Synthesis, Structural and Electrochemical Properties of a New Family of Amino Acid-Based Coordination Complexes

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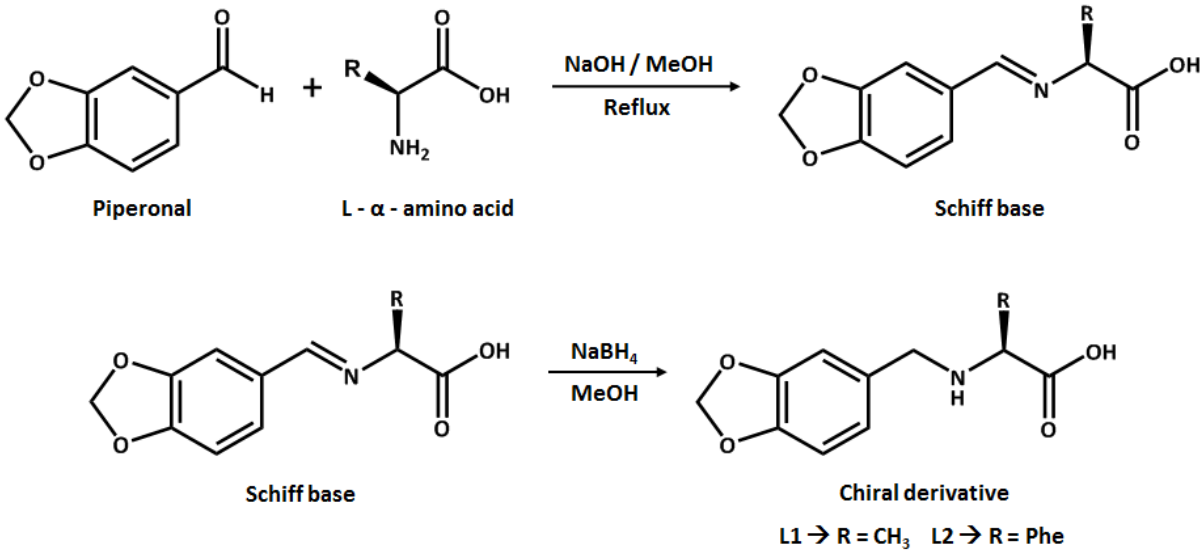
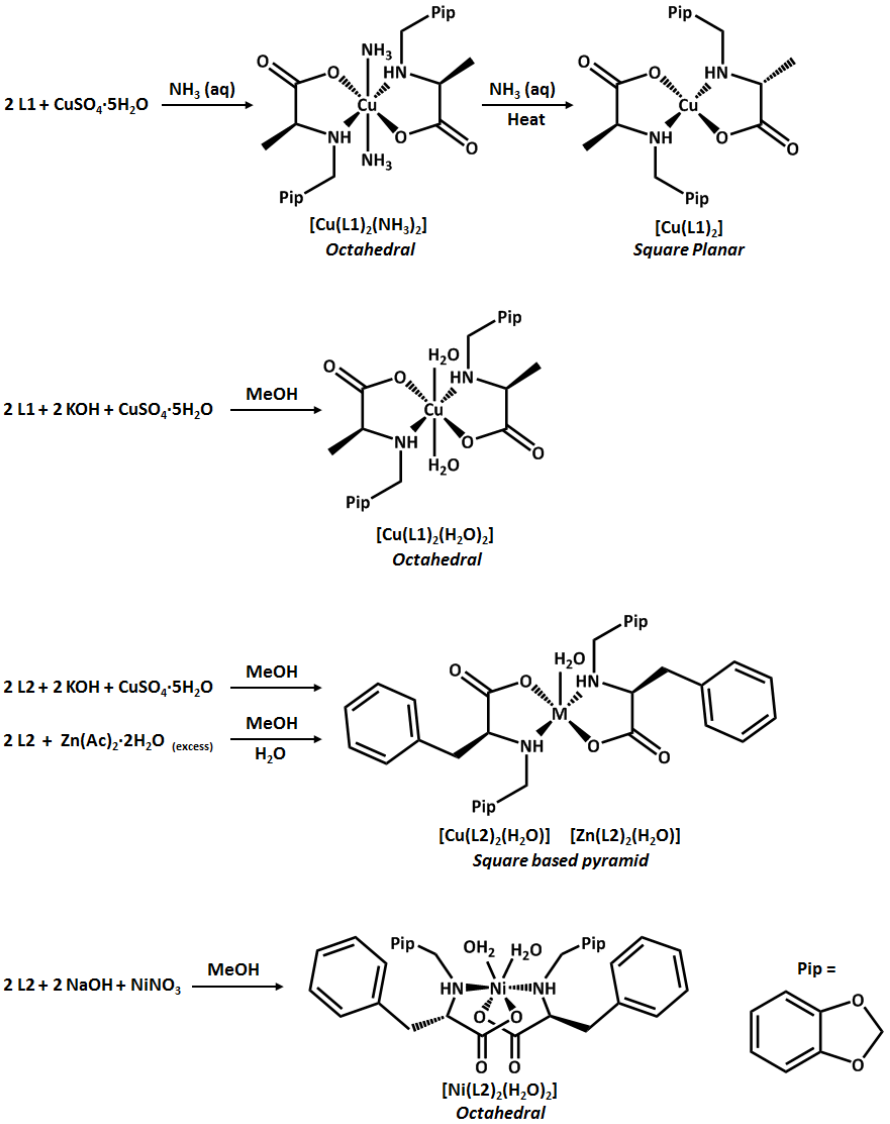
Synthesis and characterization

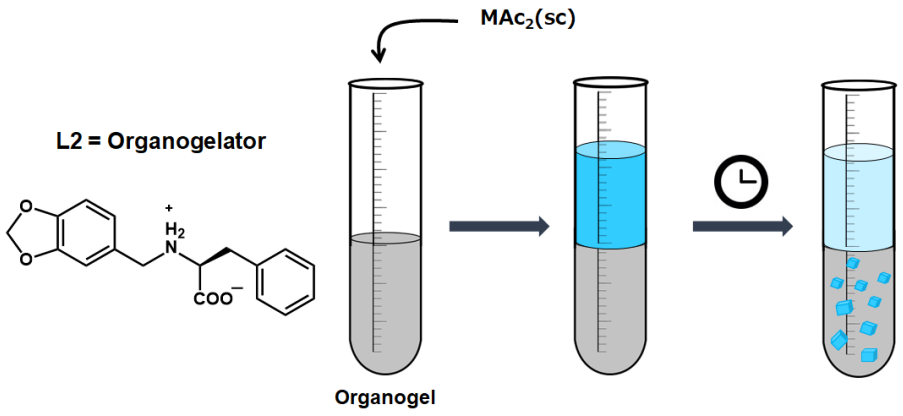
Scheme S1. Synthesis of L-amino acid derivatives **L1** and **L2** through a Schiff base formation and the subsequent reduction.



Scheme S2. Synthesis of the complexes from the L-amino acid derivatives and the corresponding metal ions.



Scheme S3. Schematic representation of the synthetic procedure for the obtention of crystalline material for [M(**L2**)$_2$(H$_2$O)], M = Cu^{2+} and Zn^{2+}.



Chirality inversion of L1

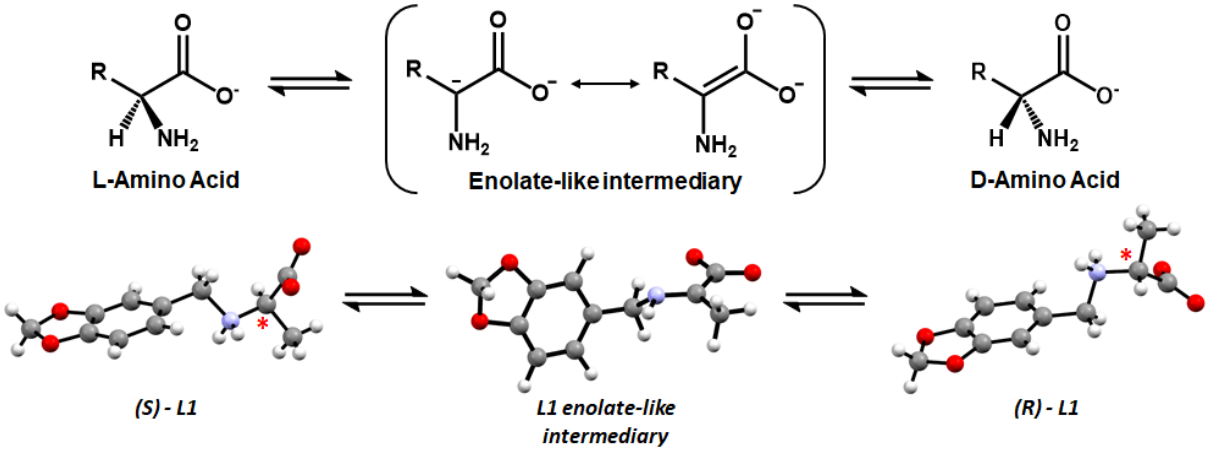


Figure S1. Proposed mechanism for the base-catalyzed racemization of amino acids through keto/enol tautomerism (top); DFT optimized species for **L1** (functional: BP86, basis: def2-SVP with def2/J as auxiliary basis set) (bottom).

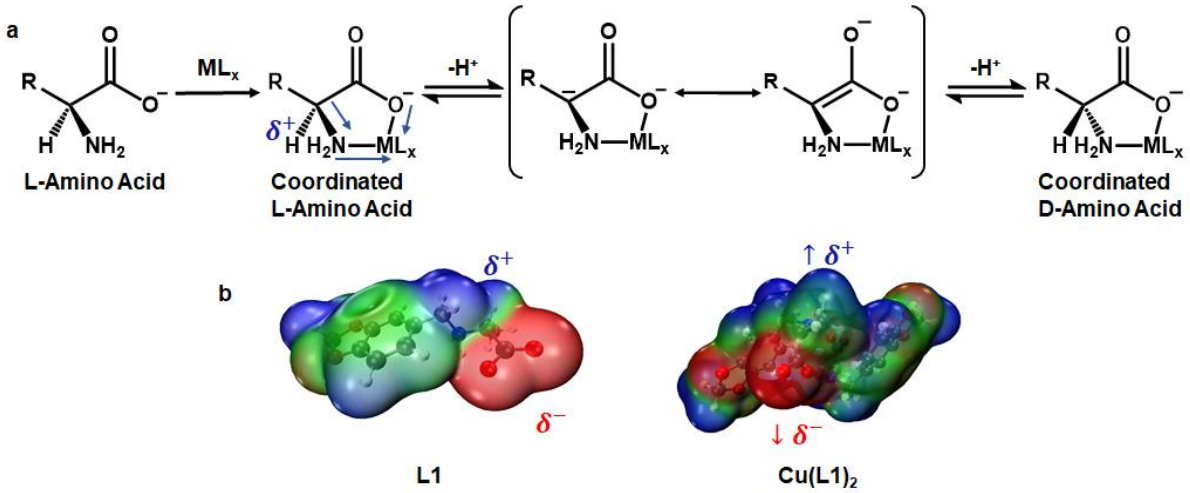


Figure S2. Schematic representation of the proposed mechanism for the metal ion-mediated racemization of **L1** in basic media (a); Electrostatic potential over the Van der Waals surface calculated by DFT for the optimized structures of the ligand and [Cu(**L1**)$_2$], blue and red areas represent negative and positive electrostatic potential, respectively.

XRD Studies

Crystallographic Tables

Table S1. Bond Lengths for [Cu(**L1**)$_2$(NH$_3$)$_2$]

Atom	Atom	Length / Å
Cu1	O4	1.943(3)
Cu1	O5	1.935(3)
Cu1	N1	2.017(3)
Cu1	N2	2.020(3)
O1	C1	1.431(9)
O1	C4	1.381(6)
O2	C1	1.405(8)
O2	C5	1.377(7)
O3	C11	1.223(6)
O4	C11	1.265(6)
O5	C12	1.266(6)
O6	C12	1.239(5)
O7	C18	1.366(6)
O7	C22	1.418(7)
O8	C19	1.377(6)
O8	C22	1.420(7)
N1	C8	1.493(6)
N1	C9	1.481(8)
N2	C14	1.479(7)
N2	C15	1.496(6)
C2	C3	1.404(7)
C2	C7	1.373(7)
C3	C4	1.352(9)

T**able S2**. Bond Angles for [Cu(**L1**)$_2$(NH$_3$)$_2$]

Atom	Atom	Atom	Angle / °
O4	Cu1	N1	84.75(18)
O4	Cu1	N2	94.62(15)
O5	Cu1	O4	178.62(16)
O5	Cu1	N1	95.54(17)
O5	Cu1	N2	84.95(16)
N1	Cu1	N2	173.97(16)
C4	O1	C1	104.6(5)
C5	O2	C1	105.5(5)
C11	O4	Cu1	115.6(3)
C12	O5	Cu1	116.6(3)
C18	O7	C22	106.1(4)
C19	O8	C22	105.9(4)
C8	N1	Cu1	114.5(3)
C9	N1	Cu1	109.1(3)
C9	N1	C8	113.4(4)
C14	N2	Cu1	109.5(3)
C14	N2	C15	113.1(3)
C15	N2	Cu1	113.2(3)
O2	C1	O1	108.8(5)
C7	C2	C3	122.3(5)
C4	C3	C2	116.4(5)
C3	C4	O1	127.7(5)
C3	C4	C5	122.2(5)

C4	C5	1.359(8)
C5	C6	1.366(7)
C6	C7	1.393(7)
C7	C8	1.505(7)
C9	C10	1.523(7)
C9	C11	1.528(7)
C12	C14	1.537(7)
C13	C14	1.522(8)
C15	C16	1.512(6)
C16	C17	1.405(7)
C16	C21	1.376(6)
C17	C18	1.359(7)
C18	C19	1.373(7)
C19	C20	1.353(7)
C20	C21	1.400(7)

C5	C4	O1	110.1(5)
C4	C5	O2	110.1(5)
C4	C5	C6	121.9(5)
C6	C5	O2	127.9(5)
C5	C6	C7	118.0(5)
C2	C7	C6	119.2(4)
C2	C7	C8	120.1(5)
C6	C7	C8	120.6(5)
N1	C8	C7	115.3(4)
N1	C9	C10	113.0(5)
N1	C9	C11	110.4(4)
C10	C9	C11	110.4(4)
O3	C11	O4	123.0(5)
O3	C11	C9	118.3(5)
O4	C11	C9	118.6(5)
O5	C12	C14	117.8(4)
O6	C12	O5	123.8(5)
O6	C12	C14	118.4(4)
N2	C14	C12	111.0(4)
N2	C14	C13	112.0(5)
C13	C14	C12	110.6(4)
N2	C15	C16	113.7(4)
C17	C16	C15	119.2(4)
C21	C16	C15	121.0(4)
C21	C16	C17	119.8(4)
C18	C17	C16	117.3(4)
O7	C18	C19	110.0(4)

C17	C18	O7	127.5(4)
C17	C18	C19	122.5(4)
C18	C19	O8	109.4(4)
C20	C19	O8	129.0(4)
C20	C19	C18	121.6(4)
C19	C20	C21	117.0(4)
C16	C21	C20	121.9(4)
O7	C22	O8	108.1(4)

Table S3. Hydrogen Bond Information for [Cu(**L1**)$_2$(NH$_3$)$_2$]

D	H	A	d(D-H) / Å	d(H-A) / Å	d(D-A) / Å	D-H-A / °
N3	H3A	O1[1]	0.89	2.22	2.871(13)	129.2
N3	H3B	O7[2]	0.89	1.89	2.740(14)	160.3
N4	H4A	O2[3]	0.89	1.99	2.864(12)	168.5
N4	H4C	O9	0.89	1.95	2.791(18)	155.9
O9	H9B	O2[4]	0.85	1.92	2.737(14)	159.8

[1]1-x,1/2+y,1-z; [2]+x,1+y,+z; [3]+x,-1+y,+z; [4]2-x,-1/2+y,1-z

Table S4. Bond Lengths for [Cu(**L1**)$_2$]

Atom	Atom	Length / Å
Cu1	O2	1.918(2)
Cu1	O2[1]	1.918(2)
Cu1	N2[1]	2.002(3)
Cu1	N2	2.002(3)
O2	C12	1.296(4)
O4	C12	1.222(4)
O6	C15	1.382(5)

Table S5. Bond Angles for [Cu(**L1**)$_2$]

Atom	Atom	Atom	Angle / °
O2	Cu1	O2[1]	180.0
O2[1]	Cu1	N2[1]	85.78(12)
O2[1]	Cu1	N2	94.22(11)
O2	Cu1	N2[1]	94.22(12)
O2	Cu1	N2	85.78(12)
N2[1]	Cu1	N2	180.0
C12	O2	Cu1	114.9(2)

O6	C22	1.414(6)
O8	C17	1.370(5)
O8	C22	1.423(6)
N2	C14	1.478(5)
N2	C16	1.511(4)
C12	C14	1.535(5)
C13	C16	1.504(5)
C13	C19	1.381(5)
C13	C20	1.394(6)
C14	C21	1.520(5)
C15	C17	1.376(6)
C15	C18	1.358(6)
C17	C20	1.371(6)
C18	C19	1.377(6)

[1]-x,1-y,1-z

C15	O6	C22	105.1(3)
C17	O8	C22	105.6(4)
C14	N2	Cu1	107.8(2)
C14	N2	C16	112.4(3)
C16	N2	Cu1	110.7(2)
O2	C12	C14	116.2(3)
O4	C12	O2	123.5(4)
O4	C12	C14	120.3(3)
C19	C13	C16	120.6(4)
C19	C13	C20	119.3(4)
C20	C13	C16	120.0(4)
N2	C14	C12	109.4(3)
N2	C14	C21	110.6(3)
C21	C14	C12	108.2(3)
C17	C15	O6	109.9(4)
C18	C15	O6	128.9(4)
C18	C15	C17	121.2(4)
C13	C16	N2	113.4(3)
O8	C17	C15	109.6(4)
O8	C17	C20	128.4(4)
C20	C17	C15	122.0(4)
C15	C18	C19	117.3(4)
C18	C19	C13	122.7(4)
C17	C20	C13	117.5(4)
O6	C22	O8	108.7(4)

[1]-x,1-y,1-z

Table S6. Bond Lengths for [Cu(**L1**)$_2$(H$_2$O)$_2$]

Atom	Atom	Length / Å
Cu1	O1	1.953(8)
Cu1	O3	1.949(7)
Cu1	N1	2.014(7)
Cu1	N2	2.030(7)
Cu1	N3	2.456(10)
Cu1	N4	2.440(9)
O1	C9	1.236(13)
O2	C13	1.234(13)
O3	C13	1.250(13)
O4	C3	1.388(15)
O4	C21	1.42(2)
O5	C4	1.389(14)
O5	C19	1.445(15)
O6	C11	1.376(14)
O6	C19	1.426(16)
O7	C9	1.231(14)
O8	C12	1.397(16)
O8	C21	1.43(2)
N1	C10	1.467(17)
N1	C15	1.498(13)
N2	C2	1.460(14)
N2	C16	1.488(15)
C1	C2	1.540(14)
C1	C6	1.414(15)
C1	C8	1.382(14)

Table S7. Bond Angles for [Cu(**L1**)$_2$(H$_2$O)$_2$]

Atom	Atom	Atom	Angle / °
O1	Cu1	N1	84.4(4)
O1	Cu1	N2	95.1(4)
O1	Cu1	N3	89.3(4)
O1	Cu1	N4	88.1(3)
O3	Cu1	O1	179.0(4)
O3	Cu1	N1	95.5(4)
O3	Cu1	N2	84.9(4)
O3	Cu1	N3	89.7(3)
O3	Cu1	N4	92.9(4)
N1	Cu1	N2	174.6(4)
N1	Cu1	N3	83.6(4)
N1	Cu1	N4	87.9(4)
N2	Cu1	N3	91.1(3)
N2	Cu1	N4	97.4(3)
N4	Cu1	N3	171.3(4)
C9	O1	Cu1	116.8(8)
C13	O3	Cu1	116.2(7)
C3	O4	C21	104.2(12)
C4	O5	C19	106.6(9)
C11	O6	C19	106.6(9)
C12	O8	C21	105.4(12)
C10	N1	Cu1	109.4(8)
C10	N1	C15	113.1(9)
C15	N1	Cu1	115.6(6)
C2	N2	Cu1	112.8(7)

C3	C12	1.377(18)	C2	N2	C16	114.2(7)
C3	C17	1.36(2)	C16	N2	Cu1	109.7(7)
C4	C7	1.342(16)	C6	C1	C2	116.9(9)
C4	C11	1.357(15)	C8	C1	C2	122.2(9)
C5	C14	1.330(16)	C8	C1	C6	120.9(9)
C5	C15	1.502(16)	N2	C2	C1	114.0(8)
C5	C18	1.399(18)	C12	C3	O4	111.5(12)
C6	C11	1.371(16)	C17	C3	O4	127.8(12)
C7	C8	1.399(16)	C17	C3	C12	120.8(11)
C9	C10	1.558(17)	C7	C4	O5	127.8(10)
C10	C22	1.525(15)	C7	C4	C11	123.2(10)
C12	C18	1.332(18)	C11	C4	O5	108.9(10)
C13	C16	1.549(16)	C14	C5	C15	120.6(12)
C14	C17	1.422(17)	C14	C5	C18	121.1(11)
C16	C20	1.480(19)	C18	C5	C15	118.3(11)
			C11	C6	C1	115.1(9)
			C4	C7	C8	116.2(9)
			C1	C8	C7	121.5(10)
			O1	C9	C10	117.5(10)
			O7	C9	O1	124.7(12)
			O7	C9	C10	117.8(10)
			N1	C10	C9	110.6(9)
			N1	C10	C22	113.1(12)
			C22	C10	C9	110.8(11)
			C4	C11	O6	110.9(10)
			C4	C11	C6	123.0(10)
			C6	C11	O6	126.0(10)

C3	C12	O8	108.3(11)
C18	C12	O8	129.5(12)
C18	C12	C3	122.2(12)
O2	C13	O3	123.9(11)
O2	C13	C16	117.0(10)
O3	C13	C16	119.1(10)
C5	C14	C17	120.8(12)
N1	C15	C5	117.0(8)
N2	C16	C13	110.1(9)
C20	C16	N2	112.6(10)
C20	C16	C13	110.8(10)
C3	C17	C14	117.1(12)
C12	C18	C5	118.0(11)
O6	C19	O5	106.5(10)
O4	C21	O8	109.6(12)

Table S8. Occupancy for $[Cu(L1)_2(H_2O)_2]$

Atom	Occupancy
O12	0.50(4)
H12A	0.50(4)
H12B	0.50(4)
O13	0.50(4)
H13D	0.50(4)
H13E	0.50(4)

Table S9. Hydrogen Bond Information for $[Cu(\mathbf{L1})_2(H_2O)_2]$

D	H	A	d(D-H) / Å	d(H-A) / Å	d(D-A) / Å	D-H-A / °
O10	H10D	O4[1]	0.85	2.01	2.835(5)	162.2
O9	H9A	O11	0.85	1.97	2.785(8)	160.2
O9	H9B	O6[2]	0.85	2.03	2.861(5)	166.2
O11	H11A	O12	0.85	2.01	2.795(17)	153.0
O11	H11A	O13	0.85	2.04	2.89(2)	170.6

[1]1-x,1/2+y,1-z; [2]+x,-1+y,+z

Table S10. Bond Lengths for [Cu(**L2**)$_2$(H$_2$O)]

Atom	Atom	Length / Å
Cu1	O2	1.920(7)
Cu1	O5	1.938(7)
Cu1	O9	2.125(8)
Cu1	N1	2.026(6)
Cu1	N2	2.015(7)
O1	C21	1.241(13)
O2	C21	1.288(12)
O3	C1	1.385(13)
O3	C27	1.425(12)
O4	C2	1.379(11)
O4	C27	1.428(13)
O5	C15	1.283(12)
O6	C5	1.376(11)
O6	C28	1.437(12)
O7	C15	1.209(13)
O8	C14	1.369(11)
O8	C28	1.432(12)
N1	C9	1.498(10)
N1	C18	1.468(12)
N2	C3	1.487(10)
N2	C30	1.497(9)
C1	C2	1.389(12)
C1	C8	1.370(12)
C2	C23	1.367(14)
C3	C12	1.538(11)

Table S11. Bond Angles for [Cu(**L2**)$_2$(H$_2$O)]

Atom	Atom	Atom	Angle / °
O2	Cu1	O5	175.8(3)
O2	Cu1	O9	92.0(3)
O2	Cu1	N1	94.4(3)
O2	Cu1	N2	84.4(3)
O5	Cu1	O9	92.1(3)
O5	Cu1	N1	84.3(3)
O5	Cu1	N2	94.4(3)
N1	Cu1	O9	107.7(4)
N2	Cu1	O9	107.5(4)
N2	Cu1	N1	144.8(3)
C21	O2	Cu1	115.8(6)
C1	O3	C27	104.6(7)
C2	O4	C27	104.8(7)
C15	O5	Cu1	115.8(6)
C5	O6	C28	105.5(7)
C14	O8	C28	105.7(7)
C9	N1	Cu1	106.6(5)
C18	N1	Cu1	107.5(5)
C18	N1	C9	113.1(6)
C3	N2	Cu1	107.6(5)
C3	N2	C30	112.5(6)
C30	N2	Cu1	107.2(5)
O3	C1	C2	109.8(8)
C8	C1	O3	127.5(8)
C8	C1	C2	122.7(9)

