Electronic Supplementary Material (ESI) for Dalton Transactions

A 1D Schiff base zinc polymer as a versatile metallo-ligand for the synthesis of polynuclear zinc cages

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Supporting Information

SI1. Table 1. Crystal Data for Compounds 1 - 4:

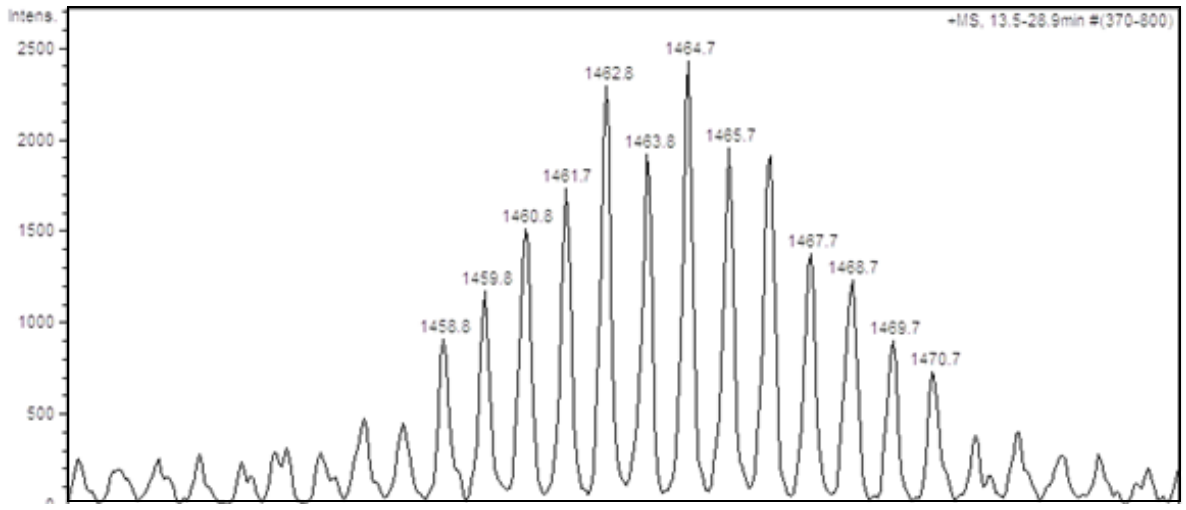
Compound Name	**1**	**2**	**3**	**4**
Chemical Formula	$C_{28}H_{46}N_4O_4Zn_4CdI_4$	$C_{38}H_{69}N_4O_7Zn_6I$	$C_{76}H_{92}N_4O_{16}Zn_8Fe_4$	$C_{48}H_{84}N_6O_{10}Zn_{10}$
CCDC No.	873629	873630	873631	873632
Formula Weight	1384.17	1213.09	2063.90	1558.19
Crystal System	Monoclinic	Orthorhombic	Triclinic	Trigonal
Space Group	P21/c	Pca21	P-1	R-3
T(K)	173(2)	173(2)	173(2)	173(2)
a (Å)	8.8739(2)	21.7613(10)	12.9401(11)	21.0729(12)
b (Å)	17.6026(5)	12.3586(8)	14.8409(13)	21.0729(12)
c (Å)	26.5306(5)	18.5174(9)	25.1129(18)	24.0603(18)
α (^{o})	90	90	78.762(7)	90
β (^{o})	92.250(2)	90	85.067(7)	90
γ (^{o})	90	90	87.677(7)	120
V (Å ^{3})	4140.98(17)	4980.1(5)	4711.4(7)	9252.9(10)

