Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Unveiling the reaction mechanism of novel copper N-alkylated tetra-azacyclophanes with outstanding superoxide dismutase activity

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Content

I. Experimental section

2.1 Synthesis of L1 and L2

All reagents were obtained from commercial sources and used as received. Solvents used for the chemical synthesis were of analytical grade and used without further purification.

Synthesis of 6-(*N*-methyl)-3,6,9-triaza-1(2,6)-pyridinecyclodecaphane (L2). The synthesis of the starting material 6-(*N*-methyl)-3,9-(p-tolylsulfonyl)-3,6,9-triaza-1(2,6)-pyridinecyclodecaphane was carried out following a procedure described previously in the literature.[1] 6-(*N*-methyl)-3,9-(p-tolylsulfonyl)-3,6,9-triaza-1(2,6)-pyridinecyclodecaphane (0.79 g, 1.49 mmol) and phenol (3.41 g, 35.72 mmol) were suspended in HBr-AcOH 33% (36 cm^3). The mixture was stirred at 90 ºC for further 24 h and cooled. The resulting suspension was filtered and washed several times with EtOH anhydrous to give the product **L2** in a salt form (0.45 g, 65%). Characterization data of the compound are included in the supplementary materials (Figures S1-S4). ^{1}H NMR (300 MHz, D_2O), δ (ppm): 7.99 (t, J=7.84 Hz, 1H), 7.51 (d, J=7.81 Hz, 2H), 4.63 (m, 4H), 3.32 (m, 4H), 2.66 (t, J=5.53 Hz, 4H), 2.45 (s, 3H). ^{13}C NMR (75.43 MHz, D_2O) δ (ppm): 149.76, 140.15, 122.73, 52.99, 50.49, 46.19, 42.20. Anal. Calc. for $C_{18}H_{32}N_4 \cdot 3HBr \cdot 0.3H_2O \cdot 0.05(C_4H_8O_2)$: C 31.0 %, H 5.1 %, N 11.8 %. Found: C 31.0 %, H 4.6%, N 11.7%. MS (ESI) m/z 221.2 $[M + H]^+$.

The synthesis of **6-(*N*-methyl)-3,9-(N-isopropyl)-3,6,9-triaza-1(2,6)-pyridinacyclodecaphane hydrochloride (L1)** has been carried out as previously described in bibliography.[2] Characterization data of the compound are included in the supplementary materials (Figures S5-S8). ^{1}H NMR (300 MHz, D_2O), δ (ppm): 8.01 (t, J=7.8 Hz, 1H), 7.53 (d, J=7.8 Hz, 2H), 4.83 (s, 2H), 4.59 (s, 2H), 3.96 (hept, J=6.7 Hz,

2H), 3.55 (s, 4H), 2.71 (s, 2H), 2.43 (s, 3H), 3.05-2.00 (m, 2H), 1.48 (s, 6H), 1.46 (s, 6H). ^{13}C NMR (75.43 MHz, D_2O) δ (ppm): 150.5 140.6, 122.9, 60.5, 54.9, 53.2, 51.6, 40.3, 16.7. Anal. Calc. for $C_{18}H_{32}N_4 \cdot 3.3HCl \cdot 4H_2O \cdot 0.4(C_4H_8O_2)$: C 44.2 %, H 8.8 %, N 10.5 %. Found: C 44.4 %, H 8.5 %, N 10.6 %. MS (ESI) m/z 305.1 $[M + H]^+$.

2.2 *In vitro* McCord-Fridovich SOD activity assays

SOD-like activity of the Cu-based complexes was determined by measuring the amount of blue formazane that is produced by reduction of nitro blue tetrazolium (NBT) after reaction with $\mathbf{O_2^{\cdot-}}$ in the presence of the tested inhibitor.[3–7] A reproducible and constant flux of superoxide anions was generated using xanthine ($1.5\ 10^{-4}$ M) and xanthine oxidase (50 mM in TRIS pH=7.4). The rate of reduction of NBT ($5.6\ 10^{-5}$ M) to blue formazane was followed spectrophotometrically at 560 nm. Data in the absence of the complex were used as reference. The rate of NBT reduction was progressively inhibited after the addition of the complex solutions at increasing concentrations prepared in 50 mM Tris buffer, pH 7.4. Thus, the percentage of inhibition of the NBT reduction was used as a measure of the SOD activity of the tested compounds. The half maximum inhibitory concentration (IC_{50}) was determined from a plot of percentage inhibition versus complex concentration. The IC_{50} data have been calculated from the mean values of three independent measurements. The catalytic constant was calculated from IC_{50} values using the equation $k_{cat}=k_{NBT}$ [NBT]/IC_{50} where $k_{NBT} = (5.9 \pm 0.5) \times 10^5\ M^{-1}\ s^{-1}$.[8–10]

2.3 Quantum mechanical calculations

The available crystal structure of $[Cu(C_{18}H_{32}N_4)(OH_2)]^{2+}$ (Figure 1) in the Cambridge Crystal Database (CCD id. 1827336) was used as starting geometry for the ground state geometry optimization. As initial benchmarking, the GGA functional BP86,[11,12] the

Becke three-parameter Lee-Yang-Parr hybrid functional (B3LYP),[11,13,14] and the meta-hybrid GGA functional M06[15] of Truhlar and Zhao were tested. The influence of the dispersion was also taken into account by means of the Grimme's dispersion (D3) correction.[16] All the gas-phase optimizations were carried out using the Ahlrichs' basis set def2-SV(P)[17] for all atoms except for copper for which we used the MDF10 Stuttgart-Dresden effective core potential.[18] A larger basis set (def2-TZV(P)) for all atoms except copper was also tested to check its influence over the geometry. Vibrational frequencies were computed on each stationary point for identification as either a transition state (TS) (single imaginary frequency) or an intermediate (all frequencies positive) on the potential energy surface. The zero-point correction was calculated and applied to all the stationary structures. The atomic polar tensor (APT) charges and the spin density were also computed for each stationary structure in order to elucidate the oxidation state of the metal ion and the dioxygen molecules. Finally, the energies were recalculated taking into account the effect of the polarizable solvent (water) by using the default SCRF method of the Polarizable Continuum Model.[19] gMolden[20] and PyMOL[21] were used for visual inspection and to create the molecular graphics. Computations were carried out using the program Gaussian09 E.01.[22]

2.4 Hybrid quantum mechanics/molecular dynamics (QM/MD) simulation

The QM-optimized geometry of 1 was embedded in a box of 4175 TIP3P water molecules[23] that extended 20 Å away from any solute atom and two Cl- ions were added to ensure electrical neutrality. The system was relaxed by energy minimization in three consecutive steps (3x5000 cycles) in which after the first 1000 cycles the minimization method was switched from steepest descendent to conjugate graduate. The resulting system was heated from 100 to 300 K during 20 ps with the position of the solute atoms were restrained (20 kcal mol^{-1} $Å^{-2}$) using the weak-coupled algorithm for

the temperature regulation and with fixed volume (NVT ensemble). These harmonic restraints were gradually reduced in five steps (5 x 20 ps) until they were completely removed. In the latter equilibrating step, the pressure was fixed (NPT ensemble). The system was further simulated under the same conditions up to a total time of 200 ps with a time step of 2 fs. System coordinates were printed every 10 ps for further analysis. The step time used for the minimizations, as well as for the heating and the equilibration steps, was fixed in 1 fs. The cutoff distance for the non-bonded interactions was 10 Å and periodic boundary conditions were used. Electrostatic interactions were treated by using the smooth particle mesh Ewald (PME) method[24] with a grid spacing of 1 Å. The SHAKE algorithm[25] was applied to all bonds involving hydrogen atoms in the classical region. The molecular dynamics (MD) simulation protocol made use of the pmemd_cuda.SPFP module in the AMBER16 suite of programs.[26] All the MD simulations were performed using one NVIDIA GPU.

The square pyramid coordination sphere of 1 and 2 was described using the Metal Centre Parameter Builder (MCPB)[27] module within Amber16. Briefly, the force field parameters (bond, angle, dihedral, electrostatic, van der Waals terms) were obtained at the B3LYP/6-31G*[28] level of theory and the ESP punctual charges were derived by fitting the electrostatic potential according to the Merz-Singh-Kollman[29,30] scheme. Some additional parameters for the coordination sphere of 1 and 2 were taken from previous works.[31–33]

The final equilibrated snapshots of 1 and 2 within the box of TIP3P water molecules obtained in the former MD simulation step were subjected to a hybrid quantum mechanics/molecular mechanics molecular dynamics (QM/MM-MD) simulation. All the QM/MM-MD calculations were performed within the *sander* module of AMBER16, which also includes a complete treatment of long-range electrostatic interactions. The

external ORCA package[34] was used for the quantum mechanical calculations. The QM region encompassed the complex and the different diatomic oxygen species ($O_2^{\cdot-}$ for steps *b* and *d*, O_2 for step *c* and O^{2-} for step *e*), whereas the MM region included all the remaining solvent and counter ions. Therefore, no covalent bond had been cut when defining the QM/MM-MD boundary. The inner QM region was treated at the B3LYP-D3/def2-SV(P) level of theory. A cutoff of 10 Å was employed for the evaluation of the electrostatic interactions within the MM-MD region and of 10 Å for the QM region. All the simulations were run up to 2 ps (2000 steps, 1 fm/step) at 300 K. The system coordinates were printed every 10 steps for further analysis. The MD and QM/MM-MD simulation trajectories were analysed using the cpptraj module[35] within AmberTools17.

2.5 Crystal structure determination

$3.6 \cdot 10^{-3}$ mmol of $[Cu\mathbf{L1}(H_2O)]^{2+}$ and $18 \cdot 10^{-3}$ mmol of NaN_3 were dissolved in pure water and, after slow evaporation, green crystals suitable for X-ray diffraction were obtained. The crystals were measured in a Bruker D8 Venture X-ray diffractometer using MoKα radiation (λ=0.71073 Å) equipped with an Oxford low temperature unit operating at 120 K. Indexing, strategy and data collection were performed with APEX3 software suite. OLEX2 was used as frontend for solving and refining.[36] The initial structure was solved with direct methods using SHELXS.[37] The resulting structure was refined using SHELXL2014.[38] Initially, an isotropic refinement was performed on the non-hydrogen atoms and then anisotropic refinement was introduced. The hydrogen atoms were found in the Fourier map and positions and isotropic thermal factors were left free to refine.

II. Figures

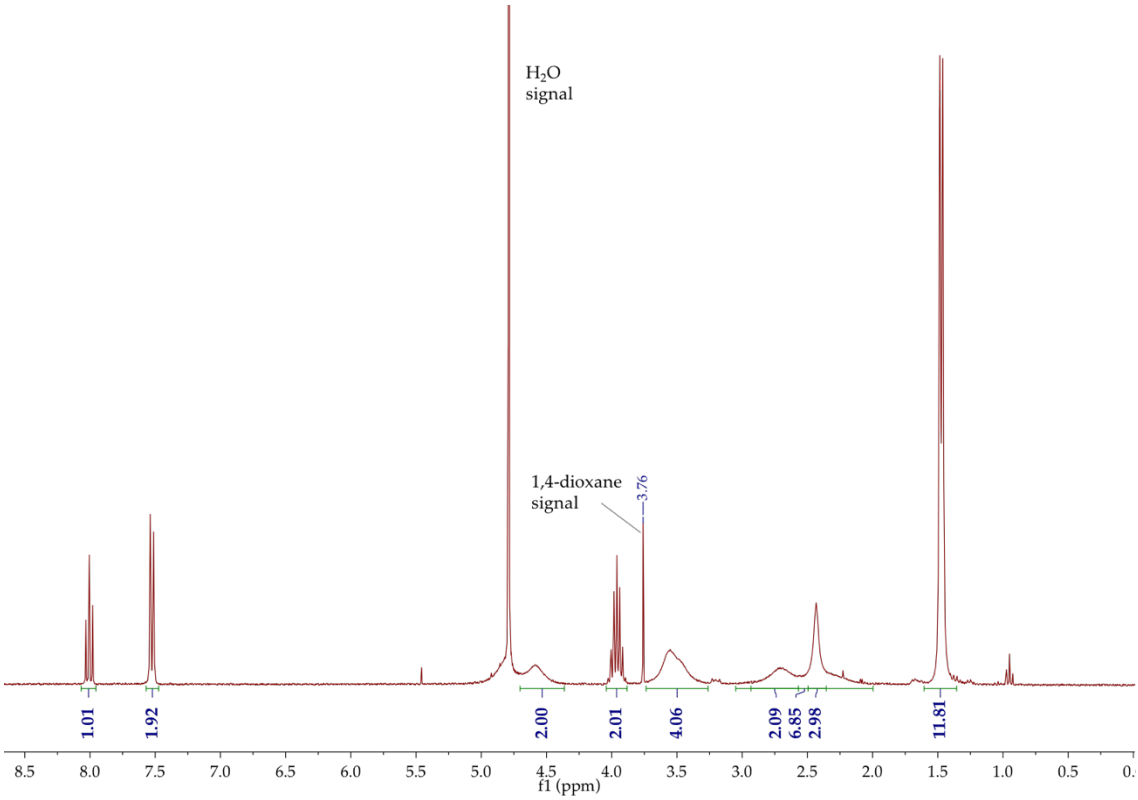

Figure S1. ^{1}H-NMR spectrum of **L1** in D_2O at 298 K.

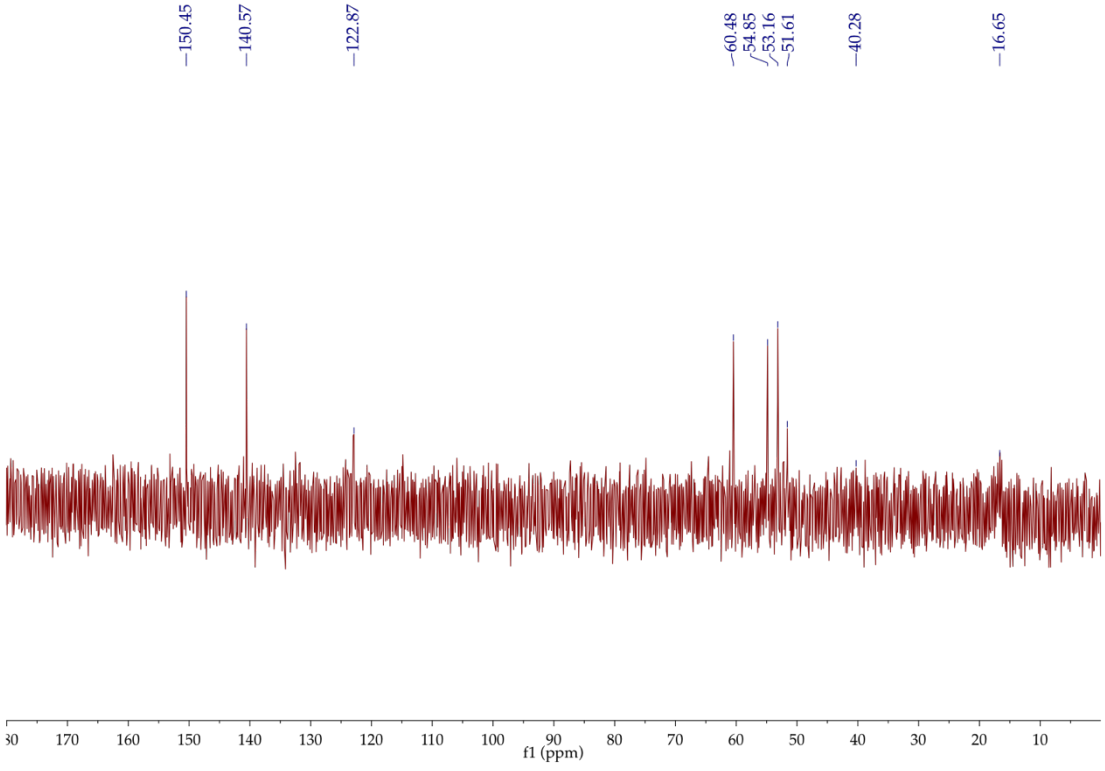

Figure S2. ^{13}C-NMR spectrum of **L1** in D_2O at 298 K.

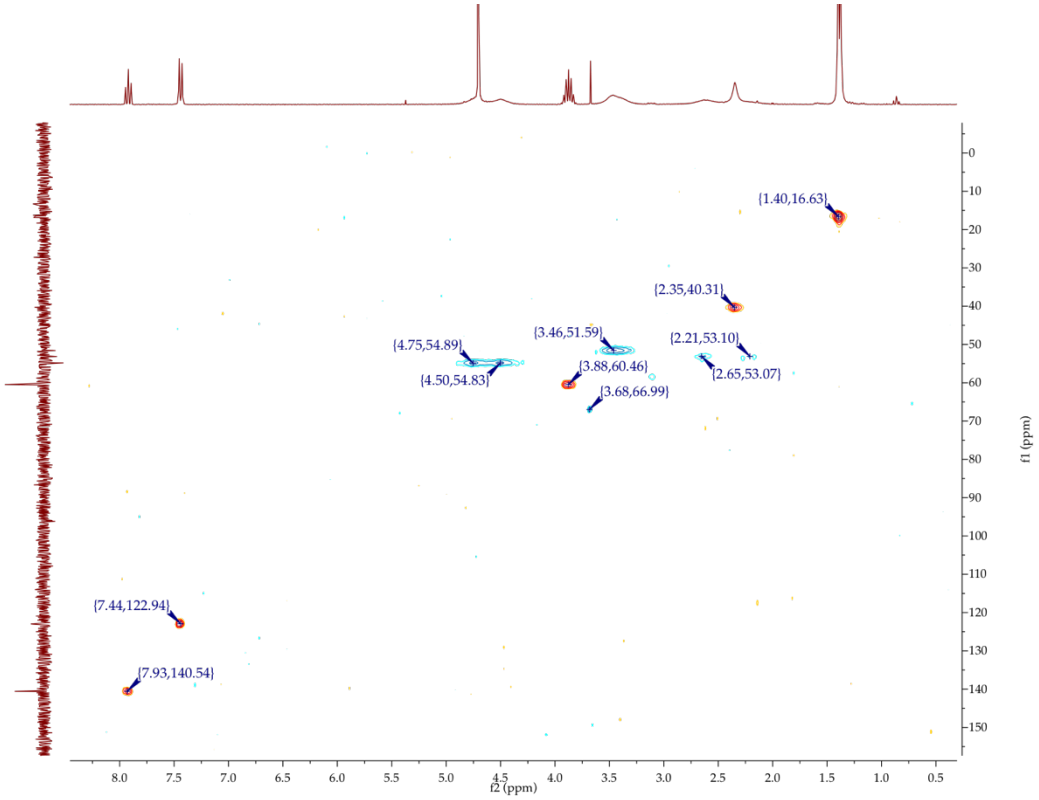

Figure S3. 2D ^{1}H-^{13}C HSQC-NMR spectrum of **L1** in D_2O at 298 K.