C3	C21	1.533(12)	O4	C2	C1	109.9(9)
C4	C6	1.391(12)	C23	C2	O4	127.9(8)
C4	C9	1.536(11)	C23	C2	C1	122.2(8)
C4	C17	1.403(12)	N2	C3	C12	110.6(7)
C5	C11	1.367(13)	N2	C3	C21	109.2(7)
C5	C14	1.394(12)	C21	C3	C12	110.2(7)
C6	C11	1.388(13)	C6	C4	C9	120.4(7)
C7	C12	1.537(12)	C6	C4	C17	120.3(8)
	C22	1.406(16)	C17	C4	C9	119.2(7)
	C32	1.377(15)	O6	C5	C14	109.4(8)
	C10	1.404(13)	C11	C5	O6	129.7(8)
	C20	1.387(12)	C11	C5	C14	121.0(8)
	C30	1.520(11)	C11	C6	C4	122.1(8)
	C16	1.384(15)	C22	C7	C12	119.9(9)
	C19	1.518(13)	C32	C7	C12	119.8(9)
	C31	1.397(16)	C32	C7	C22	120.3(10)
	C17	1.367(12)	C1	C8	C10	116.3(8)
	C18	1.548(12)	N1	C9	C4	111.5(6)
	C25	1.392(14)	C8	C10	C30	119.7(7)
	C19	1.540(12)	C20	C10	C8	120.9(8)
	C23	1.410(13)	C20	C10	C30	119.3(8)
	C26	1.421(17)	C5	C11	C6	117.1(8)
	C25	1.378(15)	C7	C12	C3	110.7(7)
	C29	1.403(17)	C16	C13	C19	120.2(9)
	C34	1.38(2)	C16	C13	C31	118.4(9)
	C31	1.374(17)	C31	C13	C19	121.2(9)
	C33	1.384(16)	O8	C14	C5	109.6(8)

C34	1.40(2)		C17	C14	O8	127.6(8)
			C17	C14	C5	122.7(8)
			O5	C15	C18	116.4(9)
			O7	C15	O5	124.9(9)
			O7	C15	C18	118.7(8)
			C13	C16	C25	121.5(9)
			C14	C17	C4	116.7(7)
			N1	C18	C15	110.4(7)
			N1	C18	C19	111.4(7)
			C19	C18	C15	108.7(7)
			C13	C19	C18	110.0(7)
			C10	C20	C23	122.1(9)
			O1	C21	O2	124.9(9)
			O1	C21	C3	118.0(8)
			O2	C21	C3	117.0(8)
			C7	C22	C26	117.6(12)
			C2	C23	C20	115.9(8)
			C25	C24	C29	119.5(9)
			C24	C25	C16	119.5(10)
			C34	C26	C22	121.0(13)
			O3	C27	O4	109.4(7)
			O8	C28	O6	107.3(7)
			C31	C29	C24	120.4(11)
			N2	C30	C10	112.5(6)
			C29	C31	C13	120.6(12)
			C7	C32	C33	121.9(12)
			C32	C33	C34	118.9(13)

C26	C34	C33	120.3(11)

Table S12. Hydrogen Bond Information for [Cu(**L2**)$_2$(H$_2$O)]

D	H	A	d(D-H) / Å	d(H-A) / Å	d(D-A) / Å	D-H-A / °
O9	H9A	O1[1]	0.87	1.88	2.738(11)	167.1
O9	H9B	O7[2]	0.87	1.93	2.739(10)	152.7

[1]1+x,+y,+z; [2]+x,1+y,+z

Table S13. Bond Lengths for [Zn(**L2**)$_2$(H$_2$O)]

Atom	**Atom**	**Length/Å**
Zn1	O4	2.066(11)
Zn1	O4[1]	2.066(11)
Zn1	O24[1]	1.97(2)
Zn1	O24	1.97(2)
Zn1	N4	2.094(12)
Zn1	N4[1]	2.094(12)
O4	C24	1.222(18)
O8	C24	1.261(17)
O12	C8	1.443(19)
O12	C40	1.382(19)
O16	C8	1.417(18)
O16	C56	1.392(18)
O24	O24[1]	0.82(7)
N4	C16	1.499(17)
N4	C36	1.52(2)
C4	C28	1.35(2)
C4	C44	1.37(2)
C12	C32	1.41(2)

Table S14. Bond Angles for [Zn(**L2**)$_2$(H$_2$O)]

Atom	**Atom**	**Atom**	**Angle / °**
O4[1]	Zn1	O4	167.8(7)
O4	Zn1	N4[1]	93.9(4)
O4[1]	Zn1	N4[1]	81.0(4)
O4[1]	Zn1	N4	93.9(4)
O4	Zn1	N4	81.0(4)
O24[1]	Zn1	O4	100.3(14)
O24	Zn1	O4[1]	100.3(13)
O24[1]	Zn1	O4[1]	91.7(13)
O24	Zn1	O4	91.7(13)
O24	Zn1	O24[1]	24.0(19)
O24	Zn1	N4	125.0(12)
O24[1]	Zn1	N4[1]	125.0(12)
O24	Zn1	N4[1]	103.9(12)
O24[1]	Zn1	N4	103.9(12)
N4[1]	Zn1	N4	130.7(6)
C24	O4	Zn1	114.2(9)
C40	O12	C8	105.4(11)
C56	O16	C8	105.9(11)

C12	C68	1.37(2)	O24[1]	O24	Zn1	78.0(9)
C16	C24	1.541(19)	C16	N4	Zn1	107.0(8)
C16	C60	1.52(2)	C16	N4	C36	113.7(11)
C20	C28	1.44(2)	C36	N4	Zn1	111.9(8)
C20	C56	1.37(2)	C28	C4	C44	126.0(15)
C28	C36	1.50(2)	O16	C8	O12	107.1(12)
C32	C64	1.39(3)	C68	C12	C32	119.5(16)
C40	C44	1.38(2)	N4	C16	C24	108.8(12)
C40	C56	1.37(2)	N4	C16	C60	112.2(11)
C48	C52	1.42(2)	C60	C16	C24	110.1(11)
C48	C60	1.52(2)	C56	C20	C28	115.6(12)
C48	C68	1.37(2)	O4	C24	O8	124.6(13)
C52	C64	1.39(2)	O4	C24	C16	120.6(12)
Zn2	O18	1.967(13)	O8	C24	C16	114.8(14)
Zn2	O21	2.041(9)	C4	C28	C20	118.5(13)
Zn2	O21[2]	2.041(9)	C4	C28	C36	123.2(14)
Zn2	N5[2]	2.069(12)	C20	C28	C36	117.8(12)
Zn2	N5	2.069(12)	C64	C32	C12	118.6(15)
O17	C74	1.280(18)	C28	C36	N4	112.0(11)
O19	C70	1.41(2)	C44	C40	O12	129.1(14)
O19	C82	1.428(18)	C56	C40	O12	109.6(14)
O20	C70	1.444(18)	C56	C40	C44	121.2(15)
O20	C79	1.394(19)	C4	C44	C40	115.0(14)
O21	C74	1.267(19)	C52	C48	C60	119.3(15)
N5	C71	1.499(15)	C68	C48	C52	118.9(14)
N5	C73	1.507(17)	C68	C48	C60	121.8(16)
C69	C72	1.39(3)	C64	C52	C48	118.8(15)

C69	C75	1.41(3)	C20	C56	O16	126.8(12)
C71	C80	1.53(2)	C20	C56	C40	123.6(14)
C72	C77	1.36(3)	C40	C56	O16	109.6(13)
C73	C74	1.52(2)	C48	C60	C16	111.2(13)
C73	C76	1.554(19)	C52	C64	C32	121.6(16)
C75	C83	1.42(2)	C48	C68	C12	122.5(17)
C76	C83	1.48(2)	O18	Zn2	O21	96.0(3)
C77	C84	1.41(2)	O18	Zn2	$O21^2$	96.0(3)
C78	C80	1.40(2)	O18	Zn2	N5	115.5(3)
C78	C82	1.32(2)	O18	Zn2	$N5^2$	115.5(3)
C79	C82	1.35(2)	O21	Zn2	$O21^2$	168.1(5)
C79	C85	1.39(2)	$O21^2$	Zn2	$N5^2$	81.4(4)
C80	C81	1.38(2)	O21	Zn2	N5	81.4(4)
C81	C85	1.39(2)	O21	Zn2	$N5^2$	93.5(4)
C83	C84	1.37(2)	$O21^2$	Zn2	N5	93.5(4)
			$N5^2$	Zn2	N5	129.1(6)
			C70	O19	C82	106.4(11)
			C79	O20	C70	103.3(12)
			C74	O21	Zn2	114.0(9)
			C71	N5	Zn2	112.6(9)
			C71	N5	C73	112.2(9)
			C73	N5	Zn2	107.2(8)
			C72	C69	C75	119.5(18)
			O19	C70	O20	109.0(11)
			N5	C71	C80	112.3(11)
			C77	C72	C69	121.8(18)
			N5	C73	C74	109.1(13)

N5	C73	C76	108.8(11)
C74	C73	C76	111.4(11)
O17	C74	C73	115.4(14)
O21	C74	O17	125.0(14)
O21	C74	C73	119.5(13)
C69	C75	C83	118.9(17)
C83	C76	C73	114.2(12)
C72	C77	C84	118.6(19)
C82	C78	C80	115.6(13)
C82	C79	O20	113.2(13)
C82	C79	C85	120.6(15)
C85	C79	O20	126.2(13)
C78	C80	C71	120.0(13)
C81	C80	C71	119.6(13)
C81	C80	C78	120.3(14)
C80	C81	C85	122.6(14)
C78	C82	O19	127.2(13)
C78	C82	C79	125.8(14)
C79	C82	O19	107.0(14)
C75	C83	C76	119.1(15)
C84	C83	C75	119.4(15)
C84	C83	C76	121.3(15)
C83	C84	C77	121.6(18)
C79	C85	C81	115.1(13)

[1]1-x,+y,1-z; [2]1-x,+y,2-z

Table S15. Occupancy for [Zn(**L2**)$_2$(H$_2$O)]

Atom	**Occupancy**
O24	0.5
H24	0.5
H18A	0.5
H18B	0.5

Table S16. Hydrogen Bond Information for [Zn(**L2**)$_2$(H_2O)]

D	H	A	d(D-H) / Å	d(H-A) / Å	d(D-A) / Å	D-H-A / °
O24	H24	O8[1]	0.98	1.83	2.68(4)	143.6
O18	H18A	O17[1]	1.04	1.67	2.600(12)	146.1
O18	H18B	O17[2]	1.04	1.67	2.600(12)	146.2

[1]-1/2+x,1/2+y,+z; [2]3/2-x,1/2+y,2-z

Powder XRD Studies

The powder XRD pattern of samples obtained from bulk showed an excellent agreement with simulated data from single-crystal X-ray diffraction. For $[Cu(\mathbf{L1})_2(X)_2]$ X = NH_3, H_2O, the agreement was not good enough due to the bulk samples and single crystals corresponding to different hydrates (data not shown).

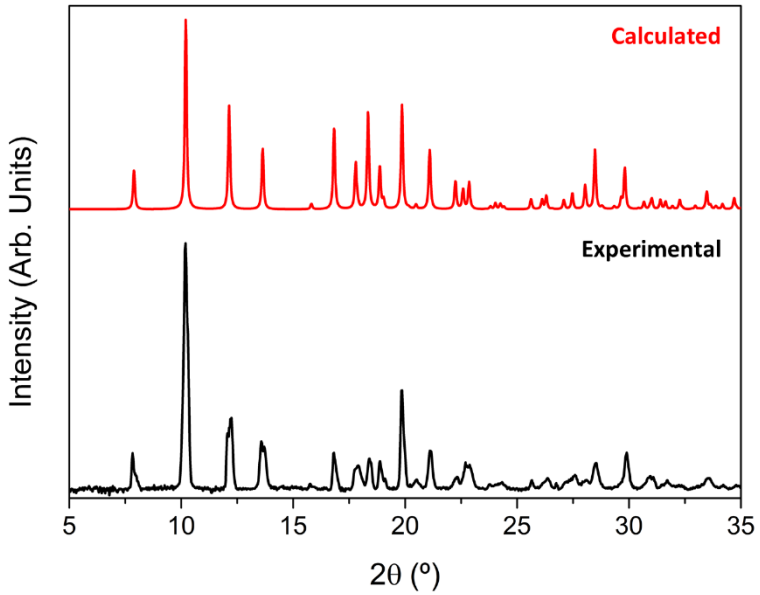


Figure S3. Calculated (red) and measured (black) powder X-ray diffractogram for $[Cu(\mathbf{L1})_2]$.

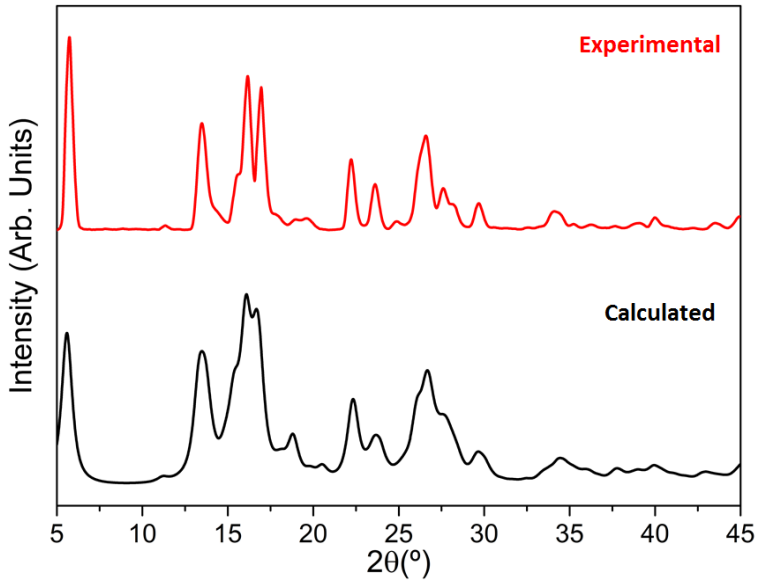


Figure S4. Calculated with 0.75 full width at half maximum (black) and measured (red) powder diffraction pattern of $[Cu(\mathbf{L2})_2H_2O]$.

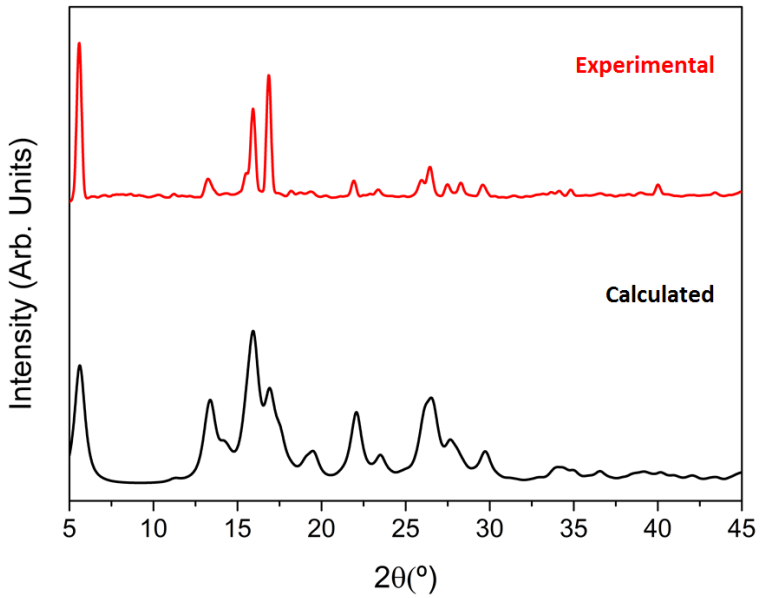


Figure S5. Calculated with 0.75 full width at half maximum (black) and measured (red) powder diffraction pattern of [Zn(**L2**)$_2$H$_2$O].

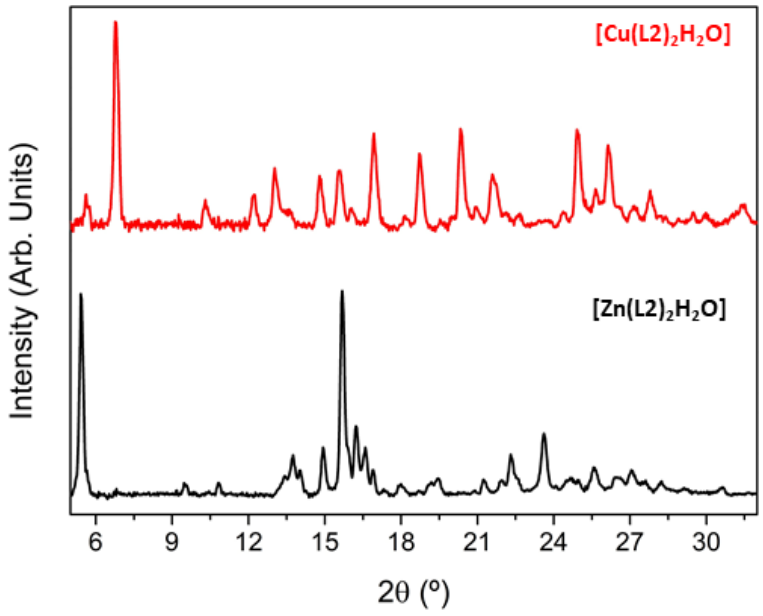


Figure S6. Powder diffraction pattern of milled samples of [Cu(**L2**)$_2$H$_2$O] (red) and [Zn(**L2**)$_2$H$_2$O] (black)

IR and UV-Vis Spectra

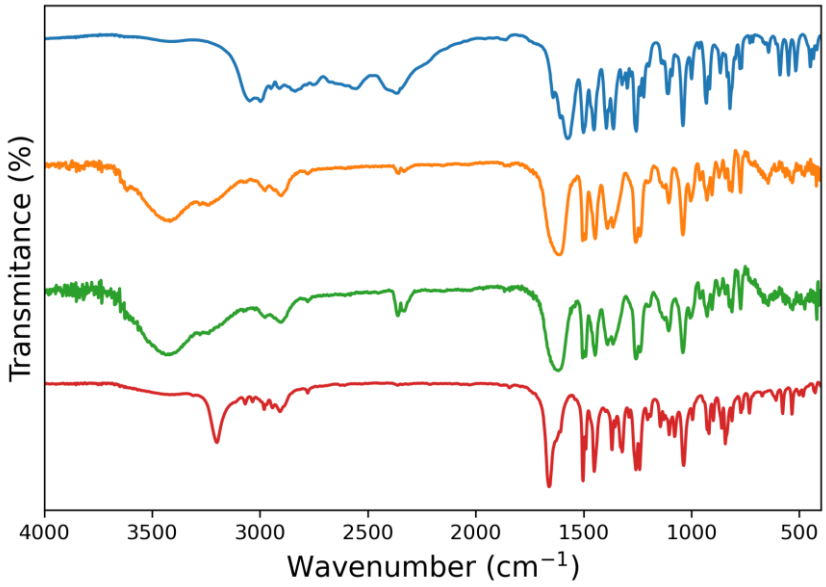


Figure S7. FT-IR spectra of **L1** (blue), [Cu(**L1**)$_2$(NH$_3$)$_2$] (orange), [Cu(**L1**)$_2$(H$_2$O)$_2$] (green) and [Cu(**L1**)$_2$] (red) in KBr pellet.

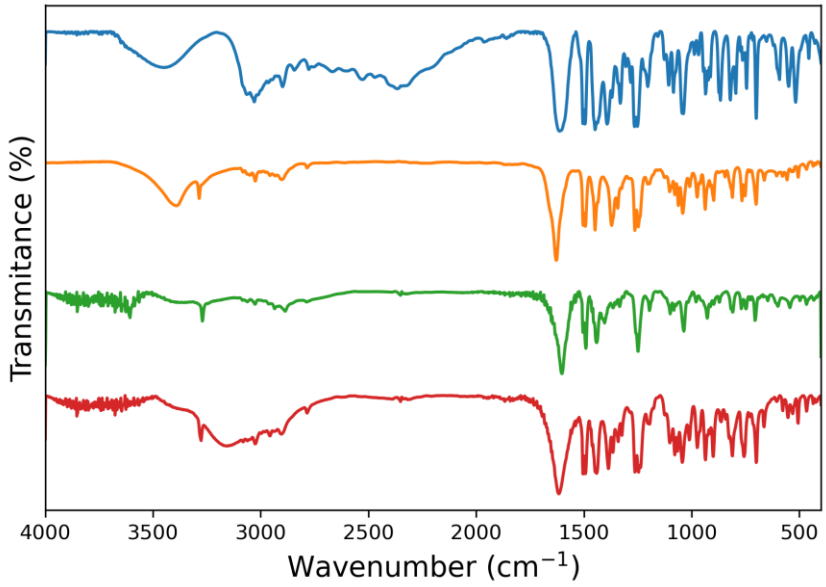


Figure S8. FT-IR spectra of **L2** (blue), [Cu(**L2**)$_2$H$_2$O] (orange), [Ni(**L2**)$_2$(H$_2$O)$_2$] (green) and [Zn(**L2**)$_2$H$_2$O] (red) in KBr pellet.

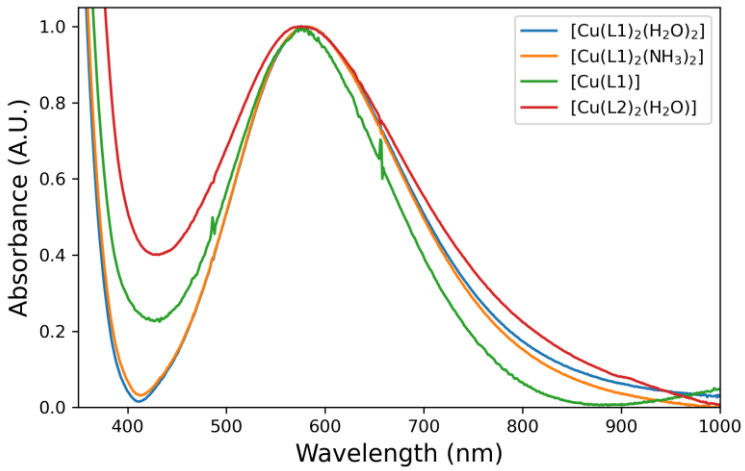


Figure S9. Normalized UV-Vis spectra of the synthesized complexes in DMSO. Bands at about 600 nm correspond to d-d transitions of the Cu^{2+} complexes. It is suggested that all complexes in DMSO show a tetragonal six-coordinate geometry due to the coordination of the solvent.

NMR ^{1}H Spectroscopy.

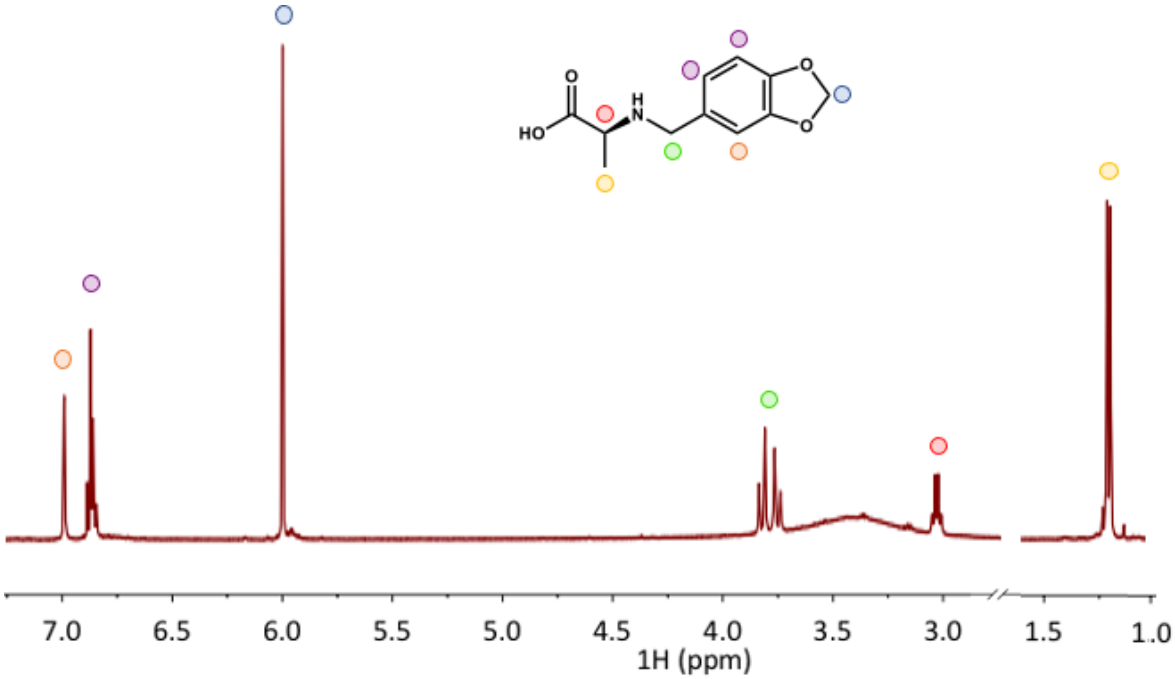


Figure S10. ^{1}H NMR spectra of **L1** in DMSO-d_6.