Z	4	4	2	6
Reflections collected	16560	36004	299918	12536
Independent reflections	7449	11058	16860	3566
Data/restraints/parameter ratio	7449/0/416	11058/7/493	16860/3/985	3566/0/229
R int	0.0540	0.0594	0.0560	0.0476
Dcalc (Mg/m^3)	2.220	1.618	1.455	1.679
F(000)	2616	2456	2096	4764
R indices (all data)	R1 = 0.0709, wR2 = 0.1120	R1 = 0.0818, wR2 = 0.1637	R1 = 0.0941, wR2 = 0.1872	R1 = 0.0517, wR2 = 0.0683
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0469, wR2 = 0.1014	R1 = 0.0659, wR2 = 0.1532	R1 = 0.0627, wR2 = 0.1631	R1 = 0.0313, wR2 = 0.0623
Largest difference in peak and hole ($e Å^{-3}$)	1.470[#] and -1.115	2.610[#] and -1.094	0.872 and -0.729	0.519 and -0.345

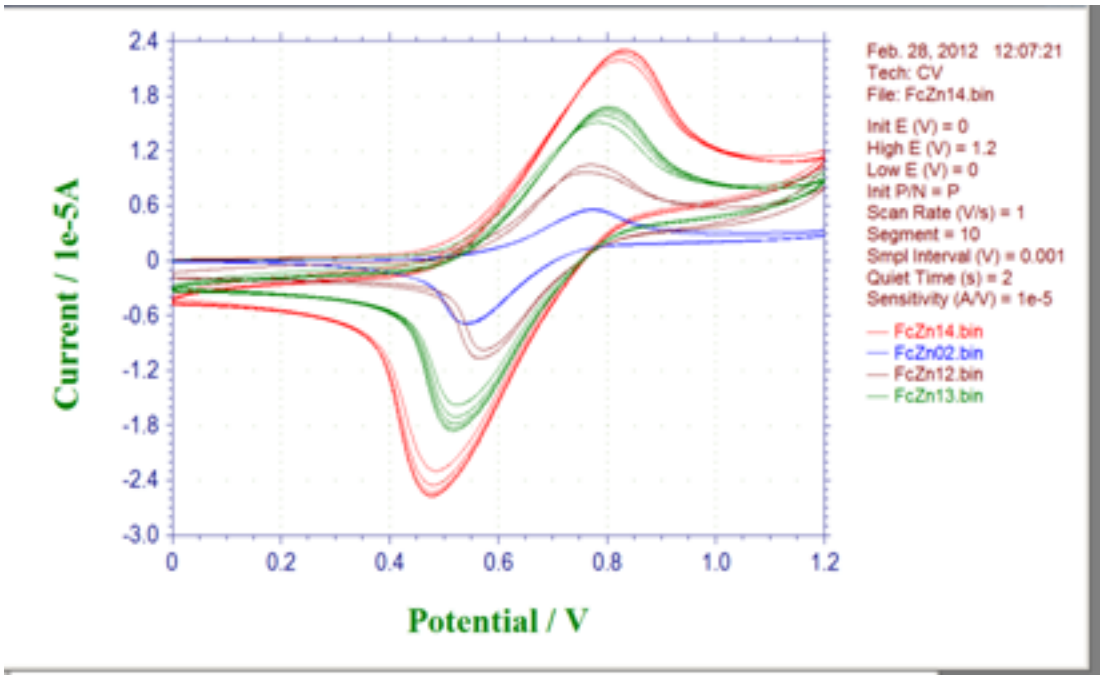
[#] Residual electron density is located close to the iodide atoms.

SI2. Mass spectral analysis of complex 1:

Isotope pattern consistent with the presence of Cd and Zn atoms, but a molecular ion peak was not observed.



SI 3. Electrochemical study on complex 3 with a 2 mm electrode



Solution phase voltammetry of 1 mM solution of **3** disolved in THF containing 0.1 M $TBAPF_6$ using a 3 mm diameter platinum working electrode. The scan rates are 0.05, 0.2, 0.5 and 1.0 Vs^{-1}.

SI4. UV/Vis data for complexes 1, 2 and 4.

Samples were dissolved in thf and run on a Carey UV-Vis spectrometer