

## Supporting Information

### Recurrent $\pi(\text{arene})\cdots\pi(\text{chelate ring})$ motifs in four trinuclear $\text{Cu}^{\text{II}}\text{M}^{\text{II}}$ ( $\text{M} = \text{Cd}/\text{Zn}$ ) complexes derived from an unsymmetrical $\text{N}_2\text{O}_2$ donor ligand: structural and theoretical investigations

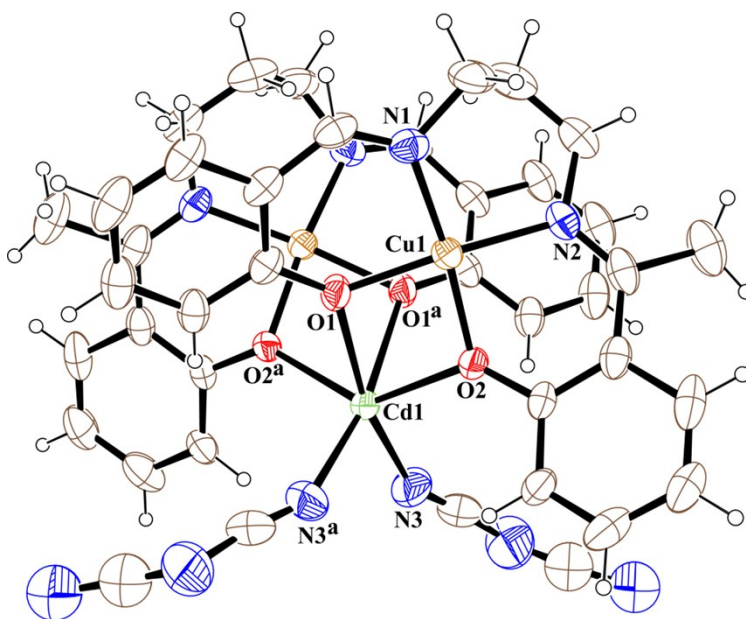
Souvik Maity,<sup>1</sup> Tanmoy Kumar Ghosh,<sup>1</sup> Rosa M. Gomila,<sup>2</sup> Antonio Frontera\*<sup>3</sup> and Ashutosh Ghosh\*<sup>1, 4</sup>

1. Department of Chemistry, University College of Science, University of Calcutta, 92 A.P.C. Road, Kolkata 700009, India. E-mail: [ghosh\\_59@yahoo.com](mailto:ghosh_59@yahoo.com)

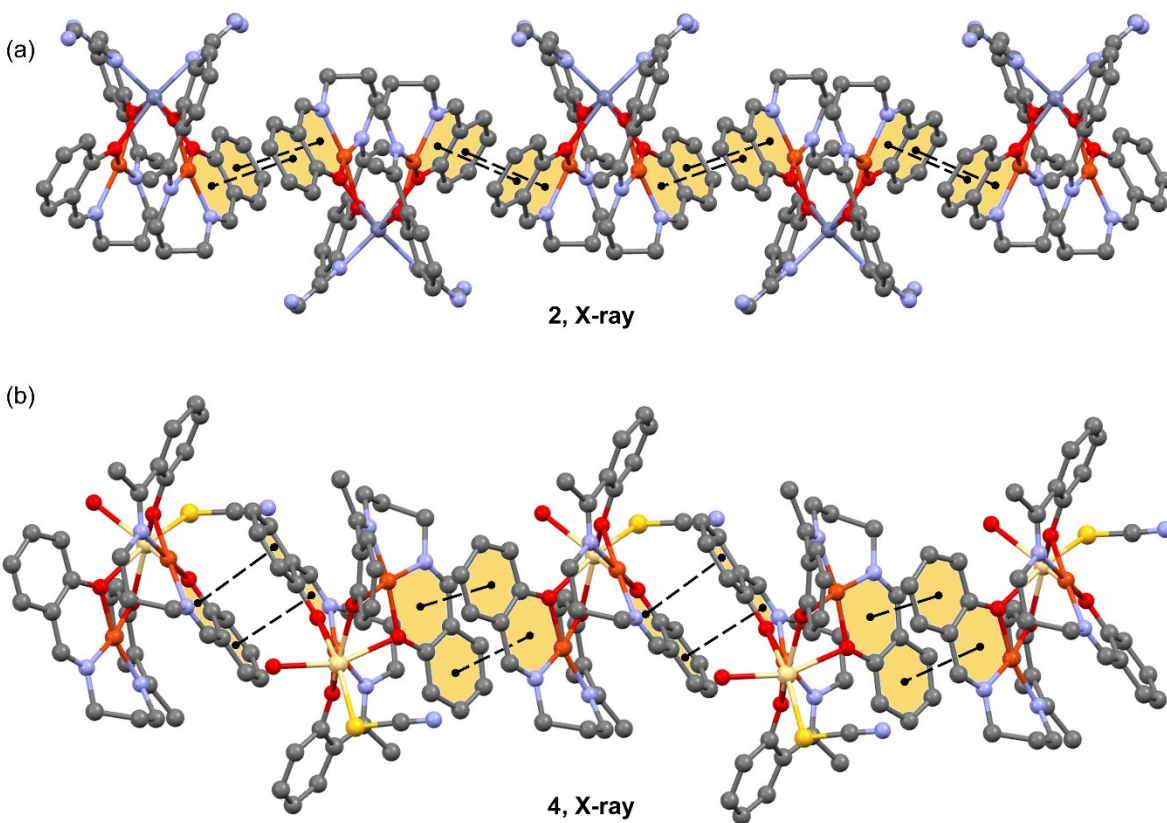
2. Serveis Científico-Tècnics, Universitat de les Illes Balears, Crta de Valldemossa km 7.5, 07122 Palma de Mallorca (Balears), SPAIN