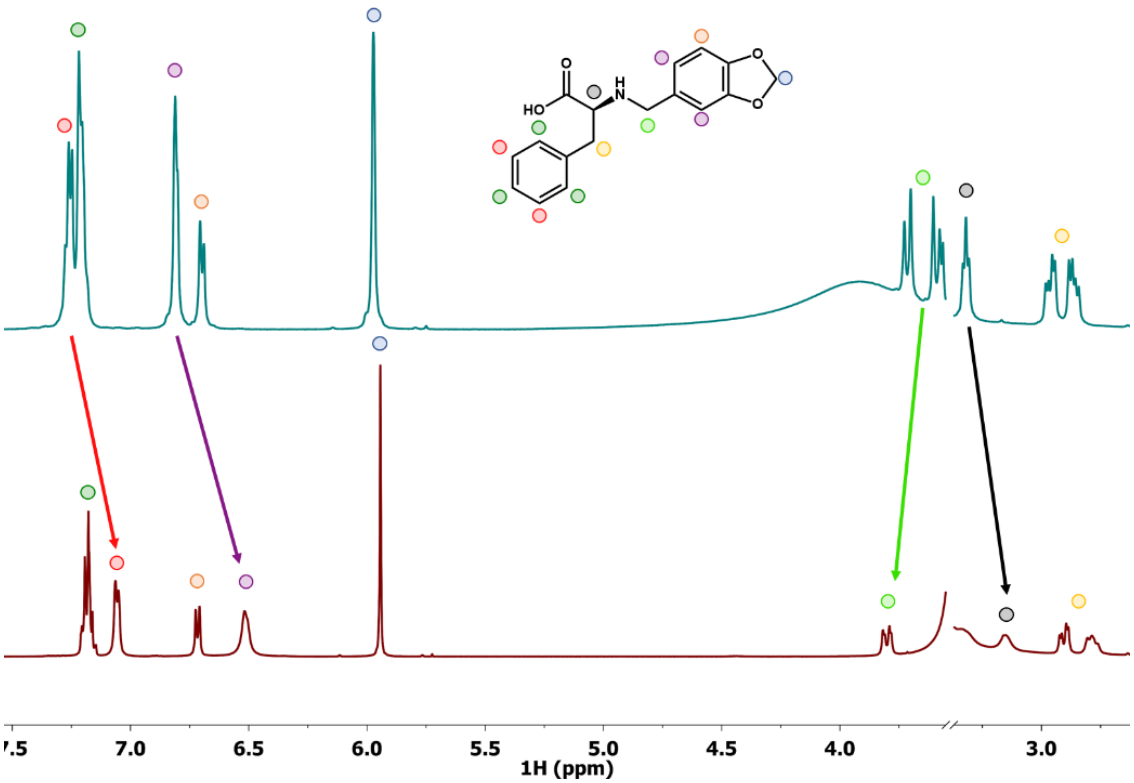


Figure S11. ^{1}H NMR spectra of **L2** (blue) and [Zn(**L2**)$_2$H$_2$O] (red) in DMSO-d_6.

CSD statistical analysis

Queries construction.

All searches were done over the CSD structural database employing the ConQuest November-2019 version. In all queries, all bonds were set to "Any" to avoid bond misinterpretation or omission. Polymeric and structures with the error were omitted for all hits in the query. For six-, five- and four-coordinate complexes, metal ions were linked to six, five and four atoms, being two of them, nitrogen atoms and the other two, oxygen atoms for all cases. The number of the remaining bonds were assigned to oxygen atoms changing in each query, from zero, one and two, respectively (Figure S12). The maximum number of linked atoms for each metal in every query was fixed to the corresponding coordination number. Hits that did not present 3D coordinates or contained disordered fragments were manually omitted when performing statistical analysis.

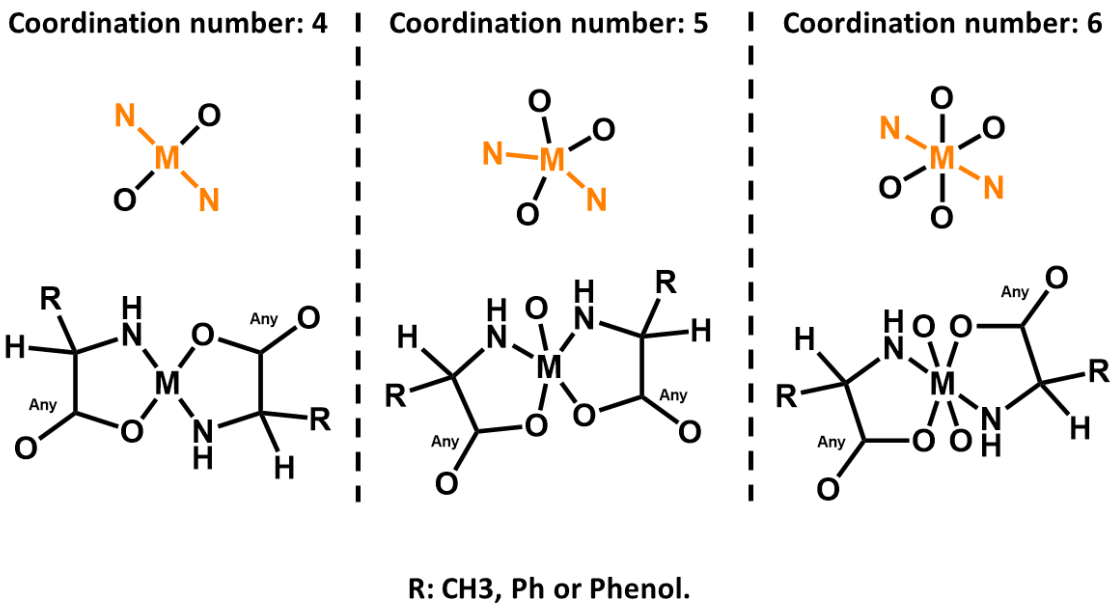


Figure S12. Structures used as queries for CSD searches, M = Ni, Cu, Zn, coordination number: 4-6 and amino acids: Ala, Phe for R = CH_3, Phe

MOGUL statistical analysis of structural parameters for [M(L2)$_2$H$_2$O].

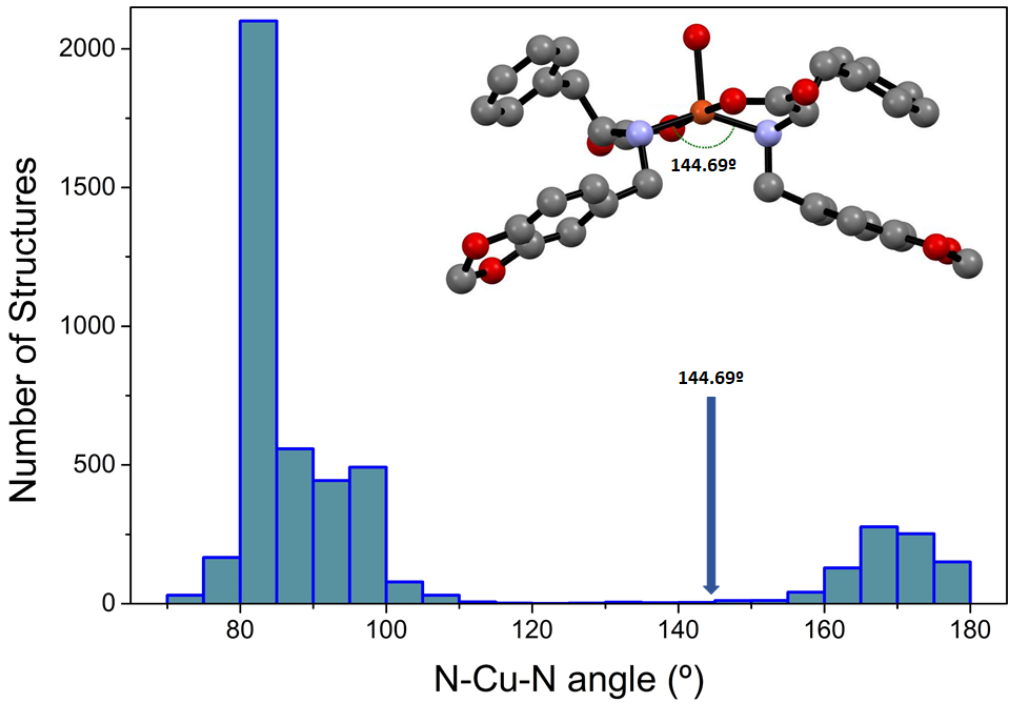


Figure S13. Distribution of the N–M–N angle (used as reference) in Cu five-coordinated complexes. Values found for [Cu(**L2**)$_2$H$_2$O] lie far from the most frequent values. Hydrogen atoms are not shown for clarity.

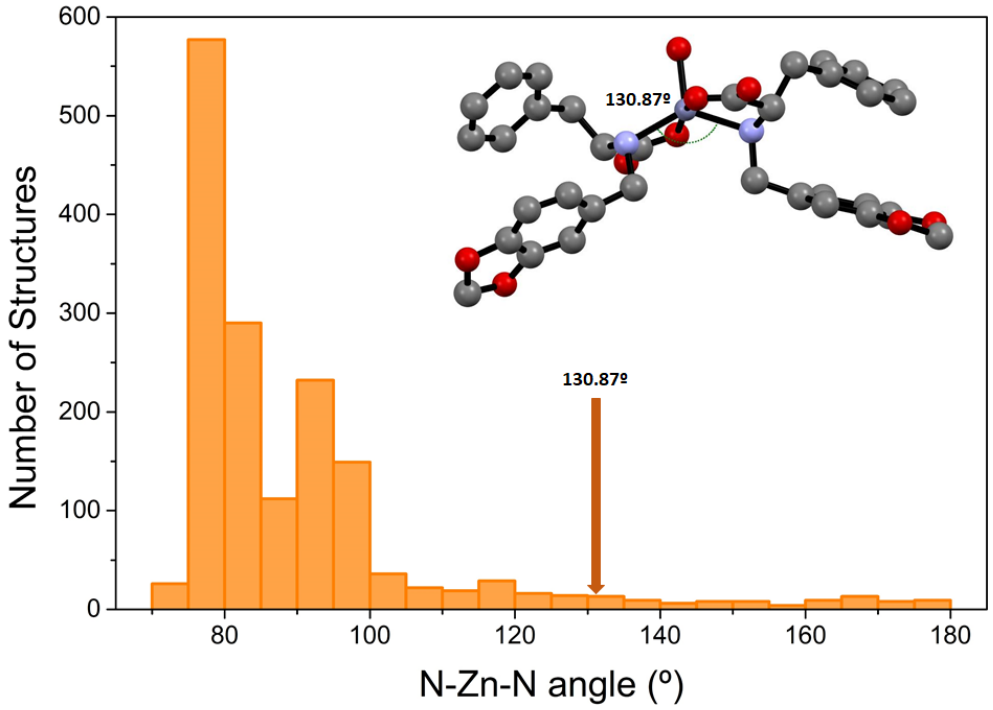


Figure S14. Distribution of the N–M–N angle (used as reference) in Zn five-coordinated complexes. Values found for [Zn(**L2**)$_2$H$_2$O] lie far from the most frequent values. Hydrogen atoms are not shown for clarity.

Supramolecular Analysis

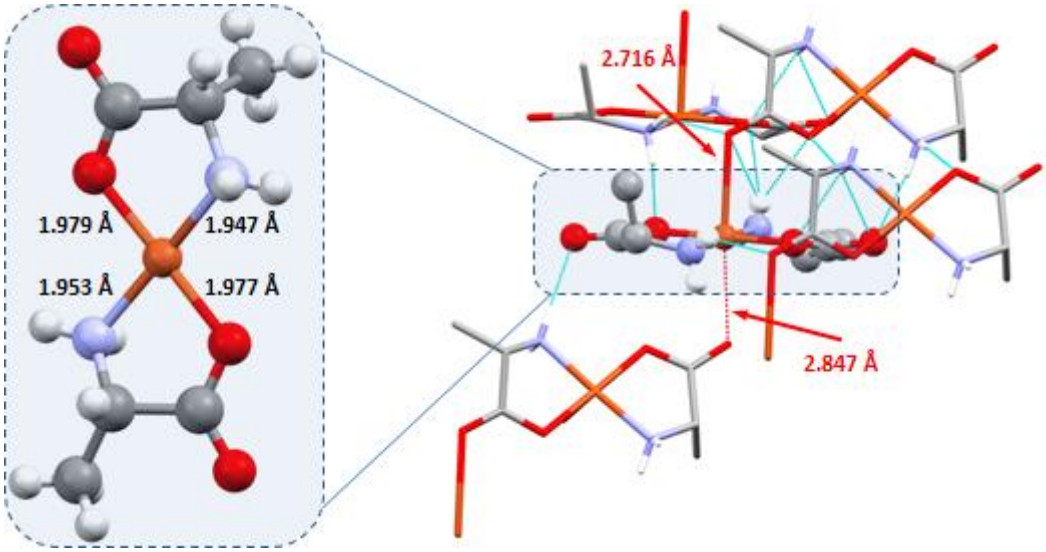


Figure S15. Supramolecular analysis for the complex *trans*-bis(L-α-Alaninato)-copper(II) ID: CUALTE01.

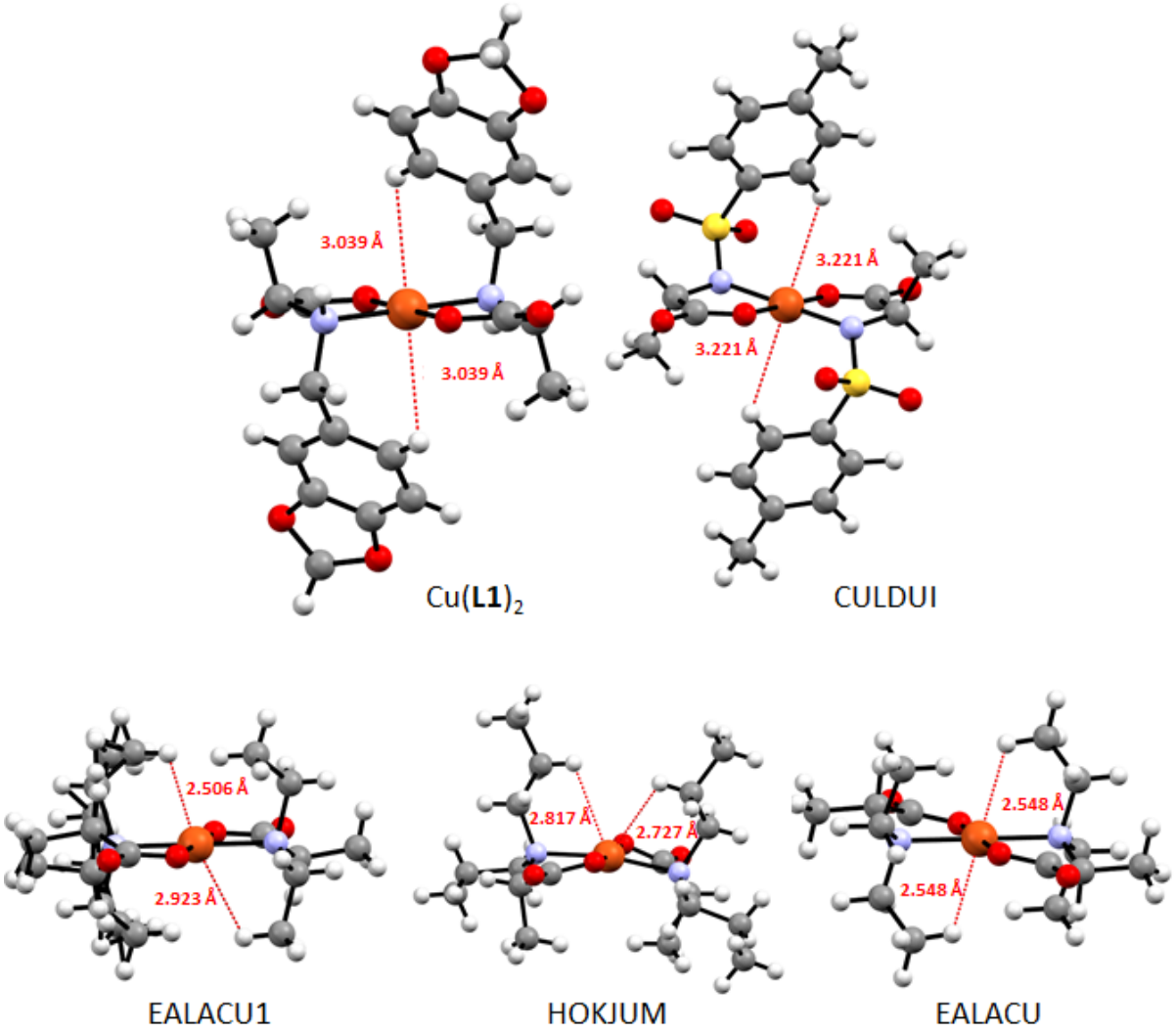


Figure S16. Square planar Cu^{2+} complexes with flexible ligands showing structural features similar to **Cu(L1)$_2$**; interatomic distance between the metal center and the nearest atom in the apical position are indicated in red dashed lines.

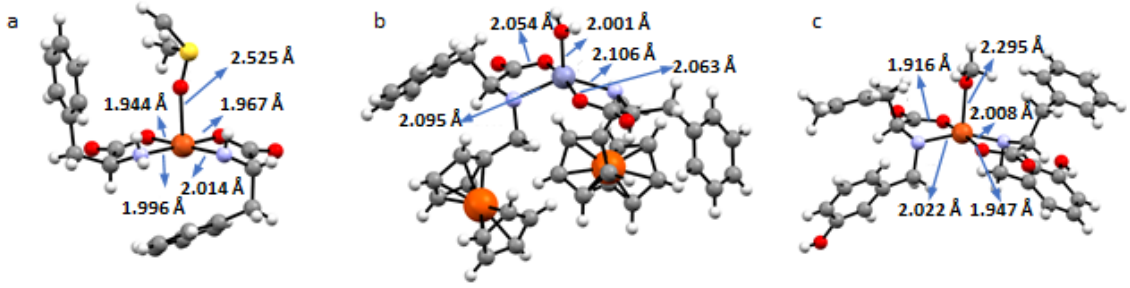


Figure S17. Five-coordinate complexes with similar features than [M(**L2**)$_2$(H$_2$O)] M = Cu, Zn, ID codes: CEBREG (a), NEPLIE (b), and TIFSIM ; bond distances involving the metal centers are indicated.

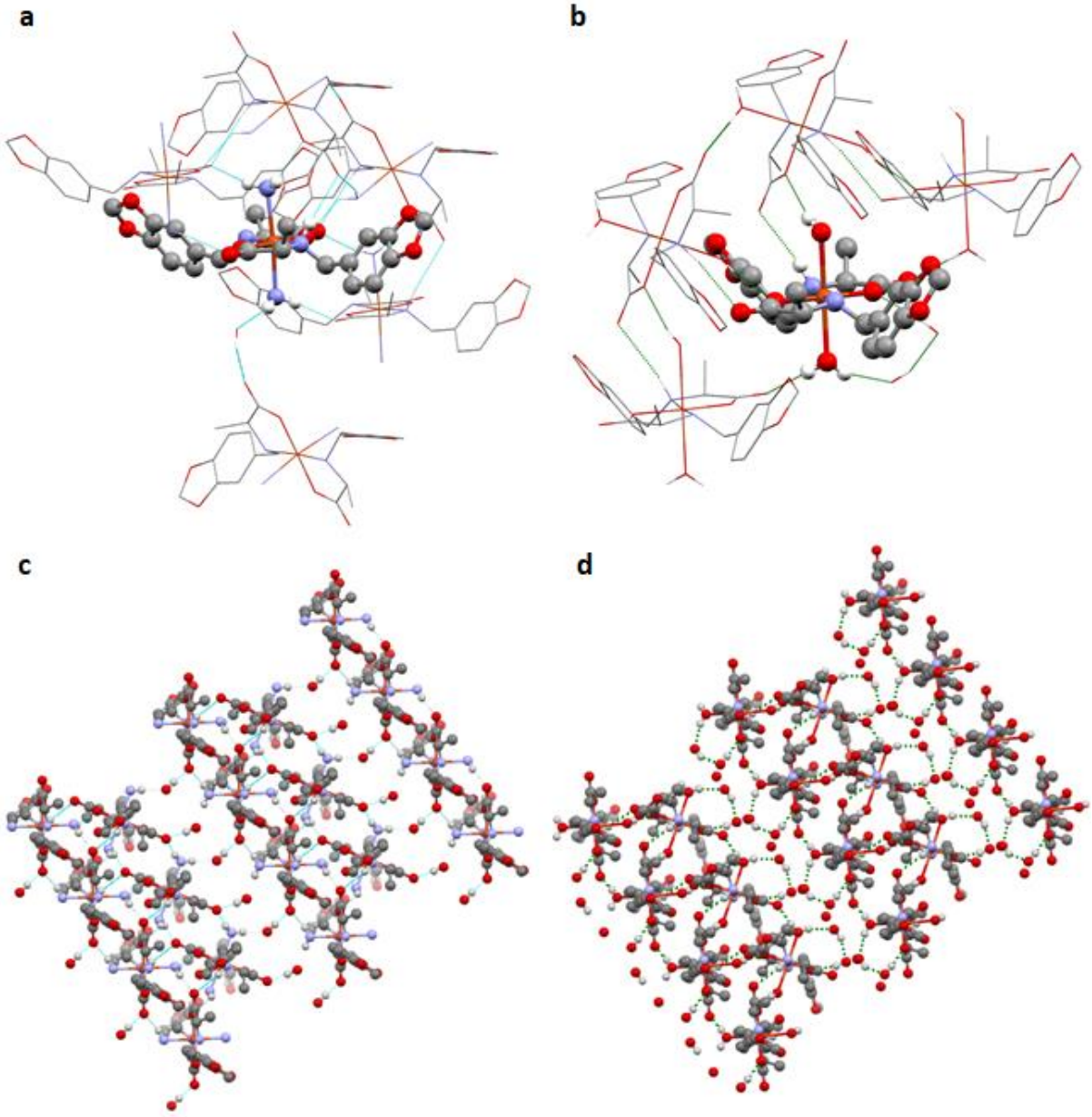


Figure S18. Short contacts present in the crystal structures of [Cu(**L1**)$_2$(X)$_2$], with X = NH_3 (a) or H_2O (b). Detail of the 3D supramolecular architecture developed due to connection of the linear arrangements by different C–H···O contacts ((c) for X = NH_3, and (d) for X = H_2O).

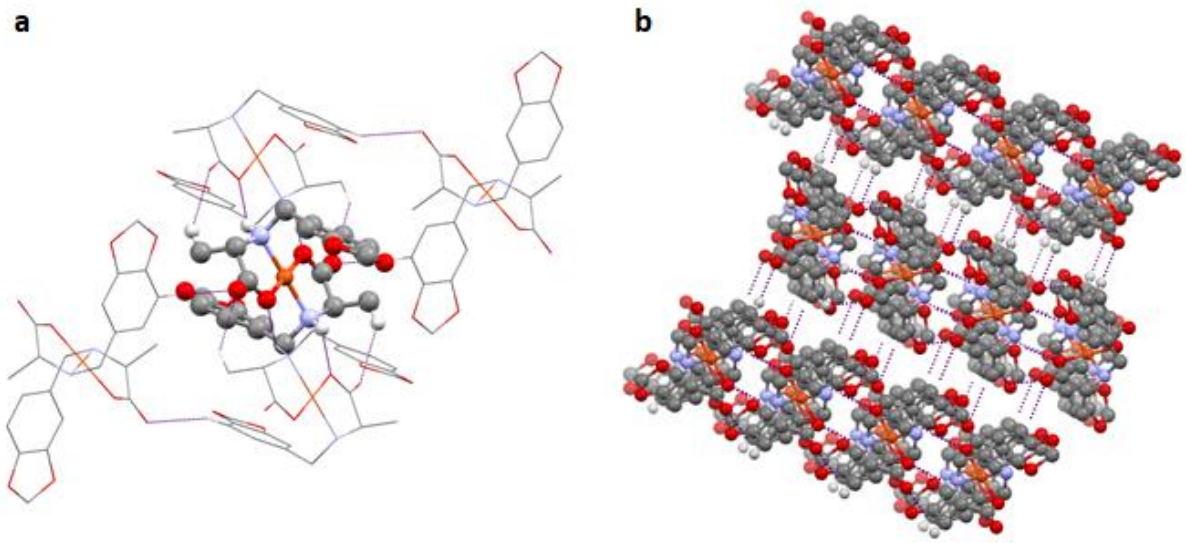


Figure S19. Short contacts present in the crystal structure of [Cu(**L1**)$_2$] (a). 1D arrangements are connected through different C–H···O H-bonds to assemble a 3D supramolecular structure (b).

