthesis and Characterization of Cu(II)-amidoquinoline complexes

Synthesis of 1A

A CHCl₃ solution (1 mL) of L1 (100 mg, 0.26 mmol) was added dropwise to a pre-dissolved MeOH solution (1 mL) of CuCl₂.2H₂O (61 mg, 0.26 mmol) which resulted in a dark green solution and within few minutes a dark green precipitate started to form. This solution was stirred for 1 hour at RT and then the precipitate was filtered washed with cold MeOH (1 \times 2 mL) and diethyl ether (2 \times 5 mL) and dried under vacuum. Crystals of **1A** were obtained by slow diffusion of diethyl ether into the DCM solution.

Complex (1A) [Cu(L1)]²⁺

Dark green crystals; Yield 64 mg (50%). Analytically calculated elements for C, 57.26; H, 3.90; N, 11.61. Found: C, 57.08; H, 3.80; N, 11.51. HR-MS (m/z) [Found (calcd)]: [481.0592 (481.0493)]; UV-Vis {CHCl₃, λ_{max} , nm ($\epsilon/10^{-4}$ M⁻¹ cm⁻¹)}: 312 (11260 M⁻¹ cm⁻¹), 383 (4600 M⁻¹ cm⁻¹).

Synthesis of **1B** and **2**

The respective ligands were dissolved in DMF under N_2 and to it, 2 equivalents of trimethylamine were added resulting in a dark yellow coloured solution. After stirring for 30 minutes solid CuCl₂.2H₂O (61 mg, 0.26 mmol) was added resulting in a dark green solution. After stirring for 4 hours at RT. Then this solution was filtered over celite and the solution was directly kept for crystallization. Crystals of pure complexes were obtained within 10 days.

Complex (1B) [Cu(L1)]²⁺

Dark green crystals; Yield 58 mg (47%). Analytically calculated elements for C, 61.74; H, 4.04; N, 12.56. Found: C, 58.41; H, 3.79; N, 11.79. HR-MS (m/z) [Found (calcd)]: [446.0782 (446.0799)]; UV-Vis {CHCl₃, λ_{max} , nm ($\epsilon/10^{-4}$ M⁻¹ cm⁻¹)}: 318 (7230 M⁻¹ cm⁻¹), 388 (6480 M⁻¹ cm⁻¹).

Complex (2) [Cu(L2)]²⁺

Dark green crystals; Yield 50 mg (43%). For complex **2**: analytically calculated elements for C, 58.20; H, 3.46; N, 16.16. Found: C, 57.98; H, 3.30; N, 15.98. HR-MS (m/z) [Found (calcd): 433.0591 (433.0595)]. UV-Vis {CHCl₃, λ_{max} , nm ($\epsilon/10^{-4}$ M⁻¹ cm⁻¹)}: 395 (3880 M⁻¹ cm⁻¹).



Figure S1: Crystal structure of complex **2**.



Figure S2: Top (left) HR-MS of 1A, top, (right) HR-MS of 1B, and bottom HR-MS of 2.



Figure S3: EPR spectra of **1A**, **1B** and **2** in DMF at 80 K at X-band frequency and magnetic field modulation of 100 kHz, with a microwave power of 2.25 mW and modulation amplitude of 1 G at 80 K. For **1A**: $S = \frac{1}{2}$, $g = [2.031 \ 2.071 \ 2.196]$, $A(Cu) = [40 \ 38 \ 548]$ MHz, $lw = [5.7 \ 12.6 \ 6.2]$ mT; for **1B**: $S = \frac{1}{2}$, $g = [2.034 \ 2.071 \ 2.197]$, $A(Cu) = [40 \ 10 \ 549]$ MHz, lw (full width at half maximum) = [5.8 \ 12.5 \ 6.3] mT and for **2**: $S = \frac{1}{2}$, $g = [2.055 \ 2.246]$, $A(Cu) = [10 \ 455]$ MHz, $lw = [4 \ 5]$ mT Voigtian broadening (Gaussian + Lorentzian). The spectra were simulated using the EasySpin package, (S. Stoll, A. Schweiger, *J. Magn. Reson.* **2006**, *178*, 42-55).