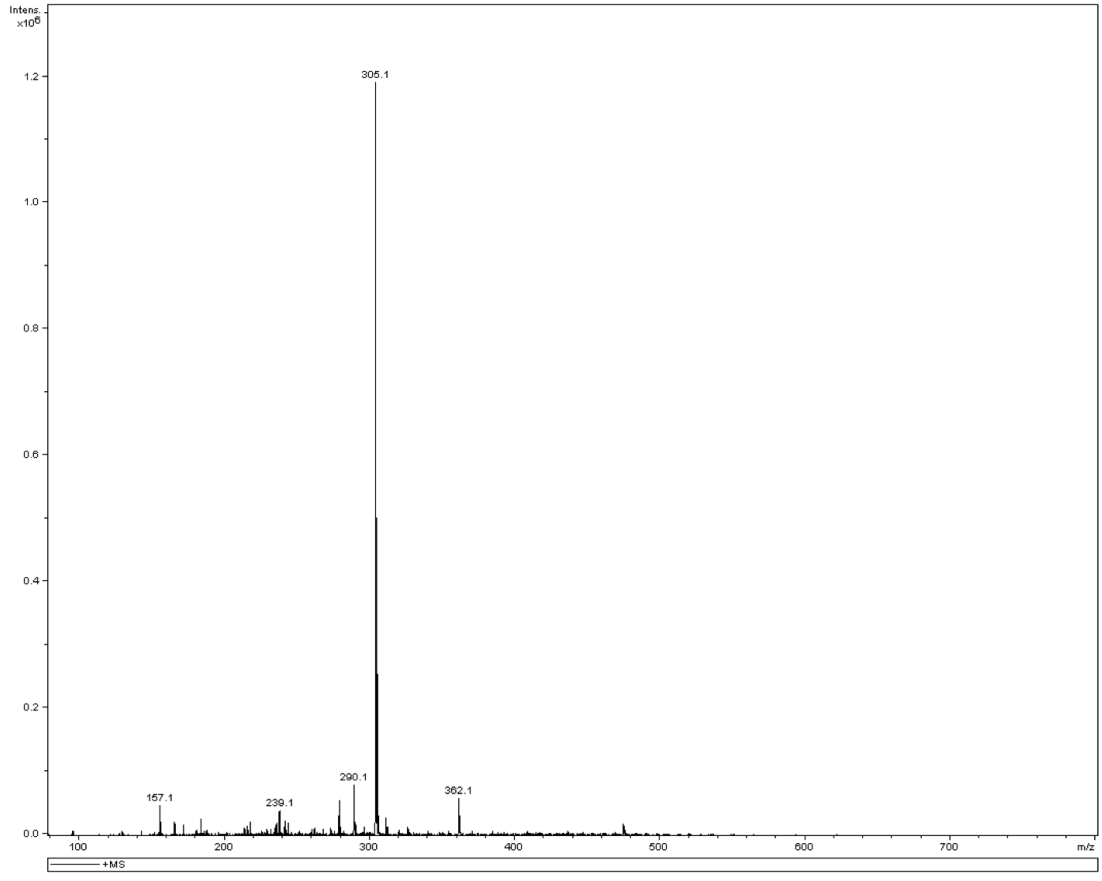

Figure S4. LC-MS (ESI/APCI-TOF) of **L1** in H_2O.

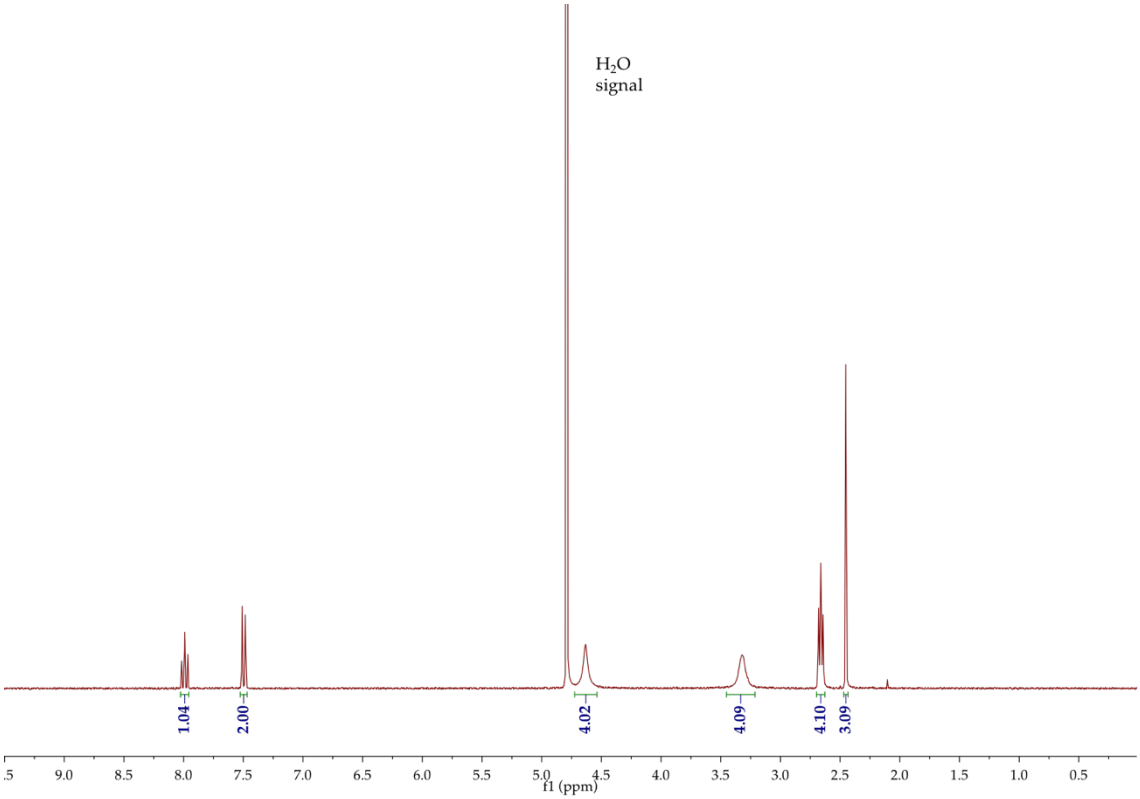

Figure S5. ^{1}H-NMR spectrum of **L2** in D_2O at 298 K.

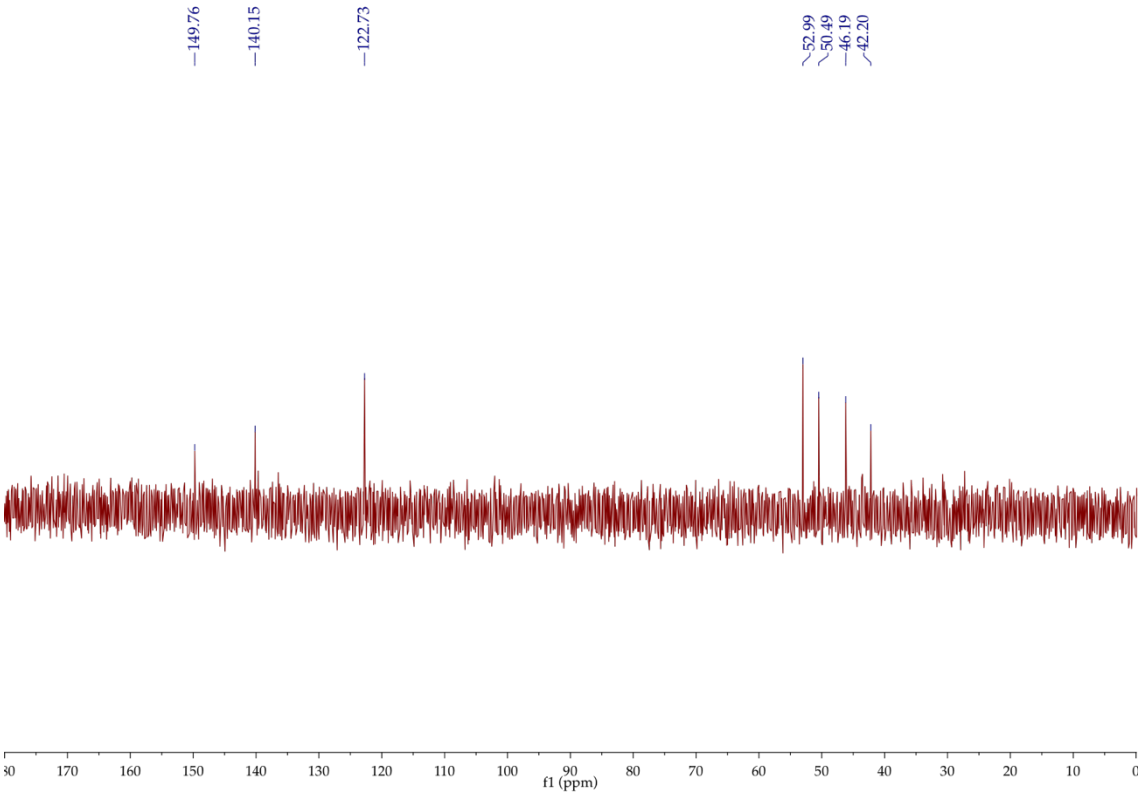

Figure S6. ^{13}C-NMR spectrum of **L2** in D_2O at 298 K.

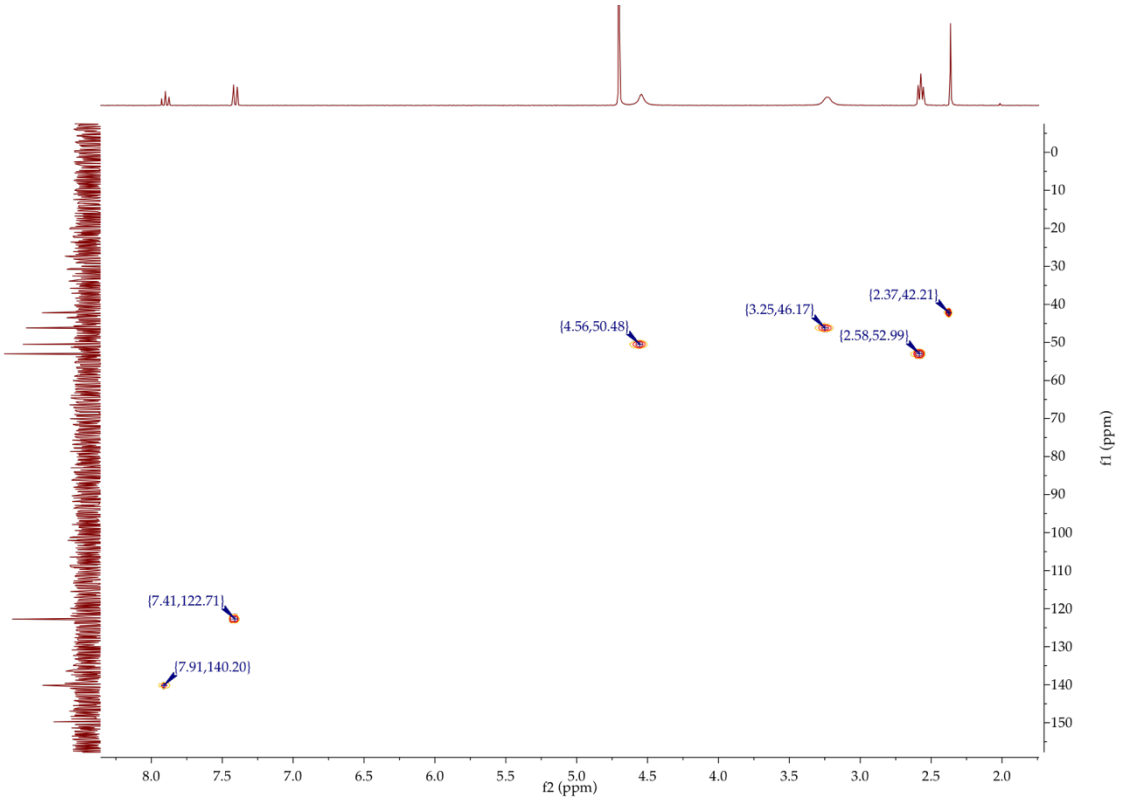

Figure S7. 2D ^{1}H-^{13}C HSQC-NMR spectrum of **L2** in D_2O at 298 K.

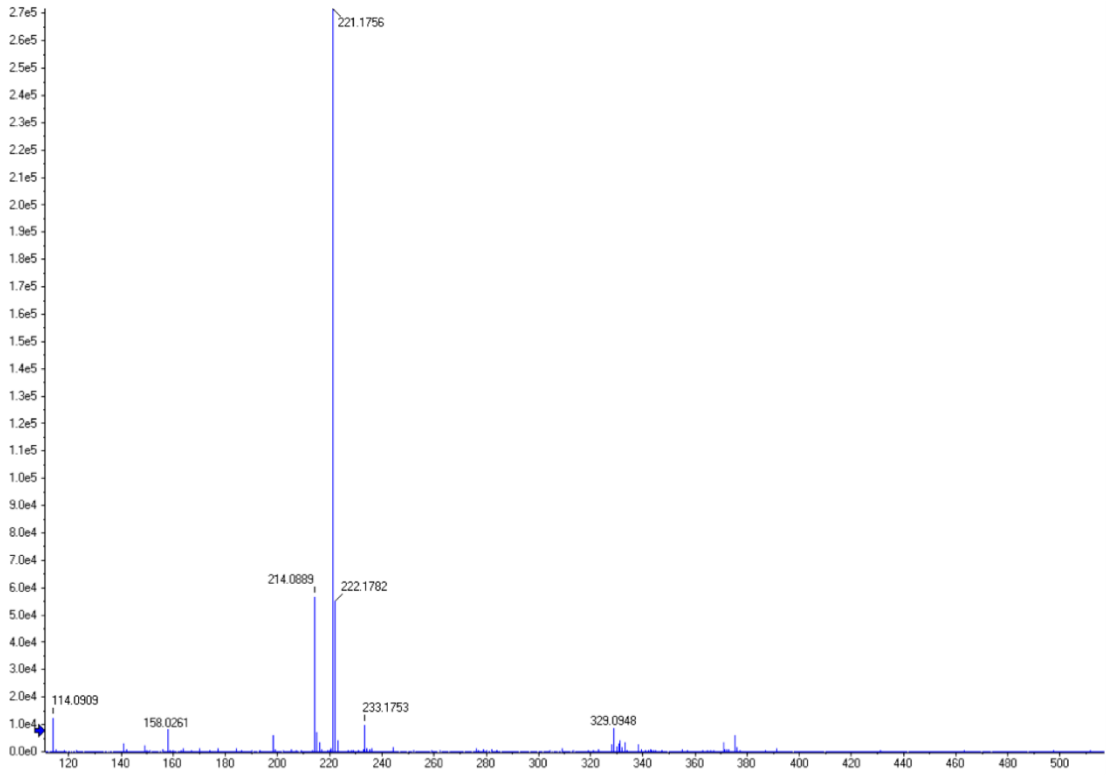

Figure S8. LC-MS (ESI/APCI-TOF) of **L2** in H_2O.

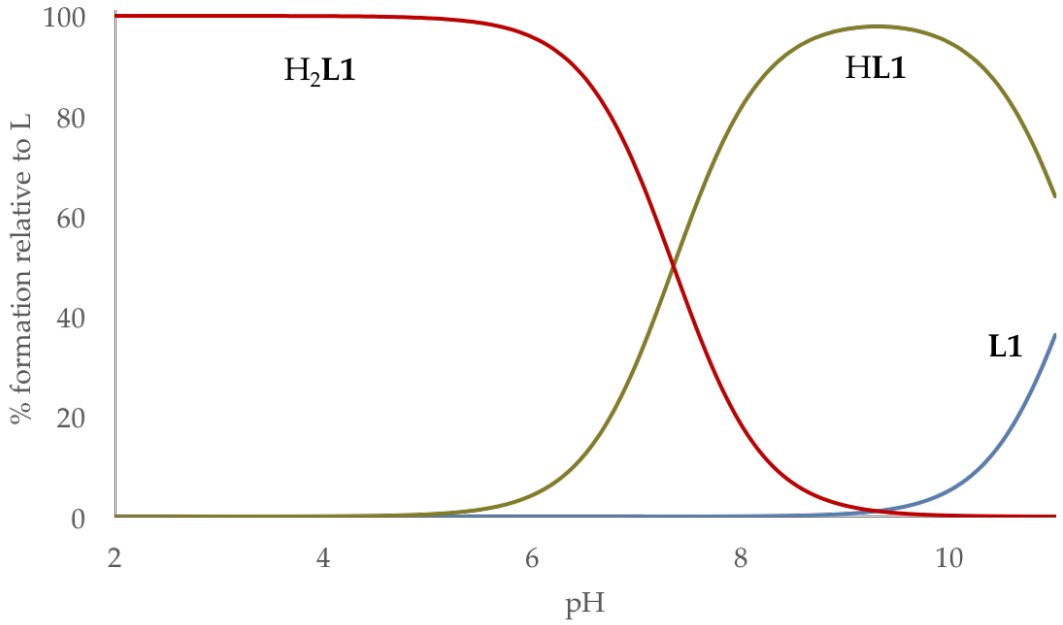

Figure S9. Distribution diagram of **L1** as a function of the pH in aqueous solution.