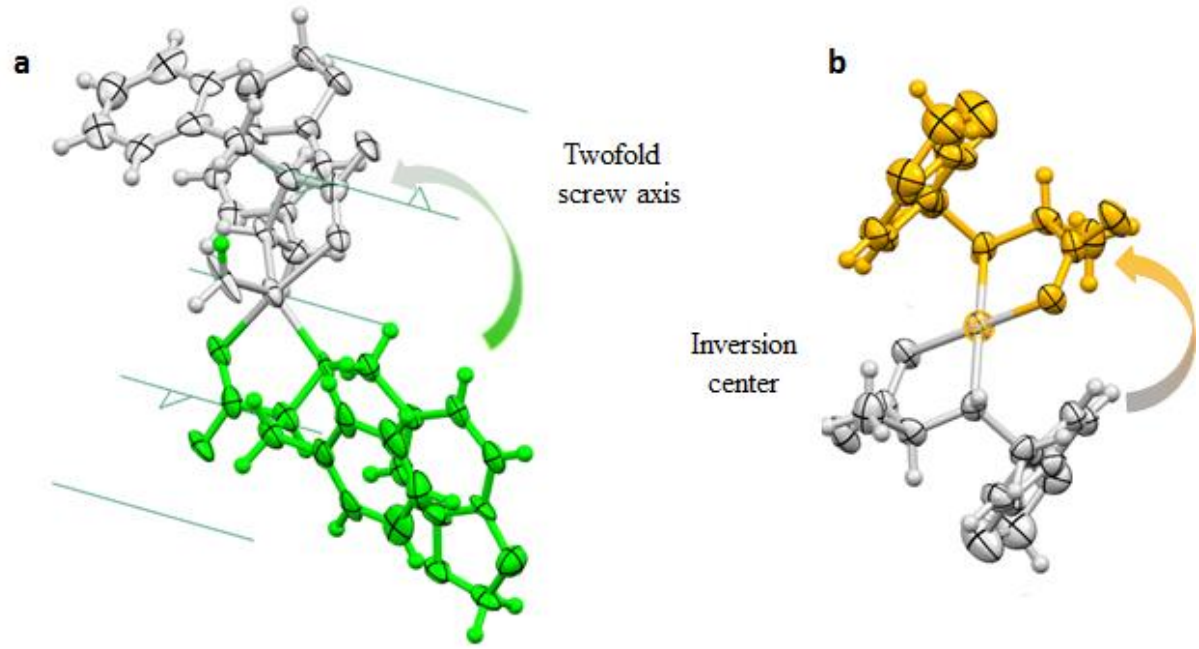


Figure S20. Symmetry operations in the molecular structures of [Zn(**L2**)$_2$(H$_2$O)] (a) and [Cu(**L1**)$_2$] (b)

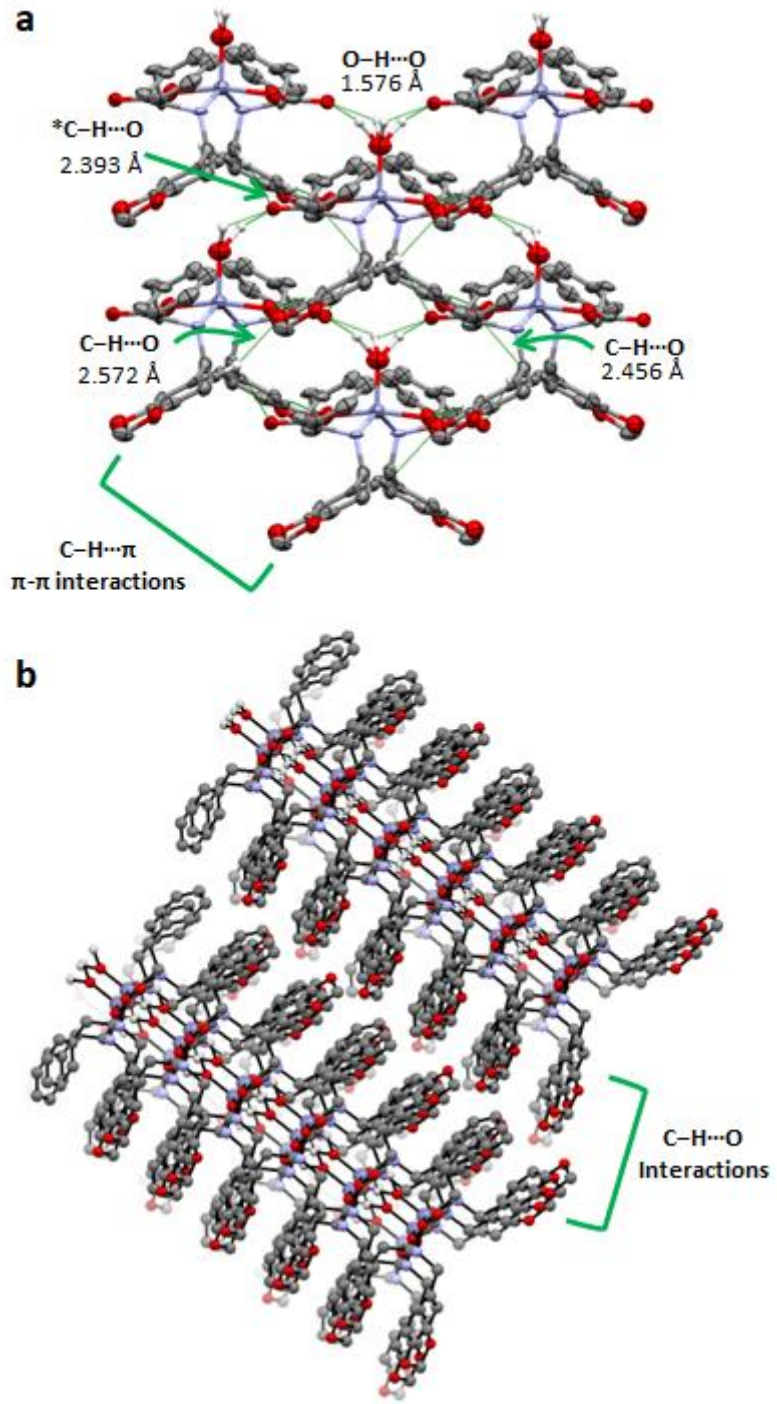


Figure S21. Short contacts present in the crystal structure of [Zn(**L2**)$_2$(H_2O)] (a). Detail of the different C–H···O H-bonds to assemble the 2D and 3D supramolecular structure (b).

DFT electronic structure calculations

Geometry optimizations

When comparing the single-crystal X-ray diffraction structures with the results obtained after geometry optimization, some changes are observed in the $MN_2O_2O_x$ moiety related to angles and, to a lesser extent, to bond lengths. The greatest differences were obtained for copper complexes in comparison with [Zn(**L2**)$_2$(H_2O)]; for the last one, only the angle between N-Zn-O planes showed some differences (from 51.1° to 48.7° after optimization). In contrast, the analogous complex [Cu(**L2**)$_2$(H_2O) showed a more pronounced variation of the interplanar angle after geometry optimization (from 35.2° to 18.3°), and as a result, an increase of the symmetry in the MN_2O_2 moiety is also observed. Finally, as mentioned in the manuscript complexes [Cu(**L1**)2($X)_2$] with X = NH_3 and H_2O, showed the most drastic change, since the octahedral geometry did not correspond to an energy minimum.

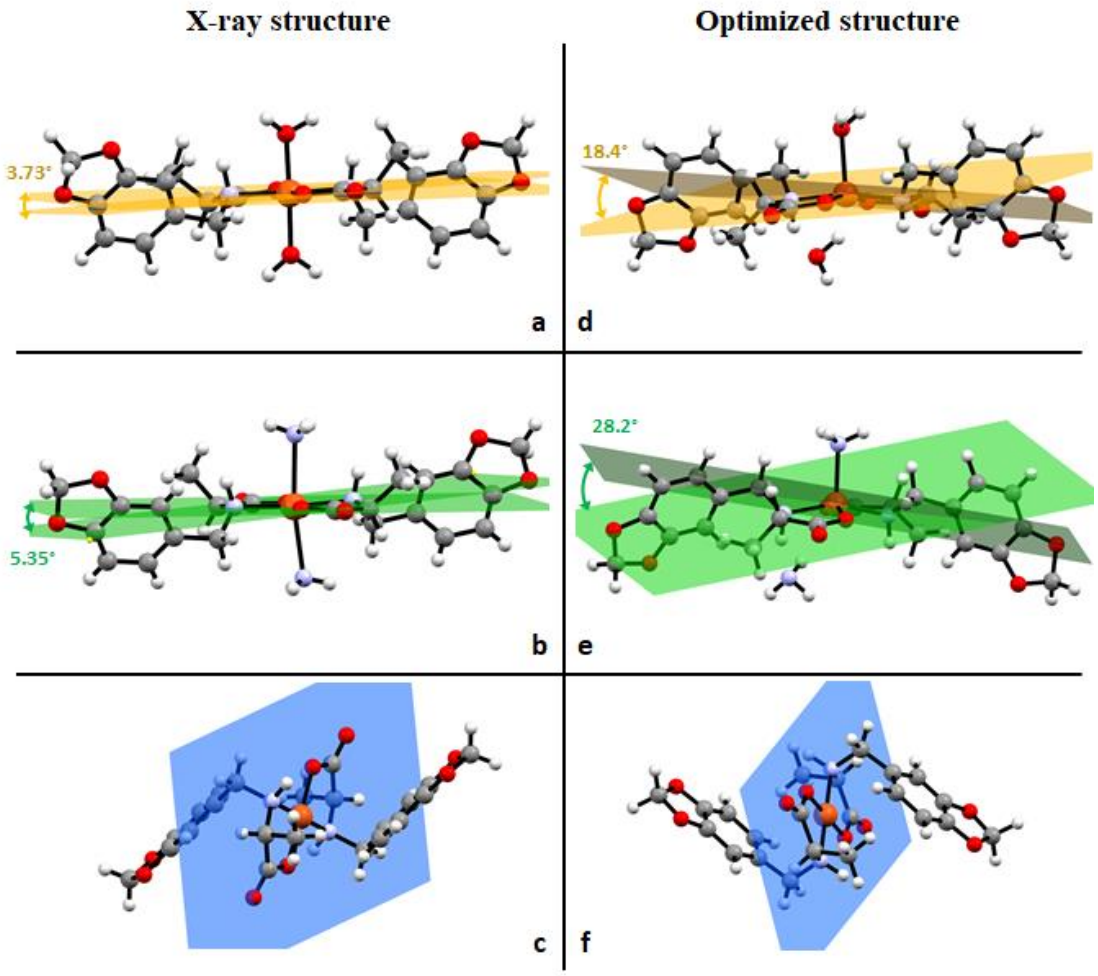


Figure S22. Crystal structures obtained by single-crystal X-ray diffraction experiments (left) and DFT optimized geometries at the BP86/def2-SVP for all light atoms/def2-TZVP for Cu (right) for

Cu(**L1**)$_2$H$_2$O (a and d), Cu(**L1**)$_2$NH$_3$ (b and e) and Cu(**L1**)$_2$ (c and f). For each structure two plains containing N-M-O atoms of the MN_2O_2 moiety are plotted.

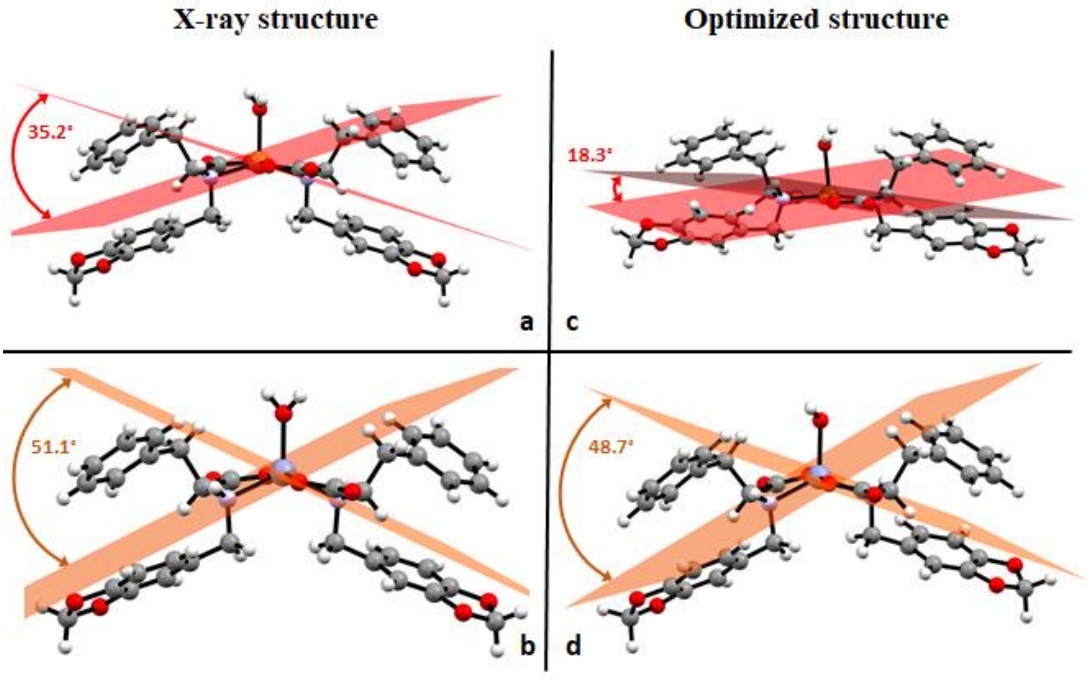


Figure S23. Crystal structures obtained by single-crystal X-ray diffraction experiments (left) and DFT optimized geometries at the BP86/def2-SVP for all light atoms/def2-TZVP for metals (right) for Cu(**L2**)$_2$H$_2$O (a and c) and Zn(**L2**)$_2$H$_2$O (b and d). For each structure two plains containing N-M-O atoms of the MN_2O_2 moiety are plotted.

Molecular Orbitals Calculations

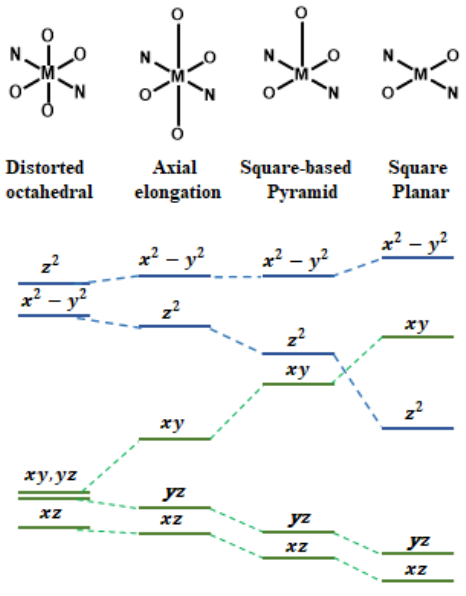


Figure S24. Schematic representation of the molecular orbital diagram on a distorted six-coordinate environment, axially elongated octahedra, square-based pyramid and square planar.

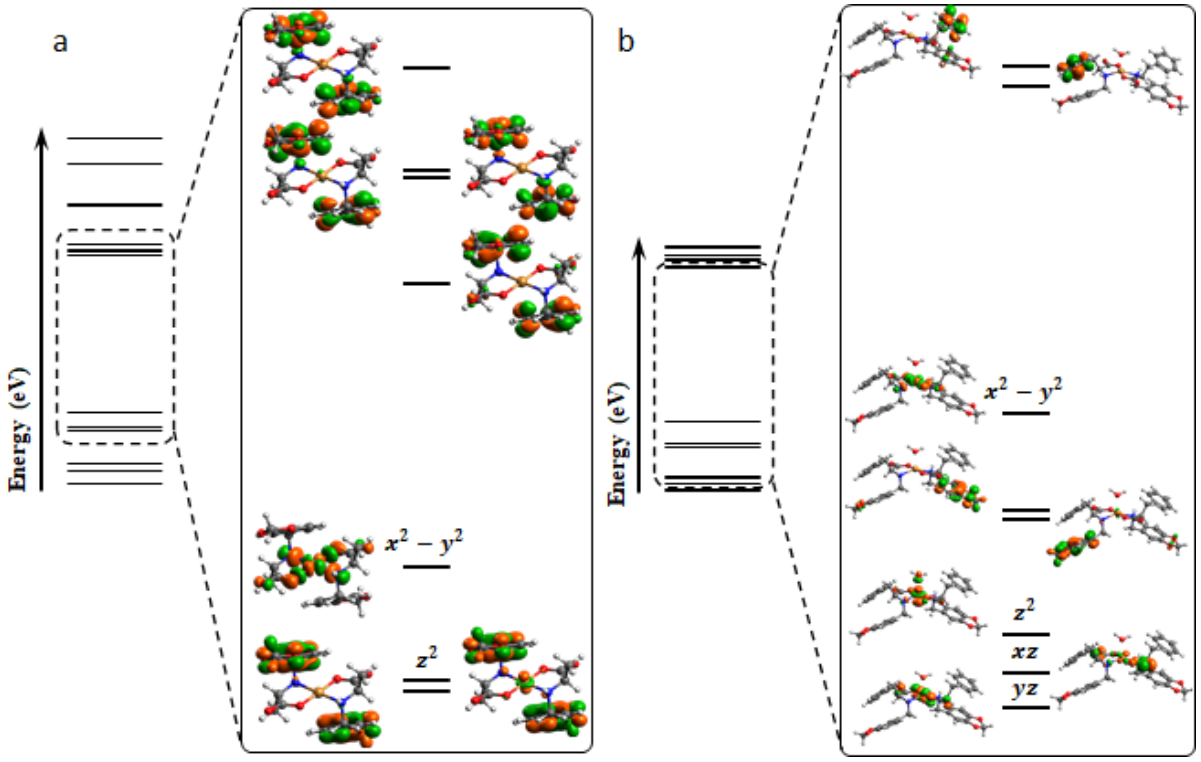


Figure S25. Calculated molecular orbital diagram (left) at the BP86/def2-SVP for all light atoms/def2-TZVP for [Cu(**L1**)$_2$] (a) and [Cu(**L2**)$_2$H$_2$O] (b) and detailed diagram for the frontier orbitals gap (right); molecular orbitals are plotted with isosurface=0.04 and 0.05 respectively.

Energy Framework Analysis

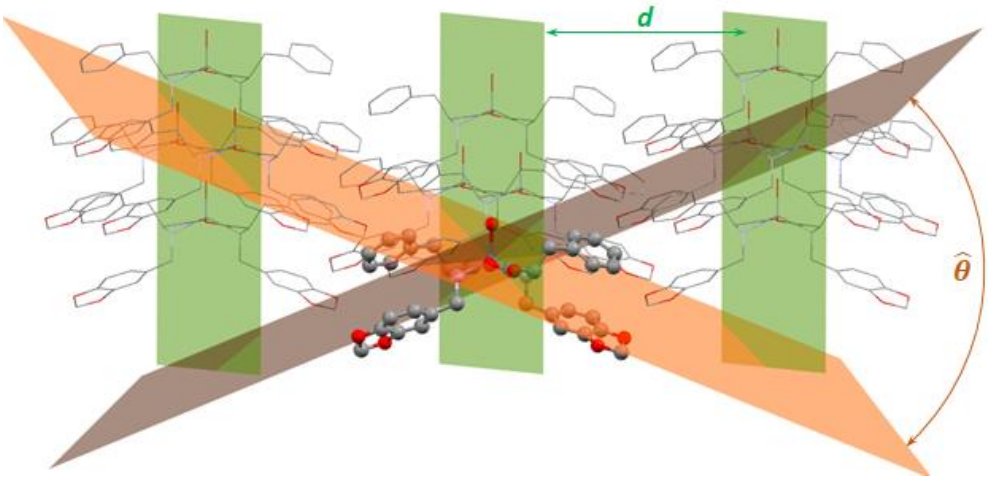
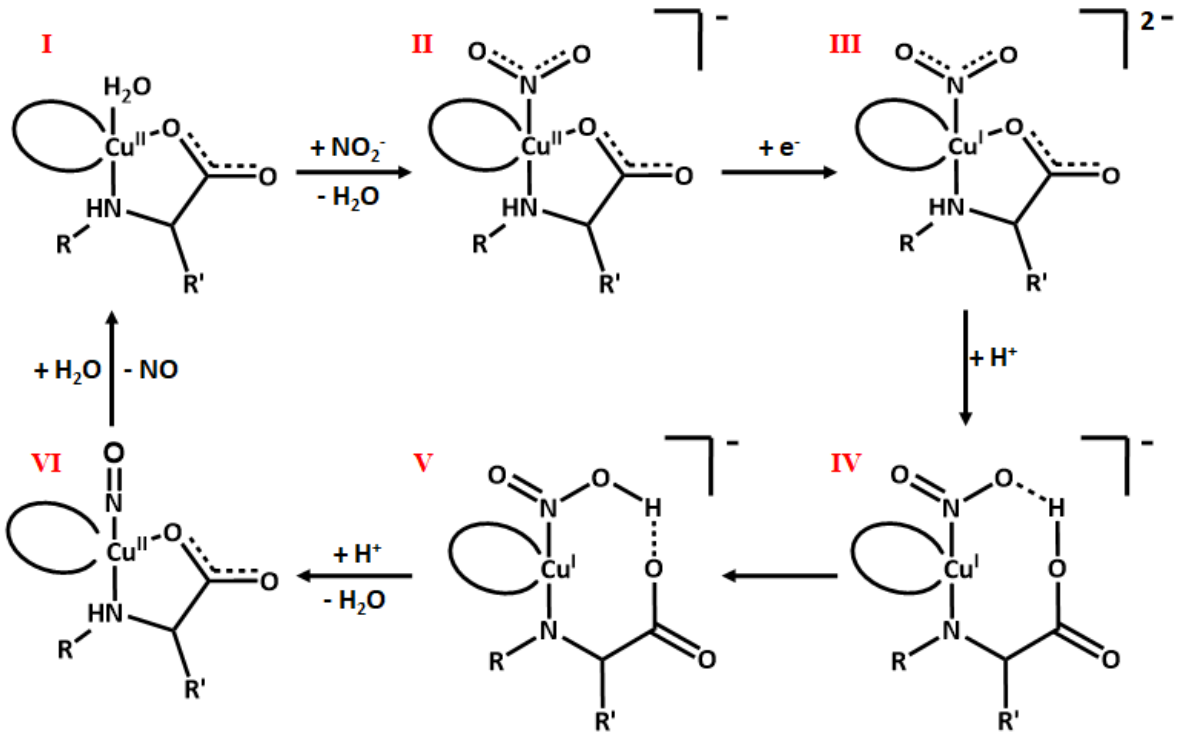


Figure S26. Representation of distance between 1D-layer planes(***d***) and interplanar angles (**θ**) exemplified for [Zn(**L2**)$_2$H$_2$O] structure.

Electrochemical characterization and catalytic studies

Scheme S4. Proposed mechanism of the electrocatalytic cycle for the reduction of nitrite to nitric oxide by copper complexes.



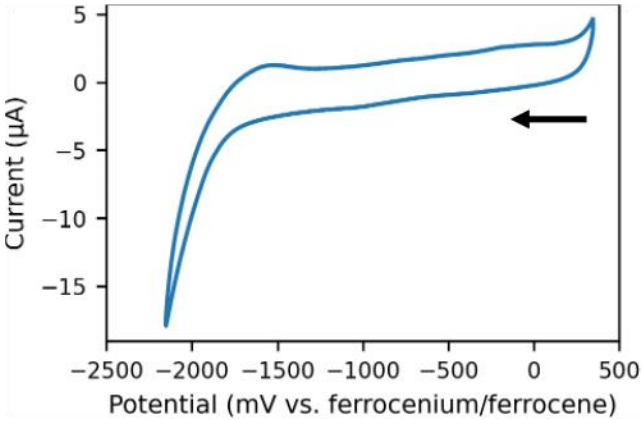


Figure S27. Cyclic voltammogram of $[Zn(L2)_2(H_2O)]$ (7.4 mM) in DMSO, with $[TBAPF_6]$ = 0.2 M, glassy carbon as working electrode and Pt as counter electrode, at 100 mV/s. No redox-assigned signals are observed in the scan range studied, except for the decomposition of the solvent at extreme potentials.

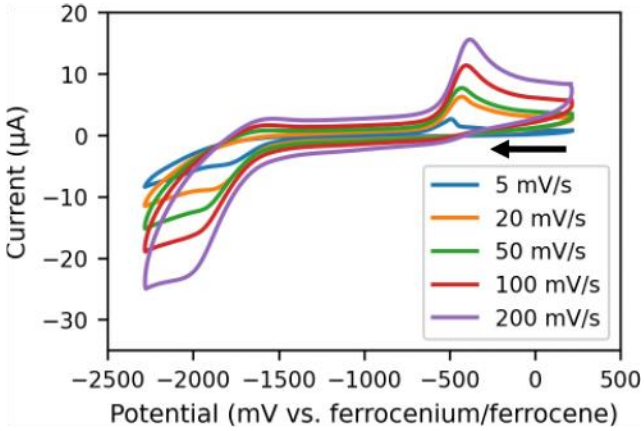


Figure S28. Cyclic voltammograms of [Ni(**L2**)$_2$(H$_2$O)$_2$] (7.4 mM) in DMSO, with [TBAPF$_6$] = 0.2 M, glassy carbon as working electrode and Pt as counter electrode, at different scan rates (5 to 200 mV/s).