Figure S4: Cyclic voltamogram of Cu(II) amido-quinoline complexes (4 mM) in DMF at 25 °C Supporting electrolyte: $^{n}Bu_{4}NPF_{6}$ (0.1 M); Reference electrode: Ag/Ag⁺ (0.54V *vs.* NHE); Working electrode: glassy carbon; Counter electrode: Pt wire; Scan rate: 0.05 V s⁻¹.



Figure S5: UV-Vis spectra of Cu(II) complexes (0.1mM) in CHCl₃.

Compounds	1A	1B	2
Empirical formula	C ₂₃ H ₁₉ N ₄ O ₂ ClCu	$\mathrm{C}_{23}\mathrm{H}_{24}\mathrm{N}_{4}\mathrm{O}_{3}\mathrm{Cu}$	$C_{42}H_{34}Cu_2N_{10}O_6$
Formula weight	482.41	496.01	901.89
Temperature (K)	296(2)	299(2)	297.12
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	triclinic	monoclinic	triclinic
Space group	P^{-1}	$P2_{l}/c$	P^{-1}
a (Å)/α (°)	10.1783(5)/72.660(2)	7.7535(8)/90	7.2592(2)/91.6400(10)
b (Å)/β (°)	10.5304(4)/73.038(2)	10.0540(10)/97.94	13.9102(4)/ 90.9330(10)
c (Å)/γ (°)	10.9027(5)/73.118(2)	28.075(3)/90	17.9303(5)/ 95.7430(10)
Volume (Å ³)	1040.11(8)	2167.57	1800.39(9)
Ζ	2	4	2
Density (calc) (Mg/m ⁻³)	1.540	1.520	1.6635
Absorption coefficient (μ) (mm ⁻¹)	1.207	1.048	1.250
F(000)	494	1028	925.7
Crystal size (mm ³)	0.21 x 0.13 x 0.06	0.23 x 0.15 x 0.07	0.23 x 0.10 x 0.05
Theta ranges for data collection	2.008-26.022°	2.500-25.675°	2.28 - 52.86°
Index ranges	-12<=h<=12, - 12<=k<=12, - 13<=l<=13	-9<=h<=9, -12<=k<=12, - 34<=l<=34	-9<=h<=9, -17<=k<=17, -22<=l<=22
Reflections collected	33568	20692	46118
Independent reflections	4094 [R(int) = 0.0281]	3972 [R(int) = 0.1267]	7355[R(int) = 0.0267]
Data/restraints/parameters	4094/0/280	3972/0/303	7355/0/549
Goodness-of-fit on F ²	1.094	1.041	1.058
Final R indices [I>2sigma(I)]	$\begin{array}{c} R1 = 0.0263 \ wR_2 = \\ 0.0705 \end{array}$	$R1 = 0.127 \ wR_2 = 0.1288$	$\begin{array}{c} R1 = 0.0326 \ wR_2 = \\ 0.1026 \end{array}$
R indices (all data)	$\begin{array}{c} R1 = 0.0300 \ wR_2 = \\ 0.0734 \end{array}$	$R1 = 0.0687 \text{ w}R_2 = 0.1490$	$R1 = 0.0378 wR_2 = 0.1126$
Largest diff peak and hole (e Å-3)	0.275 and -0.301	0.613 and -0.744	0.42 and -0.57
CCDC No.	2184057	2184058	2184059

Table S1 Crystal data and structure refinement parameters of complexes.

	Bond lengths (Å)	Bond a	ngles [°]	
	(1A)			
Cu-N1	1.960(1)	N1-Cu-N2	84.35(7)	
Cu-N2	1.939(1)	N1-Cu-Cl1	98.07(5)	
Cu-Cl1	2.207(5)	Cl1-Cu-O1	93.97(5)	
Cu-O1	1.948(1)	N2-Cu-O1	92.54(7)	
		N2-Cu-Cl1	160.68(5)	
		N1-Cu-O1	151.99(7)	
		Tetrahedral distortion parameter	0.33	
		(τ_4)		
Cu-N1	2 039(4)	(1B) N1_Cu_N2	83.26(6)	
Cu-N2	1.039(4)	N2-Cu-N2	93.86(6)	
Cu-N3	1.971(2) 1.946(1)	N3-Cu-N4	93.80(0) 81.69(6)	
Cu-NJ	2.025(2)	N1 Cu N4	08.48(6)	
Cu-IN4	2.055(2)	N2-Cu-N4	98.48(0) 176.2(6)	
		N1-Cu-N3	146.5(6)	
		Tetrahedral distortion parameter (τ_4)	0.27	
		(2)		
Cu-N1	1.970(3)	N1-Cu-N2	84.64(1)	
Cu-N2	1.921(3)	N2-Cu-N3	94.19(1)	
Cu-N3	1.907(3)	N3-Cu-N4	83.55(1)	
Cu-N4	1.986(3)	N1-Cu-N4	101.01(1)	
		N2-Cu-N4	170.34(1)	
		N1-Cu-N3	157.71(1)	
		Tetrahedral distortion parameter (τ_4)	0.24	