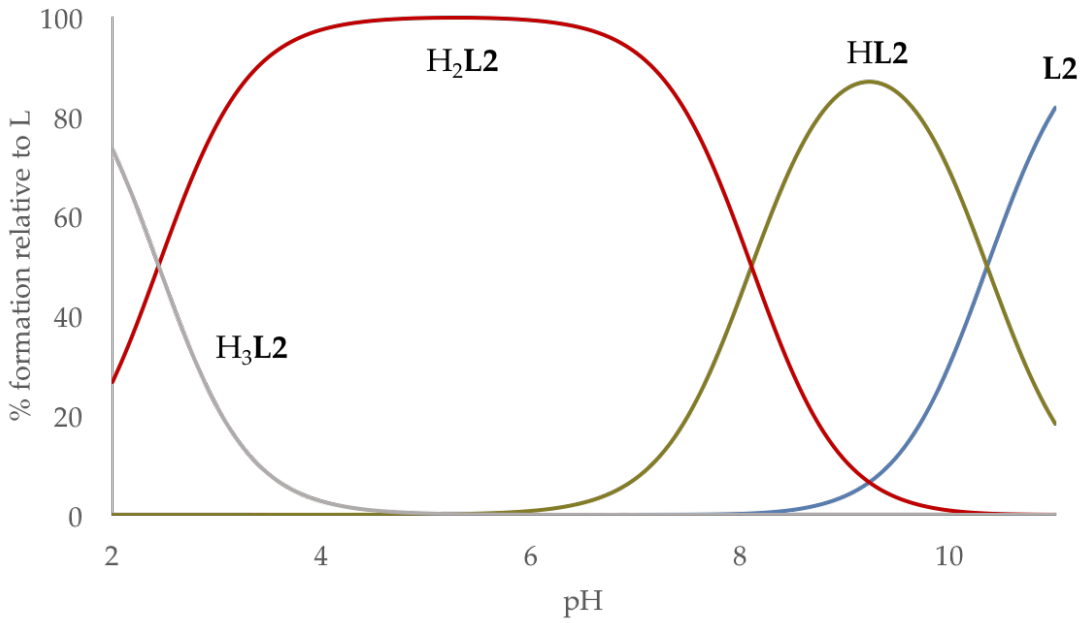

Figure S10. Distribution diagram of **L2** as a function of the pH in aqueous solution.

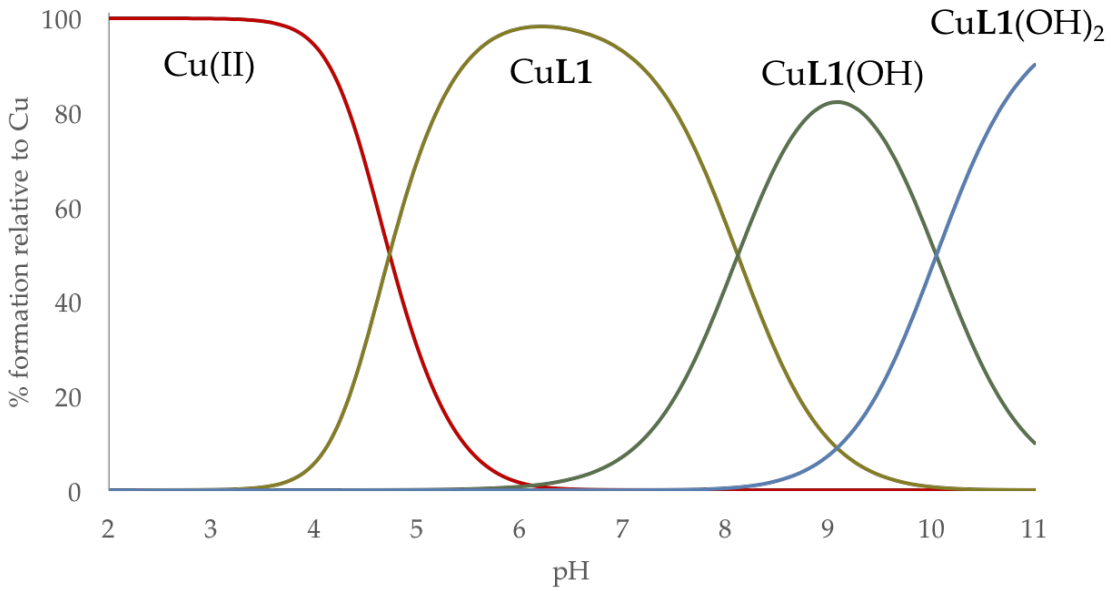

Figure S11. Distribution diagram of the Cu^{2+}:**L1** system as a function of the pH in aqueous solution.

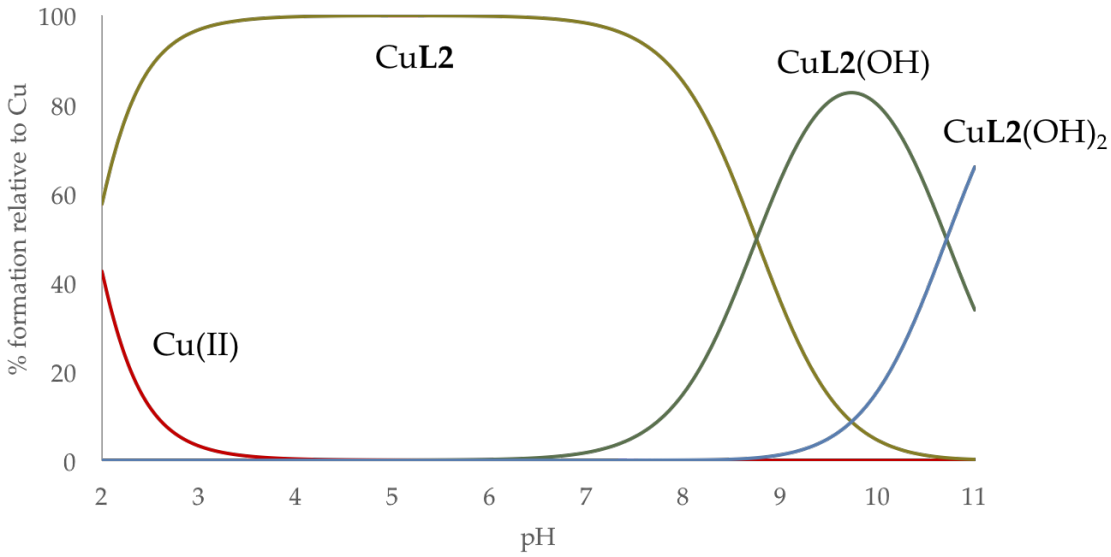

Figure S12. Distribution diagram of the Cu^{2+}:**L2** system as a function of the pH in aqueous solution.

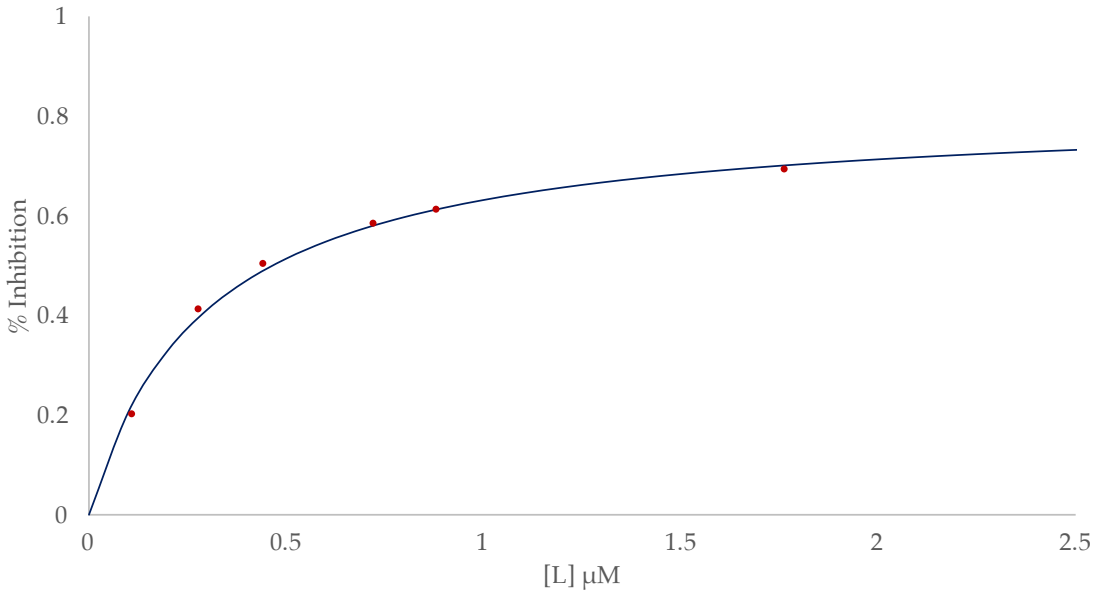

Figure S13. Fitting of the SOD activity data obtained by the McCord-Fridovich method for the system Cu-**L1**-N_3^-, 1:1:1 molar ratio.

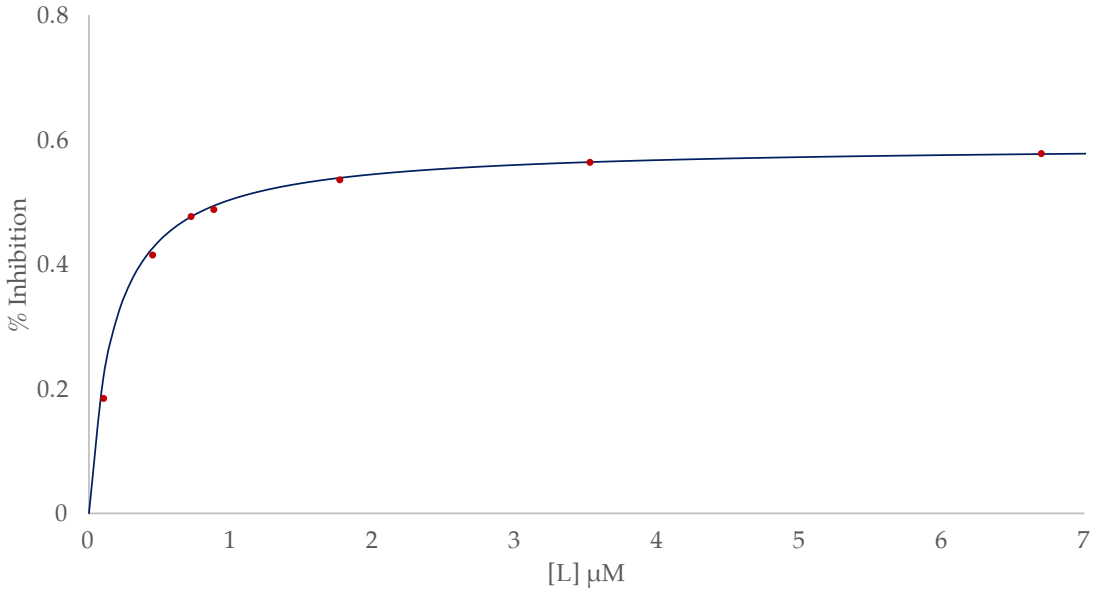

Figure S14. Fitting of the SOD activity data obtained by the McCord-Fridovich method for the system Cu-**L1**-N_3^-, 1:1:6 molar ratio.

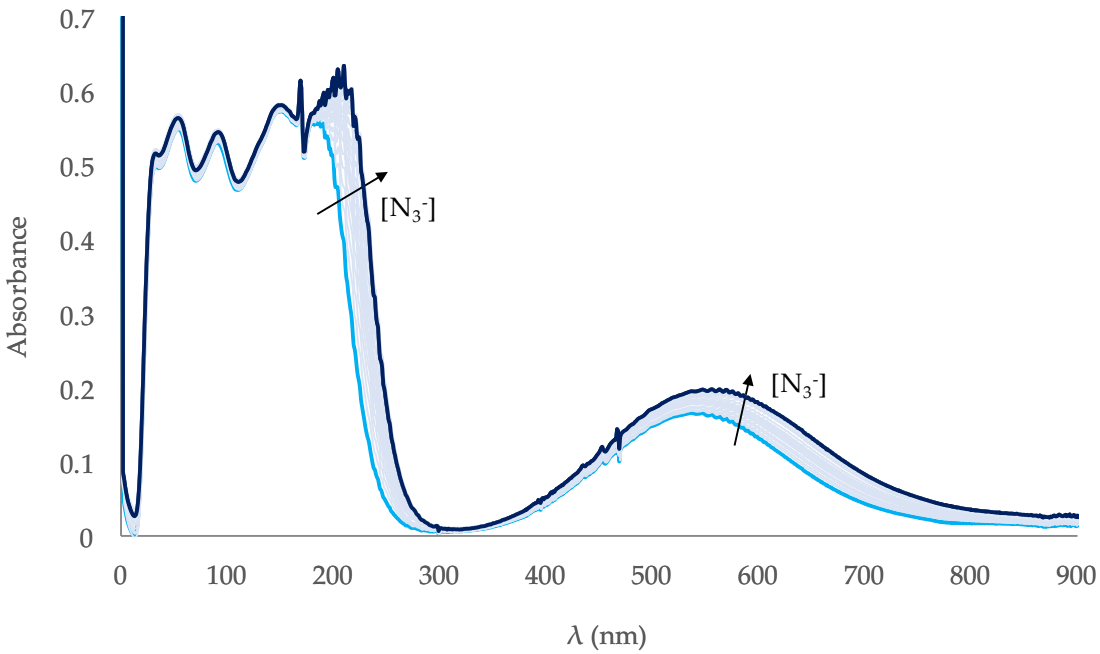

Figure S15. UV Vis spectra of $[Cu\mathbf{L1}(H_2O)]^{2+}$ versus $[N_3^-]$.

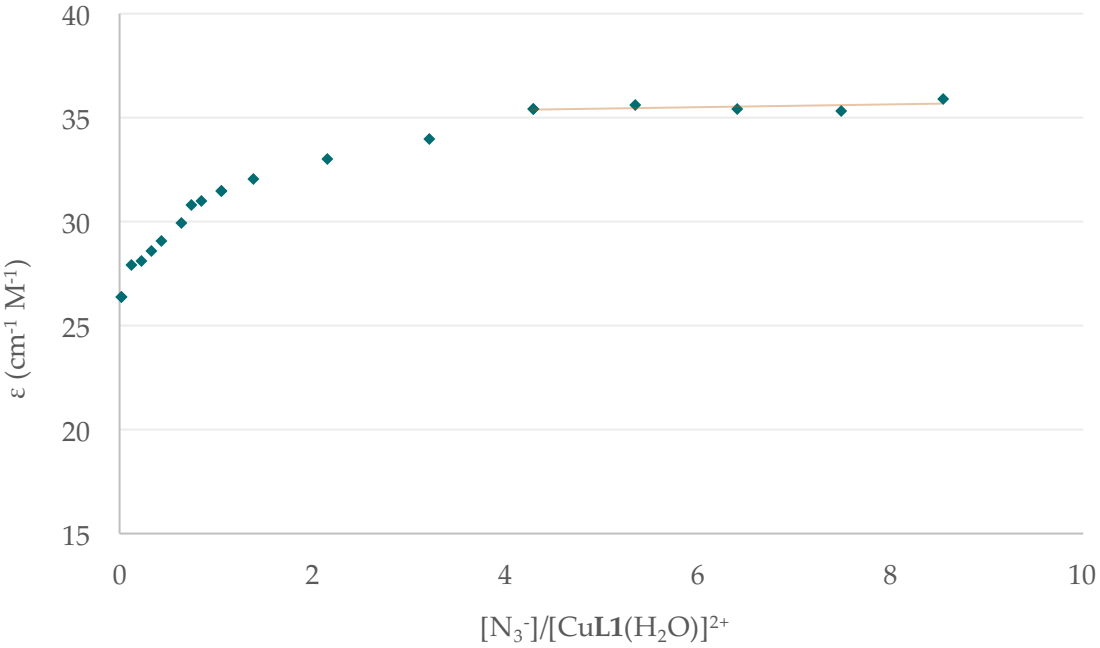

Figure S16 Absorbance at 573 nm versus $[N_3^-]/[Cu\mathbf{L1}(H_2O)]^{2+}$ ratio.

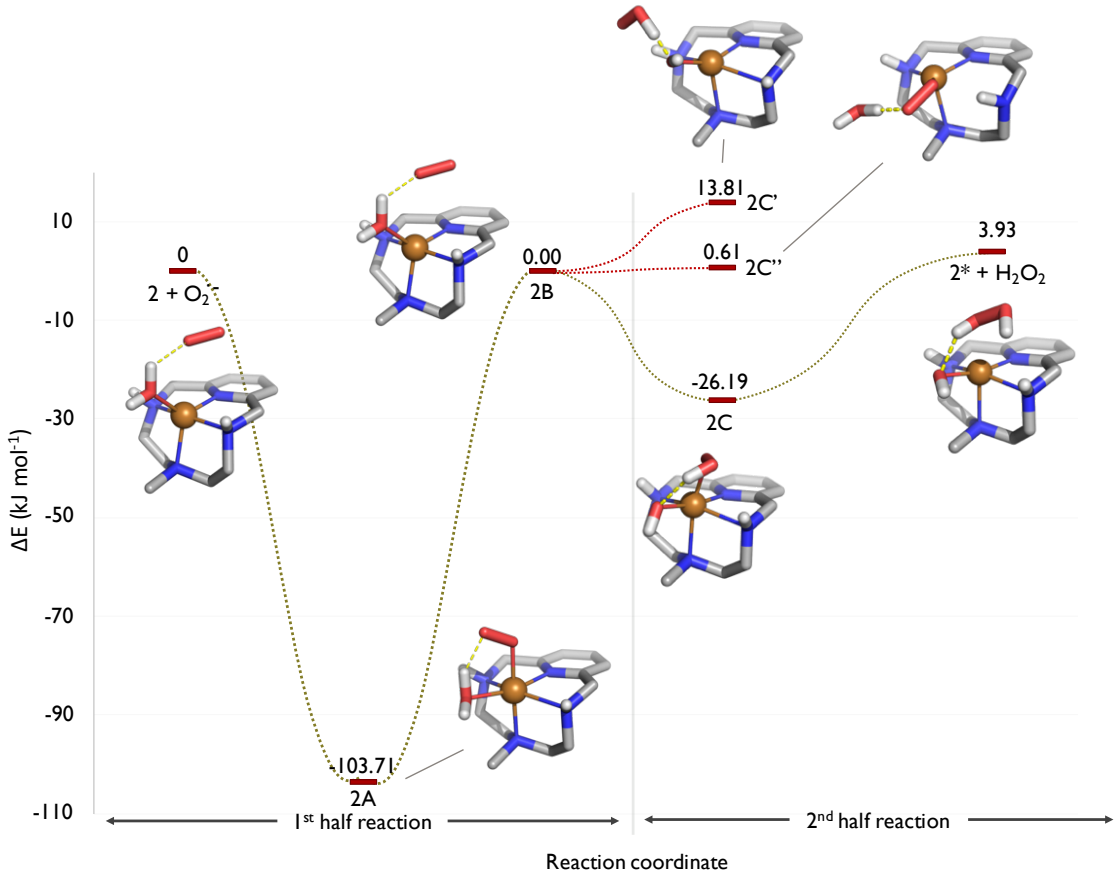

Figure S17. Energy profile (kJ mol^{-1}, B3LYP-D3/def2-svp/Cu(MDF10)) for the reaction mechanism of the catalytic oxidation and reduction of two species of superoxide by complex **2**. Structure **2*** corresponds to the hydroxylated form of **2**.

