Supplementary Material

Solvent Switchable Nuclearity of Cu^{II} Complexes with 2,6-bis((2-(acetylamino)phenylimino)methyl)-4-*tert*-butylphenol (H_3L) Ligand

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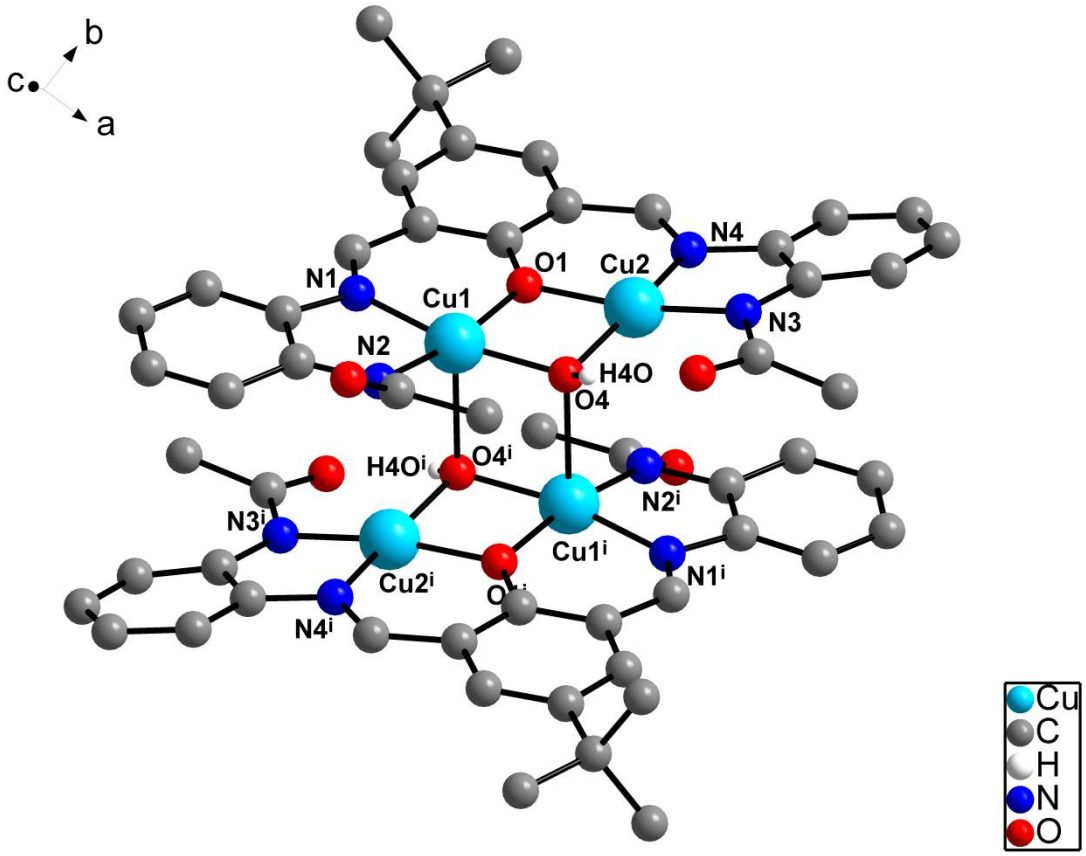

Figure S1. Scheme of the tetranuclear complex $[Cu_2L(OH)]_2$. Hydrogen atoms, methanol and water molecule have been omitted for the sake of clarity.