Table S2 Selected bond lengths (Å) and bond angles (°) of complexes.

Chromatographic methods

Separation of the various products shown here was performed using the following GC methods:

Column: Agilent 7890B GC system equipped with a HP-5 capillary column (30 m \times 0.32 mm \times 0.25 µm); Agilent 5977B GC/MSD equipped with a HP-5 MS capillary column (30 m \times 0.32 mm \times 0.25 µm)- Detector: FID (280 °C)

			1		
Inlet			Detector		
Septum purge fl	ow 3ml/	min	Zero air Flo	w 3	00ml/min
Split ratio	20:1		H ₂ fuel flow	v 3	0ml/min
Split flow	30m	l/min	Makeup N ₂	flow	25ml/min
Substrates	Initial	Final oven	Heating	Hold time	Total run time
	oven temp	temp (°C)	rate (°C)	(min)	(min)
	(°C)				
RC ₆ H ₅	60	100	10	1	5
	100	220	10	1	18
R=NO ₂ , NMe ₂	60	220	10	2	16
	220	300	10	0	24

For RC₆H₅ oxidation reactions, where R= H, OH, Cl, CH₃, CH₂CH₃, ^{*i*}Pr, Cl.

General procedure for benzene hydroxylation

In a typical reaction 100 μ L of a 1mM solution of Cu(II) catalyst in CH₃CN: CH₂Cl₂ (8:2 v/v) and benzene 89 μ L, 1 mmol was added to a solution of dry CH₃CN 504 μ L. Then, 307 μ L of 30% H₂O₂, was slowly added to the reaction mixture. The final concentrations of the reagents were 0.1 mM Cu(II) catalyst, 1M benzene, and 3M H₂O₂. This solution was vigorously stirred at 60 °C for 5 hr. After completion of the reaction, a fraction of the resulting mixture was analyzed by GC (FID), and the products were identified by GC-MS. The products were quantified from the calibration curve of authentic compounds.

Benzene hydroxylation in presence of radical trap CCl₄

In a typical reaction 100 μ L of a 1mM solution of **1B** in CH₃CN: CH₂Cl₂ (8:2 v/v) and benzene 89 μ L, 1 mmol was added to a solution of dry CH₃CN 214 μ L. Then, 307 μ L of 30% H₂O₂ and 290 μ L CCl₄ were slowly added to the reaction mixture. This solution was vigorously stirred at 60 °C for 5 hr. After completion of the reaction, a fraction of the resulting mixture was analyzed by GC (FID), and the products were identified by GC-MS. The products were quantified from the calibration curve of authentic compounds.



Scheme S1: Catalytic oxidation of benzene using 1B in presence of H₂O₂ and CCl₄.



Figure S6: HR-MS spectra for in situ generated $[LCu^{II} - Et_3N]^+$ by the reaction of complex **1B** with 0.5 eq of Et_3N in CH_3CN .



Figure S7: Bar plot of phenol conversion, selectivity, and yield from hydroxylation of benzene (1 M) catalysed by **1A**, **1B**, and **2** (0.1 mM) at 60 °C in the presence of aqueous H_2O_2 (3 M).



Figure S8: (A) Effect of H_2O_2 amount on benzene hydroxylation where 3M H_2O_2 was found to be optimal. (B) Temperature dependant catalytic hydroxylation of benzene using **1B** as catalyst where 60 °C was found to be the optimal temperature for the reaction.



Figure S9: The standard calibration curve using GC peak areas (unit: pico Ampere or pA) of known concentrations of (A) benzene, (B) phenol, and (C) benzoquinone.