3. Departament de Química, Universitat de les Illes Balears, Crta de Valldemossa km 7.5, 07122 Palma de Mallorca (Balears), SPAIN

4. Rani Rashmoni Green University, Tarakeswar, Hooghly 712410, West Bengal, India



**Fig. S1** ORTEP view of complex **2** with 30% ellipsoid probability. Disordered atoms have been omitted for clarity.



**Fig. S2.** 1D supramolecular polymers in **2** (a) and **4** (b) with indication of the  $\pi(\text{arene})\cdots\pi(\text{chelate ring})$  interactions.

**Table S1.** Bond lengths ( $\text{\AA}$ ) and bond angles ( $^\circ$ ) of complexes **1** and **2**.

	<b>Complex 1</b>	<b>Complex 2</b>
M(1)–O(1)	2.319(3)	2.389(4)
M(1)–O(2)	2.034(3)	2.213(4)
M(1)–N(3)	2.025(4)	2.208(9)
Cu(1)–O(1)	1.909(3)	1.908(4)
Cu(1)–O(2)	1.916(3)	1.888(4)
Cu(1)–N(1)	1.944(3)	1.940(5)
Cu(1)–N(2)	1.983(4)	1.983(5)
O(1)–M(1)–O(2)	70.51(11)	66.41(14)

O(1)–M(1)–N(3)	167.67(14)	168.3(2)
O(1)–M(1)–O(1) <sup>a</sup>	76.03(11)	75.32(15)
O(1)–M(1)–O(2) <sup>a</sup>	79.19(11)	78.59(15)
O(1)–M(1)–N(3) <sup>a</sup>	93.95(14)	95.4(2)
O(2)–M(1)–N(3)	100.87(15)	105.1(2)
O(2)–M(1)–O(2) <sup>a</sup>	141.36(12)	135.61(15)
O(2)–M(1)–N(3) <sup>a</sup>	104.51(15)	104.5(2)
N(3)–M(1)–N(3) <sup>a</sup>	96.83(18)	94.7(3)
O(1)–Cu(1)–O(2)	82.56(13)	83.37(17)
O(1)–Cu(1)–N(1)	91.55(15)	91.2(2)
O(1)–Cu(1)–N(2)	166.07(13)	164.7(2)
O(2)–Cu(1)–N(1)	169.29(13)	169.7(2)
O(2)–Cu(1)–N(2)	90.45(14)	89.7(2)
N(1)–Cu(1)–N(2)	97.11(16)	97.6(2)
M(1)–O(1)–Cu(1)	94.29(12)	97.54(17)
M(1)–O(2)–Cu(1)	103.94(13)	104.40(18)

<sup>a</sup> = 1-x, y, 1/2-z, M = Zn for complex **1** and Cd for complex **2**.

**Table S2.** Bond lengths (Å) and bond angles (°) of complex **3**.

	Complex <b>3</b>
Zn(1)–O(1)	2.572(3)
Zn(1)–O(2)	2.031(3)
Zn(1)–O(3)	2.308(3)
Zn(1)–O(4)	2.014(3)
Zn(1)–N(5)	2.018(4)
Zn(1)–N(6)	1.985(4)
Cu(1)–O(1)	1.907(3)
Cu(1)–O(2)	1.912(3)