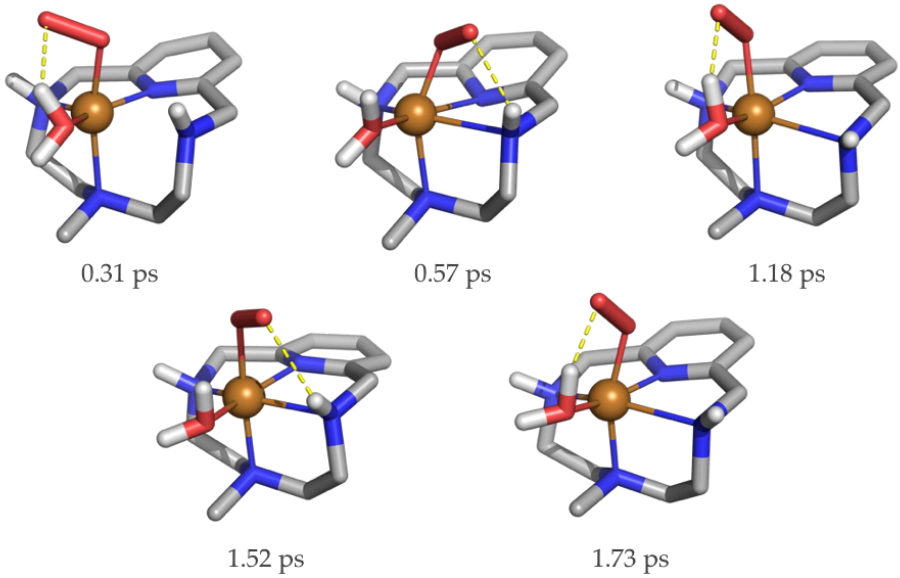

Figure S18. Representation of the different conformations adopted by adduct **2A** all along the QM/MM MD modelling. Structures taken at 0.31, 0.57, 1.18, 1.52 and 1.73 ps since the starting of the calculation.

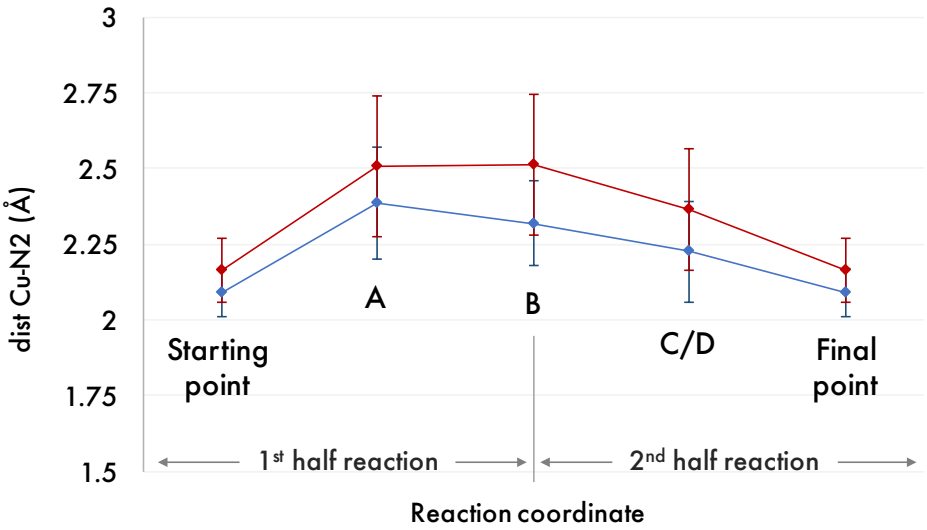

Figure S19. Distance Cu-N2 (Å) for complex **1** (red line) and **2** (blue line) along the catalytic mechanism.

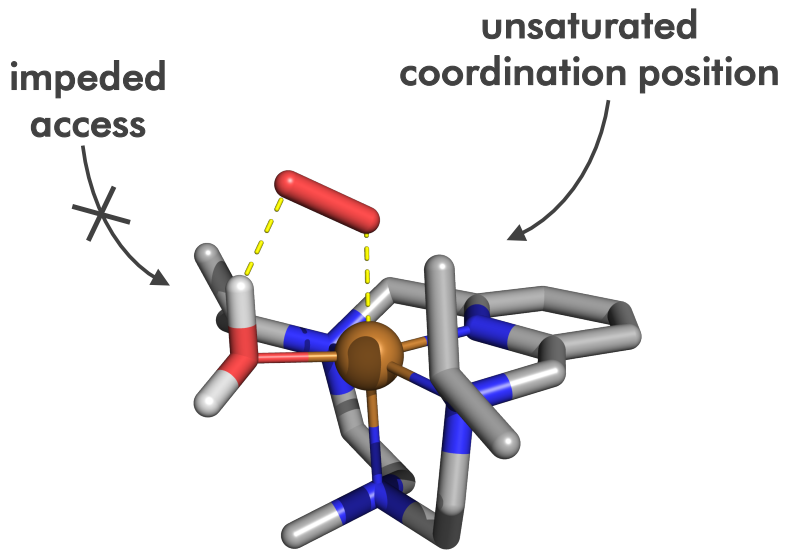

Figure S20. Entering of the superoxide into **1**. The water molecule prevents the entering by face A but orientates the entrance by a hydrogen-bond with the superoxide.

III. Tables

Table S1. Stepwise protonation logarithm constants for **L1** and **L2** measured in 0.15 M $NaClO_4$ at 298.1 K.

Reaction[a]	log K_a (**L1**)	log K_a (**L2**)
$H + L \rightleftarrows HL$	11.25(1)	10.35(1)[b]
$H + HL \rightleftarrows H_2L$	7.345(7)	8.09(2)
$H + H_2L \rightleftarrows H_3L$	-	2.47(6)

a) Charges omitted. b) Values in parenthesis are standard deviations in the last significant figure.

Table S2. Distribution of the Cu(II)-N and Cu(II)-O distances (Å) in complexes **1** and **2** along QM/MM-MD trajectories in the absence of superoxide. The variation between the values of the two complexes (noted as **Δd**) is shown.

		distance (Å)				
cmp	value	**Cu-N1**	**Cu-N2**	**Cu-N3**	**Cu-N4**	**Cu-O5**
1	mean	1.97 ± 0.13	2.28 ± 0.17	2.19 ± 0.15	2.16 ± 0.19	2.02 ± 0.12
2	mean	1.97 ± 0.12	2.19 ± 0.16	2.08 ± 0.16	1.97 ± 0.19	2.04 ± 0.11
	Δd*	**0.00**	**-0.09**	**-0.11**	**-0.19**	**0.02**
1	width**	0.66	1.21	1.23	0.78	0.82
2	width**	0.63	0.99	0.44	0.52	0.64
	Δwidth	**-0.03**	**-0.22**	**-0.79**	**-0.26**	**-0.18**

(*) Δd is defined as the difference between the distance found in **2** and **1**.
(**) Difference between maximum and minimum value of the distribution.

Table S3. Crystal data and structure refinement for [Cu**L1**(N_3^-)](ClO_4).

	[Cu**L1**(N_3^-)](ClO_4)
Empirical formula	$C_{18}H_{32}ClCuN_7O_4$
Formula weight	509.49
Temperature/K	120.0(1)
Crystal system	monoclinic
Space group	C*c*
a/Å	9.682(2)
b/Å	18.886(6)
c/Å	24.789(7)
α/°	90
β/°	99.902(11)
γ/°	90
Volume/Å^3	4465(2)
Z	8
d(calc) /g cm^{-3}	1.516
μ/mm^{-1}	1.138
F(000)	2136.0
2Θ range	2.400 to 36.327
Radiation	0.71073
Refl. collected	118824
Independent refl.	21612
R_{int}	0.0365
restraints/param	2/803
GOF	1.037
R_1, wR_2[I>=2σ (I)]	0.0276, 0.0615
R_1, wR_2[all data]	0.0349, 0.0654

IV.- Gas phase geometry optimization

An initial small benchmarking for the ground state geometry optimization of complex 1 was carried out using three different functionals (BP86, B3LYP and M06). The most relevant geometrical parameters are shown in Tables S5 and S6. All the geometries were compared with the crystal structure of **1**.

For the smallest basis set, all the computed geometries are in reasonably good agreement with the experimental structure obtained by X-Ray analysis (RMSd values < 0.20). The distances Cu-alkylated nitrogens (N2-N4) in all the computed structures differ less than a 3 % from the experimental model. In contrast, the distance Cu-pyridine nitrogen deviates less than a 1 % from the experimental data. Larger differences were found for the distance Cu-O (up to a 8 %) that could be due to the crystal packing effect. The geometry index (τ_5)[39] defines the trigonal bipyramidal/square pyramid molecular geometry of the coordination sphere. The closer to 0 the value of τ_5, the more trigonal bipyramidal the geometry is. On the other side, a closer value to 1 corresponds to square pyramid geometry. 1 has a distorted square pyramidal molecular geometry in the solved crystal structure ($\tau_5 = 0.24$) like in all the optimized geometries. However, the use of the hybrid functionals B3LYP and M06 give results more in consonant with the crystallographic data (Tables S5 and S6).

Table S4. Measured Cu(II)-N and Cu(II)-O distances (Å) in the optimized ground state geometries of 1 at different levels of theory and deviation from the X-Ray structure values (%). Deviations higher than 1 % are highlighted in red.

	X-Ray	BP86		M06		B3LYP		B3LYP-D3 (SVP)		B3LYP-D3 (TZVP)	
	d (Å)	d (Å)	% desv.	d (Å)	% desv.	d (Å)	% desv.	d (Å)	% desv.	d (Å)	% desv.
Cu-N1	1.935	1.955	1.03	1.952	0.88	1.958	1.19	1.954	0.98	1.948	0.67
Cu-N2	2.102	2.167	3.09	2.117	0.71	2.151	2.33	2.131	1.38	2.119	0.81
Cu-N3	2.191	2.186	-0.23	2.163	-1.28	2.203	0.55	2.184	-0.32	2.174	-0.78
Cu-N4	2.103	2.165	2.95	2.114	0.52	2.151	2.28	2.129	1.24	2.119	0.76
Cu-O	1.977	2.138	8.14	2.123	7.38	2.125	7.49	2.103	6.37	2.128	7.64
RMSd (Å)	-	0.201		0.174		0.184		0.170		0.155	

Table S5. Measured angles (º), geometry index in the optimized ground state geometries of 1 at different levels of theory and deviation from the X-Ray structure values (%). Deviations higher than 1 % are highlighted in red.

	X-Ray	BP86		M06		B3LYP		B3LYP-D3 (def2-SVP)		B3LYP-D3 (def2-TZVP)	
	Angle (º)	Angle (º)	% desv	Angle (º)	% desv	Angle (º)	% desv	Angle (º)	% desv	Angle (º)	% desv
N1-Cu-N2	82.48	82.78	0.36	82.78	0.36	82.68	0.24	82.83	0.42	83.00	0.63
N1-Cu-N3	100.03	104.44	4.41	104.36	4.33	104.12	4.09	103.42	3.39	104.29	4.26
N1-Cu-N4	82.39	82.79	0.49	82.86	0.57	82.68	0.35	82.89	0.61	83.00	0.74
N1-Cu-O	160.68	157.54	-1.95	159.47	-0.75	159.26	-0.88	160.69	0.01	159.83	-0.53
N2-Cu-N3	86.66	87.56	1.04	87.55	1.03	87.56	1.04	87.64	1.13	87.73	1.23
N2-Cu-N4	162.14	163.18	0.64	163.24	0.68	162.94	0.49	163.55	0.87	163.73	0.98
N2-Cu-O	99.23	100.35	1.13	99.23	0.00	98.35	-0.89	98.85	-0.38	98.01	-1.23
N3-Cu-N4	86.70	87.71	1.16	87.68	1.13	87.56	0.99	87.78	1.25	87.74	1.20
N3-Cu-O	99.29	97.93	-1.37	96.14	-3.17	96.62	-2.69	95.88	-3.43	95.88	-3.43
N4-Cu-O	98.20	111.17	13.21	97.25	-0.97	98.45	0.25	97.33	-0.89	97.99	-0.21
τ	0.024	0.094	-	0.063	-	0.061	-	0.048	-	0.065	-

We also expanded the size of the basis set and we introduced the Grimm's dispersion correction.[16] For the latter case, the deviation respect to the crystal structure is reduced up to a 50% using B3LYP-D3/def2-SVP. As example, the deviation distances Cu-N2 and Cu-N4 with respect to the X-Ray structure decreases from 0.049 Å to 0.026 Å, respectively. These observations are in accordance to previous works which show an insufficiently account for dispersion for the B3LYP functional.[40] On the other hand, the inclusion of the extra valence basis (triple zeta) in the basis set [17,41–43] shows a marginal influence on the optimized geometries since we are using in all case an ECP for the copper atom. Thus, as result of our benchmarking, we chose B3LYP-D3/def2-SVP as method for the following computations.

V.- Geometries and energies of the optimized structures

Geometry and energy of **1** + $O_2^{\cdot -}$ structure in z-matrix format.
Energy = -1346.985569 Hartrees

Geometry:
C
C 1 r2
C 2 r3 1 a3
C 2 r4 1 a4 3 d4
C 2 r5 1 a5 3 d5
C 3 r6 2 a6 1 d6
C 1 r7 2 a7 3 d7
C 7 r8 1 a8 2 d8
C 1 r9 2 a9 3 d9
C 2 r10 1 a10 3 d10
C 4 r11 2 a11 1 d11
C 4 r12 2 a12 1 d12
C 8 r13 7 a13 1 d13
C 9 r14 1 a14 2 d14
C 3 r15 2 a15 1 d15
C 10 r16 2 a16 1 d16
C 7 r17 1 a17 2 d17
C 9 r18 1 a18 2 d18
O 14 r19 9 a19 1 d19
N 4 r20 2 a20 1 d20
N 17 r21 7 a21 1 d21
N 5 r22 2 a22 1 d22
N 11 r23 4 a23 2 d23
H 15 r24 3 a24 2 d24
H 15 r25 3 a25 2 d25
H 17 r26 7 a26 1 d26
H 18 r27 9 a27 1 d27
H 17 r28 7 a28 1 d28
H 18 r29 9 a29 1 d29
H 17 r30 7 a30 1 d30
H 19 r31 14 a31 9 d31
H 19 r32 14 a32 9 d32
H 5 r33 2 a33 1 d33
H 3 r34 2 a34 1 d34
H 5 r35 2 a35 1 d35
H 6 r36 3 a36 2 d36
H 6 r37 3 a37 2 d37
H 6 r38 3 a38 2 d38

H 7 r39 1 a39 2 d39
H 7 r40 1 a40 2 d40
H 8 r41 7 a41 1 d41
H 8 r42 7 a42 1 d42
H 9 r43 1 a43 2 d43
H 10 r44 2 a44 1 d44
H 11 r45 4 a45 2 d45
H 11 r46 4 a46 2 d46
H 1 r47 2 a47 3 d47
H 1 r48 2 a48 3 d48
H 12 r49 4 a49 2 d49
H 13 r50 8 a50 7 d50
H 13 r51 8 a51 7 d51
H 14 r52 9 a52 1 d52
H 14 r53 9 a53 1 d53
H 14 r54 9 a54 1 d54
H 15 r55 3 a55 2 d55
H 16 r56 10 a56 2 d56
H 18 r57 9 a57 1 d57
C 20 r58 4 a58 2 d58
O 52 r59 14 a59 9 d59
O 59 r60 52 a60 14 d60
Variables:
r2= 3.2196
r3= 5.4259
a3= 86.46
r4= 2.3320
a4= 113.86
d4= 23.71
r5= 1.5216
a5= 47.31
d5= 236.71
r6= 1.5304
a6= 85.73
d6= 250.33
r7= 1.5349
a7= 76.33
d7= 298.62
r8= 2.4460
a8= 143.80
d8= 67.41
r9= 2.4588
a9= 82.29
d9= 88.49

r10= 1.3971
a10= 126.93
d10= 135.33
r11= 1.5200
a11= 146.81
d11= 312.98
r12= 1.3974
a12= 91.57
d12= 131.99
r13= 1.5345
a13= 144.04
d13= 1.04
r14= 1.5314
a14= 144.50
d14= 329.05
r15= 1.5348
a15= 131.31
d15= 135.66
r16= 1.3961
a16= 118.95
d16= 237.52
r17= 2.4384
a17= 102.01
d17= 122.27
r18= 1.5349
a18= 97.38
d18= 112.27
r19= 3.3503
a19= 80.09
d19= 301.97
r20= 1.3428
a20= 29.75
d20= 309.62
r21= 1.4655
a21= 34.02
d21= 244.47
r22= 1.4652
a22= 114.34
d22= 34.29
r23= 1.4676
a23= 114.44
d23= 33.30
r24= 1.1001
a24= 110.33

d24= 161.58
r25= 1.1017
a25= 111.18
d25= 42.59
r26= 1.0978
a26= 90.51
d26= 11.52
r27= 1.1002
a27= 110.37
d27= 145.88
r28= 1.1082
a28= 94.47
d28= 120.49
r29= 1.1007
a29= 112.17
d29= 26.12
r30= 1.0981
a30= 144.00
d30= 250.95
r31= 0.9700
a31= 47.79
d31= 215.47
r32= 0.9683
a32= 150.75
d32= 188.24
r33= 1.1003
a33= 106.46
d33= 153.86
r34= 1.1040
a34= 109.81
d34= 356.87
r35= 1.1066
a35= 108.78
d35= 267.98
r36= 1.1001
a36= 112.57
d36= 284.58
r37= 1.1015
a37= 109.71
d37= 165.90
r38= 1.0998
a38= 111.18
d38= 45.37
r39= 1.1085

a39= 108.00
d39= 212.95
r40= 1.0988
a40= 109.25
d40= 328.13
r41= 1.0982
a41= 80.03
d41= 251.85
r42= 1.1087
a42= 102.05
d42= 147.11
r43= 1.1034
a43= 82.63
d43= 219.85
r44= 1.0928
a44= 120.09
d44= 56.80
r45= 1.1004
a45= 106.40
d45= 273.72
r46= 1.1065
a46= 108.77
d46= 159.46
r47= 1.1080
a47= 97.76
d47= 192.71
r48= 1.0998
a48= 152.07
d48= 43.67
r49= 1.0923
a49= 120.10
d49= 181.52
r50= 1.1002
a50= 109.13
d50= 85.11
r51= 1.1079
a51= 107.22
d51= 199.49
r52= 1.1006
a52= 111.34
d52= 329.53
r53= 1.1011
a53= 109.84
d53= 208.31

r54= 1.1008
a54= 112.64
d54= 89.58
r55= 1.1006
a55= 112.02
d55= 281.37
r56= 1.0922
a56= 120.47
d56= 179.86
r57= 1.1020
a57= 111.20
d57= 264.91
r58= 2.0305
a58= 117.87
d58= 158.46
r59= 2.5610
a59= 139.26
d59= 115.28
r60= 1.2029
a60= 156.81
d60= 288.96