Figure S10: Effect of ligand framework in the benzene hydroxylation.

Entry	Substrate	sp ² :sp ³ :q ^a	Product (o/ p/ m) ^b	Selectivity,%°
1.	Toluene	70:30:0	ОН (65:35:0)	70
2.	Ethylbenzene	96:4	(19:68:13)	96
3.	Cumene	94:6	(40:52:8)	94

Table S3: Product Distributions in Catalytic Oxidation of alkyl-substituted benzenes with 1B.

Reaction conditions: substrate (1 M), H_2O_2 (3 M), **1B** (0.1 mM) in $CH_3CN:CH_2Cl_2$ (8:2 v/v) at 60 °C for 5 hr. aRatio of products given by (sp²) aromatic hydroxylation, (sp³) oxidation of alkyl-substituent oxygenation and (q) quinone derivatives. bRatio of ortho, para and meta products of hydroxylation. cSelectivity for aromatic hydroxylation products.



Product Distribution of catalytic hydroxylation of benzene with H_2O_2 using catalyst $\mathbf{1B}$

Figure S11: GC profile for the formation of phenol.





Figure S12: GC profile for the oxidation of phenol.

Scheme S3: Product distribution of catalytic hydroxylation of toluene with H_2O_2 using catalyst **1B**.



Figure S13: GC profile for the oxidation of toluene.

Scheme S4: Product Distribution of catalytic hydroxylation of ethylbenzene with H_2O_2 using catalyst **1B**.



Figure S14: GC profile for the oxidation of ethylbenzene.

Scheme S5: Product distribution of catalytic hydroxylation of cumene with H_2O_2 using catalyst **1B**.



Figure S15: GC profile for the oxidation of cumene.

General procedure for oxidation of anthracene

In a typical reaction, 100 μ L of a 1mM solution of **1B** in CHCl₃:CH₃CN (8:2 v/v) and anthracene 1 mmol was added to a solution of dry CHCl₃ 214 μ L. Then, 512 μ L of 30% H₂O₂ was slowly added to the reaction mixture. This solution was vigorously stirred at 60 °C for 4 hr. After completion of the reaction, a fraction of the resulting mixture was analyzed by GC (FID), and the products were identified by GC-MS.



Figure S16: GC-MS trace for oxidation of anthracene using **1B**. Inset shows the GC-MS spectra for anthracene and 9,10-anthraquinone.

Scheme S6: Product Distribution of catalytic hydroxylation of chlorobenzene with H_2O_2 using catalyst **1B**.



Figure S17: GC profile for the oxidation of chlorobenzene.





Figure S18: GC profile for the oxidation of N, N-dimethylaniline.

Scheme S8: Rate equation of Benzene hydroxylation with Cu complexes using H_2O_2 as an oxidant.

$$\mathbf{1B} + \mathbf{H}_2\mathbf{O}_2 \stackrel{K}{\longleftarrow} \operatorname{Int} \qquad \operatorname{Rate} = \frac{kK[\mathbf{1B}][S][\mathbf{H}_2\mathbf{O}_2]}{1 + K[\mathbf{H}_2\mathbf{O}_2]}$$

$$\operatorname{Int} + S \stackrel{k}{\longrightarrow} P$$

Table S4: Variation of H_2O_2 concentration in catalytic hydroxylation of benzene on using **1A** or **1B** as the catayst at 60 °C in CH₃CN:CH₂Cl₂ (8:2 v/v) 1mL. Rate was measured using GC.

[CuL]/ mM	[H ₂ O ₂]/ M	[S]/ M	Rate _{1A} (M Min ⁻¹)	$Rate_{1B} (M Min^{-1})$
0.1	0.5	1.0	3.00 × 10 ⁻⁵	5.95 × 10 ⁻⁵
0.1	1.0	1.0	4.67 × 10 ⁻⁵	8.15 × 10 ⁻⁵
0.1	2.0	1.0	8.33 × 10 ⁻⁵	1.08 × 10 ⁻⁴
0.1	3.0	1.0	1.17×10^{-4}	1.30×10^{-4}
0.1	4.0	1.0	1.33 × 10 ⁻⁴	1.37 × 10 ⁻⁴
0.1	5.0	1.0	1.40×10^{-4}	1.47×10^{-4}



Fig. S19: rate vs. $[H_2O_2]$ for **1B**.