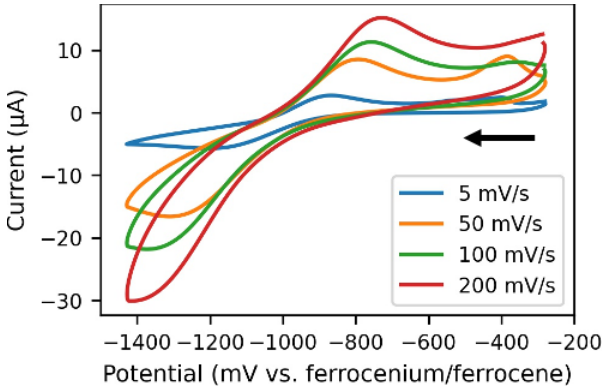


Figure 29. Cyclic voltammograms of [Cu(**L1**)$_2$] (7.4 mM) in DMSO, with [TBAPF$_6$] = 0.2 M, glassy carbon as working electrode and Pt as counter electrode, at different scan rates (5 to 200 mV/s).

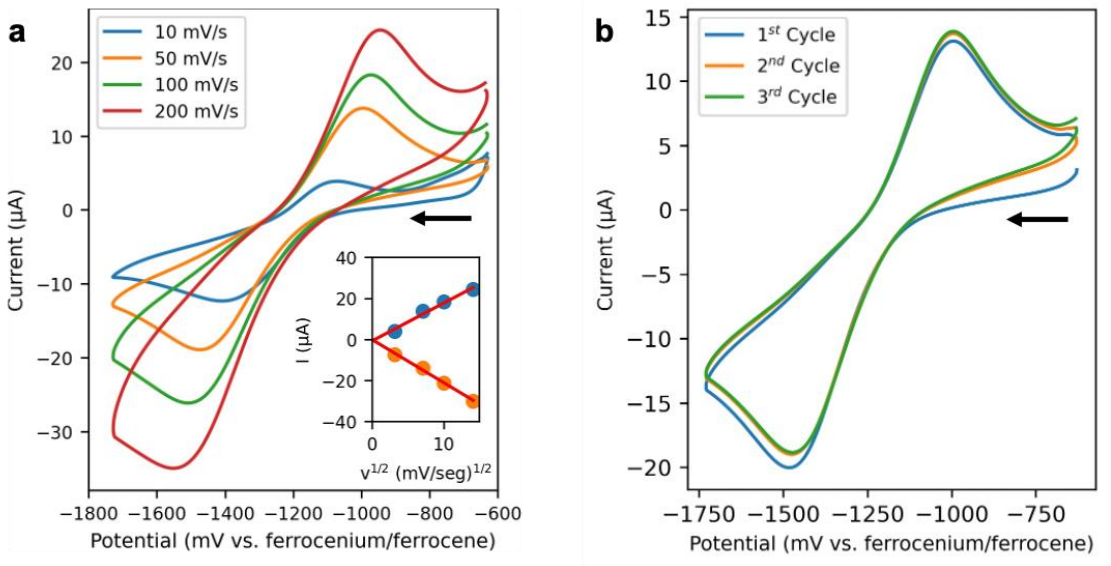


Figure 30. a) Cyclic voltammograms of [Cu(**L1**)$_2$(NH$_3$)$_2$] (7.4 mM) in DMSO, with [TBAPF$_6$] = 0.2 M, glassy carbon as working electrode and Pt as counter electrode, at different scan rates (10 to 200 mV/s). Inset: Plot of the anodic peak current (blue) and the cathodic peak current (orange) vs square root of the scan rate. b) Three consecutive cyclic voltammograms of [Cu(**L1**)$_2$(NH$_3$)$_2$] in the same conditions at a scan rate = 50 mV/s. Analogues results were obtained for the other scans rates.

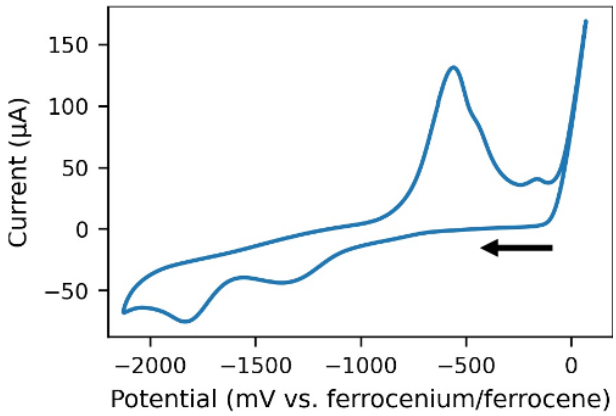


Figure S31. Cyclic voltammograms of [Cu(**L2**)$_2$(H$_2$O)] (7.4 mM) in DMSO, with [TBAPF$_6$] = 0.2 M, glassy-carbon as working electrode and Pt as counter electrode, at 100 mV/s.

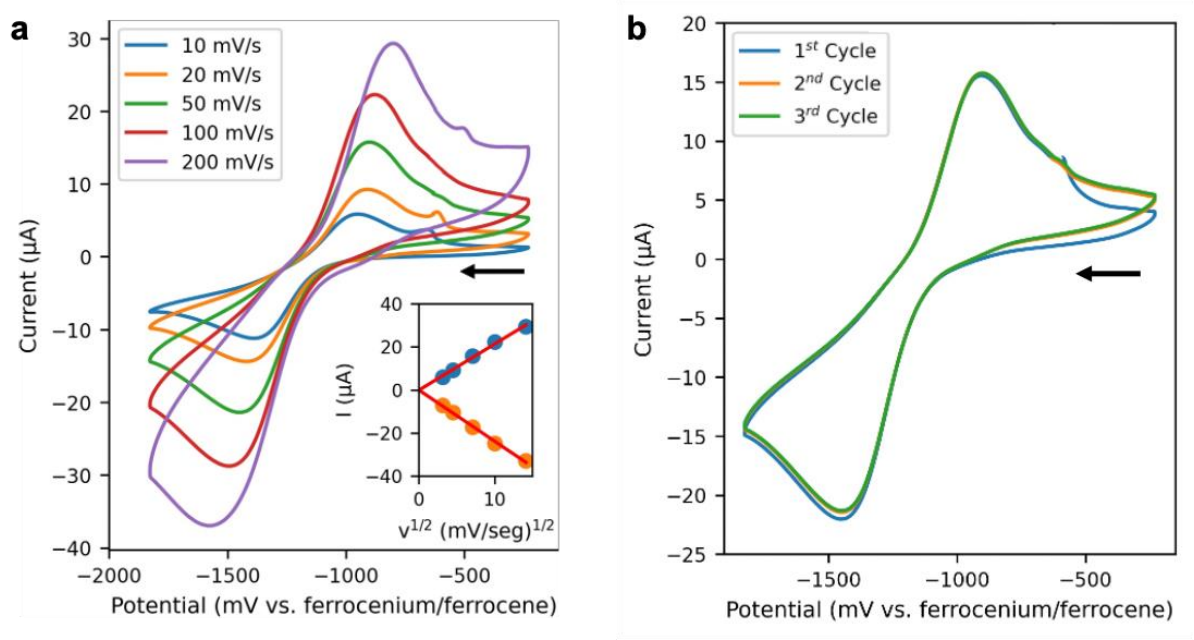


Figure S32. a) Cyclic voltammograms of [Cu(**L2**)$_2$(H$_2$O)] (7.4 mM) in DMSO, with [TBAPF$_6$] = 0.2 M, glassy carbon as working electrode and Pt as counter electrode, at different scan rates (10 to 200 mV/s). Inset: Plot of the anodic peak current (blue) and the cathodic peak current (orange) vs square root of the scan rate. b) Three consecutive cyclic voltammograms of [Cu(**L2**)$_2$(H$_2$O)] in the same conditions at a scan rate = 50 mV/s. Analogues results were obtained for the other scans rates.

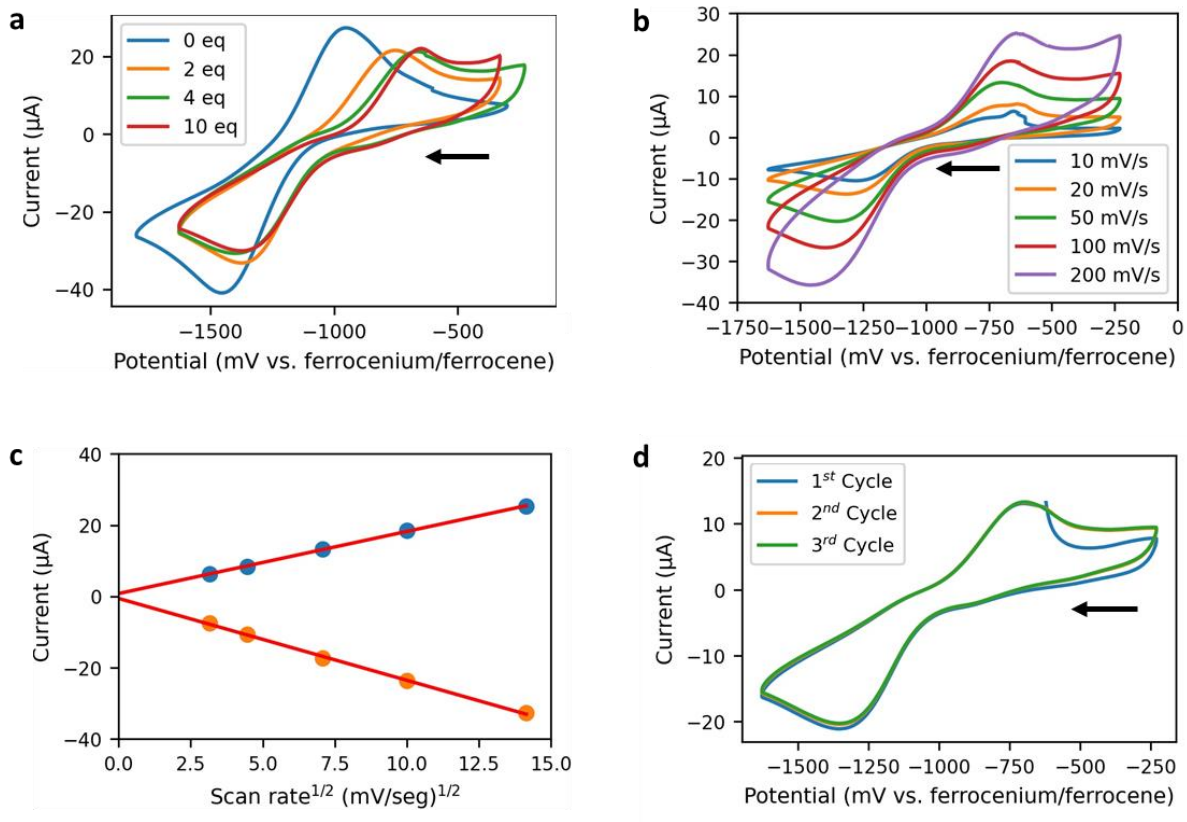


Figure S33. a) Cyclic voltammograms of [Cu(**L2**)$_2$(H$_2$O)] (7.4 mM) in DMSO with the addition of different equivalents of $NaNO_2$ in DMSO, with [$TBAPF_6$] = 0.2 M, glassy-carbon as working electrode and Pt as counter electrode, at 100 mV/s. b) Cyclic voltammograms of [Cu(**L2**)$_2$(H$_2$O)] with 4 equivalents of $NaNO_2$ in the same conditions at different scan rates (10 to 200 mV/s). c) Plot of the anodic peak current (orange) and the cathodic peak current (blue) vs square root of the scan rate. d) Three consecutive cyclic voltammograms of [Cu(**L2**)$_2$(H$_2$O)] with 4 equivalents of $NaNO_2$ in the same conditions at a scan rate = 50 mV/s. Analogues results were obtained for the other scans rates.

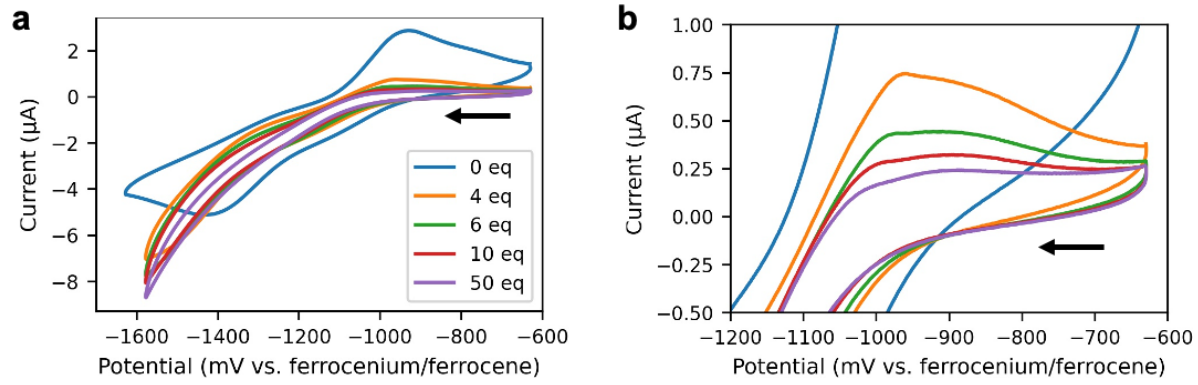


Figure S34. a) Cyclic voltammograms of [Cu(**L2**)$_2$(H$_2$O)] in DMSO (7.4 mM) with the addition of 100 equivalents of $NaNO_2$ and different amounts of benzoic acid, with [$TBAPF_6$] = 0.2 M, glassy-carbon as working electrode and Pt as counter electrode, at 100 mV/s. b) Amplification of the region from -1200 mV to - 600 mV to observe the diminution of the anodic peak. The colours refer to the same experiments as the ones informed in Figure S34 a.

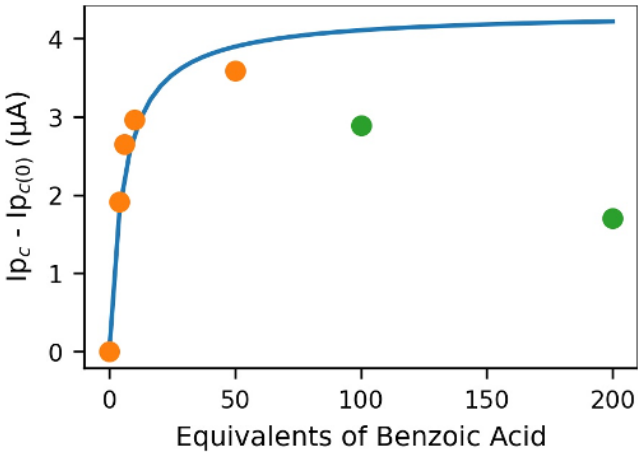


Figure S35. Plot of the difference between the catalytic peak current (Ip_c) and the cathodic peak current ($Ip_{c(0)}$) vs. the concentration of benzoic acid added for the voltammograms of Figure S34.

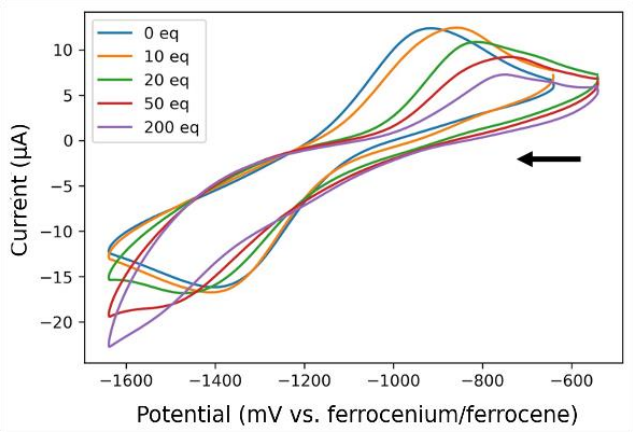


Figure S36. Cyclic voltammograms of [Cu(**L2**)$_2$(H_2O)] in DMSO (7.4 mM) with the addition of different amounts of benzoic acid, with [$TBAPF_6$] = 0.2 M, glassy-carbon as working electrode and Pt as counter electrode, at 100 mV/s.

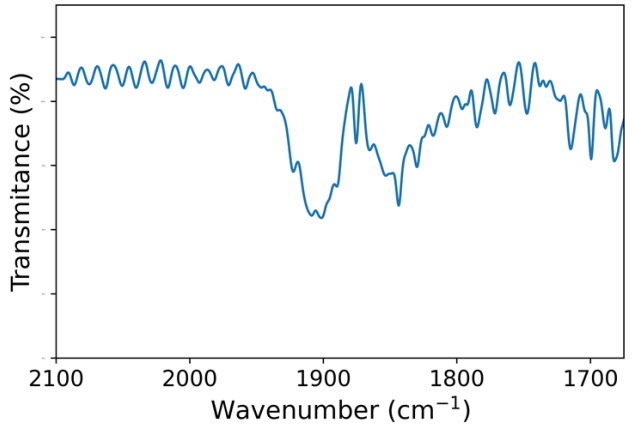


Figure S37. FTIR spectrum of the headspace from the electrolysis, which shows the distinctive bands of the NO centered at 1876 cm^{-1} (Dinerman & Ewing, 1970).

Study of the proposed intermediaries. NO-specie

A solution of [Cu(**L2**)$_2$(H$_2$O)] 7.4 mM in DMSO was degassed and bubbled with NO(g). The NO(g) was prepared following known procedures (Suarez *et al.*, 2015). The reaction was followed by UV-Visible spectroscopy, observing a shift of the λ_{max} from 573 nm to 745 nm with a color change from blue to green-yellow and a characteristic band between 325 and 400 nm which has been previously observed in the reduction of Cu^{2+} complexes to Cu^{+} mediated by nitric oxide (Figure S43) (Sarma *et al.*, 2010).

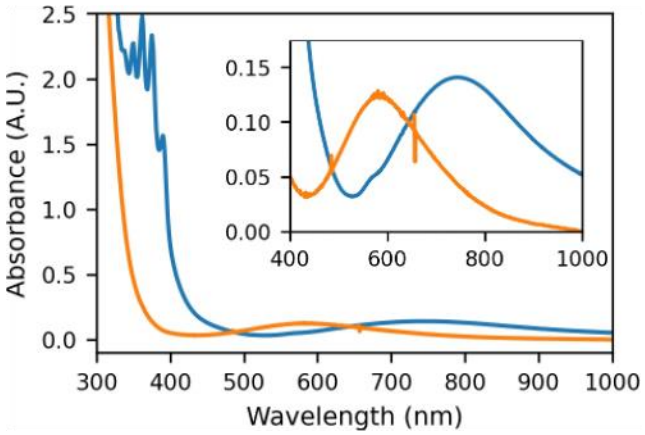


Figure S38. UV-Visible of a solution 7.4 mM [Cu(**L2**)$_2$(H$_2$O)] in DMSO (blue) and the product of the reaction with nitric oxide (orange).

Study of the proposed intermediaries. Nitrite-species

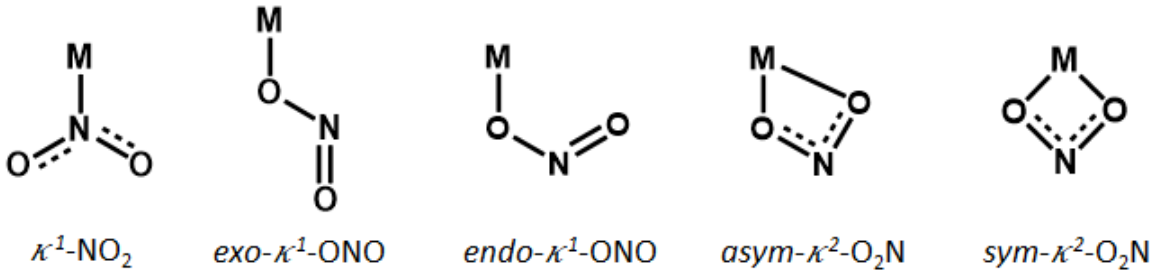


Figure S39. Most frequent monodentate or bidentate coordination modes for nitrite complexes.

Evaluation of the coordination modes of the nitrite in $[Cu(L2)_2(NO_2)]^-$, after acid addition.

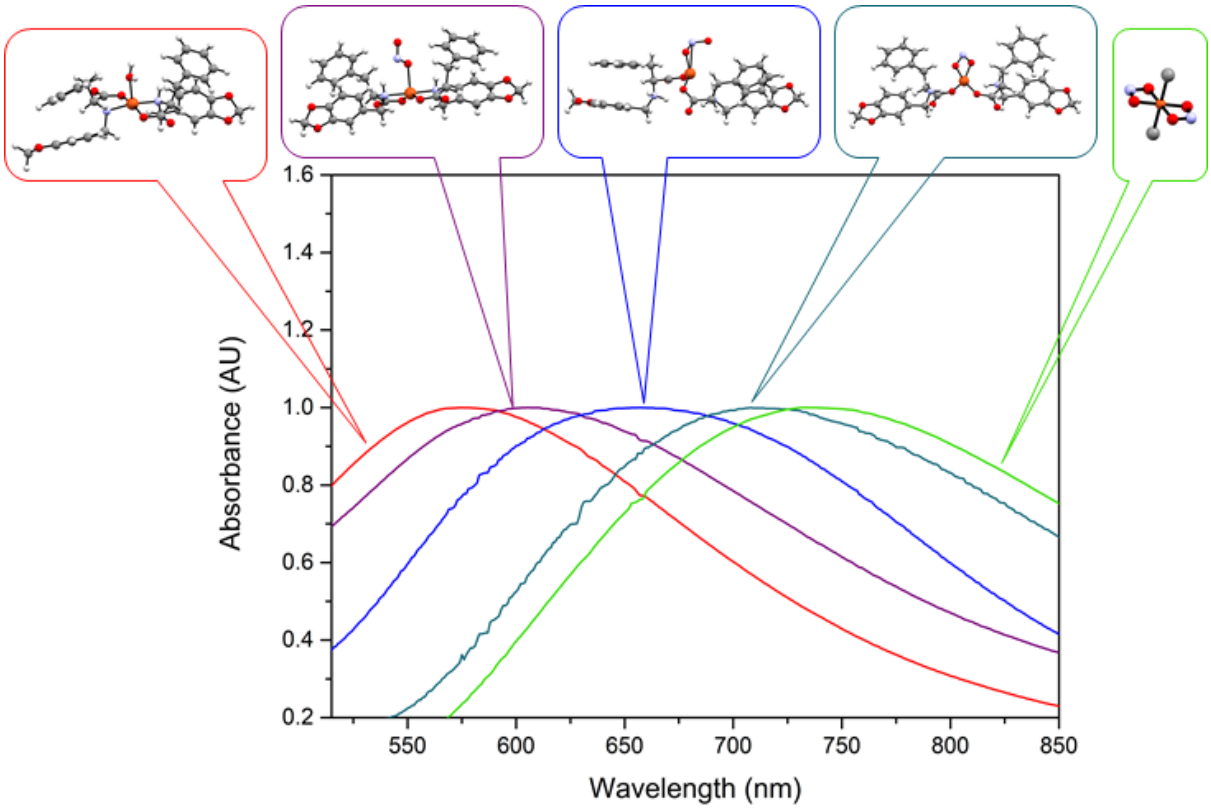


Figure S40. Normalized UV-Vis spectra of the reaction evolution for the addition of acid to $[Cu(\mathbf{L2})_2(NO_2)]^-$ in DMSO. Reference complex $[Cu(\mathbf{L2})_2(H_2O)]^-$ (red), $[Cu(\mathbf{L2})_2(NO_2)]^-$ (purple), spectrum of $[Cu(\mathbf{L2})_2(NO_2)]^-$ immediately after acid addition (blue), spectrum after 24 hours (dark green) and Cu(II)-nitrite solution in DMSO (light green). On top of each spectrum, suggested species are shown. For the last spectrum, an octahedral Cu(II)-nitrite-solvent species is proposed. Grey spheres in the *trans* positions represent either solvents or other ligands.

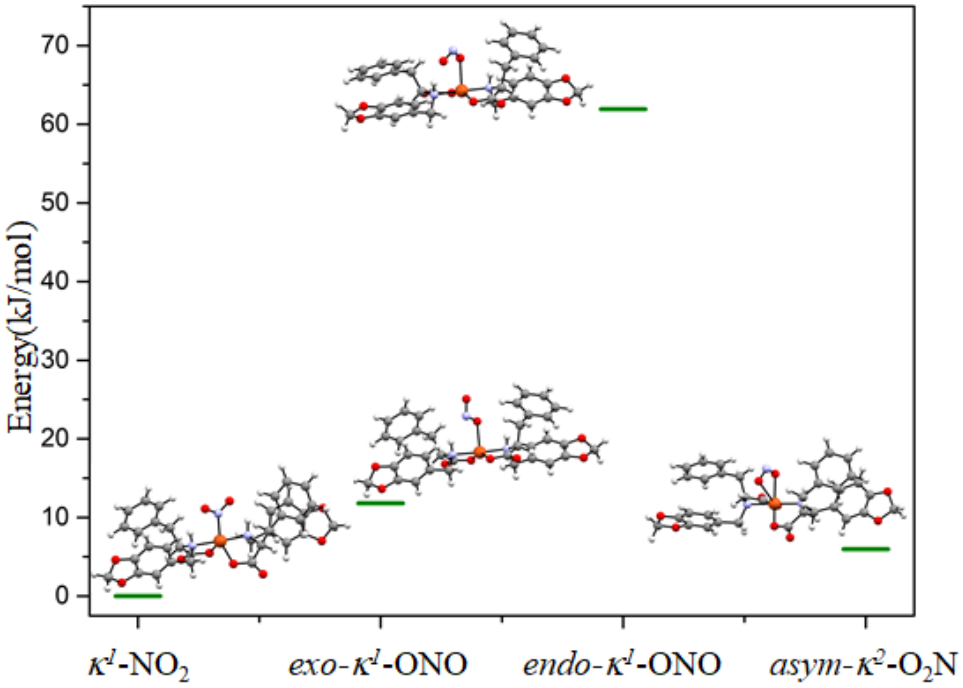


Figure S41. DFT calculated energies at the BP86/def2-SVP for all light atoms/def2-TZVP for Cu with CPCM model (DMSO) (in kJ/mol) for$[Cu(\mathbf{L2})_2(NO_2)]^-$ with different coordination modes for the nitrite.