Geometry and energy of **1A** structure in z-matrix format.
Energy = -1346.998916 Hartrees

Geometry:
N
C 1 r2
C 2 r3 1 a3
C 3 r4 2 a4 1 d4
C 4 r5 3 a5 2 d5
C 1 r6 2 a6 3 d6
C 2 r7 1 a7 3 d7
N 7 r8 2 a8 1 d8
C 1 r9 2 a9 3 d9
O 9 r10 1 a10 2 d10
O 10 r11 9 a11 1 d11
C 6 r12 1 a12 2 d12
N 12 r13 6 a13 1 d13
C 13 r14 12 a14 6 d14
C 14 r15 13 a15 12 d15

N 15 r16 14 a16 13 d16
C 16 r17 15 a17 14 d17
C 16 r18 15 a18 14 d18
C 8 r19 7 a19 2 d19
C 8 r20 7 a20 2 d20
C 20 r21 8 a21 7 d21
C 20 r22 8 a22 7 d22
C 13 r23 12 a23 6 d23
C 23 r24 13 a24 12 d24
C 23 r25 13 a25 12 d25
O 9 r26 1 a26 2 d26
H 24 r27 23 a27 13 d27
H 24 r28 23 a28 13 d28
H 17 r29 16 a29 15 d29
H 21 r30 20 a30 8 d30
H 17 r31 16 a31 15 d31
H 21 r32 20 a32 8 d32
H 17 r33 16 a33 15 d33
H 26 r34 9 a34 1 d34
H 26 r35 9 a35 1 d35
H 7 r36 2 a36 1 d36
H 23 r37 13 a37 12 d37
H 7 r38 2 a38 1 d38
H 25 r39 23 a39 13 d39
H 25 r40 23 a40 13 d40
H 25 r41 23 a41 13 d41
H 18 r42 16 a42 15 d42
H 18 r43 16 a43 15 d43
H 15 r44 14 a44 13 d44
H 15 r45 14 a45 13 d45
H 20 r46 8 a46 7 d46
H 3 r47 2 a47 1 d47
H 12 r48 6 a48 1 d48
H 12 r49 6 a49 1 d49
H 19 r50 8 a50 7 d50
H 19 r51 8 a51 7 d51
H 5 r52 4 a52 3 d52
H 14 r53 13 a53 12 d53
H 14 r54 13 a54 12 d54
H 22 r55 20 a55 8 d55
H 22 r56 20 a56 8 d56
H 22 r57 20 a57 8 d57
H 24 r58 23 a58 13 d58
H 4 r59 3 a59 2 d59

H 21 r60 20 a60 8 d60
Variables:
r2= 1.3363
r3= 1.4001
a3= 120.50
r4= 1.3947
a4= 118.79
d4= 0.05
r5= 1.3986
a5= 119.55
d5= 0.66
r6= 1.3421
a6= 121.89
d6= 359.17
r7= 1.5258
a7= 118.80
d7= 182.34
r8= 1.4648
a8= 116.06
d8= 339.50
r9= 2.0396
a9= 120.64
d9= 186.46
r10= 2.0069
a10= 92.62
d10= 260.58
r11= 1.2635
a11= 120.13
d11= 334.23
r12= 1.5203
a12= 117.74
d12= 178.93
r13= 1.4714
a13= 115.48
d13= 35.20
r14= 1.4746
a14= 112.92
d14= 72.44
r15= 1.5283
a15= 114.64
d15= 278.92
r16= 1.4795
a16= 113.95
d16= 309.46

r17= 1.4712
a17= 111.65
d17= 288.62
r18= 1.4799
a18= 110.13
d18= 164.22
r19= 1.4699
a19= 113.20
d19= 272.61
r20= 1.5005
a20= 113.93
d20= 144.95
r21= 1.5359
a21= 113.52
d21= 65.40
r22= 1.5277
a22= 112.74
d22= 298.55
r23= 1.5020
a23= 112.77
d23= 198.81
r24= 1.5350
a24= 113.51
d24= 306.30
r25= 1.5262
a25= 112.88
d25= 74.45
r26= 2.1741
a26= 166.85
d26= 309.99
r27= 1.1001
a27= 109.92
d27= 190.81
r28= 1.1015
a28= 111.56
d28= 72.06
r29= 1.0966
a29= 109.85
d29= 179.04
r30= 1.1007
a30= 109.91
d30= 177.04
r31= 1.1064
a31= 111.65

d31= 300.03
r32= 1.1001
a32= 112.78
d32= 57.51
r33= 1.0979
a33= 109.93
d33= 60.49
r34= 0.9729
a34= 103.10
d34= 315.80
r35= 0.9684
a35= 120.19
d35= 199.30
r36= 1.0995
a36= 105.67
d36= 99.81
r37= 1.1024
a37= 104.06
d37= 189.67
r38= 1.1075
a38= 108.19
d38= 212.65
r39= 1.0996
a39= 112.76
d39= 298.12
r40= 1.1000
a40= 109.48
d40= 178.43
r41= 1.0976
a41= 111.05
d41= 58.58
r42= 1.1066
a42= 110.43
d42= 79.84
r43= 1.0979
a43= 107.75
d43= 324.19
r44= 1.0971
a44= 109.81
d44= 70.10
r45= 1.1069
a45= 108.43
d45= 186.06
r46= 1.1022

a46= 103.81
d46= 183.02
r47= 1.0919
a47= 120.21
d47= 179.78
r48= 1.1012
a48= 105.80
d48= 276.11
r49= 1.1052
a49= 108.29
d49= 161.38
r50= 1.1086
a50= 111.80
d50= 307.93
r51= 1.0995
a51= 107.43
d51= 191.61
r52= 1.0916
a52= 120.97
d52= 178.91
r53= 1.0997
a53= 107.53
d53= 157.41
r54= 1.1074
a54= 111.94
d54= 41.57
r55= 1.0974
a55= 111.89
d55= 311.18
r56= 1.0996
a56= 109.19
d56= 190.95
r57= 1.1013
a57= 112.54
d57= 72.92
r58= 1.1009
a58= 112.25
d58= 310.35
r59= 1.0924
a59= 120.26
d59= 179.86
r60= 1.1018
a60= 111.30
d60= 295.63

Geometry and energy of **1B** structure in z-matrix format.
Energy = -1346.985562 Hartrees

Geometry:
C
C 1 r2
C 2 r3 1 a3
N 3 r4 2 a4 1 d4
C 4 r5 3 a5 2 d5
C 1 r6 2 a6 3 d6
C 3 r7 2 a7 1 d7
N 7 r8 3 a8 2 d8
C 8 r9 7 a9 3 d9
C 9 r10 8 a10 7 d10
C 4 r11 3 a11 2 d11
O 11 r12 4 a12 3 d12
C 5 r13 4 a13 3 d13
N 13 r14 5 a14 4 d14
C 14 r15 13 a15 5 d15
C 15 r16 14 a16 13 d16
C 8 r17 7 a17 3 d17
C 17 r18 8 a18 7 d18
N 18 r19 17 a19 8 d19
C 19 r20 18 a20 17 d20
C 14 r21 13 a21 5 d21
C 19 r22 18 a22 17 d22
C 15 r23 14 a23 13 d23
C 9 r24 8 a24 7 d24
O 4 r25 3 a25 2 d25
O 25 r26 4 a26 3 d26
H 24 r27 9 a27 8 d27
H 24 r28 9 a28 8 d28
H 22 r29 19 a29 18 d29
H 23 r30 15 a30 14 d30
H 22 r31 19 a31 18 d31
H 23 r32 15 a32 14 d32
H 22 r33 19 a33 18 d33
H 12 r34 11 a34 4 d34
H 12 r35 11 a35 4 d35
H 13 r36 5 a36 4 d36
H 9 r37 8 a37 7 d37
H 13 r38 5 a38 4 d38
H 10 r39 9 a39 8 d39
H 10 r40 9 a40 8 d40

H 10 r41 9 a41 8 d41
H 20 r42 19 a42 18 d42
H 20 r43 19 a43 18 d43
H 18 r44 17 a44 8 d44
H 18 r45 17 a45 8 d45
H 15 r46 14 a46 13 d46
H 6 r47 1 a47 2 d47
H 7 r48 3 a48 2 d48
H 7 r49 3 a49 2 d49
H 21 r50 14 a50 13 d50
H 21 r51 14 a51 13 d51
H 2 r52 1 a52 3 d52
H 17 r53 8 a53 7 d53
H 17 r54 8 a54 7 d54
H 16 r55 15 a55 14 d55
H 16 r56 15 a56 14 d56
H 16 r57 15 a57 14 d57
H 24 r58 9 a58 8 d58
H 1 r59 2 a59 3 d59
H 23 r60 15 a60 14 d60
Variables:
r2= 1.3968
r3= 1.3975
a3= 118.88
r4= 1.3428
a4= 121.24
d4= 359.29
r5= 1.3421
a5= 120.59
d5= 2.88
r6= 1.3965
a6= 119.10
d6= 358.60
r7= 1.5195
a7= 121.60
d7= 180.09
r8= 1.4677
a8= 114.36
d8= 214.52
r9= 1.4925
a9= 113.63
d9= 208.72
r10= 1.5299
a10= 112.18

d10= 65.86
r11= 2.0317
a11= 117.69
d11= 161.32
r12= 2.1231
a12= 156.64
d12= 109.84
r13= 1.5213
a13= 117.29
d13= 178.03
r14= 1.4655
a14= 114.35
d14= 326.73
r15= 1.4907
a15= 114.32
d15= 147.88
r16= 1.5323
a16= 112.05
d16= 298.83
r17= 1.4740
a17= 113.27
d17= 79.36
r18= 1.5349
a18= 114.99
d18= 282.54
r19= 1.4723
a19= 114.05
d19= 303.49
r20= 1.4728
a20= 112.38
d20= 157.90
r21= 1.4707
a21= 113.65
d21= 278.50
r22= 1.4659
a22= 112.40
d22= 285.62
r23= 1.5346
a23= 113.92
d23= 65.69
r24= 1.5358
a24= 113.84
d24= 298.43
r25= 3.1319

a25= 103.99
d25= 241.45
r26= 1.2028
a26= 79.22
d26= 26.00
r27= 1.1005
a27= 110.31
d27= 186.00
r28= 1.1019
a28= 111.18
d28= 67.00
r29= 1.0979
a29= 110.06
d29= 173.95
r30= 1.1007
a30= 110.34
d30= 176.53
r31= 1.1089
a31= 112.07
d31= 295.31
r32= 1.1011
a32= 112.11
d32= 56.87
r33= 1.0979
a33= 110.12
d33= 56.25
r34= 0.9689
a34= 115.58
d34= 22.58
r35= 0.9684
a35= 117.80
d35= 256.85
r36= 1.1001
a36= 106.52
d36= 86.40
r37= 1.1041
a37= 104.18
d37= 181.22
r38= 1.1076
a38= 108.77
d38= 200.43
r39= 1.1010
a39= 112.50
d39= 288.96

r40= 1.1003
a40= 109.78
d40= 170.25
r41= 1.0999
a41= 111.12
d41= 49.64
r42= 1.1087
a42= 111.05
d42= 80.58
r43= 1.0985
a43= 107.86
d43= 324.52
r44= 1.0983
a44= 109.34
d44= 64.24
r45= 1.1089
a45= 107.93
d45= 179.44
r46= 1.1021
a46= 104.08
d46= 183.52
r47= 1.0917
a47= 120.99
d47= 182.26
r48= 1.0999
a48= 106.48
d48= 95.02
r49= 1.1067
a49= 108.79
d49= 340.59
r50= 1.1083
a50= 111.73
d50= 313.07
r51= 1.0999
a51= 107.38
d51= 197.08
r52= 1.0914
a52= 120.98
d52= 179.15
r53= 1.0994
a53= 107.47
d53= 160.86
r54= 1.1081
a54= 111.64

d54= 44.96
r55= 1.1006
a55= 111.34
d55= 317.69
r56= 1.1005
a56= 109.85
d56= 196.36
r57= 1.1014
a57= 112.62
d57= 77.68
r58= 1.0999
a58= 112.08
d58= 305.77
r59= 1.0922
a59= 120.44
d59= 180.19
r60= 1.1017
a60= 111.25
d60= 295.63

Geometry and energy of **1C** structure in z-matrix format.
Energy = -1423.48637 Hartrees

Geometry:
C
C 1 r2
C 2 r3 1 a3
C 2 r4 1 a4 3 d4
C 2 r5 1 a5 3 d5
C 3 r6 2 a6 1 d6
C 1 r7 2 a7 3 d7
C 7 r8 1 a8 2 d8
C 1 r9 2 a9 3 d9
C 2 r10 1 a10 3 d10
C 4 r11 2 a11 1 d11
C 4 r12 2 a12 1 d12
C 8 r13 7 a13 1 d13
C 9 r14 1 a14 2 d14
C 3 r15 2 a15 1 d15
C 10 r16 2 a16 1 d16
C 8 r17 7 a17 1 d17

C 9 r18 1 a18 2 d18
O 6 r19 3 a19 2 d19
O 19 r20 6 a20 3 d20
O 19 r21 6 a21 3 d21
N 2 r22 1 a22 3 d22
N 8 r23 7 a23 1 d23
N 5 r24 2 a24 1 d24
N 11 r25 4 a25 2 d25
C 22 r26 2 a26 1 d26
H 15 r27 3 a27 2 d27
H 15 r28 3 a28 2 d28
H 17 r29 8 a29 7 d29
H 18 r30 9 a30 1 d30
H 17 r31 8 a31 7 d31
H 18 r32 9 a32 1 d32
H 17 r33 8 a33 7 d33
H 21 r34 19 a34 6 d34
H 21 r35 19 a35 6 d35
H 5 r36 2 a36 1 d36
H 3 r37 2 a37 1 d37
H 5 r38 2 a38 1 d38
H 6 r39 3 a39 2 d39
H 6 r40 3 a40 2 d40
H 6 r41 3 a41 2 d41
H 7 r42 1 a42 2 d42
H 7 r43 1 a43 2 d43
H 8 r44 7 a44 1 d44
H 8 r45 7 a45 1 d45
H 9 r46 1 a46 2 d46
H 10 r47 2 a47 1 d47
H 11 r48 4 a48 2 d48
H 11 r49 4 a49 2 d49
H 1 r50 2 a50 3 d50
H 1 r51 2 a51 3 d51
H 12 r52 4 a52 2 d52
H 13 r53 8 a53 7 d53
H 13 r54 8 a54 7 d54
H 14 r55 9 a55 1 d55
H 14 r56 9 a56 1 d56
H 14 r57 9 a57 1 d57
H 15 r58 3 a58 2 d58
H 16 r59 10 a59 2 d59
H 18 r60 9 a60 1 d60
O 51 r61 1 a61 2 d61

H 61 r62 51 a62 1 d62
H 61 r63 51 a63 1 d63
Variables:
r2= 3.2268
r3= 5.5551
a3= 84.65
r4= 2.3306
a4= 114.16
d4= 15.13
r5= 1.5204
a5= 46.88
d5= 227.15
r6= 1.5289
a6= 92.77
d6= 257.97
r7= 1.5324
a7= 73.64
d7= 298.09
r8= 2.4281
a8= 143.31
d8= 63.15
r9= 2.4448
a9= 82.70
d9= 99.06
r10= 1.3997
a10= 129.14
d10= 128.78
r11= 1.5162
a11= 147.20
d11= 317.72
r12= 1.3982
a12= 91.44
d12= 135.23
r13= 1.5384
a13= 145.78
d13= 12.12
r14= 1.5307
a14= 147.00
d14= 337.05
r15= 1.5390
a15= 128.32
d15= 138.49
r16= 1.3937
a16= 119.12

d16= 235.64
r17= 2.4219
a17= 59.97
d17= 72.17
r18= 1.5386
a18= 94.25
d18= 115.24
r19= 3.4980
a19= 122.29
d19= 46.41
r20= 1.3262
a20= 74.96
d20= 286.53
r21= 2.4633
a21= 73.92
d21= 20.76
r22= 1.3431
a22= 92.54
d22= 353.65
r23= 1.4519
a23= 33.44
d23= 42.91
r24= 1.4594
a24= 114.68
d24= 34.68
r25= 1.4551
a25= 114.30
d25= 46.25
r26= 2.0285
a26= 116.84
d26= 323.46
r27= 1.1027
a27= 111.11
d27= 49.99
r28= 1.1013
a28= 112.21
d28= 288.90
r29= 1.0955
a29= 144.52
d29= 327.15
r30= 1.1005
a30= 109.70
d30= 150.15
r31= 1.1142

a31= 93.66
d31= 96.60
r32= 1.1000
a32= 112.75
d32= 30.70
r33= 1.1001
a33= 91.52
d33= 204.53
r34= 1.0582
a34= 10.76
d34= 100.10
r35= 0.9644
a35= 110.56
d35= 29.29
r36= 1.1002
a36= 106.04
d36= 154.07
r37= 1.1043
a37= 108.44
d37= 6.59
r38= 1.1101
a38= 108.43
d38= 267.95
r39= 1.1009
a39= 109.45
d39= 165.84
r40= 1.0963
a40= 111.83
d40= 45.41
r41= 1.1020
a41= 112.34
d41= 284.26
r42= 1.1140
a42= 106.56
d42= 211.81
r43= 1.1002
a43= 109.41
d43= 325.20
r44= 1.0968
a44= 81.56
d44= 259.58
r45= 1.1165
a45= 101.32
d45= 155.37

r46= 1.0991
a46= 83.91
d46= 223.19
r47= 1.0928
a47= 119.71
d47= 55.04
r48= 1.1010
a48= 106.51
d48= 287.21
r49= 1.1113
a49= 107.93
d49= 172.35
r50= 1.1101
a50= 103.49
d50= 195.27
r51= 1.0983
a51= 146.60
d51= 39.58
r52= 1.0923
a52= 119.74
d52= 181.45
r53= 1.1000
a53= 108.35
d53= 86.99
r54= 1.1133
a54= 106.65
d54= 200.05
r55= 1.0984
a55= 112.08
d55= 320.91
r56= 1.1001
a56= 108.95
d56= 201.70
r57= 1.1027
a57= 112.32
d57= 83.82
r58= 1.1010
a58= 110.41
d58= 168.84
r59= 1.0932
a59= 120.62
d59= 180.14
r60= 1.1037
a60= 111.38

d60= 268.71
r61= 2.2857
a61= 155.20
d61= 5.39
r62= 0.9643
a62= 138.00
d62= 93.82
r63= 0.9879
a63= 93.29
d63= 337.91