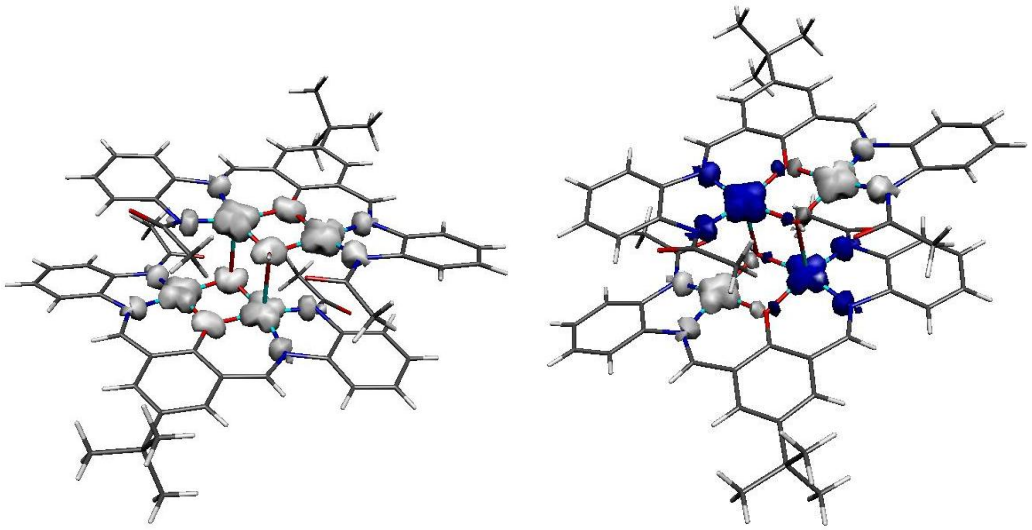

Figure S2. Spin density surfaces for the different spin solutions. Gray: alpha spin density; Blue: beta spin density.

Table S1. Bond distances (Å) for $[Cu_2L(OH)]_2 \cdot 2CH_3OH \cdot H_2O$ (1)

Cu1	Cu2	3.0389(9)	C13	C14	1.384(7)
Cu1	N1	1.954(4)	C13	C21	1.402(7)
Cu1	N2	1.972(4)	C14	C15	1.374(8)
Cu1	O1	2.017(3)	C15	C16	1.367(8)
Cu1	O4	1.925(3)	C16	C24	1.419(7)
Cu1	$O4^i$	2.425(3)	C17	C18	1.377(7)
Cu2	N3	1.960(4)	C17	C20	1.383(7)
Cu2	N4	1.916(4)	C18	C19	1.367(7)
Cu2	O1	1.946(3)	C19	C23	1.399(7)
Cu2	O4	1.899(3)	C20	C22	1.398(7)
C1	C2	1.403(6)	C21	C24	1.394(7)
C1	C6	1.423(6)	C21	N1	1.435(6)
C1	O1	1.322(5)	C22	C23	1.406(7)
C2	C3	1.413(6)	C22	N4	1.421(6)
C2	C11	1.445(6)	C23	N3	1.408(6)
C3	C4	1.385(6)	C24	N2	1.412(6)
C4	C5	1.388(7)	C25	C27	1.519(7)
C4	C7	1.531(6)	C26	C28	1.512(7)
C5	C6	1.399(7)	C27	N3	1.347(6)
C6	C12	1.442(7)	C27	O2	1.246(6)
C7	C8	1.520(7)	C28	N2	1.380(7)
C7	C9	1.546(7)	C28	O3	1.236(6)
C7	C10	1.520(7)			
C11	N4	1.291(6)			
C12	N1	1.292(6)			

Symmetry code: (i) 1/2-x, 3/2-y, 1-z

Table S2. Selected bond angles (º) for $[Cu_2L(OH)]_2 \cdot 2CH_3OH \cdot H_2O$ (1)

N1	Cu1	Cu2	127.57(12)	Cu1	O1	Cu2	100.12(13)
N1	Cu1	N2	85.21(16)	Cu1	O4	$Cu1^i$	97.54(14)
N1	Cu1	O1	89.12(14)	Cu2	O4	$Cu1^i$	100.95(14)
N1	Cu1	$O4^i$	99.57(14)	Cu1	O4	Cu2	105.23(15)
N2	Cu1	Cu2	144.29(12)				
N2	Cu1	O1	170.23(14)				
N2	Cu1	$O4^i$	96.14(14)				
O1	Cu1	Cu2	39.09(8)				
O1	Cu1	$O4^i$	92.64(12)				
$O4^i$	Cu1	Cu2	92.03(8)				
O4	Cu1	Cu2	37.08(10)				
O4	Cu1	N1	164.61(15)				
O4	Cu1	N2	109.84(15)				
O4	Cu1	O1	75.53(13)				
O4	Cu1	$O4^i$	82.46(14)				
N3	Cu2	Cu1	139.50(12)				
N4	Cu2	Cu1	134.30(11)				
N4	Cu2	N3	85.42(16)				
N4	Cu2	O1	93.51(14)				
O1	Cu2	Cu1	40.80(9)				
O1	Cu2	N3	170.48(15)				
O4	Cu2	Cu1	37.69(10)				
O4	Cu2	N3	104.61(15)				
O4	Cu2	N4	167.56(16)				
O4	Cu2	O1	77.82(14)				

Symmetry code: (i) 1/2-x, 3/2-y, 1-z