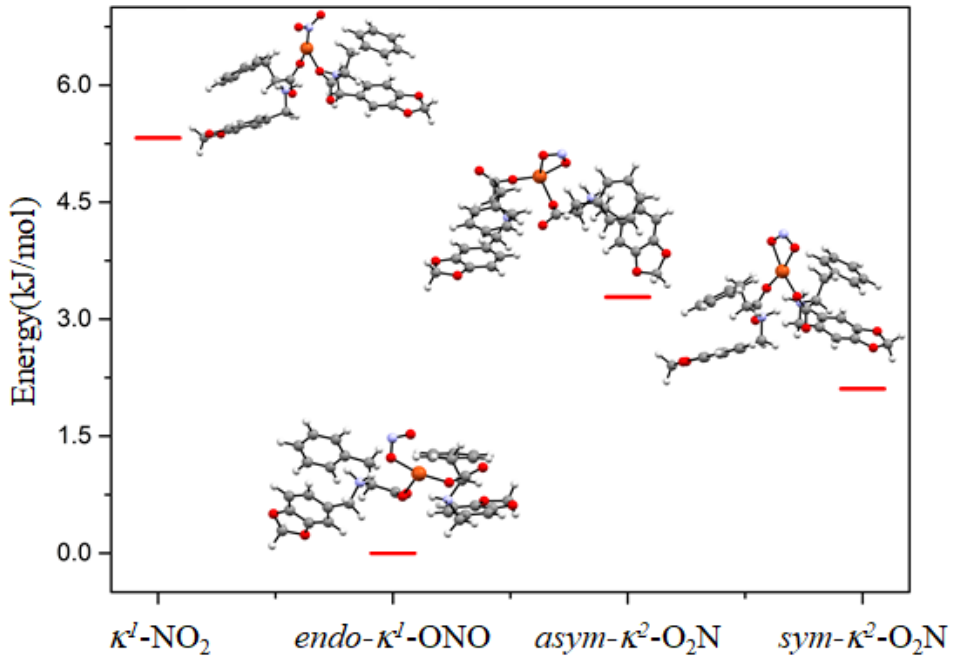


Figure S42. DFT calculated energies at the BP86/def2-SVP for all light atoms/def2-TZVP for Cu with CPCM model (DMSO) in (kJ/mol) for protonated species of $[Cu(\mathbf{L2})_2NO_2]^-$ with different coordination modes. For the calculations, only the protonation of the amino acid-based ligands was evaluated, thus $[Cu(\mathbf{L2H})_2NO_2]^+$ represents the studied species.

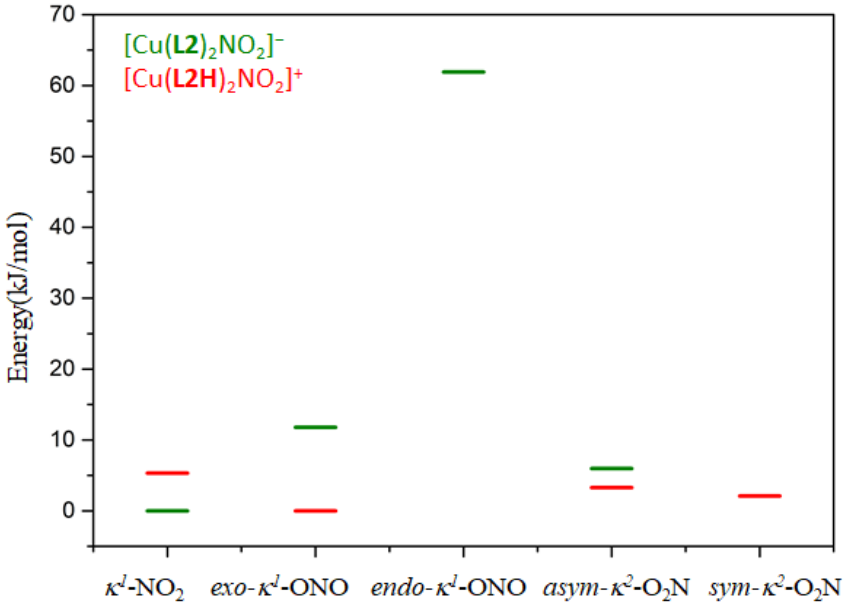


Figure S43. Comparative results of DFT calculated at the BP86/def2-SVP for all light atoms/def2-TZVP for Cu with CPCM model (DMSO) energies (in kJ/mol) for the family of species $[Cu(\mathbf{L2})_2(NO_2)]^-$ (red) and $[Cu(\mathbf{HL2})_2(NO_2)]^+$ (green) bearing different coordination modes for the nitrite ligand.

Cartesian Coordinates of DFT optimized structures.

[Cu(**L1**)2]		CPCM(WATER)			[Cu(**L1**)2(NH3)2]		CPCM(WATER)	
Cu	10.239252	2.767486	8.658699		**Cu**	7.717145	3.245588	7.924413
O	9.200147	1.364214	9.520556		**O**	6.27415	1.850325	7.904374
O	7.434437	1.019018	10.861952		**O**	9.403345	6.633263	6.5753
N	8.901821	4.052362	9.513619		**O**	8.574131	5.038383	7.911442
H	9.417259	4.836415	9.938687		**N**	7.147479	3.430562	9.895493
O	6.187679	0.11885	5.522689		**H**	6.502412	4.234446	9.852304
C	8.233337	1.774588	10.295996		**N**	7.665098	3.507582	5.904949
C	8.033314	4.595727	8.425222		**H**	6.640052	3.780241	5.827092
H	8.66161	5.287835	7.833763		**O**	6.635417	5.128169	15.988313
H	7.200638	5.175165	8.878321		**O**	6.799699	2.777715	-0.33483
C	7.509114	3.477351	7.553858		**O**	4.998216	2.78154	1.130748
O	4.894248	0.845305	7.313598		**O**	5.010698	0.554713	9.228934
C	8.164936	3.298557	10.563158		**C**	7.659084	2.310922	3.693126
H	7.094495	3.591384	10.545259		**N**	9.461943	1.877807	8.133476
C	6.750516	1.241476	6.070239		**H**	9.269412	0.964815	7.698702
C	7.910982	1.907871	5.688955		**H**	9.740751	1.661156	9.100364
H	8.504725	1.569883	4.828516		**H**	10.31521	2.23127	7.678692
C	5.967468	1.681595	7.153718		**C**	7.894409	2.231854	5.186635
C	8.277773	3.039123	6.456442		**H**	7.213724	1.492183	5.653626
H	9.180531	3.60636	6.18375		**H**	8.935186	1.904504	5.382034
C	6.315574	2.79484	7.910281		**C**	7.109008	4.637857	14.798048
H	5.69298	3.121291	8.754499		**C**	7.25739	2.63641	0.951792

C	8.72097	3.60751	11.956319		**C**	7.942554	4.130852	12.185635
H	9.792626	3.340622	12.028588		**O**	6.209826	6.661257	14.295869
H	8.166093	3.019711	12.71163		**C**	6.330478	2.472465	3.210418
H	8.607483	4.68418	12.193845		**H**	5.47374	2.491854	3.898092
C	4.930359	-0.074098	6.202928		**C**	8.562945	2.461807	1.399405
H	4.092643	0.152136	5.505755		**H**	9.411093	2.450036	0.700498
H	4.867739	-1.11463	6.580255		**C**	8.74293	2.301974	2.796155
O	11.280862	4.171095	7.800165		**C**	5.825747	1.475331	9.064528
O	13.048815	4.517294	6.46184		**C**	6.377575	2.22873	10.309084
N	11.574274	1.482566	7.799843		**H**	7.105581	1.528521	10.775662
H	11.057548	0.701224	7.371331		**C**	6.164545	2.639117	1.841873
O	14.294198	5.376806	11.83638		**C**	6.849941	5.567324	13.770559
C	12.248304	3.76147	7.025087		**C**	8.86088	5.529487	6.742314
C	12.438885	0.932833	8.888079		**C**	8.204278	3.213152	13.219853
H	11.807812	0.238486	9.473877		**H**	8.73198	2.276454	12.983558
H	13.271748	0.353652	8.434626		**C**	8.305198	3.802028	10.755612
C	12.963035	2.044469	9.768257		**H**	9.021104	2.958256	10.731022
O	15.579065	4.673675	10.030045		**H**	8.785575	4.6646	10.254152
C	12.314667	2.238067	6.753954		**C**	8.529309	4.641877	5.511312
H	13.38462	1.943136	6.772881		**H**	9.510209	4.219087	5.194953
C	13.728559	4.261562	11.276833		**C**	7.79442	3.451618	14.554919
C	12.569764	3.590348	11.654538		**H**	8.005492	2.736595	15.362314
H	11.980312	3.917001	12.522273		**C**	7.259314	5.348317	12.461266
C	14.506449	3.835505	10.184057		**H**	7.05404	6.085277	11.670784
C	12.198904	2.46917	10.874142		**C**	5.396026	3.083289	-0.220786
H	11.296683	1.899631	11.143676		**H**	5.234543	4.167316	-0.422213
C	14.155106	2.731747	9.415377		**H**	4.820056	2.454145	-0.927697
H	14.774938	2.416113	8.565101		**C**	7.957408	5.489251	4.36813
C	11.762346	1.934759	5.35802		**H**	7.888852	4.912652	3.427181
H	10.69265	2.208124	5.280626		**H**	8.613658	6.366457	4.210795
H	12.324014	2.520774	4.606369		**H**	6.943626	5.85526	4.630139
H	11.870679	0.857925	5.118936		**C**	5.889725	6.316777	15.658212
C	15.548282	5.578604	11.152691		**H**	4.798989	6.106019	15.74158
H	16.389304	5.343382	11.842876		**H**	6.190926	7.143535	16.331492
H	15.609102	6.623959	10.788619		**C**	5.248728	2.524026	11.302121
					H	5.63386	2.899404	12.267862
					H	4.676688	1.593077	11.475481
					H	4.553455	3.280008	10.880873
					H	9.763111	2.180591	3.191721
					N	4.872138	3.982993	6.197154
					H	4.064953	3.912894	5.562672
					H	4.675301	4.786443	6.81078
					H	4.840646	3.15092	6.8087
[Cu(**L2**)2(H2O)]		CPCM(WATER)			[Zn(**L2**)2(H2O)]		CPCM(WATER)	
Cu	1.305656	3.639952	7.965814		**O**	3.466647	2.239126	14.988749
O	-2.159302	5.61425	7.780864		**O**	1.338806	1.878522	15.646124
O	-0.355537	4.399248	7.211101		**O**	3.308063	-1.60275	22.713596
O	-3.331049	3.705171	14.008949		**O**	1.832407	-2.085312	20.988908
O	-1.669478	3.747833	15.6284		**N**	4.482389	1.4504	17.405113

O	2.721995	2.506006	8.727579		**H**	4.874928	1.896488	18.251273
O	2.402949	1.307848	0.160432		**C**	5.382112	-0.26362	19.942953
O	4.48433	1.236337	8.150748		**H**	6.331533	0.247907	19.721232
O	3.093249	-0.323378	1.658537		**C**	3.036969	1.760643	17.335236
N	1.972365	2.957557	6.186032		**H**	2.443075	0.928572	17.766979
H	2.031403	3.781095	5.565203		**C**	2.55686	1.955512	15.869573
C	-2.127496	3.366989	13.43869		**C**	4.488842	-0.541773	18.887981
N	0.415198	3.981585	9.74622		**C**	2.973867	-1.522553	20.470215
H	1.126467	4.347778	10.400594		**C**	2.91619	1.88553	21.793285
C	-1.121804	3.388422	14.420503		**H**	2.361775	1.225182	22.477053
C	-0.634245	5.007085	9.541613		**C**	4.80384	-0.007243	17.510216
H	-1.512318	4.781496	10.181434		**H**	4.239122	-0.539169	16.720158
C	1.257653	1.790855	4.111179		**H**	5.884161	-0.116386	17.289026
C	1.901066	1.591466	1.408292		**C**	5.089354	-0.607486	21.281305
C	0.837832	2.772264	3.189926		**H**	5.778201	-0.371505	22.103478
H	0.253196	3.631997	3.552598		**C**	2.457718	2.075611	20.482154
C	0.331029	6.461731	11.370153		**H**	1.543699	1.563434	20.141659
C	-1.847601	3.09509	12.103806		**C**	2.718705	3.040148	18.147436
H	-2.645533	3.081274	11.347656		**H**	3.21588	3.9108	17.671078
C	0.98859	2.007164	5.582765		**H**	1.62465	3.199137	18.078931
H	-0.013653	2.449767	5.74033		**C**	4.347837	3.53226	20.032084
H	1.040114	1.060221	6.15464		**H**	4.907108	4.185057	19.341743
C	-0.490415	2.845784	11.761948		**C**	4.094447	2.518662	22.230691
C	1.151608	2.69059	1.81518		**H**	4.457062	2.360279	23.257791
H	0.839748	3.466164	1.102872		**C**	3.25279	-1.192805	19.14774
C	-0.120871	6.412399	9.929516		**H**	2.539254	-1.42146	18.343282
H	-0.952488	7.120014	9.743569		**C**	3.869812	-1.234594	21.514263
H	0.716519	6.687867	9.257561		**C**	4.810759	3.340812	21.347252
C	4.255141	3.92963	4.581936		**H**	5.735709	3.837386	21.678955
C	2.322318	0.604871	2.316664		**C**	2.130563	-2.359918	22.371677
C	3.541018	1.982749	7.858189		**H**	2.339162	-3.44764	22.497818
C	3.693773	5.200551	4.333265		**H**	1.283228	-2.035897	23.006202
H	3.429924	5.843494	5.188362		**C**	3.164852	2.906141	19.584713
C	2.015656	0.672019	3.67162		**Zn**	5.367485	2.318225	15.727114
H	2.352527	-0.10658	4.370554		**O**	5.346807	4.409732	15.918117
C	3.33196	2.402182	6.384318		**H**	4.884846	4.946556	15.24303
H	3.469735	1.503307	5.748582		**H**	6.211996	4.846618	16.0544
C	4.423747	3.429563	5.998031		**O**	7.277906	2.201187	16.446494
H	4.385591	4.278335	6.708846		**O**	9.396203	1.81924	15.769164
H	5.398138	2.918995	6.12832		**O**	7.371385	-1.616068	8.726813
C	0.508581	2.864964	12.756807		**O**	8.831103	-2.124283	10.457663
H	1.554292	2.671445	12.471514		**N**	6.234537	1.466054	14.027768
C	-1.117664	5.010962	8.071767		**H**	5.845218	1.919493	13.184189
C	-0.61344	6.470271	12.419907		**C**	5.313029	-0.233257	11.487544
H	-1.68867	6.490484	12.181774		**H**	4.372045	0.29547	11.704767
C	0.210321	3.13478	14.110746		**C**	7.684977	1.749189	14.091466
H	0.992953	3.165486	14.880724		**H**	8.261831	0.911843	13.646892
C	3.815338	4.819057	1.931687		**C**	8.177978	1.917166	15.556173
H	3.640016	5.15969	0.899694		**C**	6.196859	-0.526955	12.546197
C	3.475863	5.643679	3.015724		**C**	7.699169	-1.538327	10.971177
H	3.037643	6.638222	2.83892		**C**	7.833147	1.871761	9.642318

C	-0.195533	6.442926	13.7578		**H**	8.38566	1.204025	8.964207
H	-0.943266	6.439563	14.56522		**C**	5.886334	0.014106	13.922306
C	-3.09667	3.71495	15.430685		**H**	6.437998	-0.527274	14.715191
H	-3.554648	4.618881	15.876701		**H**	4.803304	-0.073821	14.139067
H	-3.512308	2.784492	15.882131		**C**	5.604444	-0.584294	10.150728
C	2.943867	-0.024258	0.257184		**H**	4.923117	-0.336984	9.325645
H	2.231986	-0.74795	-0.203414		**C**	8.28424	2.060617	10.956126
H	3.933054	-0.060689	-0.238334		**H**	9.190604	1.539854	11.303887
C	4.36914	3.547443	2.169624		**C**	8.016037	3.029157	13.287333
H	4.618	2.890266	1.322854		**H**	7.520319	3.903027	13.761729
C	-0.081286	2.688439	10.315491		**H**	9.109682	3.186296	13.365162
H	0.747471	1.961939	10.212187		**C**	6.406076	3.537468	11.388831
H	-0.922321	2.343998	9.682874		**H**	5.847895	4.198706	12.072143
C	4.583466	3.105918	3.482969		**C**	6.664508	2.515605	9.194932
H	5.006265	2.104876	3.662351		**H**	6.307627	2.358029	8.165743
C	1.703378	6.413945	11.694906		**C**	7.42151	-1.201436	12.292081
H	2.451637	6.411144	10.884999		**H**	8.127251	-1.442587	13.099814
C	2.124853	6.383012	13.03709		**C**	6.812807	-1.234623	9.923312
H	3.199806	6.346454	13.272059		**C**	5.950472	3.347465	10.070932
C	1.175721	6.399457	14.070793		**H**	5.033091	3.852716	9.731626
H	1.500591	6.368365	15.121997		**C**	8.532791	-2.395297	9.074249
O	2.440735	5.664818	7.617238		**H**	8.30358	-3.478966	8.949022
H	1.912982	6.412046	7.272725		**H**	9.388559	-2.08875	8.442351
H	3.119173	6.090847	8.177203		**C**	7.578992	2.900508	11.846426
[Cu(**L2**)2(NO2)]−		CPCM(DMSO)			[Cu(**L2**)2(NO2)]−		CPCM(DMSO)	
exo-*κ*1-ONO					**endo-*κ*1-ONO**			
Cu	0.818701	3.211536	8.015824		**Cu**	0.920956	3.280419	8.063018
O	-2.955392	4.59921	8.028637		**O**	-2.866949	4.626669	7.973742
O	-1.014526	3.684616	7.351117		**O**	-0.921638	3.668327	7.372592
O	-2.905593	3.727782	14.702842		**O**	-3.083247	3.696414	14.573813
O	-1.016081	4.187956	15.968135		**O**	-1.272288	4.19619	15.935454
O	2.12016	1.837612	8.653189		**O**	2.310766	2.062495	8.821655
O	2.836431	2.11422	0.040387		**O**	2.39559	2.587347	0.021202
O	3.943487	0.697357	8.002854		**O**	4.184774	0.95808	8.263654
O	2.897018	0.132305	1.243396		**O**	3.240579	0.77296	1.204099
N	1.6412	2.867403	6.198982		**N**	1.725199	2.7749	6.27947
H	1.79569	3.85122	5.89791		**H**	1.802138	3.759748	5.938876
C	-1.781318	3.410122	13.978023		**C**	-1.915956	3.41182	13.905222
N	0.032562	3.628942	9.832082		**N**	0.089985	3.708899	9.857785
H	0.768859	4.184346	10.299122		**H**	0.794795	4.274996	10.358567
C	-0.636718	3.685002	14.745725		**C**	-0.819177	3.710142	14.731527
C	-1.1568	4.4909	9.626615		**C**	-1.114255	4.53888	9.621479
H	-1.920322	4.270908	10.400943		**H**	-1.89222	4.300115	10.376089
C	1.190751	2.18382	3.840567		**C**	1.132824	2.147911	3.94228
C	2.210039	2.294979	1.251076		**C**	1.858634	2.571847	1.284726
C	1.165494	3.383348	3.100376		**C**	0.612236	3.234146	3.21092
H	0.739684	4.288584	3.56033		**H**	-0.080821	3.928655	3.710191
C	-0.10048	6.329186	11.027495		**C**	-0.178211	6.378333	11.086837
C	-1.696899	2.951882	12.667441		**C**	-1.753554	2.963104	12.598833

H	-2.6021	2.743504	12.079454		**H**	-2.621817	2.733458	11.964936
C	0.698249	2.187573	5.270039		**C**	0.789826	2.013377	5.408253
H	-0.267939	2.719046	5.363644		**H**	-0.220895	2.417483	5.605805
H	0.547125	1.15414	5.639908		**H**	0.80399	0.954889	5.736029
C	-0.396322	2.777157	12.122171		**C**	-0.422884	2.824204	12.119409
C	1.67478	3.462248	1.786283		**C**	0.961398	3.465541	1.860459
H	1.671337	4.402515	1.219076		**H**	0.561253	4.318776	1.295367
C	-0.794953	5.992533	9.727774		**C**	-0.792922	6.046982	9.746417
H	-1.745967	6.552094	9.62583		**H**	-1.748442	6.587652	9.599411
H	-0.143035	6.264884	8.875324		**H**	-0.103827	6.338379	8.930162
C	4.346358	3.635317	4.809985		**C**	4.467128	3.311858	4.691524
C	2.246329	1.095222	1.98051		**C**	2.376184	1.479478	2.001568
C	3.019329	1.495454	7.781131		**C**	3.209662	1.668568	7.972276
C	4.144796	4.99089	4.476301		**C**	3.878337	4.376646	3.978779
H	3.801438	5.695067	5.248985		**H**	3.227626	5.088358	4.510753
C	1.743819	1.004741	3.27457		**C**	2.03412	1.238964	3.326017
H	1.783952	0.061813	3.838445		**H**	2.451158	0.379734	3.869283
C	2.939366	2.175886	6.389124		**C**	3.054122	2.161435	6.506689
H	3.039666	1.368568	5.633341		**H**	3.161161	1.26143	5.86682
C	4.144332	3.127338	6.2221		**C**	4.224378	3.116604	6.171548
H	4.035334	3.97322	6.929572		**H**	4.040868	4.086141	6.678144
H	5.033746	2.54534	6.539054		**H**	5.124946	2.66649	6.634355
C	0.744185	3.05239	12.904168		**C**	0.669115	3.120475	12.960577
H	1.743041	2.913427	12.462016		**H**	1.692216	3.00876	12.56925
C	-1.789684	4.229858	8.239229		**C**	-1.710092	4.252231	8.222611
C	-0.815722	6.355815	12.244609		**C**	-0.975988	6.451496	12.249482
H	-1.899575	6.159119	12.24299		**H**	-2.065304	6.306682	12.170725
C	0.646039	3.511374	14.236419		**C**	0.491642	3.56867	14.288324
H	1.5365	3.742927	14.836312		**H**	1.344436	3.81698	14.934326
C	4.796314	4.55765	2.167871		**C**	4.954708	3.635596	1.919382
H	4.965265	4.912243	1.139413		**H**	5.145797	3.768246	0.843531
C	4.369675	5.448463	3.165212		**C**	4.116397	4.532043	2.602693
H	4.20596	6.510533	2.923731		**H**	3.642477	5.363975	2.059363
C	-0.158058	6.623172	13.45384		**C**	-0.394529	6.699665	13.501216
H	-0.725546	6.631232	14.396658		**H**	-1.027303	6.742234	14.400658
C	-2.440504	3.984574	16.04199		**C**	-2.693335	3.959389	15.935315
H	-2.926643	4.897952	16.435639		**H**	-3.220294	4.859916	16.305735
H	-2.655965	3.100512	16.686054		**H**	-2.921157	3.06867	16.565963
C	3.043492	0.693729	-0.074585		**C**	3.184854	1.387694	-0.096212
H	2.271176	0.259695	-0.751994		**H**	2.698802	0.691569	-0.816681
H	4.06552	0.495865	-0.451605		**H**	4.210741	1.649058	-0.42749
C	4.988233	3.201349	2.487		**C**	5.538173	2.563937	2.617711
H	5.305206	2.491913	1.70766		**H**	6.189536	1.850181	2.09026
C	-0.213342	2.415258	10.665757		**C**	-0.157704	2.480436	10.671254
H	0.664247	1.756185	10.524755		**H**	0.745897	1.850442	10.568663
H	-1.100791	1.895781	10.254628		**H**	-1.008269	1.938142	10.214018
C	4.761517	2.746711	3.793666		**C**	5.290715	2.403833	3.990219
H	4.914606	1.682137	4.033051		**H**	5.751185	1.563188	4.534819
C	1.291862	6.563631	11.048761		**C**	1.21907	6.54079	11.210278
H	1.847003	6.521221	10.096042		**H**	1.844603	6.46003	10.305483
C	1.951521	6.828517	12.263275		**C**	1.802671	6.788158	12.466477