Cu(1)–N(1)	1.934(4)
Cu(1)–N(2)	1.973(4)
Cu(2)–O(1)	2.606(3)
Cu(2)–O(3)	1.902(4)
Cu(2)–O(4)	1.919(3)
Cu(2)–N(3)	1.949(5)
Cu(2)–N(4)	1.953(4)
O(1)– Zn(1)–O(2)	66.80(10)
O(1)– Zn(1)–O(3)	72.17(12)
O(1)– Zn(1)–O(4)	75.99(12)
O(1)– Zn(1)–N(5)	90.04(15)
O(1)– Zn(1)–N(6)	162.91(12)
O(2)– Zn(1)–O(3)	81.70(12)
O(2)– Zn(1)–O(4)	138.74(12)
O(2)– Zn(1)–N(5)	100.36(17)
O(2)– Zn(1)–N(6)	99.95(14)
O(3)– Zn(1)–O(4)	70.18(12)
O(3)– Zn(1)–N(5)	159.81(16)
O(3)– Zn(1)–N(6)	95.94(14)
O(4)– Zn(1)–N(5)	96.76(14)
O(4)– Zn(1)–N(6)	112.17(15)
N(5)– Zn(1)–N(6)	103.40(17)
O(1)–Cu(1)–O(2)	84.78(12)
O(1)–Cu(1)–N(1)	91.88(15)
O(1)–Cu(1)–N(2)	163.35(16)
O(2)–Cu(1)–N(1)	164.90(14)
O(2)–Cu(1)–N(2)	90.82(14)
N(1)–Cu(1)–N(2)	96.30(16)

O(3)–Cu(2)–O(4)	81.58(12)
O(3)–Cu(2)–N(3)	92.28(18)
O(3)–Cu(2)–N(4)	169.67(19)
O(4)–Cu(2)–N(3)	172.84(19)
O(4)–Cu(2)–N(4)	88.78(17)
N(3)–Cu(2)–N(4)	97.1(2)
Zn(1)–O(1)–Cu(1)	91.84(11)
Zn(1)–O(1)–Cu(2)	72.32(9)
Zn(1)–O(2)–Cu(1)	111.01(13)
Zn(1)–O(3)–Cu(2)	92.57(13)
Zn(1)–O(4)–Cu(2)	101.93(13)

**Table S3.** Bond lengths (Å) and bond angles (°) of complex **4**.

	Complex <b>4</b>
Cd(1)–O(1)	2.462(9)
Cd(1)–O(2)	2.237(10)
Cd(1)–O(3)	2.327(8)
Cd(1)–O(4)	2.233(10)
Cd(1)–O(5)	2.315(12)
Cd(1)–S(1)	2.587(5)
Cu(1)–O(1)	1.925(10)
Cu(1)–O(2)	1.923(8)
Cu(1)–N(1)	1.918(11)
Cu(1)–N(2)	1.987(13)
Cu(2)–O(3)	1.934(10)
Cu(2)–O(4)	1.903(9)
Cu(2)–N(3)	1.960(11)

Cu(2)–N(4)	1.996(15)
O(1)– Cd(1)–O(2)	65.7(3)
O(1)– Cd(1)–O(3)	75.9(3)
O(1)– Cd(1)–O(4)	81.2(3)
S(1)– Cd(1)–O(1)	163.8(3)
S(1)– Cd(1)–O(2)	98.3(3)
S(1)– Cd(1)–O(3)	107.2(2)
S(1)– Cd(1)–O(4)	114.9(3)
S(1)– Cd(1)–O(5)	89.4(3)
O(2)– Cd(1)–O(3)	86.8(3)
O(2)– Cd(1)–O(4)	142.3(3)
O(2)– Cd(1)–O(5)	103.6(4)
O(3)– Cd(1)–O(4)	67.3(3)
O(3)– Cd(1)–O(5)	159.2(4)
O(4)– Cd(1)–O(5)	94.5(4)
O(1)–Cu(1)–O(2)	83.3(4)
O(1)–Cu(1)–N(1)	92.0(5)
O(1)–Cu(1)–N(2)	166.1(4)
O(2)–Cu(1)–N(1)	170.4(4)
O(2)–Cu(1)–N(2)	90.0(4)
N(1)–Cu(1)–N(2)	96.4(5)
O(3)–Cu(2)–O(4)	82.5(4)
O(3)–Cu(2)–N(3)	91.9(5)
O(3)–Cu(2)–N(4)	170.2(4)
O(4)–Cu(2)–N(3)	174.4(5)
O(4)–Cu(2)–N(4)	88.6(5)
N(3)–Cu(2)–N(4)	96.8(6)
Cd(1)–O(1)–Cu(1)	97.0(5)

Cd(1)–O(2)–Cu(1)	105.6(4)
Cd(1)–O(3)–Cu(2)	97.6(4)
Cd(1)–O(4)–Cu(2)	101.8(4)