Supplementary Material (ESI) for Dalton Transactions

Supporting Information
for

Unsymmetrical dizinc complexes as models for the active sites of phosphohydrolases

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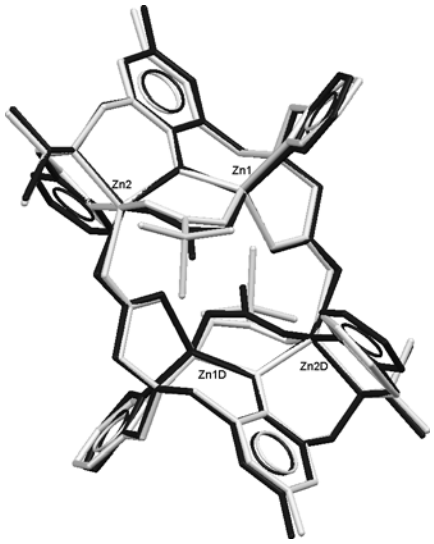

Figure S1: An overlay calculation of the structures of $[\{Zn_2IPCPMP(OAc)\}_2]^{2+}$ 2 and $[\{Zn_2IPCPMP(Piv)\}_2]^{2+}$ 3 made in Mercury (C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler and J. van de Streek, *J. Appl. Crystallogr.*, 2006, 39, 453-457) with a calculated RMS deviation of 0.27.

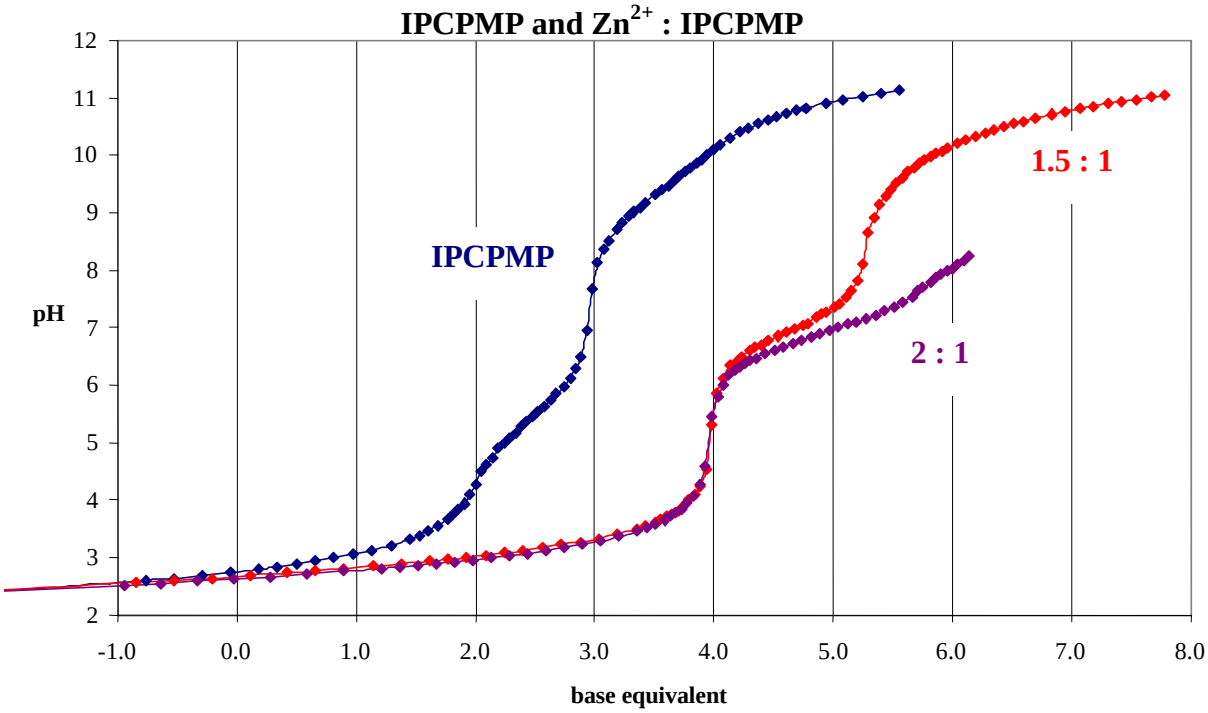

Figure S2: Plot of the data from the potentiometric titration for IPCPMP (blue), 1.5:1 Zn^{2+}:IPCPMP (red) and 2:1 Zn^{2+}:IPCPMP (purple).

