Electronic Supplementary Information for Dalton Transactions

Symmetrical and unsymmetrical dizinc complexes as models for the active sites of hydrolytic enzymes†

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Supplementary Information

Figure S1: An ORTEP representation of the molecular structure of the cation of complex **2**, $[\{Zn_2(IPCPMP)(OAc)\}_2]^{2+}$

Table S1: Relevant crystallographic details for the crystal structure of $[\{Zn_2(IPCPMP)(OAc)\}_2](PF_6)_2$

Figure S2: FAB+ mass spectrum of complex **2** dissolved in a 1:1 $MeCN/H_2O$ solution

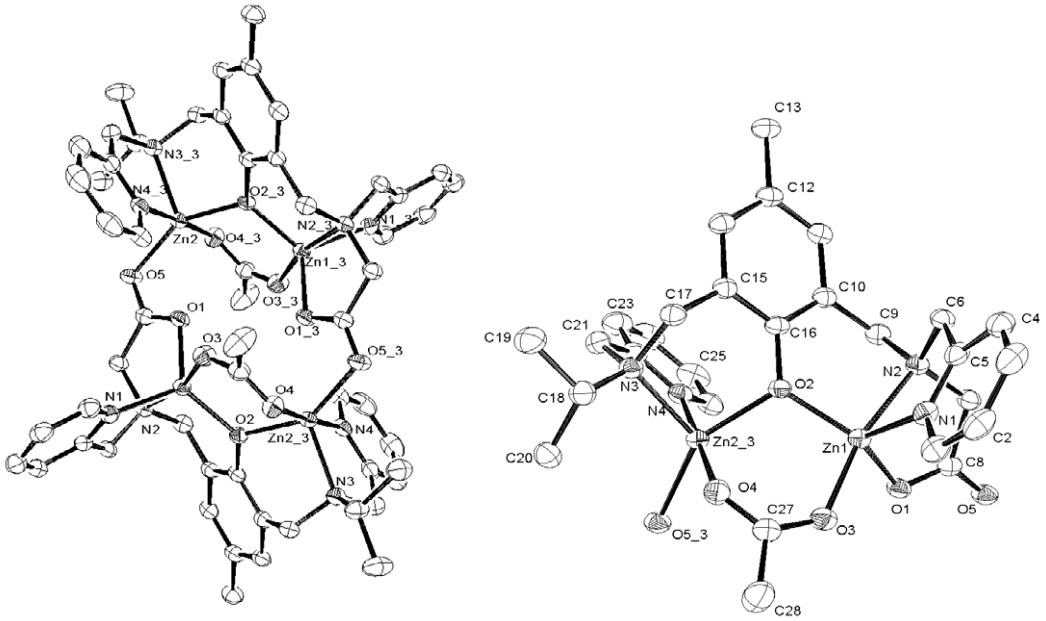
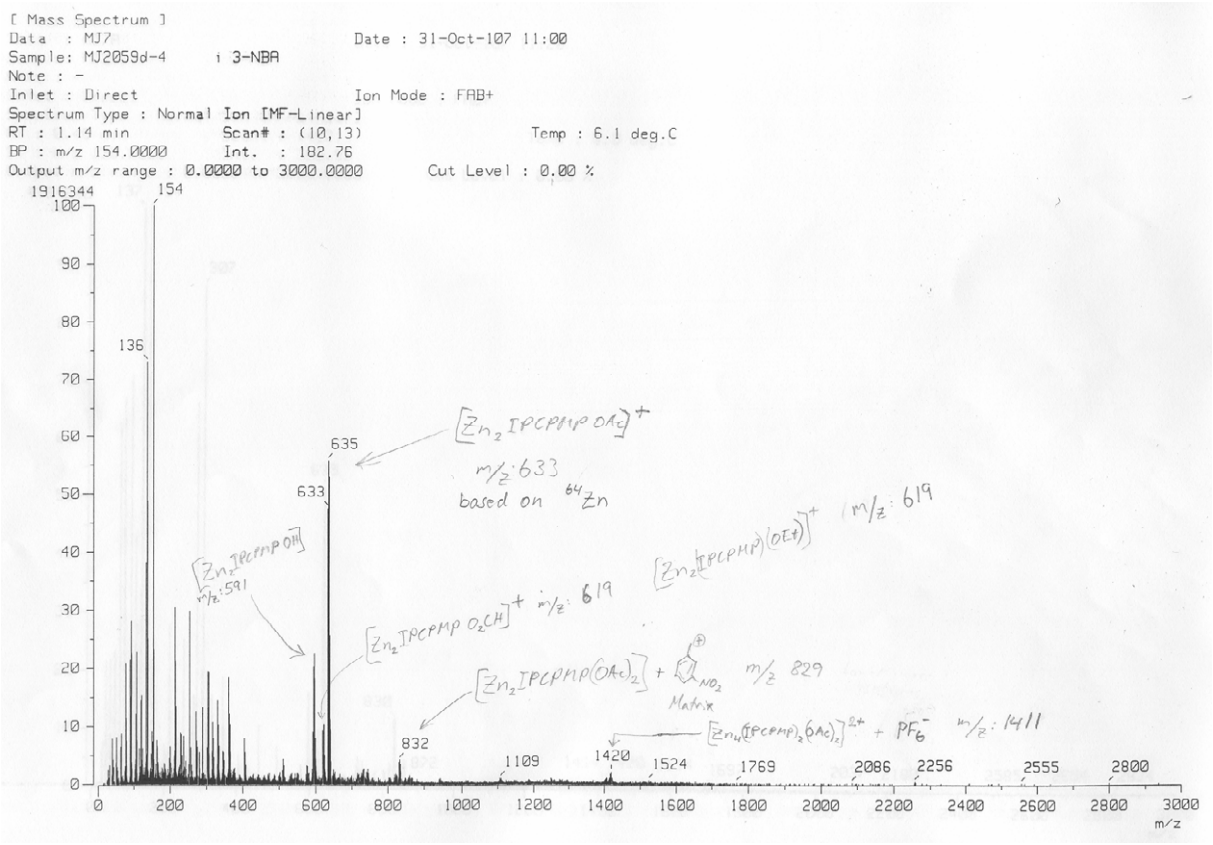