Determination of Kinetic Isotopic Effect (KIE)

100 μ L of a 1mM solution of **1B** in CH₃CN: CH₂Cl₂ (8:2 v/v) and benzene 44.5 μ L, 0.5 mmol and deuterated benzene 44.2 μ L, 0.5 mmol was added to a solution of dry CH₃CN 214 μ L. Then, 307 μ L of 30% H₂O₂ was slowly added to the reaction mixture. This solution was vigorously stirred at 60 °C for 5 h. After completion of the reaction, a fraction of the resulting mixture was analyzed by GC (FID), and the products were identified by GC-MS.



Figure S20: GC-MS profile for the measurement of KIE using C_6H_6 and C_6D_6 (a) Isotopic pattern of phenol to phenol-*d5* ratio (b) benzoquinone to benzoquinone-*d4* obtained after the reaction.

Scheme S9: Plausible mechanism of TEMPO mediated oxidation of phenol.



Figure S21: GC profile for the oxidation of phenol. Reaction conditions: catalyst (0.1 mM), Phenol (1 M), TEMPO (3 M), temp 60 °C, time 5h in 1 mL of CH_3CN/CH_2Cl_2 (8:2 v/v).

Spectroscopic characterization of the Cu(II)-OOH intermediate

In a conventional Bruker spectrometer (Bruker, EMXmicro) operating at X-band frequency and magnetic field modulation of 100 kHz, with a microwave power of 2.25 mW and modulation amplitude of 1 G at 100 K, electron paramagnetic resonance (EPR) spectroscopic measurements were performed. The Bruker WINEPR SimFonia software was used to simulate the resonance lines. The EPR spectra of the Cu(II)-OOH intermediate were recorded on a frozen solution of DMF (0.1mM) in an EPR tube by adding 10 equiv. of H_2O_2 (20 µL, 50 mM). The respective EPR spectra are shown in Fig. 3 and S23. Other than EPR, Cu(II)-OOH intermediate was also characterized by UV-Vis (Fig. S21) and HR-MS (Fig. S22).



Figure S22: Electronic spectral changes for the reaction of **1A** with H_2O_2 in CH_3CN/CH_2Cl_2 (8:2 v/v) at RT.



Figure S23: Mass spectra for in situ generated [LCu^{II} -OOH] by the reaction of complex **1B** with 10 equiv. of H_2O_2 in CH₃CN.

Substituents	[substrate] ^a _{t=0}	[substrate] ^b _{t=5 hr}	Δ [substrate] ^c	r ^d =∆Subs./5 hr	r'= r/replacable
					hydrogens
-NMe ₂	100	10	90	18	3.6
-OH	100	30	70	14	2.8
-H	100	19	81	16.2	2.7
-Cl	100	42.2	57.8	11.6	2.3
-NO ₂	100	52.3	47.7	9.54	1.9

Table S5: Effect of substituents in the benzene ring on the rate of oxidation rection using **1B** as the catayst.

Reaction conditions: catalyst (0.1 M), substrate (1 M), H_2O_2 (3 M), temp 60 °C, time 5 hr in 1 mL of CH₃CN:CH₂Cl₂ (8:2 v/v).^{a,b} Concentration of substrates in mM at t = 0 hours and t = 5 hours respectively determined by GC. ^dRate of change of concentration of substrate (average rate) with respect to time. ^e Rate divided by replaceable hydrogens in each substrate.

S.No.	Catalyst	Temp (°C)	Time (hr)	TON	Conversion %	Selectivity %	C/S/O ^a	Ref. in the manuscript
1 ^b	Tp*Cu(NCMe)	80	2	11	25	92	1/200/300	9
2°	[Cu(N ₄)] diazepane	60	5	740	37	98	1/2000/5000	12
3 ^d	[Cu ₂ (µ-OH) ₆ - hpa] ³⁺	50	40	12000	22	82	1/60000/12000	10
4	[CuL(HOCH ₃)C lO ₄] ⁺	80	6	48.7	14.6	_	1/200/600	11(a)
5 ^e	[Cu(L1– 7) ₂](ClO ₄)	60	5	740		98	1/2000/4000	11(b)
6 ^f	Cu(L)(ClO ₄) ₂	25	24	Not mentio ned	Not mentioned	95	1/500/5000	S5
7	This work	60	5	810	22	91	1/10000/30000	

Table S6: Comparison of catalytic activity of various catalysts employed for hydroxylation of benzene using H_2O_2 as the oxidant.