ESI-MS results

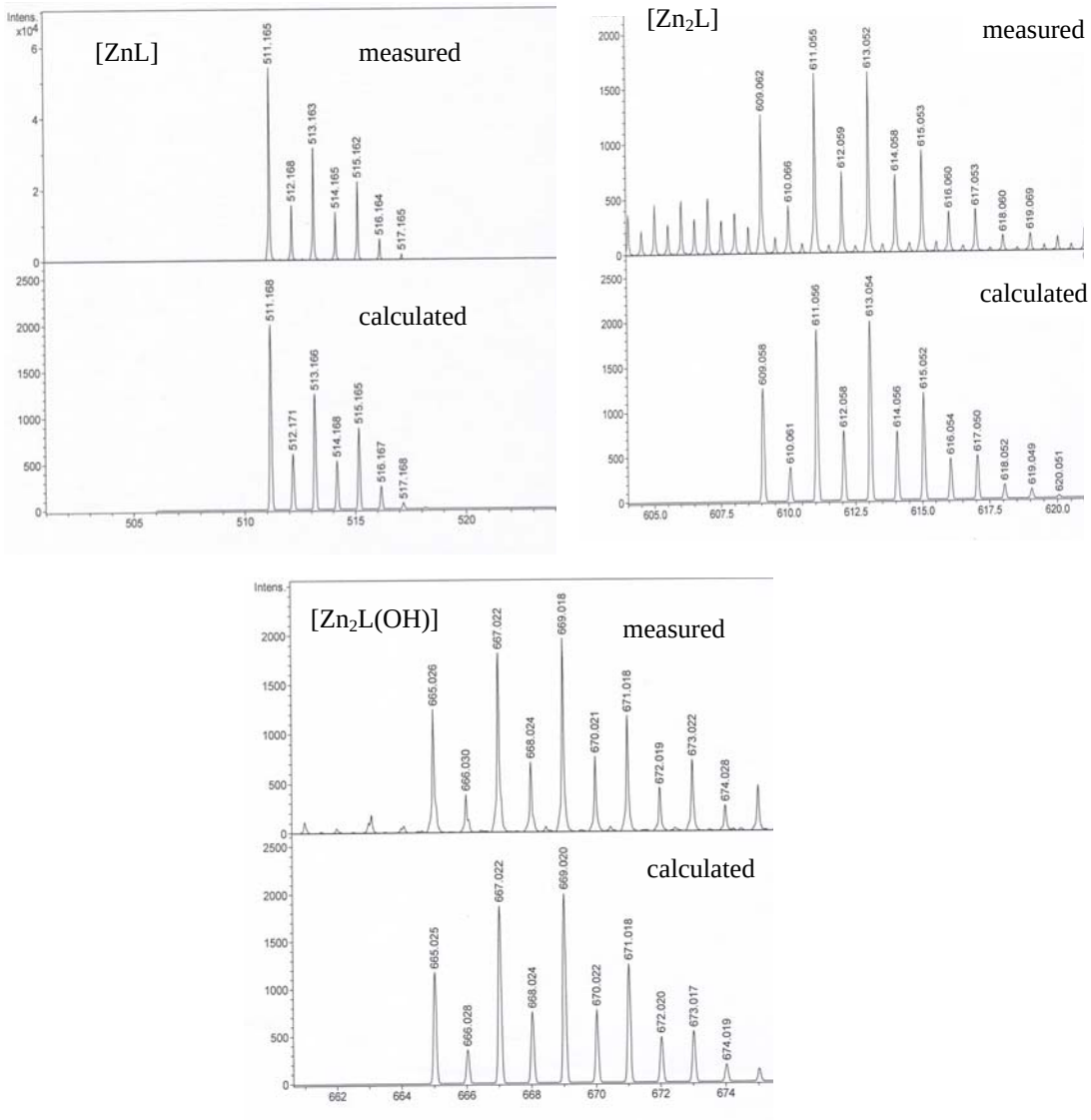

Figure S3: ESI-MS spectra of a solution with 2:1 ratio of $ZnCl_2$ to IPCPMP at pH 7.8. Details on the measurements are given in the experimental part of the paper.

