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Supporting information for article:

**Self-assembling of three rare structurally various
homomultinuclear Cu(II) complexes derived from a bis-
(salamo)-based multioxime ligand**

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Materials and general methods. 5-Nitrosalicylic aldehyde (99%) and 2-hydroxy-5-methylbenzene-1,3-dicarbaldehyde (99%) were purchased from Alfa Aesar and used without further purification. The other solvents and reagents were analytical grade reagents. C, H and N analyses were performed via a GmbH VarioEL V3.00 automatic elemental analyses instrument. Elemental analyses for Cu(II) were conducted using an IRIS ER/S·WP-1 ICP atomic emission spectrometer. ¹H NMR spectra were recorded using a Bruker AVANCE DRX-400 spectrometer (Bruker AVANCE, Billerica, MA, USA). Melting points were made via microscopic melting point instrument made in Beijing Tektronix Instruments Limited Company. FT-IR spectra were gained via a VERTEX70 FT-IR spectrophotometer, with samples prepared as KBr (4000-400 cm⁻¹) pellets. UV/Vis absorption spectra were obtained via a Shimadzu UV-2550 spectrometer. X-ray single crystal structures were carried out on a Bruker D8 Venture diffractometer. Fluorescence spectra were measured via an F-7000 FL spectrophotometer.

Table S1

Selected bond lengths (Å) and angles (°) for complexes **1-3**.

1		2		3	
Cu1-O1	1.9477(16)	Cu1-O1	1.9535(18)	Cu2-Br1	2.4819(7)
Cu1-O1 ^{#1}	2.3618(17)	Cu1-O1 ^{#1}	2.3845(19)	Cu2-Br2	2.4445(7)
Cu1-O6	1.9530(16)	Cu1-O6	1.946(2)	Cu1-N2	1.976(4)
Cu1-N2	1.960(2)	Cu1-N2	1.945(2)	Cu1-N3	1.943(4)
Cu1-N3	2.0048(19)	Cu1-N3	2.004(2)	Cu1-O1	1.959(3)
Cu2-O6	1.9476(16)	Cu2-O6	1.9455(19)	Cu1-O6	1.943(3)
Cu2-O9	1.9618(18)	Cu2-O9	1.961(2)	Cu1-O12	2.337(4)
Cu2-O12	2.286(2)	Cu2-O12	2.240(2)	Cu2-N4	1.962(4)
Cu2-N4	2.048(2)	Cu2-N4	2.043(2)	Cu2-O1	1.987(3)
Cu2-N5	1.938(2)	Cu2-N5	1.941(2)	Cu2-O6	2.100(3)
O1-Cu1-O1 ^{#1}	80.36(6)	O1-Cu1-O1 ^{#1}	81.00(8)	N2-Cu1-O12	103.70(15)
O1-Cu1-O6	88.36(7)	O1-Cu1-N3	172.59(9)	N3-Cu1-N2	100.05(15)
O1-Cu1-N2	87.94(7)	O6-Cu1-O1	87.40(8)	N3-Cu1-O1	169.97(14)
O1-Cu1-N3	170.57(7)	O6-Cu1-O1 ^{#1}	99.04(19)	N3-Cu1-O12	90.91(16)
O6-Cu1-O1 ^{#1}	101.60(6)	O6-Cu1-N3	86.54(9)	O1-Cu1-N2	89.85(13)
O6-Cu1-N2	163.80(8)	N2-Cu1-O1	88.29(9)	O1-Cu1-O12	85.06(13)
O6-Cu1-N3	85.73(7)	N2-Cu1-O1 ^{#1}	93.27(8)	O6-Cu1-N2	159.56(14)
N2-Cu1-O1 ^{#1}	93.31(7)	N2-Cu1-O6	166.15(9)	O6-Cu1-N3	90.64(14)
N2-Cu1-N3	99.73(8)	N2-Cu1-N3	98.58(3)	O6-Cu1-O1	80.45(11)
N3-Cu1-O1 ^{#1}	93.63(7)	N3-Cu1-O1 ^{#1}	95.75(8)	O6-Cu1-O12	93.41(13)
O6-Cu2-O9	86.06(7)	O6-Cu2-O9	85.97(8)	Br2-Cu2-Br1	144.07(3)
O6-Cu2-O12	91.04(7)	O6-Cu2-O12	92.41(8)	N4-Cu2-Br1	91.63(11)
O6-Cu2-N4	86.32(7)	O6-Cu2-N4	85.57(9)	N4-Cu2-Br2	91.86(11)
O9-Cu2-O12	96.91(8)	O9-Cu2-O12	97.09(8)	N4-Cu2-O1	164.60(13)
O9-Cu2-N4	165.70(8)	O9-Cu2-N4	168.30(9)	N4-Cu2-O6	88.83(13)
N4-Cu2-O12	95.31(8)	N4-Cu2-O12	91.33(9)	O1-Cu2-Br1	93.70(9)
N5-Cu2-O6	173.61(8)	N5-Cu2-O6	171.65(9)	O1-Cu2-Br2	92.27(9)
N5-Cu2-O9	90.07(8)	N5-Cu2-O9	89.83(9)	O1-Cu2-O6	76.08(11)
N5-Cu2-O12	94.48(8)	N5-Cu2-O12	95.28(9)	O6-Cu2-Br1	98.87(9)
N5-Cu2-N4	96.36(9)	N5-Cu2-N4	97.49(10)	O6-Cu2-Br2	116.95(9)