H	3.038041	7.009196	12.266577		**H**	2.893915	6.912816	12.546781
C	1.228757	6.861357	13.466865		**C**	0.997389	6.872065	13.613299
H	1.744505	7.062763	14.418503		**H**	1.452265	7.059021	14.598201
N	2.006624	5.703052	7.008209		**N**	2.073162	6.096567	7.175764
O	2.38033	6.888264	7.006912		**O**	1.713438	5.638704	6.059842
O	1.947254	5.139879	8.165081		**O**	2.057181	5.278285	8.15613
[Cu(**HL2**)2(NO2)]+		CPCM(DMSO)			[Cu(**HL2**)2(NO2)]+		CPCM(DMSO)	
asym-*κ*2-O2N					**sym-*κ*2-O2N**			
Cu	4.626345	2.735545	9.486209		**Cu**	2.779457	5.831801	8.001563
O	1.425734	2.953261	7.725114		**O**	-0.777892	4.010573	7.975541
O	2.647156	2.254581	9.493328		**O**	0.881202	5.466242	7.602234
O	-4.042996	3.475733	11.506042		**O**	-3.764645	3.471468	12.98929
O	-4.205693	5.179345	13.079548		**O**	-2.742013	3.344172	15.073642
O	5.504949	1.516287	8.342369		**O**	3.039526	3.898371	8.323259
O	0.720202	2.169593	1.016642		**O**	2.42926	0.109997	0.661833
O	6.884128	1.628567	6.56538		**O**	2.199661	1.88196	7.833332
O	2.6064	0.821254	0.924704		**O**	2.829978	-0.901129	2.716974
N	3.315832	1.336143	6.72298		**N**	1.347208	3.754067	5.512172
H	2.528418	2.036756	6.978173		**H**	1.484607	4.27941	4.621505
C	-2.821219	3.692896	12.074336		**C**	-2.458693	3.104185	12.837429
N	1.557063	4.000602	11.214003		**N**	1.205408	3.714187	10.352281
H	1.401555	4.949271	11.619059		**H**	1.632735	3.978906	11.266264
C	-2.920996	4.721468	13.032943		**C**	-1.840438	3.021183	14.10192
C	1.018828	4.014426	9.814181		**C**	0.334811	4.870961	9.918553
H	-0.046275	3.712368	9.873561		**H**	-0.651381	4.709323	10.392236
C	2.177192	0.749714	4.595217		**C**	0.781623	1.919925	3.985229
C	1.057151	1.77753	2.271048		**C**	1.799444	0.812682	1.647267
C	1.032407	1.589758	4.640945		**C**	0.528877	2.516031	2.729757
H	0.591888	1.844877	5.615821		**H**	-0.071157	3.437649	2.681786
C	0.347339	6.405726	10.144825		**C**	0.98562	6.122097	11.9673
C	-1.611756	3.065308	11.790349		**C**	-1.760544	2.857782	11.659127
H	-1.550244	2.263905	11.04076		**H**	-2.248842	2.933202	10.677282
C	2.754735	0.224677	5.883698		**C**	0.356184	2.643102	5.23513
H	1.977483	-0.261121	6.504883		**H**	-0.627015	3.13578	5.129089
H	3.56268	-0.507762	5.704156		**H**	0.339382	1.995667	6.129211
C	-0.47235	3.511802	12.510034		**C**	-0.387166	2.519186	11.785763
C	0.445494	2.113614	3.478635		**C**	1.031547	1.968588	1.531527
H	-0.435161	2.766989	3.513423		**H**	0.844213	2.436865	0.556454
C	1.072713	5.443552	9.231641		**C**	0.917152	6.183488	10.456449
H	0.593191	5.390938	8.235944		**H**	0.269614	7.010173	10.105414
H	2.12606	5.755385	9.079441		**H**	1.933635	6.371348	10.036298
C	3.451958	4.023969	4.967818		**C**	3.732653	4.412158	3.991577
C	2.204775	0.952587	2.216873		**C**	2.047317	0.203208	2.894288
C	5.763603	1.689591	7.065537		**C**	2.646401	2.976886	7.476353
C	2.314037	4.801788	5.260039		**C**	3.10193	5.506303	3.362421
H	2.057334	5.003177	6.309721		**H**	2.729638	6.346808	3.971069
C	2.786031	0.417519	3.364179		**C**	1.551684	0.730724	4.082769
H	3.677651	-0.22159	3.308778		**H**	1.75761	0.253978	5.051436
C	4.543071	2.015002	6.172316		**C**	2.7141	3.296473	5.966685

H	4.743935	1.59599	5.168553		**H**	2.904167	2.333963	5.455912
C	4.374687	3.543918	6.068588		**C**	3.772545	4.303701	5.501004
H	4.057822	3.953045	7.051135		**H**	3.599935	5.306461	5.959361
H	5.391991	3.948433	5.88575		**H**	4.757641	3.952037	5.864247
C	-0.585436	4.53485	13.477525		**C**	0.219787	2.427301	13.057981
H	0.313224	4.86209	14.022518		**H**	1.286081	2.163625	13.128004
C	1.754102	2.988338	8.936872		**C**	0.104333	4.766564	8.394904
C	-1.064432	6.40762	10.198926		**C**	-0.201323	6.189906	12.730562
H	-1.636345	5.76164	9.514198		**H**	-1.163376	6.376994	12.227963
C	-1.817684	5.159017	13.760706		**C**	-0.499698	2.673338	14.245335
H	-1.903318	5.962109	14.50424		**H**	-0.026058	2.612122	15.233797
C	1.828883	5.0495	2.88781		**C**	3.440179	4.478249	1.181462
H	1.197961	5.44314	2.076656		**H**	3.321361	4.498445	0.087662
C	1.507825	5.313225	4.228719		**C**	2.957373	5.539288	1.962435
H	0.622708	5.918591	4.477286		**H**	2.464341	6.399831	1.485552
C	-1.739522	7.221535	11.119422		**C**	-0.162994	6.013281	14.120704
H	-2.839262	7.212066	11.154727		**H**	-1.095055	6.061816	14.703531
C	-4.969493	4.357969	12.172176		**C**	-3.997749	3.591384	14.407401
H	-5.472499	5.002325	11.422561		**H**	-4.344745	4.619092	14.640992
H	-5.7062	3.756697	12.747279		**H**	-4.74286	2.831801	14.727115
C	1.673488	1.5671	0.119917		**C**	3.059472	-1.021173	1.298254
H	1.145681	0.878257	-0.572462		**H**	2.598447	-1.960735	0.925353
H	2.214389	2.36182	-0.434531		**H**	4.150181	-0.999977	1.095521
C	2.9573	4.264458	2.585784		**C**	4.070783	3.383549	1.801559
H	3.21951	4.054839	1.537393		**H**	4.443668	2.546184	1.192789
C	0.898993	3.005475	12.147282		**C**	0.47434	2.403775	10.556496
H	1.560862	2.930697	13.02937		**H**	1.259646	1.633277	10.656972
H	0.885803	2.031557	11.626196		**H**	-0.103632	2.210318	9.636016
C	3.758946	3.753541	3.616955		**C**	4.213978	3.348727	3.195639
H	4.645956	3.150519	3.365615		**H**	4.69969	2.484697	3.675945
C	1.066384	7.226274	11.040441		**C**	2.207903	5.868517	12.624536
H	2.168523	7.235721	11.006192		**H**	3.142504	5.822165	12.041545
C	0.387508	8.040261	11.967005		**C**	2.24485	5.689363	14.020388
H	0.961748	8.675772	12.658015		**H**	3.205884	5.493562	14.519506
C	-1.015134	8.039269	12.006688		**C**	1.060252	5.760574	14.769048
H	-1.548122	8.669813	12.734243		**H**	1.085862	5.613743	15.859342
N	4.637492	5.277918	10.330425		**N**	4.237842	7.868695	8.076491
O	5.049402	5.20138	9.172696		**O**	4.633888	6.686972	8.33318
O	4.364974	4.110493	10.86956		**O**	3.002967	7.887942	7.775641
H	3.578842	0.962012	7.659617		**H**	0.962536	4.463017	6.211174
H	2.603164	3.873924	11.192958		**H**	2.020819	3.609308	9.67084
[CuI(**L2**)2]- + NO2-		CPCM(DMSO)			[CuI(**L2**)2NO2]		CPCM(DMSO)	
					asym-*κ*2-O2N			
Cu	-1.08093	2.49543	7.16942		**Cu**	1.305971	4.475348	7.439883
O	-4.3421	3.41442	9.35947		**O**	-2.762666	5.529477	7.429425
O	-2.97636	2.69964	7.71886		**O**	-0.80569	4.742579	6.60691
O	0.12246	4.19384	14.70269		**O**	-1.897897	3.625939	14.229309
O	2.28764	5.00853	14.47166		**O**	0.188944	3.258243	15.192471
O	-0.41543	0.37813	7.37646		**O**	2.054948	0.65359	8.527171
O	4.3622	3.6671	1.10779		**O**	1.568536	2.52562	0.456799

O	1.68117	-0.42435	7.64025		**O**	3.485222	2.21611	9.334392
O	4.2457	1.46041	1.83632		**O**	2.617932	0.731842	1.500349
N	0.40654	2.50719	5.829		**N**	1.907964	2.804313	6.456268
H	0.75952	3.48524	5.84957		**H**	2.215557	3.289898	5.596821
C	0.61091	3.85499	13.46408		**C**	-1.001857	3.246582	13.257648
N	-0.69589	3.31626	9.16788		**N**	0.151989	4.191425	9.136802
H	-0.061	4.1019	8.94168		**H**	0.781262	4.57012	9.859885
C	1.92361	4.33631	13.32788		**C**	0.25616	3.019511	13.838258
C	-1.98909	3.80169	9.67161		**C**	-1.013537	5.082188	9.006835
H	-2.15869	3.45069	10.71223		**H**	-1.847673	4.744059	9.662847
C	1.08399	2.62253	3.42577		**C**	0.781155	1.976162	4.489876
C	3.21035	3.48109	1.83427		**C**	1.198058	2.482749	1.781542
C	1.16165	3.9536	2.96809		**C**	0.13477	3.053496	3.847357
H	0.39072	4.66867	3.29097		**H**	-0.489814	3.723312	4.461302
C	-1.31667	5.97731	10.84904		**C**	-0.2982	6.560857	10.920726
C	-0.0341	3.17144	12.44148		**C**	-1.219181	3.110155	11.892595
H	-1.06187	2.80411	12.56858		**H**	-2.206463	3.311911	11.454003
C	0.00033	2.24375	4.41453		**C**	0.778908	1.926021	5.997562
H	-0.91341	2.83718	4.21855		**H**	-0.166011	2.332185	6.405945
H	-0.27257	1.17256	4.33373		**H**	0.943132	0.914456	6.414197
C	0.68244	2.97736	11.22922		**C**	-0.107321	2.735729	11.088596
C	2.22115	4.40696	2.14953		**C**	0.325439	3.320241	2.469537
H	2.28221	5.44833	1.80352		**H**	-0.169973	4.16362	1.967652
C	-2.06957	5.34964	9.69752		**C**	-0.649813	6.52019	9.452075
H	-3.14357	5.61032	9.77736		**H**	-1.531402	7.156242	9.239583
H	-1.68957	5.72963	8.72436		**H**	0.198359	6.875316	8.830453
C	3.62174	2.84472	6.11892		**C**	4.481465	3.337513	5.27054
C	3.14238	2.15083	2.2776		**C**	1.834846	1.399512	2.411765
C	0.84858	0.40836	7.20009		**C**	2.880176	1.611677	8.405978
C	3.5313	4.13905	5.56592		**C**	3.898059	4.507387	4.730099
H	2.69133	4.78589	5.86738		**H**	3.438522	5.242201	5.412058
C	2.08868	1.68615	3.05536		**C**	1.644187	1.114127	3.757271
H	2.04629	0.63565	3.37533		**H**	2.168583	0.278673	4.241898
C	1.44175	1.56962	6.33439		**C**	3.116525	2.087275	6.942256
H	1.92686	1.04832	5.48091		**H**	3.265982	1.171939	6.320347
C	2.57033	2.32327	7.07268		**C**	4.335777	3.006579	6.739829
H	2.12134	3.15981	7.64827		**H**	4.182105	3.918961	7.351822
H	3.02707	1.60157	7.77761		**H**	5.231798	2.479955	7.124011
C	2.00418	3.45257	11.11061		**C**	1.150295	2.490826	11.681568
H	2.54136	3.29141	10.16311		**H**	1.998862	2.22748	11.023026
C	-3.20669	3.25429	8.86115		**C**	-1.584664	5.109535	7.551141
C	-1.95596	6.16265	12.09498		**C**	-1.311862	6.682496	11.896022
H	-3.00966	5.85783	12.20901		**H**	-2.355028	6.829808	11.571565
C	2.65574	4.13986	12.16156		**C**	1.351105	2.623272	13.076808
H	3.68273	4.5179	12.05951		**H**	2.332485	2.446629	13.540395
C	5.53766	3.7444	4.23398		**C**	4.442276	3.782941	2.466759
H	6.27934	4.09713	3.50079		**H**	4.417475	3.953113	1.379281
C	4.48235	4.5827	4.63161		**C**	3.870691	4.722346	3.340295
H	4.39218	5.59225	4.20101		**H**	3.393044	5.629528	2.938488
C	-1.2728	6.73232	13.18168		**C**	-1.010129	6.610278	13.264909
H	-1.78974	6.87142	14.14403		**H**	-1.814867	6.709293	14.009488

C	1.21038	4.8174	15.40782		**C**	-1.171366	3.639941	15.471656
H	0.88212	5.80113	15.80174		**H**	-1.189417	4.665279	15.900881
H	1.54852	4.15122	16.2344		**H**	-1.626097	2.910462	16.177508
C	5.01048	2.38251	1.03887		**C**	2.567363	1.50212	0.285508
H	5.03217	2.03319	-0.01781		**H**	2.284491	0.843716	-0.561847
H	6.03887	2.46361	1.44965		**H**	3.558828	1.975334	0.104498
C	5.62957	2.44692	4.76941		**C**	5.046527	2.626064	2.99215
H	6.44627	1.7771	4.45715		**H**	5.495934	1.882756	2.315588
C	0.01149	2.34604	10.02758		**C**	-0.187344	2.803698	9.580723
H	0.77525	1.83693	9.40756		**H**	0.525709	2.08589	9.131721
H	-0.71402	1.56553	10.33453		**H**	-1.201348	2.560833	9.204356
C	4.67825	2.00434	5.70265		**C**	5.059315	2.406014	4.378441
H	4.74661	0.98456	6.11685		**H**	5.511589	1.485057	4.781508
C	0.03535	6.35972	10.72221		**C**	1.0328	6.364393	11.352835
H	0.5437	6.19702	9.75689		**H**	1.839988	6.28973	10.602943
C	0.72144	6.92432	11.8107		**C**	1.332595	6.26718	12.723038
H	1.77921	7.20933	11.69889		**H**	2.371813	6.092889	13.042588
C	0.0703	7.12318	13.03979		**C**	0.314942	6.392564	13.683111
H	0.61148	7.57141	13.88729		**H**	0.55404	6.316713	14.754924
N	0.12894	5.68564	6.99221		**N**	2.95708	6.728692	7.869735
O	0.34448	5.43989	5.77377		**O**	3.230482	5.956694	8.818969
O	1.03099	5.2959	7.80098		**O**	2.064076	6.277757	7.039966
[CuI(**HL2**)2]+ + NO2-		CPCM(DMSO)			[CuI(**HL2**)2NO2]		CPCM(DMSO)	
					asym-*κ*2-O2N			
Cu	-0.88003	2.092943	7.367512		**Cu**	2.816385	5.73528	7.951913
O	-4.058089	3.046758	9.646911		**O**	-0.823933	3.846478	7.887681
O	-2.740879	2.154572	8.053363		**O**	0.822844	5.335744	7.5048
O	-0.166736	3.440928	15.069113		**O**	-3.571504	3.196198	13.216946
O	1.331712	5.206927	14.96997		**O**	-2.46252	3.27751	15.254946
O	0.025233	0.106691	7.497614		**O**	3.021201	3.726873	8.305651
O	4.317553	3.61433	1.026647		**O**	2.325854	0.245054	0.450247
O	2.093974	-0.73264	7.161141		**O**	2.130232	1.713374	7.82314
O	3.525174	1.435382	1.024445		**O**	2.712402	-0.873114	2.449317
N	0.541511	2.378348	5.977258		**N**	1.434798	3.668423	5.503367
H	0.799008	3.359896	6.221758		**H**	1.621506	4.214716	4.636666
C	0.369378	3.515547	13.799125		**C**	-2.236042	2.951254	13.021729
N	-0.434307	3.163379	9.224535		**N**	1.224253	3.869664	10.299204
H	0.170227	3.931447	8.875908		**H**	1.65075	4.261027	11.163495
C	1.276674	4.583518	13.740454		**C**	-1.56458	2.995516	14.257215
C	-1.730121	3.640605	9.717337		**C**	0.194794	4.861978	9.806593
H	-1.816371	3.461083	10.812192		**H**	-0.763343	4.570964	10.274264
C	1.156704	2.771486	3.575777		**C**	0.762443	1.953607	3.876962
C	3.243524	3.517376	1.884314		**C**	1.708452	0.914094	1.475437
C	1.660581	4.089112	3.579184		**C**	0.518836	2.61465	2.656408
H	1.237687	4.8163	4.290256		**H**	-0.042391	3.561877	2.659232
C	-1.200762	6.027781	10.512277		**C**	0.628078	6.323328	11.785469
C	0.062822	2.746509	12.679265		**C**	-1.559427	2.745584	11.824705
H	-0.651305	1.911672	12.737516		**H**	-2.091527	2.720389	10.863003
C	0.073384	2.385945	4.567286		**C**	0.38677	2.632886	5.167774

H	-0.768525	3.10529	4.517495		**H**	-0.571108	3.179461	5.099964
H	-0.334379	1.384243	4.322291		**H**	0.338617	1.941796	6.027758
C	0.695007	3.091728	11.455755		**C**	-0.148513	2.585133	11.898408
C	2.712542	4.48884	2.72718		**C**	0.987386	2.102649	1.425884
H	3.117364	5.50972	2.747437		**H**	0.81217	2.627137	0.477138
C	-1.907391	5.158726	9.491594		**C**	0.564641	6.274795	10.272575
H	-2.996993	5.367362	9.542361		**H**	-0.208328	6.964526	9.878384
H	-1.570548	5.409918	8.463559		**H**	1.539093	6.577047	9.829632
C	3.79619	2.838622	6.01043		**C**	3.871125	4.218672	4.040137
C	2.760831	2.199694	1.881984		**C**	1.947383	0.239747	2.686976
C	1.215723	0.158102	7.036718		**C**	2.631862	2.796822	7.483509
C	4.114731	4.199929	6.190699		**C**	3.359867	5.402045	3.465643
H	3.619492	4.754859	7.001273		**H**	3.06928	6.241507	4.118708
C	1.716624	1.796267	2.70903		**C**	1.487327	0.730162	3.904083
H	1.352047	0.758411	2.703617		**H**	1.687525	0.201728	4.847086
C	1.650592	1.43118	6.238753		**C**	2.754922	3.101497	5.969808
H	2.026225	1.032241	5.271032		**H**	2.878622	2.131386	5.453993
C	2.839046	2.121008	6.940495		**C**	3.893831	4.034721	5.541608
H	2.444687	2.830342	7.697421		**H**	3.796132	5.017596	6.064782
H	3.396335	1.321361	7.471718		**H**	4.844924	3.582121	5.884852
C	1.589846	4.182259	11.406074		**C**	0.51331	2.622689	13.142062
H	2.018665	4.476748	10.436354		**H**	1.60655	2.496617	13.174779
C	-2.945576	2.882603	9.099447		**C**	0.025174	4.662321	8.281924
C	-1.51765	5.904462	11.883576		**C**	-0.549535	6.164281	12.550806
H	-2.254954	5.150343	12.202625		**H**	-1.52238	6.071871	12.04238
C	1.904435	4.943942	12.551486		**C**	-0.186862	2.827631	14.35158
H	2.584446	5.805075	12.503914		**H**	0.330919	2.875139	15.318806
C	5.668673	4.130617	4.313288		**C**	3.600431	4.45772	1.234114
H	6.385146	4.633309	3.645306		**H**	3.488346	4.545239	0.142764
C	5.042435	4.841237	5.35027		**C**	3.226872	5.521859	2.06928
H	5.271999	5.907807	5.504733		**H**	2.827038	6.451878	1.637133
C	-0.910051	6.725236	12.843719		**C**	-0.490975	6.114044	13.950324
H	-1.160574	6.600614	13.90829		**H**	-1.415033	5.979603	14.532435
C	0.646105	4.318382	15.869453		**C**	-3.766546	3.188828	14.645295
H	0.000846	4.903857	16.552526		**H**	-4.37538	4.064796	14.941814
H	1.39361	3.7153	16.438539		**H**	-4.253387	2.23409	14.949059
C	4.32224	2.380042	0.287467		**C**	2.799805	-0.994459	1.015201
H	3.866295	2.547191	-0.717498		**H**	2.149536	-1.831106	0.672467
H	5.359322	2.002545	0.198427		**H**	3.854837	-1.157124	0.719919
C	5.357909	2.772104	4.122687		**C**	4.109569	3.273033	1.797711
H	5.831903	2.20715	3.305279		**H**	4.389873	2.430451	1.147807
C	0.34172	2.352212	10.177194		**C**	0.665498	2.505185	10.63464
H	1.261515	2.028392	9.648282		**H**	1.539034	1.835663	10.734763
H	-0.228032	1.429099	10.412744		**H**	0.077688	2.183612	9.756613
C	4.430751	2.137307	4.961112		**C**	4.242092	3.154008	3.188141
H	4.195109	1.072547	4.803011		**H**	4.627823	2.218418	3.622925
C	-0.249249	6.994869	10.131872		**C**	1.866775	6.426888	12.454489
H	0.024697	7.093739	9.070448		**H**	2.786918	6.569978	11.864803
C	0.360945	7.822301	11.091734		**C**	1.924047	6.373066	13.86053
H	1.10563	8.56909	10.772891		**H**	2.896885	6.455893	14.369455
C	0.032942	7.692101	12.450866		**C**	0.748016	6.215259	14.609972

H	0.519756	8.329195	13.205545		**H**	0.793398	6.164571	15.708605
N	1.192012	5.80759	7.29631		**N**	4.302736	7.639664	9.084664
O	0.491803	5.266844	6.393646		**O**	4.021828	6.77008	9.934844
O	1.605811	5.035676	8.216785		**O**	3.837457	7.394361	7.899185
					H	1.067317	4.383576	6.234021
					H	2.027694	3.763956	9.579468
[Cu(**L1**)2(H2O)2]		CPCM(WATER)			**L1-2**		CPCM(WATER)	
Cu	7.283738	3.392633	7.763573		**O**	5.907626	9.715001	4.956834
O	6.179935	1.773521	7.804149		**O**	6.19803	9.891041	7.215918
O	8.480267	6.909168	6.247033		**N**	7.12988	7.205122	7.337214
O	7.906379	5.268776	7.662842		**H**	7.347618	6.210326	7.183704
N	6.923528	3.472999	9.757007		**C**	6.243931	9.246362	6.10599
H	6.317254	4.325047	9.791888		**C**	6.718951	7.826804	6.143566
N	7.323307	3.501716	5.723918		**C**	6.241902	7.285173	8.554156
H	6.327567	3.632126	5.485859		**H**	6.229314	8.374478	8.791212
O	6.908578	4.781719	15.949938		**H**	5.177094	7.010577	8.320583
O	7.342762	2.24298	-0.490671		**C**	6.759115	7.019223	4.89003
O	5.391329	2.004354	0.746451		**H**	7.790187	6.672128	4.571303
O	4.951714	0.465677	9.144604		**H**	6.145374	6.067082	4.925721
C	7.738532	2.156047	3.63092		**O**	8.647912	3.935805	12.471901
O	9.301706	2.280034	8.028262		**C**	7.938834	4.527584	11.383932
C	7.790897	2.210487	5.13911		**C**	6.780639	6.373907	9.60248
H	7.154683	1.426179	5.593654		**C**	9.959272	4.392269	12.221272
H	8.82549	2.051622	5.496515		**H**	10.46938	3.693678	11.485361
C	7.291302	4.367194	14.698924		**H**	10.52812	4.444524	13.177814
C	7.645563	2.255545	0.846573		**C**	8.665841	5.62542	10.923736
C	7.899921	4.016363	12.00059		**C**	8.151741	6.588115	10.040851
O	6.271773	6.371274	14.380599		**H**	8.739262	7.421578	9.634751
C	6.474682	2.050457	2.985564		**O**	9.882912	5.687045	11.64309
H	5.54304	1.933897	3.558536		**C**	6.06558	5.256235	10.06834
C	8.893373	2.338024	1.456676		**H**	5.043584	5.109679	9.672428
H	9.814352	2.436275	0.865349		**C**	6.584619	4.311297	11.000801
C	8.916138	2.289394	2.872267		**H**	6.024511	3.411931	11.300722
C	5.711069	1.428723	8.970462		**H**	6.360504	7.688875	4.09703
C	6.180327	2.264664	10.190502					
H	6.902559	1.606293	10.721973					
C	6.461382	2.111894	1.597898		**L1-1**		CPCM(WATER)	
C	6.905326	5.331067	13.745421		**O**	7.097497	10.192938	5.610903
C	8.158993	5.737795	6.465858		**O**	8.280591	8.88437	7.05168
C	8.282935	3.060097	12.958795		**N**	6.709244	6.995578	7.191178
H	8.823237	2.159074	12.629919		**H**	7.690058	7.476407	7.368047
C	8.15957	3.777914	10.529681		**H**	6.832799	6.059743	6.77403
H	8.867263	2.941303	10.378958		**C**	7.290858	9.165895	6.286363
H	8.605584	4.675315	10.056861		**C**	6.217464	8.015982	6.204605
C	8.070687	4.71703	5.299974		**H**	5.244828	8.409589	6.561545
H	9.120393	4.396808	5.115957		**C**	5.952856	6.904059	8.480658
C	7.988022	3.219201	14.336099		**H**	5.813434	7.947073	8.827311
H	8.293193	2.473868	15.083865		**H**	4.957921	6.469583	8.269007
C	7.196614	5.190339	12.395194		**C**	6.076501	7.45132	4.79642