Geometry and energy of **1** + HO_2^- structure in z-matrix format.
Energy = -1423.492007 Hartrees

Geometry:
C
C 1 r2
C 2 r3 1 a3
C 2 r4 1 a4 3 d4
C 2 r5 1 a5 3 d5
C 3 r6 2 a6 1 d6
C 1 r7 2 a7 3 d7
C 7 r8 1 a8 2 d8
C 1 r9 2 a9 3 d9
C 2 r10 1 a10 3 d10
C 4 r11 2 a11 1 d11
C 4 r12 2 a12 1 d12
C 8 r13 7 a13 1 d13
C 9 r14 1 a14 2 d14
C 3 r15 2 a15 1 d15
C 10 r16 2 a16 1 d16
C 8 r17 7 a17 1 d17
C 9 r18 1 a18 2 d18
O 14 r19 9 a19 1 d19
O 19 r20 14 a20 9 d20
O 19 r21 14 a21 9 d21
N 2 r22 1 a22 3 d22
N 8 r23 7 a23 1 d23
N 5 r24 2 a24 1 d24
N 11 r25 4 a25 2 d25
C 21 r26 19 a26 14 d26

H 15 r27 3 a27 2 d27
H 15 r28 3 a28 2 d28
H 17 r29 8 a29 7 d29
H 18 r30 9 a30 1 d30
H 17 r31 8 a31 7 d31
H 18 r32 9 a32 1 d32
H 17 r33 8 a33 7 d33
H 19 r34 14 a34 9 d34
H 21 r35 19 a35 14 d35
H 5 r36 2 a36 1 d36
H 3 r37 2 a37 1 d37
H 5 r38 2 a38 1 d38
H 6 r39 3 a39 2 d39
H 6 r40 3 a40 2 d40
H 6 r41 3 a41 2 d41
H 7 r42 1 a42 2 d42
H 7 r43 1 a43 2 d43
H 8 r44 7 a44 1 d44
H 8 r45 7 a45 1 d45
H 9 r46 1 a46 2 d46
H 10 r47 2 a47 1 d47
H 11 r48 4 a48 2 d48
H 11 r49 4 a49 2 d49
H 1 r50 2 a50 3 d50
H 1 r51 2 a51 3 d51
H 12 r52 4 a52 2 d52
H 13 r53 8 a53 7 d53
H 13 r54 8 a54 7 d54
H 14 r55 9 a55 1 d55
H 14 r56 9 a56 1 d56
H 14 r57 9 a57 1 d57
H 15 r58 3 a58 2 d58
H 16 r59 10 a59 2 d59
H 18 r60 9 a60 1 d60
O 29 r61 17 a61 8 d61
H 61 r62 29 a62 17 d62
H 61 r63 29 a63 17 d63
Variables:
r2= 3.2723
r3= 5.4795
a3= 84.56
r4= 2.3272
a4= 114.82
d4= 16.92

r5= 1.5209
a5= 45.35
d5= 227.13
r6= 1.5315
a6= 90.03
d6= 255.45
r7= 1.5356
a7= 73.99
d7= 296.89
r8= 2.4428
a8= 142.48
d8= 62.12
r9= 2.4651
a9= 80.07
d9= 93.69
r10= 1.3994
a10= 129.46
d10= 131.27
r11= 1.5153
a11= 147.44
d11= 319.07
r12= 1.3959
a12= 91.60
d12= 135.52
r13= 1.5399
a13= 145.82
d13= 13.43
r14= 1.5286
a14= 144.24
d14= 332.39
r15= 1.5384
a15= 131.38
d15= 136.91
r16= 1.3932
a16= 119.45
d16= 234.84
r17= 2.4297
a17= 59.93
d17= 72.13
r18= 1.5350
a18= 97.06
d18= 114.84
r19= 3.1535
a19= 96.93

d19= 265.08
r20= 1.3155
a20= 83.91
d20= 309.81
r21= 2.4827
a21= 79.06
d21= 58.46
r22= 1.3469
a22= 92.87
d22= 355.06
r23= 1.4609
a23= 33.52
d23= 41.98
r24= 1.4523
a24= 114.53
d24= 35.02
r25= 1.4555
a25= 113.64
d25= 41.26
r26= 1.9477
a26= 125.27
d26= 14.58
r27= 1.1016
a27= 111.04
d27= 47.60
r28= 1.1014
a28= 112.00
d28= 286.71
r29= 1.0951
a29= 144.32
d29= 331.63
r30= 1.1009
a30= 109.89
d30= 146.72
r31= 1.1121
a31= 91.63
d31= 98.50
r32= 1.1007
a32= 112.13
d32= 27.37
r33= 1.0988
a33= 93.02
d33= 207.37
r34= 1.0747

a34= 79.30
d34= 59.18
r35= 0.9647
a35= 109.54
d35= 160.34
r36= 1.1006
a36= 106.40
d36= 155.16
r37= 1.1039
a37= 106.61
d37= 2.92
r38= 1.1104
a38= 108.28
d38= 268.46
r39= 1.1021
a39= 109.41
d39= 160.98
r40= 1.0989
a40= 110.88
d40= 41.06
r41= 1.1015
a41= 112.36
d41= 279.26
r42= 1.1114
a42= 107.73
d42= 210.02
r43= 1.1008
a43= 109.43
d43= 324.57
r44= 1.0975
a44= 81.95
d44= 260.27
r45= 1.1140
a45= 100.22
d45= 155.39
r46= 1.0961
a46= 83.03
d46= 222.82
r47= 1.0931
a47= 119.49
d47= 54.00
r48= 1.1003
a48= 106.83
d48= 282.26

r49= 1.1107
a49= 108.35
d49= 167.41
r50= 1.1113
a50= 104.43
d50= 193.40
r51= 1.0996
a51= 144.80
d51= 38.38
r52= 1.0915
a52= 119.69
d52= 181.83
r53= 1.1006
a53= 108.46
d53= 83.69
r54= 1.1110
a54= 106.91
d54= 197.27
r55= 1.0995
a55= 110.84
d55= 323.88
r56= 1.0985
a56= 109.13
d56= 205.68
r57= 1.1035
a57= 112.72
d57= 86.15
r58= 1.1016
a58= 110.47
d58= 166.74
r59= 1.0919
a59= 120.76
d59= 179.78
r60= 1.1045
a60= 111.57
d60= 265.77
r61= 2.2177
a61= 150.96
d61= 282.87
r62= 0.9720
a62= 169.99
d62= 45.44
r63= 0.9882
a63= 72.90

d63= 4.16

Geometry and energy of **1D** structure in z-matrix format.
Energy = -1423.510398 Hartrees

Geometry:
C
C 1 r2
C 2 r3 1 a3
C 2 r4 1 a4 3 d4
C 2 r5 1 a5 3 d5
C 3 r6 2 a6 1 d6
C 1 r7 2 a7 3 d7
C 7 r8 1 a8 2 d8
C 1 r9 2 a9 3 d9
C 2 r10 1 a10 3 d10
C 4 r11 2 a11 1 d11
C 4 r12 2 a12 1 d12
C 8 r13 7 a13 1 d13
C 9 r14 1 a14 2 d14
C 3 r15 2 a15 1 d15
C 10 r16 2 a16 1 d16
C 8 r17 7 a17 1 d17
C 9 r18 1 a18 2 d18
O 6 r19 3 a19 2 d19
O 19 r20 6 a20 3 d20
O 19 r21 6 a21 3 d21
N 2 r22 1 a22 3 d22
N 17 r23 8 a23 7 d23
N 5 r24 2 a24 1 d24
N 11 r25 4 a25 2 d25
C 20 r26 19 a26 6 d26
H 15 r27 3 a27 2 d27
H 15 r28 3 a28 2 d28
H 17 r29 8 a29 7 d29
H 18 r30 9 a30 1 d30
H 17 r31 8 a31 7 d31
H 18 r32 9 a32 1 d32
H 17 r33 8 a33 7 d33
H 19 r34 6 a34 3 d34
H 21 r35 19 a35 6 d35
H 5 r36 2 a36 1 d36

H 3 r37 2 a37 1 d37
H 5 r38 2 a38 1 d38
H 6 r39 3 a39 2 d39
H 6 r40 3 a40 2 d40
H 6 r41 3 a41 2 d41
H 7 r42 1 a42 2 d42
H 7 r43 1 a43 2 d43
H 8 r44 7 a44 1 d44
H 8 r45 7 a45 1 d45
H 9 r46 1 a46 2 d46
H 10 r47 2 a47 1 d47
H 11 r48 4 a48 2 d48
H 11 r49 4 a49 2 d49
H 1 r50 2 a50 3 d50
H 1 r51 2 a51 3 d51
H 12 r52 4 a52 2 d52
H 13 r53 8 a53 7 d53
H 13 r54 8 a54 7 d54
H 14 r55 9 a55 1 d55
H 14 r56 9 a56 1 d56
H 14 r57 9 a57 1 d57
H 15 r58 3 a58 2 d58
H 16 r59 10 a59 2 d59
H 18 r60 9 a60 1 d60
O 29 r61 17 a61 8 d61
H 61 r62 29 a62 17 d62
H 61 r63 29 a63 17 d63

Variables:

r2= 3.3057
r3= 5.5623
a3= 84.46
r4= 2.3384
a4= 114.56
d4= 14.64
r5= 1.5225
a5= 44.02
d5= 223.87
r6= 1.5280
a6= 93.67
d6= 254.72
r7= 1.5278
a7= 73.81
d7= 300.10
r8= 2.4184

a8= 144.51
d8= 60.10
r9= 2.4507
a9= 80.11
d9= 97.67
r10= 1.4030
a10= 136.65
d10= 136.04
r11= 1.5163
a11= 146.63
d11= 320.31
r12= 1.3973
a12= 91.55
d12= 144.30
r13= 1.5335
a13= 147.95
d13= 16.51
r14= 1.5283
a14= 144.89
d14= 326.65
r15= 1.5390
a15= 128.70
d15= 134.49
r16= 1.3926
a16= 118.91
d16= 230.64
r17= 2.4271
a17= 60.29
d17= 72.74
r18= 1.5373
a18= 97.31
d18= 111.38
r19= 3.2824
a19= 119.38
d19= 29.97
r20= 1.4581
a20= 75.39
d20= 314.25
r21= 2.6795
a21= 76.05
d21= 37.34
r22= 1.3346
a22= 90.01
d22= 358.20

r23= 1.4696
a23= 34.47
d23= 326.88
r24= 1.4537
a24= 116.00
d24= 35.56
r25= 1.4583
a25= 114.92
d25= 44.38
r26= 1.9234
a26= 112.66
d26= 79.79
r27= 1.1011
a27= 110.16
d27= 169.10
r28= 1.1025
a28= 110.97
d28= 50.55
r29= 1.0937
a29= 145.14
d29= 329.24
r30= 1.1012
a30= 110.00
d30= 144.12
r31= 1.1091
a31= 90.30
d31= 95.59
r32= 1.1018
a32= 112.46
d32= 24.58
r33= 1.0979
a33= 92.40
d33= 204.49
r34= 0.9880
a34= 84.21
d34= 56.40
r35= 0.9664
a35= 107.71
d35= 29.19
r36= 1.1008
a36= 105.18
d36= 155.50
r37= 1.1052
a37= 106.86

d37= 3.60
r38= 1.1103
a38= 108.16
d38= 268.23
r39= 1.1022
a39= 108.64
d39= 163.77
r40= 1.0961
a40= 113.00
d40= 42.50
r41= 1.1023
a41= 111.87
d41= 281.36
r42= 1.1077
a42= 108.43
d42= 207.74
r43= 1.1001
a43= 109.41
d43= 322.87
r44= 1.0961
a44= 81.95
d44= 261.80
r45= 1.1106
a45= 96.76
d45= 156.49
r46= 1.0991
a46= 81.14
d46= 219.01
r47= 1.0922
a47= 119.88
d47= 50.52
r48= 1.1016
a48= 104.61
d48= 287.45
r49= 1.1099
a49= 108.34
d49= 171.55
r50= 1.1117
a50= 104.17
d50= 196.78
r51= 1.0983
a51= 145.20
d51= 41.83
r52= 1.0913

a52= 119.98
d52= 180.35
r53= 1.0996
a53= 108.51
d53= 85.64
r54= 1.1109
a54= 107.07
d54= 199.31
r55= 1.0970
a55= 112.16
d55= 321.46
r56= 1.1011
a56= 108.82
d56= 201.08
r57= 1.1033
a57= 112.45
d57= 83.22
r58= 1.1016
a58= 112.75
d58= 289.20
r59= 1.0934
a59= 120.36
d59= 179.81
r60= 1.1039
a60= 111.55
d60= 262.91
r61= 2.1964
a61= 159.01
d61= 300.51
r62= 0.9642
a62= 164.01
d62= 263.60
r63= 1.0075
a63= 72.95
d63= 347.28

Geometry and energy of **1** + H_2O_2 structure in z-matrix format.
Energy = -1499.849477 Hartrees

Geometry:
C

C 1 r2
C 2 r3 1 a3
C 2 r4 1 a4 3 d4
C 2 r5 1 a5 3 d5
C 3 r6 2 a6 1 d6
C 1 r7 2 a7 3 d7
C 7 r8 1 a8 2 d8
C 1 r9 2 a9 3 d9
C 2 r10 1 a10 3 d10
C 4 r11 2 a11 1 d11
C 4 r12 2 a12 1 d12
C 8 r13 7 a13 1 d13
C 9 r14 1 a14 2 d14
C 3 r15 2 a15 1 d15
C 12 r16 4 a16 2 d16
C 8 r17 7 a17 1 d17
C 9 r18 1 a18 2 d18
O 6 r19 3 a19 2 d19
O 19 r20 6 a20 3 d20
O 20 r21 19 a21 6 d21
N 4 r22 2 a22 1 d22
N 7 r23 1 a23 2 d23
N 5 r24 2 a24 1 d24
N 11 r25 4 a25 2 d25
C 21 r26 20 a26 19 d26
H 15 r27 3 a27 2 d27
H 15 r28 3 a28 2 d28
H 17 r29 8 a29 7 d29
H 18 r30 9 a30 1 d30
H 17 r31 8 a31 7 d31
H 18 r32 9 a32 1 d32
H 17 r33 8 a33 7 d33
H 19 r34 6 a34 3 d34
H 20 r35 19 a35 6 d35
H 5 r36 2 a36 1 d36
H 3 r37 2 a37 1 d37
H 5 r38 2 a38 1 d38
H 6 r39 3 a39 2 d39
H 6 r40 3 a40 2 d40
H 6 r41 3 a41 2 d41
H 7 r42 1 a42 2 d42
H 7 r43 1 a43 2 d43
H 8 r44 7 a44 1 d44
H 8 r45 7 a45 1 d45

H 9 r46 1 a46 2 d46
H 10 r47 2 a47 1 d47
H 11 r48 4 a48 2 d48
H 11 r49 4 a49 2 d49
H 1 r50 2 a50 3 d50
H 1 r51 2 a51 3 d51
H 12 r52 4 a52 2 d52
H 13 r53 8 a53 7 d53
H 13 r54 8 a54 7 d54
H 14 r55 9 a55 1 d55
H 14 r56 9 a56 1 d56
H 14 r57 9 a57 1 d57
H 15 r58 3 a58 2 d58
H 16 r59 12 a59 4 d59
H 18 r60 9 a60 1 d60
O 37 r61 3 a61 2 d61
H 61 r62 37 a62 3 d62
H 21 r63 20 a63 19 d63
O 34 r64 19 a64 6 d64
H 64 r65 34 a65 19 d65
H 64 r66 34 a66 19 d66
Variables:
r2= 3.2250
r3= 5.3183
a3= 85.42
r4= 2.3343
a4= 111.79
d4= 26.73
r5= 1.5121
a5= 46.54
d5= 238.07
r6= 1.5245
a6= 81.80
d6= 242.37
r7= 1.5419
a7= 77.68
d7= 293.50
r8= 2.4908
a8= 139.21
d8= 71.69
r9= 2.4829
a9= 80.69
d9= 83.16
r10= 1.3958

a10= 132.77
d10= 141.01
r11= 1.5082
a11= 146.68
d11= 316.65
r12= 1.3990
a12= 91.39
d12= 137.88
r13= 1.5376
a13= 138.72
d13= 358.80
r14= 1.5283
a14= 144.51
d14= 339.18
r15= 1.5322
a15= 133.26
d15= 130.32
r16= 1.3948
a16= 118.94
d16= 0.45
r17= 2.4269
a17= 59.40
d17= 67.44
r18= 1.5321
a18= 94.53
d18= 117.01
r19= 3.2728
a19= 118.44
d19= 74.12
r20= 1.4467
a20= 128.81
d20= 359.03
r21= 2.5609
a21= 95.41
d21= 337.78
r22= 1.3417
a22= 29.68
d22= 316.88
r23= 1.4607
a23= 112.02
d23= 92.17
r24= 1.4604
a24= 112.87
d24= 35.44

r25= 1.4643
a25= 113.98
d25= 21.81
r26= 1.8165
a26= 118.83
d26= 322.21
r27= 1.1006
a27= 112.40
d27= 275.10
r28= 1.1011
a28= 108.90
d28= 156.66
r29= 1.0946
a29= 143.70
d29= 323.87
r30= 1.1004
a30= 109.50
d30= 149.89
r31= 1.1094
a31= 93.57
d31= 95.26
r32= 1.1013
a32= 112.69
d32= 30.39
r33= 1.0994
a33= 90.48
d33= 206.67
r34= 0.9917
a34= 53.03
d34= 68.73
r35= 1.0168
a35= 99.36
d35= 335.75
r36= 1.1006
a36= 106.68
d36= 154.83
r37= 1.0991
a37= 108.76
d37= 349.14
r38= 1.1070
a38= 109.31
d38= 269.37
r39= 1.0991
a39= 108.67

d39= 159.14
r40= 1.0997
a40= 111.08
d40= 42.20
r41= 1.1045
a41= 113.24
d41= 278.89
r42= 1.1096
a42= 107.53
d42= 215.26
r43= 1.1000
a43= 110.09
d43= 330.69
r44= 1.1014
a44= 81.28
d44= 247.52
r45= 1.1091
a45= 106.01
d45= 143.06
r46= 1.0986
a46= 85.15
d46= 227.15
r47= 1.0918
a47= 119.93
d47= 56.82
r48= 1.1009
a48= 106.26
d48= 262.02
r49= 1.1065
a49= 109.20
d49= 148.09
r50= 1.1077
a50= 98.26
d50= 186.82
r51= 1.0970
a51= 149.94
d51= 39.22
r52= 1.0912
a52= 119.75
d52= 181.04
r53= 1.1014
a53= 109.85
d53= 74.43
r54= 1.1076

a54= 107.75
d54= 192.55
r55= 1.0996
a55= 112.00
d55= 321.46
r56= 1.0972
a56= 109.10
d56= 205.61
r57= 1.1037
a57= 112.59
d57= 85.52
r58= 1.1050
a58= 112.61
d58= 37.88
r59= 1.0931
a59= 120.39
d59= 180.20
r60= 1.1035
a60= 111.57
d60= 268.43
r61= 1.9276
a61= 159.41
d61= 21.26
r62= 0.9666
a62= 152.26
d62= 149.63
r63= 1.0300
a63= 104.86
d63= 85.68
r64= 1.7777
a64= 154.64
d64= 230.41
r65= 0.9689
a65= 81.79
d65= 330.93
r66= 1.0162
a66= 114.15
d66= 70.64