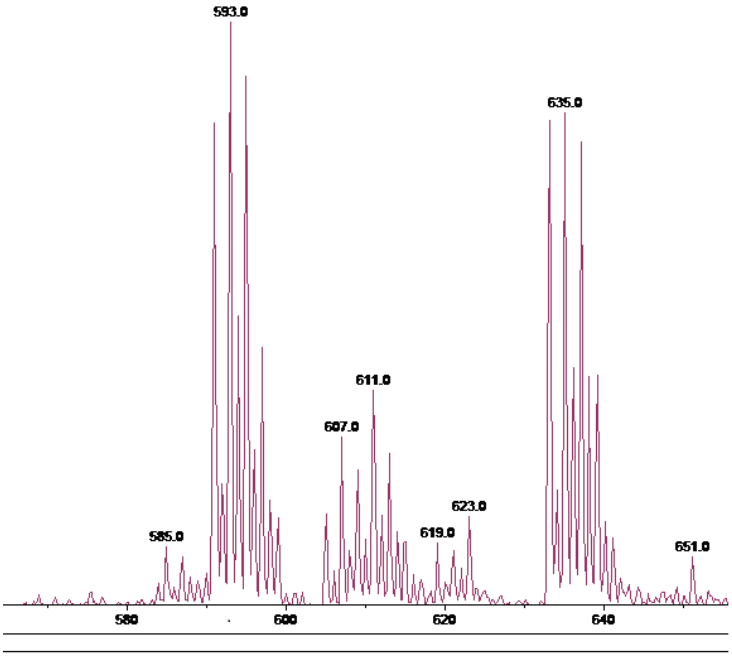

Figure S4: ESI-MS spectrum of a solution of complex **2** at pH 7.0, revealing peaks attributable to $[Zn_2(IPCPMP)(OH)]$ ($[Zn_2(IPCPMP)(O)]$), $[Zn_2(IPCPMP)(OH)_2]$ ($[Zn_2(IPCPMP)(O)(OH)]$, $[Zn_2(IPCPMP)(O)_2]$) and $[Zn_2(IPCPMP)(OAc)]$. Details on the measurements are given in the experimental part of the paper.

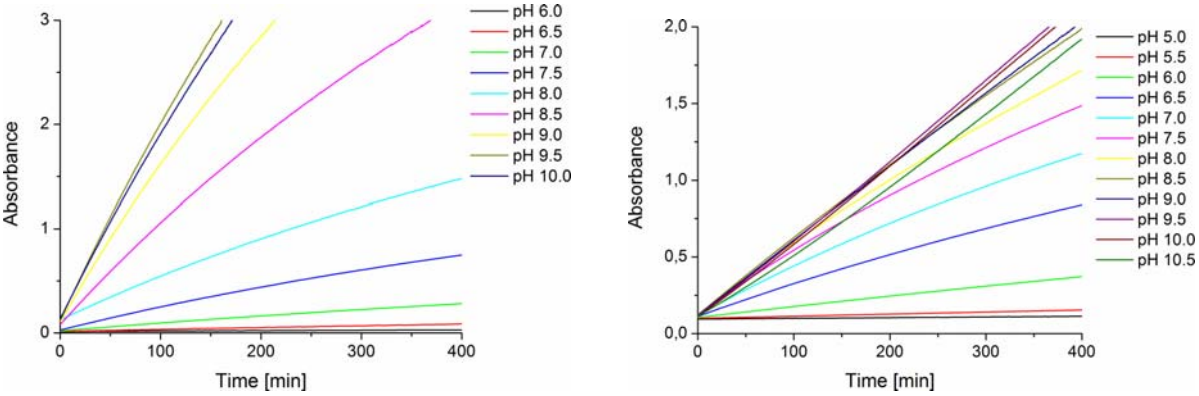

Figure S5: Kinetic traces for (a) HPNP transesterification pH 6-10 enhanced by *in situ* prepared complexes of IPCPMP (2 eq. $Zn(OAc)_2$ and 1 eq. IPCPMP) and (b) BDNPP hydrolysis pH 5.0-10.5 enhanced by complex **2**.

Table S1: Hydrogen bonds in **H_4L** (H_4IPCPMP$(PF_6)_2$.H_2O)

D-H...A	d(D-H)	d(H...A)	d(D...A)	Angle (°)
O(2)-H(2O)...O(1)#1	0.92	1.88	2.704(6)	147.5
O(3)-H(3O)...O(1)	0.96	1.78	2.724(5)	165.7
O(3)-H(3O)...N(2)	0.96	2.44	2.957(6)	113.6
O(4)-H(4O)...N(4B)#2	0.92	2.11	2.870(7)	139.5
O(4)-H(4P)...O(1B)#2	0.98	1.86	2.784(6)	156.8
N(1)-H(1N)...O(5)#5	0.90	2.58	3.066(8)	114.5
N(3)-H(3N)...O(3)	0.98	2.13	2.838(6)	127.8
O(2B)-H(2Q)...O(4)	0.98	1.60	2.545(6)	161.0
O(3B)-H(3Q)...O(1B)	0.93	1.81	2.732(6)	169.0
O(3B)-H(3Q)...N(2B)	0.93	2.53	2.970(6)	109.4
N(3B)-H(3M)...O(3B)	0.99	2.08	2.805(6)	129.1