Symmetry code (^{#1}): 1-x, 1-y, 2-z.

Table S2

Putative hydrogen bond interactions (Å) for complexes **1-3**.

Complex 1					
D-X...A	d(D-X)	d(X...A)	d(D...A)	∠D-X...A	Symmetry code
C12-H12...O13	0.871(15)	1.892(19)	2.739(7)	164(3)	
O13-H13...O14	0.84	2.07	2.900(12)	169	
C7-H7...O14	0.95	2.53	3.268(11)	135	3/2-x, -1/2+y, 1/2-z
C7-H7...O15	0.95	2.56	3.471(10)	162	3/2-x, -1/2+y, 1/2-z
C18-H18...O15	0.95	2.45	3.197(9)	135	1/2+x, 3/2-y, 1/2+z
C20-H20B...O10	0.99	2.60	3.481(4)	149	2-x, 1-y, -z
C21-H21...O2	0.95	2.22	3.125(3)	160	2-x, 1-y, -z
Complex 2					
D-X...A	d(D-X)	d(X...A)	d(D...A)	∠D-X...A	Symmetry code
C12-H12B...O13	0.99	1.79	2.707(3)	153	
O13-H13...O14	0.84	1.90	2.731(3)	170	
C5-H5...O15	0.95	2.49	3.043(4)	117	x, y, 1+z
C7-H7...O16	0.95	2.27	3.215(4)	174	1/2-x, 1/2+y, 3/2-z
C8-H8B...O13	0.99	2.45	3.409(4)	163	1/2-x, 1/2+y, 3/2-z
C20-H20B...O10	0.99	2.51	3.463(4)	162	x, 1-y, 2-z
C21-H21...O2	0.95	2.33	3.183(4)	150	x, 1-y, 2-z
Complex 3					
D-X...A	d(D-X)	d(X...A)	d(D...A)	∠D-X...A	Symmetry code
O9-H9...Br2	0.84	2.36	3.181(5)	168	1/2+x, 3/2-y, 1/2+z
O12-H12...Br1	0.91(3)	2.47(4)	3.298(4)	152(3)	
C3-H3...O10	0.95	2.58	3.426(8)	148	x, 2-y, 1/2+z
C8-H8A...O3	0.99	2.47	3.453(6)	173	x, 1-y, -1/2+z
C18-H18...O12	0.95	2.36	3.302(6)	171	x, 1-y, -1/2+z