Geometry and energy of **2** + $O_2^{\cdot -}$ structure in z-matrix format.
Energy = -1111.395403 Hartrees

Geometry:

N
N 1 r2
N 1 r3 2 a3
N 1 r4 2 a4 3 d4
C 3 r5 1 a5 2 d5
C 1 r6 2 a6 3 d6
C 1 r7 2 a7 3 d7
C 3 r8 1 a8 2 d8
C 2 r9 1 a9 3 d9
C 2 r10 1 a10 3 d10
C 6 r11 1 a11 2 d11
C 4 r12 1 a12 2 d12
C 7 r13 1 a13 2 d13
C 4 r14 1 a14 2 d14
C 11 r15 6 a15 1 d15
C 2 r16 1 a16 3 d16
O 3 r17 1 a17 2 d17
C 1 r18 2 a18 3 d18
H 16 r19 2 a19 1 d19
H 16 r20 2 a20 1 d20
H 16 r21 2 a21 1 d21
H 17 r22 3 a22 1 d22
H 17 r23 3 a23 1 d23
H 8 r24 3 a24 1 d24
H 8 r25 3 a25 1 d25
H 9 r26 2 a26 1 d26
H 9 r27 2 a27 1 d27
H 10 r28 2 a28 1 d28
H 10 r29 2 a29 1 d29
H 11 r30 6 a30 1 d30
H 12 r31 4 a31 1 d31
H 12 r32 4 a32 1 d32
H 5 r33 3 a33 1 d33
H 5 r34 3 a34 1 d34
H 13 r35 7 a35 1 d35
H 14 r36 4 a36 1 d36
H 14 r37 4 a37 1 d37
H 15 r38 11 a38 6 d38
H 4 r39 1 a39 2 d39
H 3 r40 1 a40 2 d40
O 22 r41 17 a41 3 d41
O 41 r42 22 a42 17 d42
Variables:
r2= 3.4182

r3= 2.6836
a3= 55.68
r4= 2.6843
a4= 55.70
d4= 136.17
r5= 1.4973
a5= 119.44
d5= 320.63
r6= 1.3411
a6= 109.34
d6= 316.72
r7= 1.3427
a7= 109.31
d7= 179.44
r8= 1.4982
a8= 63.06
d8= 213.73
r9= 1.4890
a9= 83.20
d9= 54.64
r10= 1.4891
a10= 83.24
d10= 169.19
r11= 1.3950
a11= 119.96
d11= 227.02
r12= 1.4963
a12= 63.07
d12= 146.27
r13= 1.3949
a13= 119.98
d13= 133.04
r14= 1.4992
a14= 119.40
d14= 39.39
r15= 1.4008
a15= 118.29
d15= 0.75
r16= 1.4805
a16= 150.32
d16= 291.91
r17= 3.2193
a17= 78.93
d17= 74.31

r18= 1.9731
a18= 35.40
d18= 68.06
r19= 1.0980
a19= 110.60
d19= 59.77
r20= 1.1041
a20= 110.98
d20= 180.02
r21= 1.0979
a21= 110.54
d21= 300.23
r22= 0.9706
a22= 115.35
d22= 81.59
r23= 0.9699
a23= 119.77
d23= 210.22
r24= 1.1035
a24= 107.93
d24= 249.67
r25= 1.1012
a25= 110.60
d25= 133.72
r26= 1.1053
a26= 111.22
d26= 164.71
r27= 1.0998
a27= 108.18
d27= 47.95
r28= 1.1000
a28= 108.18
d28= 312.14
r29= 1.1046
a29= 111.33
d29= 195.34
r30= 1.0915
a30= 120.89
d30= 180.29
r31= 1.1023
a31= 107.95
d31= 110.30
r32= 1.1032
a32= 110.67

d32= 226.30
r33= 1.1015
a33= 110.71
d33= 256.01
r34= 1.1002
a34= 107.08
d34= 140.24
r35= 1.0913
a35= 120.93
d35= 179.65
r36= 1.1006
a36= 107.08
d36= 219.77
r37= 1.1005
a37= 110.69
d37= 104.05
r38= 1.0944
a38= 119.78
d38= 180.04
r39= 1.0203
a39= 131.21
d39= 236.49
r40= 1.0207
a40= 131.21
d40= 123.61
r41= 1.9792
a41= 112.45
d41= 311.61
r42= 1.2037
a42= 145.54
d42= 274.25

Geometry and energy of **2A** structure in z-matrix format.
Energy = -1111.435292 Hartrees

Geometry:

C
C 1 r2
C 2 r3 1 a3
N 3 r4 2 a4 1 d4

C 4 r5 3 a5 2 d5
C 5 r6 4 a6 3 d6
C 4 r7 3 a7 2 d7
O 7 r8 4 a8 3 d8
C 3 r9 2 a9 1 d9
N 9 r10 3 a10 2 d10
C 10 r11 9 a11 3 d11
C 11 r12 10 a12 9 d12
N 12 r13 11 a13 10 d13
C 13 r14 12 a14 11 d14
C 5 r15 4 a15 3 d15
N 15 r16 5 a16 4 d16
C 16 r17 15 a17 5 d17
C 13 r18 12 a18 11 d18
O 7 r19 4 a19 3 d19
O 19 r20 7 a20 4 d20
H 8 r21 7 a21 4 d21
H 8 r22 7 a22 4 d22
H 16 r23 15 a23 5 d23
H 14 r24 13 a24 12 d24
H 14 r25 13 a25 12 d25
H 14 r26 13 a26 12 d26
H 9 r27 3 a27 2 d27
H 9 r28 3 a28 2 d28
H 12 r29 11 a29 10 d29
H 12 r30 11 a30 10 d30
H 18 r31 13 a31 12 d31
H 18 r32 13 a32 12 d32
H 2 r33 1 a33 3 d33
H 15 r34 5 a34 4 d34
H 15 r35 5 a35 4 d35
H 11 r36 10 a36 9 d36
H 11 r37 10 a37 9 d37
H 6 r38 5 a38 4 d38
H 17 r39 16 a39 15 d39
H 17 r40 16 a40 15 d40
H 1 r41 2 a41 3 d41
H 10 r42 9 a42 3 d42
Variables:
r2= 1.3966
r3= 1.3980
a3= 118.60
r4= 1.3374
a4= 120.66

d4= 359.55
r5= 1.3365
a5= 121.77
d5= 0.93
r6= 1.3970
a6= 120.84
d6= 359.06
r7= 2.1085
a7= 119.28
d7= 185.35
r8= 2.1154
a8= 165.37
d8= 316.44
r9= 1.5227
a9= 122.40
d9= 176.76
r10= 1.4618
a10= 113.74
d10= 157.83
r11= 1.4660
a11= 116.95
d11= 272.13
r12= 1.5303
a12= 112.16
d12= 79.34
r13= 1.4829
a13= 112.93
d13= 57.77
r14= 1.4753
a14= 110.97
d14= 77.40
r15= 1.5214
a15= 116.41
d15= 176.49
r16= 1.4661
a16= 113.62
d16= 27.85
r17= 1.4685
a17= 116.54
d17= 84.72
r18= 1.4824
a18= 111.64
d18= 202.00
r19= 2.0069

a19= 86.28
d19= 265.34
r20= 1.2832
a20= 116.25
d20= 163.28
r21= 1.0019
a21= 95.18
d21= 312.78
r22= 0.9666
a22= 122.48
d22= 200.00
r23= 1.0161
a23= 109.16
d23= 210.32
r24= 1.0956
a24= 109.98
d24= 300.84
r25= 1.1058
a25= 111.21
d25= 62.23
r26= 1.0978
a26= 109.98
d26= 182.53
r27= 1.1025
a27= 106.69
d27= 276.47
r28= 1.1066
a28= 109.24
d28= 31.35
r29= 1.1059
a29= 109.50
d29= 181.47
r30= 1.0986
a30= 109.16
d30= 298.03
r31= 1.0984
a31= 107.65
d31= 38.81
r32= 1.1056
a32= 110.78
d32= 282.30
r33= 1.0923
a33= 121.03
d33= 180.05

r34= 1.1021
a34= 106.79
d34= 269.62
r35= 1.1061
a35= 109.47
d35= 154.15
r36= 1.1072
a36= 112.19
d36= 317.60
r37= 1.0994
a37= 107.56
d37= 200.52
r38= 1.0922
a38= 120.40
d38= 180.52
r39= 1.0997
a39= 107.72
d39= 156.39
r40= 1.1065
a40= 112.07
d40= 39.61
r41= 1.0928
a41= 120.19
d41= 179.78
r42= 1.0157
a42= 110.25
d42= 144.92

Geometry and energy of **2B** structure in z-matrix format.
Energy = -1111.395403 Hartrees

Geometry:
N
N 1 r2
N 1 r3 2 a3
N 1 r4 2 a4 3 d4
C 3 r5 1 a5 2 d5
C 1 r6 2 a6 3 d6
C 1 r7 2 a7 3 d7
C 3 r8 1 a8 2 d8
C 2 r9 1 a9 3 d9
C 2 r10 1 a10 3 d10

C 6 r11 1 a11 2 d11
C 4 r12 1 a12 2 d12
C 7 r13 1 a13 2 d13
C 4 r14 1 a14 2 d14
C 11 r15 6 a15 1 d15
C 2 r16 1 a16 3 d16
O 3 r17 1 a17 2 d17
C 1 r18 2 a18 3 d18
H 16 r19 2 a19 1 d19
H 16 r20 2 a20 1 d20
H 16 r21 2 a21 1 d21
H 17 r22 3 a22 1 d22
H 17 r23 3 a23 1 d23
H 8 r24 3 a24 1 d24
H 8 r25 3 a25 1 d25
H 9 r26 2 a26 1 d26
H 9 r27 2 a27 1 d27
H 10 r28 2 a28 1 d28
H 10 r29 2 a29 1 d29
H 11 r30 6 a30 1 d30
H 12 r31 4 a31 1 d31
H 12 r32 4 a32 1 d32
H 5 r33 3 a33 1 d33
H 5 r34 3 a34 1 d34
H 13 r35 7 a35 1 d35
H 14 r36 4 a36 1 d36
H 14 r37 4 a37 1 d37
H 15 r38 11 a38 6 d38
H 4 r39 1 a39 2 d39
H 3 r40 1 a40 2 d40
O 22 r41 17 a41 3 d41
O 41 r42 22 a42 17 d42
Variables:
r2= 3.4182
r3= 2.6836
a3= 55.68
r4= 2.6843
a4= 55.70
d4= 136.17
r5= 1.4973
a5= 119.44
d5= 320.63
r6= 1.3411
a6= 109.34

d6= 316.72
r7= 1.3427
a7= 109.31
d7= 179.44
r8= 1.4982
a8= 63.06
d8= 213.73
r9= 1.4890
a9= 83.20
d9= 54.64
r10= 1.4891
a10= 83.24
d10= 169.19
r11= 1.3950
a11= 119.96
d11= 227.02
r12= 1.4963
a12= 63.07
d12= 146.27
r13= 1.3949
a13= 119.98
d13= 133.04
r14= 1.4992
a14= 119.40
d14= 39.39
r15= 1.4008
a15= 118.29
d15= 0.75
r16= 1.4805
a16= 150.32
d16= 291.91
r17= 3.2193
a17= 78.93
d17= 74.31
r18= 1.9731
a18= 35.40
d18= 68.06
r19= 1.0980
a19= 110.60
d19= 59.77
r20= 1.1041
a20= 110.98
d20= 180.02
r21= 1.0979

a21= 110.54
d21= 300.23
r22= 0.9706
a22= 115.35
d22= 81.59
r23= 0.9699
a23= 119.77
d23= 210.22
r24= 1.1035
a24= 107.93
d24= 249.67
r25= 1.1012
a25= 110.60
d25= 133.72
r26= 1.1053
a26= 111.22
d26= 164.71
r27= 1.0998
a27= 108.18
d27= 47.95
r28= 1.1000
a28= 108.18
d28= 312.14
r29= 1.1046
a29= 111.33
d29= 195.34
r30= 1.0915
a30= 120.89
d30= 180.29
r31= 1.1023
a31= 107.95
d31= 110.30
r32= 1.1032
a32= 110.67
d32= 226.30
r33= 1.1015
a33= 110.71
d33= 256.01
r34= 1.1002
a34= 107.08
d34= 140.24
r35= 1.0913
a35= 120.93
d35= 179.65

r36= 1.1006
a36= 107.08
d36= 219.77
r37= 1.1005
a37= 110.69
d37= 104.05
r38= 1.0944
a38= 119.78
d38= 180.04
r39= 1.0203
a39= 131.21
d39= 236.49
r40= 1.0207
a40= 131.21
d40= 123.61
r41= 1.9792
a41= 112.45
d41= 311.61
r42= 1.2037
a42= 145.54
d42= 274.25

Geometry and energy of **2C'** structure in z-matrix format.
Energy = -1187.927442 Hartrees

Geometry:
N
N 1 r2
N 1 r3 2 a3
N 1 r4 2 a4 3 d4
C 3 r5 1 a5 2 d5
C 1 r6 2 a6 3 d6
C 1 r7 2 a7 3 d7
C 3 r8 1 a8 2 d8
C 2 r9 1 a9 3 d9
C 2 r10 1 a10 3 d10
C 6 r11 1 a11 2 d11
C 4 r12 1 a12 2 d12
C 7 r13 1 a13 2 d13
C 4 r14 1 a14 2 d14
C 11 r15 6 a15 1 d15
C 2 r16 1 a16 3 d16
O 3 r17 1 a17 2 d17

C 1 r18 2 a18 3 d18
H 16 r19 2 a19 1 d19
H 16 r20 2 a20 1 d20
H 16 r21 2 a21 1 d21
H 17 r22 3 a22 1 d22
H 17 r23 3 a23 1 d23
H 8 r24 3 a24 1 d24
H 8 r25 3 a25 1 d25
H 9 r26 2 a26 1 d26
H 9 r27 2 a27 1 d27
H 10 r28 2 a28 1 d28
H 10 r29 2 a29 1 d29
H 11 r30 6 a30 1 d30
H 12 r31 4 a31 1 d31
H 12 r32 4 a32 1 d32
H 5 r33 3 a33 1 d33
H 5 r34 3 a34 1 d34
H 13 r35 7 a35 1 d35
H 14 r36 4 a36 1 d36
H 14 r37 4 a37 1 d37
H 15 r38 11 a38 6 d38
H 4 r39 1 a39 2 d39
H 3 r40 1 a40 2 d40
O 22 r41 17 a41 3 d41
O 41 r42 22 a42 17 d42
Variables:
r2= 3.4182
r3= 2.6836
a3= 55.68
r4= 2.6843
a4= 55.70
d4= 136.17
r5= 1.4973
a5= 119.44
d5= 320.63
r6= 1.3411
a6= 109.34
d6= 316.72
r7= 1.3427
a7= 109.31
d7= 179.44
r8= 1.4982
a8= 63.06
d8= 213.73

r9= 1.4890
a9= 83.20
d9= 54.64
r10= 1.4891
a10= 83.24
d10= 169.19
r11= 1.3950
a11= 119.96
d11= 227.02
r12= 1.4963
a12= 63.07
d12= 146.27
r13= 1.3949
a13= 119.98
d13= 133.04
r14= 1.4992
a14= 119.40
d14= 39.39
r15= 1.4008
a15= 118.29
d15=   0.75
r16= 1.4805
a16= 150.32
d16= 291.91
r17= 3.2193
a17= 78.93
d17= 74.31
r18= 1.9731
a18= 35.40
d18= 68.06
r19= 1.0980
a19= 110.60
d19= 59.77
r20= 1.1041
a20= 110.98
d20= 180.02
r21= 1.0979
a21= 110.54
d21= 300.23
r22= 0.9706
a22= 115.35
d22= 81.59
r23= 0.9699
a23= 119.77

d23= 210.22
r24= 1.1035
a24= 107.93
d24= 249.67
r25= 1.1012
a25= 110.60
d25= 133.72
r26= 1.1053
a26= 111.22
d26= 164.71
r27= 1.0998
a27= 108.18
d27= 47.95
r28= 1.1000
a28= 108.18
d28= 312.14
r29= 1.1046
a29= 111.33
d29= 195.34
r30= 1.0915
a30= 120.89
d30= 180.29
r31= 1.1023
a31= 107.95
d31= 110.30
r32= 1.1032
a32= 110.67
d32= 226.30
r33= 1.1015
a33= 110.71
d33= 256.01
r34= 1.1002
a34= 107.08
d34= 140.24
r35= 1.0913
a35= 120.93
d35= 179.65
r36= 1.1006
a36= 107.08
d36= 219.77
r37= 1.1005
a37= 110.69
d37= 104.05
r38= 1.0944

a38= 119.78
d38= 180.04
r39= 1.0203
a39= 131.21
d39= 236.49
r40= 1.0207
a40= 131.21
d40= 123.61
r41= 1.9792
a41= 112.45
d41= 311.61
r42= 1.2037
a42= 145.54
d42= 274.25