H	6.868425	5.930418	11.650148		**H**	7.034589	7.017377	4.443306
C	5.903959	2.28293	-0.571507		**H**	5.286901	6.67538	4.742897
H	5.578262	3.29954	-0.889711		**O**	9.00064	4.004042	12.240195
H	5.550015	1.508005	-1.279787		**C**	8.142848	4.552298	11.325456
C	7.510876	5.379013	4.03842		**C**	6.71324	6.088478	9.494585
H	7.606188	4.722174	3.154811		**C**	10.06117 1	4.962423	12.436743
H	8.063082	6.319478	3.853277		**H**	11.02508 9	4.523176	12.100041
H	6.439585	5.632653	4.179508		**H**	10.10639 8	5.251131	13.507984
C	6.085134	5.946767	15.744385		**C**	8.598927	5.834676	10.958924
H	5.015936	5.678836	15.90768		**C**	7.908867	6.627386	10.050988
H	6.405049	6.753907	16.432739		**H**	8.271863	7.628184	9.773996
C	5.013091	2.579376	11.129722		**O**	9.753672	6.122198	11.636601
H	5.369314	3.026675	12.076843		**C**	6.26821	4.805586	9.86086
H	4.466368	1.643443	11.352577		**H**	5.343205	4.410027	9.414385
H	4.305499	3.286489	10.649058		**C**	6.976937	4.009849	10.794297
H	9.882344	2.369757	3.393504		**H**	6.625891	3.010363	11.086097
H	10.126116	2.625257	7.632797		**H**	5.803292	8.278658	4.114446
H	9.277398	1.344192	7.747871					
O	6.044816	6.162173	9.416701					
H	5.236477	6.214288	8.869873					
H	6.76937	6.046468	8.739788					
[Cu(**L2**)2(NO2)]−		CPCM(DMSO)			[Cu(**L2**)2(NO2)]−		CPCM(DMSO)	
κ1-NO2					**asym-κ2-O2N**			
Cu	0.924616	3.21207	7.923848		**Cu**	0.935335	3.234602	7.967013
O	-3.103119	3.59201	8.399344		**O**	-2.942566	4.395112	8.075344
O	-1.102152	3.033421	7.527493		**O**	-1.039411	3.385438	7.4166
O	-2.137812	3.29183	15.030243		**O**	-2.740729	3.692964	14.680303
O	-0.52848	4.689505	15.943927		**O**	-0.873257	4.310383	15.909273
O	1.515937	1.259732	8.27318		**O**	1.893055	1.427909	8.465344
O	2.984836	2.581374	-0.075519		**O**	2.685528	2.253896	-0.049701
O	2.833875	-0.341528	7.392771		**O**	3.638833	0.182362	7.768234
O	2.288847	0.548922	0.79909		**O**	2.721182	0.235998	1.092523
N	1.643493	2.823227	6.055901		**N**	1.688021	2.791704	6.13815
H	2.137038	3.719456	5.872914		**H**	1.972171	3.708646	5.757542
C	-1.060192	3.367266	14.177588		**C**	-1.604303	3.423241	13.952269
N	0.252613	3.674087	9.794166		**N**	0.164767	3.65776	9.790936
H	0.887032	4.468784	10.009953		**H**	0.872615	4.259356	10.243222
C	-0.085231	4.212656	14.732307		**C**	-0.473397	3.796911	14.697925
C	-1.151066	4.130844	9.691886		**C**	-1.076218	4.44161	9.591054
H	-1.719323	3.789853	10.582896		**H**	-1.792019	4.229851	10.412952
C	1.13837	2.674391	3.631757		**C**	1.107631	2.243574	3.781677
C	2.353601	2.793424	1.128004		**C**	2.083975	2.412389	1.177151
C	1.569396	3.902835	3.090276		**C**	1.088737	3.463826	3.075116
H	1.428884	4.825212	3.674964		**H**	0.684263	4.362132	3.567183
C	-0.8274	6.340308	10.931895		**C**	-0.18249	6.383881	10.934012
C	-0.907564	2.792308	12.919718		**C**	-1.503073	2.934704	12.654083
H	-1.681114	2.136662	12.494631		**H**	-2.397961	2.650139	12.082523

C	0.576609	2.644776	5.035698		**C**	0.653889	2.223422	5.223293
H	-0.162144	3.453055	5.194367		**H**	-0.264135	2.821771	5.370442
H	0.05956	1.689041	5.245906		**H**	0.4353	1.193603	5.566913
C	0.281636	3.097234	12.206088		**C**	-0.199671	2.832261	12.097415
C	2.184054	3.987122	1.82225		**C**	1.578205	3.572487	1.754864
H	2.53484	4.942901	1.410843		**H**	1.579399	4.528641	1.214497
C	-1.243954	5.66982	9.640158		**C**	-0.784054	5.957777	9.613011
H	-2.303012	5.908773	9.413821		**H**	-1.751624	6.468	9.434938
H	-0.635054	6.046971	8.791993		**H**	-0.109305	6.214311	8.771149
C	4.53735	2.870443	4.965987		**C**	4.390296	3.447733	4.944102
C	1.933695	1.562747	1.658856		**C**	2.107466	1.19048	1.870147
C	2.289786	0.77817	7.359963		**C**	2.804349	1.095221	7.616578
C	4.781103	4.25794	4.917461		**C**	4.253093	4.846943	4.832039
H	4.602563	4.865882	5.81745		**H**	4.029941	5.442645	5.730406
C	1.320879	1.468546	2.904502		**C**	1.62614	1.071248	3.169739
H	1.001164	0.498011	3.310588		**H**	1.653753	0.108998	3.700788
C	2.600406	1.698199	6.145854		**C**	2.881556	1.926365	6.305607
H	2.519537	1.067682	5.235639		**H**	2.925397	1.198047	5.468226
C	4.057234	2.19763	6.23411		**C**	4.189484	2.744209	6.268291
H	4.160786	2.882165	7.101895		**H**	4.185703	3.474342	7.102188
H	4.677963	1.303944	6.447711		**H**	5.008585	2.02132	6.455679
C	1.250383	3.951474	12.771864		**C**	0.927799	3.205931	12.857663
H	2.160272	4.184558	12.19734		**H**	1.929433	3.120661	12.408125
C	-1.860436	3.526178	8.447362		**C**	-1.764879	4.043056	8.262134
C	-1.621817	6.199564	12.091339		**C**	-0.973519	6.40189	12.104485
H	-2.543502	5.597244	12.047971		**H**	-2.043551	6.147847	12.040174
C	1.086591	4.52589	14.050871		**C**	0.812723	3.695983	14.17748
H	1.833928	5.206056	14.480513		**H**	1.691765	4.004131	14.759457
C	5.43754	4.098202	2.576899		**C**	4.691338	4.738409	2.439002
H	5.781205	4.574572	1.64573		**H**	4.801332	5.236183	1.463296
C	5.22928	4.868182	3.732047		**C**	4.402304	5.489026	3.588807
H	5.412997	5.953922	3.712879		**H**	4.28966	6.582446	3.522626
C	-1.253785	6.817437	13.294646		**C**	-0.411484	6.730314	13.345855
H	-1.880214	6.689306	14.190307		**H**	-1.039084	6.726956	14.249742
C	-1.699951	3.911753	16.254156		**C**	-2.278626	4.008307	16.00733
H	-2.496696	4.576334	16.640405		**H**	-2.823269	4.892583	16.390392
H	-1.435829	3.12268	16.996813		**H**	-2.421987	3.124143	16.671378
C	2.721615	1.204949	-0.407824		**C**	2.851219	0.832284	-0.212067
H	1.908599	1.155843	-1.169592		**H**	2.050624	0.439634	-0.881701
H	3.648999	0.727421	-0.778741		**H**	3.858021	0.619147	-0.619807
C	5.186307	2.714515	2.610858		**C**	4.82666	3.341361	2.537902
H	5.328352	2.107328	1.704118		**H**	5.036908	2.745246	1.63713
C	0.478541	2.595816	10.792591		**C**	-0.009644	2.446351	10.648411
H	1.506982	2.218691	10.635899		**H**	0.890999	1.820979	10.502843
H	-0.2103	1.762016	10.557469		**H**	-0.876108	1.879796	10.255543
C	4.738122	2.109221	3.793198		**C**	4.673809	2.70405	3.776811
H	4.541243	1.025221	3.809023		**H**	4.772546	1.608834	3.842435
C	0.354914	7.103166	11.015066		**C**	1.189514	6.694083	11.043584
H	0.995582	7.199253	10.125087		**H**	1.821935	6.678812	10.14244
C	0.727808	7.722422	12.221806		**C**	1.755921	7.022687	12.289308
H	1.656368	8.31298	12.267976		**H**	2.828888	7.261373	12.354524

C	-0.077096	7.585281	13.363694		**C**	0.957058	7.042572	13.442821
H	0.215912	8.062673	14.311403		**H**	1.398779	7.290515	14.420163
N	2.060783	4.918592	7.958243		**N**	2.459863	5.699763	7.774242
O	2.50288	5.403687	6.89145		**O**	2.548934	4.622116	8.45872
O	2.31691	5.483412	9.046281		**O**	1.526185	5.76093	6.951205
[Cu(**HL2**)2(NO2)]+		CPCM(DMSO)			[Cu(**HL2**)2(NO2)]+		CPCM(DMSO)	
***κ*1-NO2**					**endo-*κ*1-ONO**			
Cu	2.152062	6.028775	7.875191		**Cu**	-2.219207	4.734142	7.520259
O	-0.944661	3.559274	8.014486		**O**	-3.814892	4.620287	11.221939
O	0.421043	5.25866	7.483458		**O**	-3.261994	4.644951	9.058508
O	-3.431153	2.778175	13.374186		**O**	-2.457499	2.930786	15.650689
O	-2.261282	3.018983	15.368241		**O**	-0.298461	2.56451	16.431948
O	2.92726	4.171329	8.260992		**O**	-1.086213	4.211179	6.07003
O	2.973583	0.099281	0.714709		**O**	5.541733	0.374908	2.379548
O	2.355285	2.040058	7.862469		**O**	0.235877	3.457869	7.74281
O	3.562349	-0.773089	2.787383		**O**	4.361423	-0.472826	4.190349
N	1.237045	3.597424	5.479		**N**	0.665128	3.847155	4.166944
H	1.268814	4.107879	4.570163		**H**	1.320283	4.445035	3.622827
C	-2.092409	2.683136	13.133329		**C**	-1.625762	2.669515	14.595655
N	1.166092	3.858731	10.312163		**N**	-0.690113	3.614772	10.27518
H	1.563443	4.288293	11.175833		**H**	0.294181	3.789874	10.567998
C	-1.382523	2.823423	14.344583		**C**	-0.317212	2.448911	15.070264
C	0.040177	4.75501	9.849566		**C**	-1.473704	4.814291	10.730674
H	-0.8672	4.414334	10.381772		**H**	-1.451339	4.787527	11.835462
C	1.031253	1.645218	4.010793		**C**	1.773055	1.934151	3.041645
C	2.227823	0.694523	1.688887		**C**	4.305953	0.961878	2.433836
C	0.665633	2.154167	2.743842		**C**	2.494166	2.435742	1.939291
H	-0.097423	2.945153	2.680805		**H**	2.046985	3.22355	1.314092
C	0.517341	6.278745	11.765086		**C**	0.710186	6.055317	10.51176
C	-1.443112	2.501036	11.915428		**C**	-1.94042	2.598476	13.24357
H	-2.005704	2.396785	10.977037		**H**	-2.955046	2.806629	12.87655
C	0.482829	2.306654	5.24771		**C**	0.450439	2.556056	3.396014
H	-0.580012	2.590475	5.142423		**H**	-0.131009	2.841045	2.500248
H	0.605342	1.695895	6.159099		**H**	-0.176234	1.908272	4.035546
C	-0.024884	2.4669	11.944968		**C**	-0.879412	2.283483	12.350491
C	1.257226	1.684443	1.553983		**C**	3.780482	1.954282	1.612535
H	0.981766	2.086915	0.570514		**H**	4.348789	2.354866	0.762813
C	0.324728	6.204601	10.266297		**C**	-0.779148	6.090668	10.228937
H	-0.526056	6.825762	9.924835		**H**	-1.272192	6.950113	10.727402
H	1.236552	6.598858	9.753636		**H**	-0.942748	6.216466	9.137601
C	3.443654	4.661409	3.918977		**C**	3.391241	4.71338	4.910621
C	2.588852	0.16955	2.947197		**C**	3.592046	0.451281	3.533867
C	2.65769	3.171784	7.462586		**C**	0.023278	3.757313	6.55055
C	2.609214	5.588419	3.258939		**C**	3.493604	5.672157	3.880801
H	2.07825	6.357835	3.843446		**H**	2.76661	6.499386	3.832482
C	2.00916	0.623293	4.128443		**C**	2.32299	0.912405	3.863904
H	2.305722	0.216498	5.105435		**H**	1.775102	0.500827	4.723442
C	2.668472	3.434707	5.939724		**C**	1.187501	3.678219	5.56389
H	3.042609	2.508659	5.463529		**H**	1.660349	2.680523	5.63698
C	3.505185	4.613915	5.430401		**C**	2.242537	4.759209	5.891738

H	3.143166	5.576891	5.861442		**H**	1.756946	5.756299	5.888095
H	4.540917	4.47553	5.796883		**H**	2.583681	4.55443	6.924896
C	0.676628	2.597174	13.16556		**C**	0.426611	2.060785	12.832408
H	1.776931	2.568296	13.158661		**H**	1.231237	1.81674	12.121561
C	-0.208716	4.491159	8.345851		**C**	-2.96511	4.686092	10.331098
C	-0.588745	6.127288	12.630481		**C**	1.194421	5.839419	11.822446
H	-1.603036	6.042688	12.209798		**H**	0.488656	5.763939	12.665114
C	0.008513	2.773841	14.393694		**C**	0.73356	2.13967	14.210233
H	0.552954	2.885249	15.340355		**H**	1.74971	1.962178	14.587904
C	3.144297	4.578181	1.10918		**C**	5.469068	4.553865	3.003056
H	3.024275	4.539486	0.015998		**H**	6.277027	4.486289	2.25893
C	2.461104	5.547216	1.85944		**C**	4.528939	5.592784	2.930791
H	1.807559	6.27752	1.358837		**H**	4.598612	6.349493	2.13465
C	-0.400808	6.076415	14.018953		**C**	2.573073	5.715992	12.062528
H	-1.268834	5.953547	14.684002		**H**	2.933819	5.543543	13.087895
C	-3.584223	2.961865	14.796143		**C**	-1.617835	3.00191	16.820838
H	-4.113875	3.917108	14.99194		**H**	-1.567895	4.053908	17.179583
H	-4.13638	2.098634	15.224686		**H**	-2.015321	2.327719	17.606003
C	3.800835	-0.884382	1.36977		**C**	5.518251	-0.68697	3.3564
H	3.513057	-1.90004	1.023255		**H**	5.425105	-1.66665	2.835575
H	4.868545	-0.672764	1.154996		**H**	6.435587	-0.642698	3.974802
C	3.978463	3.64985	1.759832		**C**	5.369951	3.589905	4.023739
H	4.509518	2.883374	1.175514		**H**	6.098357	2.766987	4.074452
C	0.75344	2.44363	10.656573		**C**	-1.121182	2.292135	10.863809
H	1.691465	1.865548	10.736595		**H**	-0.521178	1.524126	10.341485
H	0.170026	2.061191	9.800767		**H**	-2.184982	2.143787	10.602058
C	4.125517	3.689127	3.153409		**C**	4.336188	3.665154	4.967043
H	4.772102	2.953805	3.657756		**H**	4.260174	2.903948	5.759333
C	1.812988	6.372253	12.316509		**C**	1.636193	6.14542	9.451666
H	2.679369	6.504078	11.647483		**H**	1.263655	6.308089	8.430021
C	1.999669	6.317479	13.710705		**C**	3.015744	6.031353	9.692425
H	3.015177	6.392415	14.128119		**H**	3.725733	6.109223	8.854663
C	0.894085	6.168743	14.562307		**C**	3.487481	5.811077	10.99806
H	1.038598	6.119029	15.652102		**H**	4.567251	5.711839	11.186756
N	3.536524	7.2805	8.154048		**N**	-1.655618	7.323747	6.483931
O	4.055972	7.792638	7.150986		**O**	-0.524433	7.023754	6.828362
O	3.872832	7.541799	9.317287		**O**	-2.64654	6.583747	6.718437
H	0.71994	4.242134	6.156408		**H**	-0.237257	4.366047	4.248015
H	1.965797	3.866699	9.593998		**H**	-0.603732	3.558215	9.21334
[CuI(**L2**)2NO2]		CPCM(DMSO)			[CuI(**HL2**)2NO2]		CPCM(DMSO)	
***κ*1-NO2**					***κ*1-NO2**			
Cu	1.943584	4.657299	7.952423		**Cu**	2.233585	5.860905	7.924784
O	-2.081334	6.145589	7.260349		**O**	-1.186292	3.658876	7.894935
O	-0.1874	5.051095	6.66158		**O**	0.480417	5.103434	7.457133
O	-3.160483	3.372108	13.459563		**O**	-3.418198	2.998063	13.664668
O	-1.419984	3.042197	14.953623		**O**	-2.128458	3.236001	15.580463
O	2.953143	2.683333	9.226486		**O**	2.855171	3.825224	8.351053
O	1.66505	1.337717	0.789305		**O**	2.886123	0.271792	0.465237
O	4.596654	1.243816	8.61709		**O**	1.926086	1.827889	7.857938
O	2.492687	-0.295794	2.20964		**O**	3.318784	-0.781618	2.489594

N	2.222627	3.13618	6.619745		**N**	1.336503	3.559943	5.452804
H	2.331482	3.709487	5.768601		**H**	1.509878	4.125878	4.596246
C	-2.008019	3.084042	12.760334		**C**	-2.094175	2.829011	13.349301
N	0.389889	4.376647	9.253		**N**	1.013234	3.84865	10.277431
H	0.879959	4.617341	10.1286		**H**	1.42615	4.323341	11.107429
C	-0.953318	2.88199	13.665692		**C**	-1.312927	2.967256	14.511017
C	-0.644968	5.392645	9.018704		**C**	-0.119115	4.713937	9.781148
H	-1.585602	5.131955	9.557732		**H**	-1.031654	4.355387	10.291115
C	1.068889	1.90933	4.853233		**C**	0.960007	1.778239	3.800374
C	1.335602	1.653858	2.090499		**C**	2.141422	0.85999	1.454925
C	0.556221	2.892582	3.978356		**C**	0.692338	2.399989	2.56448
H	0.072439	3.777505	4.423902		**H**	0.019665	3.27097	2.53288
C	0.253133	6.618333	11.018821		**C**	0.361394	6.30375	11.658726
C	-1.814452	3.05932	11.38273		**C**	-1.522774	2.612949	12.100319
H	-2.647179	3.237498	10.687447		**H**	-2.144358	2.510116	11.199398
C	1.082569	2.222917	6.33215		**C**	0.439142	2.406636	5.065873
H	0.160222	2.760333	6.619364		**H**	-0.571622	2.83609	4.9396
H	1.184371	1.313906	6.956007		**H**	0.431072	1.714937	5.927131
C	-0.493448	2.823411	10.917071		**C**	-0.103941	2.539617	12.041653
C	0.681027	2.782311	2.575184		**C**	1.27907	1.947546	1.361549
H	0.303337	3.559399	1.896042		**H**	1.084387	2.442769	0.400906
C	-0.162234	6.757035	9.571562		**C**	0.125115	6.180279	10.170943
H	-1.001379	7.470633	9.451474		**H**	-0.758546	6.762413	9.841842
H	0.69171	7.111031	8.95767		**H**	1.005459	6.580277	9.61261
C	4.456544	3.792197	4.967728		**C**	3.774966	4.392251	4.138725
C	1.839236	0.664727	2.951572		**C**	2.406855	0.224597	2.681855
C	3.69187	2.089334	8.379625		**C**	2.482618	2.890303	7.53111
C	3.974402	5.082205	4.650844		**C**	3.20303	5.530433	3.531176
H	3.828373	5.820007	5.45687		**H**	2.812603	6.343819	4.164764
C	1.721831	0.759345	4.33473		**C**	1.829972	0.654895	3.87184
H	2.13893	-0.013607	4.995869		**H**	2.048909	0.15722	4.827024
C	3.503426	2.462777	6.874217		**C**	2.683231	3.165286	6.018773
H	3.5738	1.513963	6.292595		**H**	2.952521	2.205071	5.540036
C	4.665689	3.374831	6.406197		**C**	3.731892	4.218205	5.641142
H	4.709296	4.267353	7.064152		**H**	3.509147	5.190032	6.141241
H	5.602415	2.796877	6.533987		**H**	4.705972	3.874478	6.041913
C	0.558169	2.610137	11.836244		**C**	0.668907	2.668109	13.213372
H	1.571619	2.448441	11.432851		**H**	1.765967	2.60657	13.144071
C	-1.008612	5.530693	7.505778		**C**	-0.320148	4.457193	8.267039
C	-0.717313	6.407815	12.024455		**C**	-0.694229	6.105873	12.576138
H	-1.786125	6.436165	11.758269		**H**	-1.717078	5.938288	12.203775
C	0.346444	2.63595	13.233148		**C**	0.075325	2.88448	14.476606
H	1.169274	2.494016	13.947651		**H**	0.678718	3.002482	15.386541
C	3.78211	4.470799	2.298054		**C**	3.640881	4.606056	1.321041
H	3.50579	4.726696	1.263555		**H**	3.582507	4.683262	0.224716
C	3.644365	5.4187	3.324581		**C**	3.13669	5.637109	2.128857
H	3.263268	6.426904	3.097404		**H**	2.686378	6.530704	1.670149
C	-0.338364	6.131573	13.345859		**C**	-0.447437	6.117736	13.956188
H	-1.108706	5.946919	14.110117		**H**	-1.276465	5.955678	14.661434
C	-2.853199	3.067494	14.832637		**C**	-3.475678	3.039154	15.104624
H	-3.269621	3.854224	15.490597		**H**	-4.110493	3.88687	15.427515

H	-3.266271	2.063396	15.090777		**H**	-3.86663	2.069393	15.4886
C	2.137792	-0.020073	0.84196		**C**	3.483459	-0.897539	1.061727
H	1.320865	-0.710959	0.524507		**H**	2.956654	-1.809397	0.699344
H	3.030171	-0.130166	0.196348		**H**	4.562223	-0.930217	0.813236
C	4.258811	3.182734	2.602976		**C**	4.21361	3.467537	1.917818
H	4.350246	2.427355	1.807499		**H**	4.598378	2.650852	1.288626
C	-0.128236	2.99631	9.459874		**C**	0.593926	2.461886	10.709173
H	0.688757	2.304597	9.184293		**H**	1.522182	1.863963	10.753144
H	-0.990496	2.832957	8.784823		**H**	-0.041939	2.054493	9.903259
C	4.593368	2.849845	3.923373		**C**	4.278185	3.360592	3.314159
H	4.9438	1.831747	4.157085		**H**	4.714907	2.459981	3.773749
C	1.618407	6.545068	11.375539		**C**	1.668704	6.507941	12.150996
H	2.389322	6.672694	10.597621		**H**	2.489486	6.681788	11.434042
C	1.999299	6.274218	12.703215		**C**	1.915372	6.51397	13.536934
H	3.068391	6.214132	12.961656		**H**	2.93877	6.675388	13.908951
C	1.023862	6.06379	13.690782		**C**	0.85863	6.319143	14.440079
H	1.320649	5.833278	14.725583		**H**	1.050751	6.317359	15.523816
N	3.041201	6.190484	8.013715		**N**	3.442131	7.260976	8.161131
O	2.799999	7.22056	7.307933		**O**	4.08341	7.70442	7.174565
O	4.062928	6.24999	8.770393		**O**	3.663785	7.744134	9.301077
					H	0.840889	4.209959	6.156687
					H	1.820293	3.783758	9.543589

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