^a Molar ratio of catalyst, substrate and oxidant. ^b with sulfolane (4 mmol). ^c with Et₃N (2.5 μmol). ^d with Et₃N (5.0 μmol). ^e with Et₃N (2.5 μmol). ^f With Sulfolane and ACN taken in ratio of 1:2.

Computational Details

The structures were optimized using Gaussian 09 package.^{S6} Spin polarized calculations with the hybrid DFT functional B3LYP^{S7-9} and Gaussian basis set $6-311G+(d,p)^{S10-13}$ were performed to find the minimum energy structures. An implicit solvent environment modelled by the polarizable continuum medium (PCM) implemented in Gaussian 09 package was used to define the solvent interactions.^{S14} We used the dielectric constant equivalent to the dielectric constant of acetonitrile to model the solvent environment. Vibrational frequencies are also calculated for the complexes at the mentioned functionals and basis sets. For all the complexes we did not find any imaginary frequencies, indicating the minimum energy structures. The zero point energy and entropy corrections were added to the electronic energies to calculate the reaction free energies. The coordinates for the optimized geometry for both **1B** and **1-OOH** are given below, obtained at B3LYP/6-311G+(d,p).

Coordinates for 1B

Cu	-0.00581800 -0.19532100 0.183276
0	-2.26829500 3.17104000 -0.389782
Ο	1.99077600 3.22066000 -0.909026
Ν	-1.51703100 1.06960100 0.161886
Ν	1.41453900 1.11114600 -0.202340
Ν	-1.46459000 -1.56284300 -0.184429
Ν	1.58291500 -1.40187400 0.553752
С	-1.37403800 2.41707700 0.008328
С	-2.70241900 -0.98138200 -0.158481
C	2.72021700 -0.86010600 0.022008
C	3.93819500 -1.59337000 -0.017998
C	-2.75601600 0.43981000 0.016278
C	1.22088900 2.45099600 -0.324353
C	2.63919200 0.49290600 -0.452527
С	-3.88513000 -1.75725900 -0.324526
С	-0.00902900 3.03151800 0.436104
С	-1.35431700 -2.85947600 -0.434214
Н	-0.35380600 -3.26839700 -0.482751
C	3.78628100 1.03138100 -1.0309620
Н	3.76119400 2.04001300 -1.409011
C	3.94141000 -2.88171300 0.5677710
Н	4.85567700 -3.46478000 0.559868
С	-4.02013000 1.02328400 0.0643220
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С	-0.05681800	4.54996800	0.21378300
Н	-0.19730700	4.80082100	-0.83747300
Н	0.87698500	5.00225300	0.54969600
Н	-0.88237400	4.98294100	0.77973500
С	-5.19129400	0.24490600	-0.06159600
Н	-6.15014300	0.74896700	-0.01092700

Coordinates for 1-00H

Cu	-1.48837000	0.91761600	0.63615700
0	0.50871200	0.72892700	0.77324700
0	-0.90186600	-3.17841300	0.08736300
Ν	2.36051600	-0.50802900	0.42182100

N	-1.72086600 -1.02148500 0.20098300
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	5.15658500 5.89452500 -5.50926300 -6.48316900 -5.38300800 -5.96346300 -4.10234800 -3.66720400 -4.67295400 -4.98728100 1.31456000 1.69625000 0.76279600 2.15137900 3.89466600 3.62407100 -1.51630400 -0.26315100 0.34356800 2.81342200	5.15658500 2.16155800 5.89452500 2.82132500 -5.50926300 -1.47322200 -6.48316900 -1.55304700 -5.38300800 2.13296500 -5.96346300 3.04567500 -4.10234800 2.14633900 -3.66720400 3.04621000 -4.67295400 -2.55838200 -4.98728100 -3.51913400 1.31456000 -2.82720900 1.69625000 -3.17594000 0.76279600 -3.65696700 2.15137900 -2.59485200 3.89466600 2.61306300 3.62407100 3.64209400 -1.51630400 2.68681600 -0.26315100 3.41210400 0.34356800 2.87196800 2.81342200 -1.41369800

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