Geometry and energy of **2C''** structure in z-matrix format.
Energy = -1187.932518 Hartrees

Geometry:
C
C 1 r2
C 2 r3 1 a3
C 2 r4 1 a4 3 d4
C 1 r5 2 a5 3 d5
C 5 r6 1 a6 2 d6
C 2 r7 1 a7 3 d7
C 3 r8 2 a8 1 d8
C 3 r9 2 a9 1 d9
C 6 r10 5 a10 1 d10
C 9 r11 3 a11 2 d11
C 6 r12 5 a12 1 d12
O 12 r13 6 a13 5 d13
O 13 r14 12 a14 6 d14
O 13 r15 12 a15 6 d15
N 2 r16 1 a16 3 d16
N 12 r17 6 a17 5 d17
N 4 r18 2 a18 1 d18
H 18 r19 4 a19 2 d19
N 8 r20 3 a20 2 d20
H 20 r21 8 a21 3 d21
C 14 r22 13 a22 12 d22
H 12 r23 6 a23 5 d23
H 12 r24 6 a24 5 d24

H 12 r25 6 a25 5 d25
H 2 r26 1 a26 3 d26
H 15 r27 13 a27 12 d27
H 4 r28 2 a28 1 d28
H 4 r29 2 a29 1 d29
H 5 r30 1 a30 2 d30
H 5 r31 1 a31 2 d31
H 6 r32 5 a32 1 d32
H 6 r33 5 a33 1 d33
H 7 r34 2 a34 1 d34
H 8 r35 3 a35 2 d35
H 8 r36 3 a36 2 d36
H 1 r37 2 a37 3 d37
H 1 r38 2 a38 3 d38
H 9 r39 3 a39 2 d39
H 10 r40 6 a40 5 d40
H 10 r41 6 a41 5 d41
H 11 r42 9 a42 3 d42
O 19 r43 18 a43 4 d43
H 43 r44 19 a44 18 d44
H 43 r45 19 a45 18 d45
Variables:
r2= 3.3185
r3= 2.3301
a3= 113.69
r4= 1.5227
a4= 45.69
d4= 212.97
r5= 1.5352
a5= 77.18
d5= 317.52
r6= 2.4334
a6= 142.40
d6= 60.18
r7= 1.3990
a7= 128.85
d7= 113.69
r8= 1.5320
a8= 147.73
d8= 317.94
r9= 1.4008
a9= 91.10
d9= 134.72
r10= 1.5468

a10= 147.58
d10= 14.50
r11= 1.3955
a11= 119.34
d11= 0.31
r12= 2.4351
a12= 60.12
d12= 71.38
r13= 3.2838
a13= 107.58
d13= 251.27
r14= 1.3294
a14= 87.76
d14= 20.76
r15= 2.5917
a15= 67.79
d15= 129.74
r16= 1.3410
a16= 92.27
d16= 338.54
r17= 1.4644
a17= 33.86
d17= 329.41
r18= 1.4572
a18= 113.08
d18= 33.07
r19= 1.0305
a19= 110.61
d19= 142.66
r20= 1.4368
a20= 118.45
d20= 43.89
r21= 1.0192
a21= 115.45
d21= 273.74
r22= 1.9130
a22= 117.73
d22= 39.48
r23= 1.0959
a23= 143.84
d23= 328.14
r24= 1.1115
a24= 92.21
d24= 96.76

r25= 1.0979
a25= 92.65
d25= 206.37
r26= 5.5588
a26= 41.68
d26= 307.03
r27= 0.9657
a27= 106.36
d27= 111.91
r28= 1.1036
a28= 107.57
d28= 151.17
r29= 1.1072
a29= 109.37
d29= 266.83
r30= 1.1112
a30= 108.67
d30= 208.45
r31= 1.1003
a31= 108.64
d31= 323.74
r32= 1.0992
a32= 82.03
d32= 261.74
r33= 1.1133
a33= 97.89
d33= 156.31
r34= 1.0919
a34= 120.14
d34= 55.46
r35= 1.1048
a35= 106.99
d35= 282.46
r36= 1.1068
a36= 107.10
d36= 168.84
r37= 1.1101
a37= 100.86
d37= 211.22
r38= 1.0993
a38= 145.74
d38= 64.69
r39= 1.0926
a39= 119.77

d39= 181.41
r40= 1.1025
a40= 109.18
d40= 81.71
r41= 1.1073
a41= 105.87
d41= 194.88
r42= 1.0930
a42= 120.55
d42= 180.48
r43= 1.8686
a43= 153.86
d43= 246.26
r44= 0.9686
a44= 98.84
d44= 34.22
r45= 0.9903
a45= 87.06
d45= 292.44

Geometry and energy of **2C** structure in z-matrix format.
Energy = -1187.942826 Hartrees

Geometry:
C
C 1 r2
C 2 r3 1 a3
C 2 r4 1 a4 3 d4
C 1 r5 2 a5 3 d5
C 5 r6 1 a6 2 d6
C 2 r7 1 a7 3 d7
C 3 r8 2 a8 1 d8
C 3 r9 2 a9 1 d9
C 6 r10 5 a10 1 d10
C 7 r11 2 a11 1 d11
C 5 r12 1 a12 2 d12
O 8 r13 3 a13 2 d13
O 13 r14 8 a14 3 d14
O 13 r15 8 a15 3 d15
N 2 r16 1 a16 3 d16
N 12 r17 5 a17 1 d17
N 4 r18 2 a18 1 d18
H 18 r19 4 a19 2 d19

N 8 r20 3 a20 2 d20
H 20 r21 8 a21 3 d21
C 14 r22 13 a22 8 d22
H 12 r23 5 a23 1 d23
H 12 r24 5 a24 1 d24
H 12 r25 5 a25 1 d25
H 13 r26 8 a26 3 d26
H 15 r27 13 a27 8 d27
H 4 r28 2 a28 1 d28
H 4 r29 2 a29 1 d29
H 5 r30 1 a30 2 d30
H 5 r31 1 a31 2 d31
H 6 r32 5 a32 1 d32
H 6 r33 5 a33 1 d33
H 7 r34 2 a34 1 d34
H 8 r35 3 a35 2 d35
H 8 r36 3 a36 2 d36
H 1 r37 2 a37 3 d37
H 1 r38 2 a38 3 d38
H 9 r39 3 a39 2 d39
H 10 r40 6 a40 5 d40
H 10 r41 6 a41 5 d41
H 11 r42 7 a42 2 d42
O 19 r43 18 a43 4 d43
H 43 r44 19 a44 18 d44
H 43 r45 19 a45 18 d45

Variables:

r2= 3.3403
r3= 2.3347
a3= 112.90
r4= 1.5267
a4= 44.27
d4= 211.67
r5= 1.5406
a5= 78.32
d5= 319.39
r6= 2.4572
a6= 142.36
d6= 65.00
r7= 1.4001
a7= 138.16
d7= 121.05
r8= 1.5226
a8= 145.58

d8= 319.04
r9= 1.3972
a9= 91.58
d9= 145.00
r10= 1.5427
a10= 143.59
d10= 4.05
r11= 1.3948
a11= 118.70
d11= 232.42
r12= 2.4237
a12= 102.52
d12= 120.95
r13= 3.4685
a13= 106.32
d13= 330.94
r14= 1.4495
a14= 65.04
d14= 356.39
r15= 2.6386
a15= 96.17
d15= 68.31
r16= 1.3363
a16= 87.91
d16= 344.42
r17= 1.4639
a17= 34.55
d17= 247.06
r18= 1.4390
a18= 113.99
d18= 32.74
r19= 1.0290
a19= 113.56
d19= 124.93
r20= 1.4443
a20= 113.95
d20= 33.94
r21= 1.0170
a21= 112.38
d21= 225.82
r22= 1.9470
a22= 102.83
d22= 68.03
r23= 1.0962

a23= 89.76
d23= 14.41
r24= 1.1096
a24= 93.90
d24= 123.57
r25= 1.0971
a25= 144.47
d25= 254.24
r26= 0.9908
a26= 118.30
d26= 82.99
r27= 0.9629
a27= 130.13
d27= 88.18
r28= 1.1037
a28= 106.26
d28= 151.27
r29= 1.1097
a29= 108.85
d29= 265.55
r30= 1.1088
a30= 109.53
d30= 210.95
r31= 1.0999
a31= 108.48
d31= 327.05
r32= 1.0991
a32= 80.97
d32= 255.02
r33= 1.1094
a33= 100.90
d33= 149.57
r34= 1.0928
a34= 120.01
d34= 52.35
r35= 1.1012
a35= 105.61
d35= 277.38
r36= 1.1099
a36= 109.10
d36= 161.35
r37= 1.1107
a37= 100.77
d37= 213.81

r38= 1.1001
a38= 147.12
d38= 68.03
r39= 1.0930
a39= 120.09
d39= 179.98
r40= 1.0998
a40= 109.78
d40= 83.51
r41= 1.1108
a41= 107.21
d41= 198.57
r42= 1.0926
a42= 120.29
d42= 179.53
r43= 1.9075
a43= 149.22
d43= 274.55
r44= 0.9800
a44= 100.72
d44= 25.22
r45= 0.9905
a45= 88.73
d45= 287.94

Geometry and energy of **2** + H_2O_2 structure in z-matrix format.
Energy = -1264.296681 Hartrees

Geometry:
N
N 1 r2
N 1 r3 2 a3
N 1 r4 2 a4 3 d4
C 3 r5 1 a5 2 d5
C 1 r6 2 a6 3 d6
C 1 r7 2 a7 3 d7
C 3 r8 1 a8 2 d8
C 2 r9 1 a9 3 d9
C 2 r10 1 a10 3 d10
C 6 r11 1 a11 2 d11
C 4 r12 1 a12 2 d12
C 7 r13 1 a13 2 d13

C 4 r14 1 a14 2 d14
C 13 r15 7 a15 1 d15
C 2 r16 1 a16 3 d16
O 4 r17 1 a17 2 d17
O 16 r18 2 a18 1 d18
O 18 r19 16 a19 2 d19
O 17 r20 4 a20 1 d20
O 17 r21 4 a21 1 d21
C 18 r22 16 a22 2 d22
H 16 r23 2 a23 1 d23
H 16 r24 2 a24 1 d24
H 16 r25 2 a25 1 d25
H 17 r26 4 a26 1 d26
H 8 r27 3 a27 1 d27
H 8 r28 3 a28 1 d28
H 9 r29 2 a29 1 d29
H 9 r30 2 a30 1 d30
H 10 r31 2 a31 1 d31
H 10 r32 2 a32 1 d32
H 11 r33 6 a33 1 d33
H 12 r34 4 a34 1 d34
H 12 r35 4 a35 1 d35
H 5 r36 3 a36 1 d36
H 5 r37 3 a37 1 d37
H 13 r38 7 a38 1 d38
H 14 r39 4 a39 1 d39
H 14 r40 4 a40 1 d40
H 15 r41 13 a41 7 d41
H 19 r42 18 a42 16 d42
H 18 r43 16 a43 2 d43
H 20 r44 17 a44 4 d44
H 19 r45 18 a45 16 d45
H 21 r46 17 a46 4 d46
H 3 r47 1 a47 2 d47
H 4 r48 1 a48 2 d48
Variables:
r2= 3.1454
r3= 2.7302
a3= 60.60
r4= 2.7316
a4= 59.79
d4= 136.38
r5= 1.4609
a5= 111.71

d5= 324.99
r6= 1.3384
a6= 108.20
d6= 314.54
r7= 1.3400
a7= 108.33
d7= 180.61
r8= 1.4527
a8= 62.43
d8= 213.77
r9= 1.4613
a9= 82.74
d9= 53.33
r10= 1.4664
a10= 82.95
d10= 169.08
r11= 1.3965
a11= 120.82
d11= 234.77
r12= 1.4496
a12= 61.95
d12= 148.84
r13= 1.3990
a13= 120.39
d13= 125.43
r14= 1.4544
a14= 111.78
d14= 37.60
r15= 1.3958
a15= 118.81
d15=   0.22
r16= 1.4669
a16= 148.29
d16= 291.10
r17= 3.3240
a17= 74.71
d17= 232.81
r18= 3.0595
a18= 80.16
d18=   6.33
r19= 2.8415
a19= 68.36
d19= 246.07
r20= 2.5244

a20= 51.39
d20= 164.17
r21= 1.4471
a21= 79.91
d21= 49.53
r22= 1.8648
a22= 73.71
d22= 351.93
r23= 1.0966
a23= 109.72
d23= 56.13
r24= 1.1101
a24= 111.10
d24= 178.20
r25= 1.0965
a25= 110.05
d25= 300.66
r26= 1.0482
a26= 54.47
d26= 164.02
r27= 1.1024
a27= 107.99
d27= 255.18
r28= 1.1086
a28= 112.97
d28= 137.15
r29= 1.1106
a29= 111.72
d29= 160.46
r30= 1.1012
a30= 108.24
d30= 43.43
r31= 1.1020
a31= 107.91
d31= 316.52
r32= 1.1094
a32= 111.37
d32= 199.70
r33= 1.0924
a33= 120.21
d33= 179.24
r34= 1.1042
a34= 106.32
d34= 101.96

r35= 1.1090
a35= 113.63
d35= 220.75
r36= 1.1092
a36= 111.64
d36= 249.35
r37= 1.0984
a37= 107.23
d37= 132.28
r38= 1.0917
a38= 119.93
d38= 180.54
r39= 1.0989
a39= 106.78
d39= 224.06
r40= 1.1105
a40= 112.14
d40= 106.86
r41= 1.0927
a41= 120.27
d41= 180.49
r42= 0.9650
a42= 110.52
d42= 238.41
r43= 0.9784
a43= 70.35
d43= 234.79
r44= 0.9651
a44= 113.61
d44= 123.75
r45= 1.0263
a45= 82.18
d45= 135.51
r46= 0.9981
a46= 107.23
d46= 85.43
r47= 1.0147
a47= 131.17
d47= 116.69
r48= 1.0593
a48= 131.01
d48= 241.50

VI. QM/MM MD simulation in aqueous solution

Table S6. Distribution of Cu(II)-N and Cu(II)-O distances (Å) of complexes **1** and **2** along the QM/MM-MD trajectories. The variation between values for the two complexes (Δ) are shown.

Cmp.	Value	Distance (Å)				
		Cu-N1	**Cu-N2**	**Cu-N3**	**Cu-N4**	**Cu-O5**
1	Mean	1.97 ± 0.13	2.28 ± 0.17	2.19 ± 0.15	2.16 ± 0.19	2.02 ± 0.12
2	Mean	1.97 ± 0.12	2.19 ± 0.16	2.08 ± 0.16	1.97 ± 0.19	2.04 ± 0.11
	Δ	**0.00**	**-0.09**	**-0.11**	**-0.19**	**0.02**
1	Width	0.66	1.21	1.23	0.78	0.82
2	Width	0.63	0.99	0.44	0.52	0.64
	Δ	**-0.03**	**-0.22**	**-0.79**	**-0.26**	**-0.18**

(**) Difference btw. max and min value of the distribution.

Table S7. Distribution of Cu(I)-N and Cu(I)-O distances (Å) of complexes **1** and **2** along the QM/MM MD trajectories. The variation between values for the two complexes (Δ) are shown.

Cmp.	Value	Distance (Å)				
		Cu-N1	**Cu-N2**	**Cu-N3**	**Cu-N4**	**Cu-O5**
1	Mean	1.99 ± 0.13	2.40 ± 0.17	2.21 ± 0.15	2.40 ± 0.19	2.11 ± 0.12
2	Mean	2.03 ± 0.12	2.30 ± 0.16	2.57 ± 0.16	2.03 ± 0.19	2.04 ± 0.11
	Δ	**0.04**	**-0.10**	**0.36**	**-0.37**	**-0.07**
1	Width	0.75	1.31	0.82	1.31	0.95
2	Width	0.70	0.90	1.70	0.90	0.66
	Δ	**-0.05**	**-0.41**	**0.88**	**-0.41**	**-0.29**

(**) Difference btw. max and min value of the distribution.

Table S8. Distribution of Cu(II)-N and Cu(II)-O distances (Å) of complexes **1A** and **2A** along the QM/MM MD trajectories. The variation between values for the two complexes (Δ) are shown.

Cmp.	Value	Distance (Å)				
		Cu-N1	**Cu-N2**	**Cu-N3**	**Cu-N4**	**Cu-O5**
1	Mean	2.02 ± 0.10	2.46 ± 0.20	2.21 ± 0.10	2.50 ± 0.23	2.12 ± 0.12
2	Mean	2.14 ± 0.13	2.33 ± 0.16	2.40 ± 0.16	2.45 ± 0.19	2.10 ± 0.11
	Δ	**0.12**	**-0.13**	**0.19**	**-0.05**	**-0.02**
1	Width	0.56	1.30	0.65	1.50	0.86
2	Width	0.94	1.02	1.21	1.19	0.67
	Δ	**0.38**	**-0.28**	**0.56**	**-0.31**	**-0.19**

Table S9. Distribution of Cu(I)-N and Cu(I)-O distances (Å) of complexes **1C** and **2C''** along the QM/MM MD trajectories. The variation between values for the two complexes (Δ) are shown.

Cmp.	Value	Distance (Å)				
		Cu-N1	**Cu-N2**	**Cu-N3**	**Cu-N4**	**Cu-O5**
1	Mean	2.07 ± 0.12	2.52 ± 0.16	2.30 ± 0.23	2.55 ± 0.20	2.07 ± 0.80
2	Mean	2.07 ± 0.10	2.36 ± 0.17	2.34 ± 0.14	2.07 ± 0.18	3.04 ± 0.24
	Δ (%)	**0.0**	**-0.16**	**0.04**	**-0.48**	**0.97**
1	Width	0.60	1.25	0.97	1.13	1.32
2	Width	0.87	0.98	1.46	1.14	3.50*
	Δ (%)	**0.27**	**-0.27**	**0.49**	**0.01**	**2.18**

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