Figure S1.An ORTEP representation of the structure of **2,** showing both the dimer of dimers (left) and the simple dimer (right). Thermal ellipsoids are drawn at the 50 % probability level. Hydrogen atoms, non-coordinated counter ions and solvent molecules have been omitted for clarity. Relevant distances (Å) and angles (º): Zn(1)-O(2) 1.9680(16); Zn(1)-O(3) 2.1132(19); Zn(1)-O(2)-Zn(2) 116.86(8); O(3)-Zn(1)-N(2) 167.07(8); O(2)-Zn(1)-O(1) 121.01(7); O(4_3)-Zn(2)-N(4_3) 177.04(7); O(2_3)-Zn(2)-O(5) 146.06(7).

Table S1. Crystal data and structure refinement for complex **2**.

Identification code	2	
Empirical formula	$C_{56}H_{66}F_{12}N_8O_{10}P_2Zn_4$	
Formula weight	1562.59	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.5983(2) Å	α= 90°
	b = 19.4790(3) Å	β= 97.187(2)°
	c = 12.5532(4) Å	γ = 90°
Volume	3056.38(12) $Å^3$	
Z	2	
Density (calculated)	1.698 Mg/m^3	
Absorption coefficient	1.704 mm^{-1}	
F(000)	1592	
Crystal size	0.35 x 0.22 x 0.17 mm^3	
Theta range for data collection	3.47 to 27.48°.	
Index ranges	-16<=h<=16, -25<=k<=25, -16<=l<=16	
Reflections collected	53314	
Independent reflections	6951 [R(int) = 0.0375]	
Completeness to theta = 27.48°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7464 and 0.5744	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6951 / 0 / 419	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0349, wR2 = 0.0897	
R indices (all data)	R1 = 0.0411, wR2 = 0.0954	
Largest diff. peak and hole	1.292 and -0.726 $e.Å^{-3}$	

Figure S2


[Mass Spectrum]
Data : MJ?
Date : 31-Oct-107 11:00
Sample: MJ2059d-4 i 3-NBA
Note : -
Inlet : Direct
Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.14 min
Scan# : (10,13)
Temp : 6.1 deg.C
BP : m/z 154.0000
Int. : 182.76
Output m/z range : 0.0000 to 3000.0000
Cut Level : 0.00 %
1916344
154
136
635
633
832
1109
1420
1524
1769
2086
2256
2555
2800
m/z
m/z: 633
based on 64Zn
m/z: 619
m/z 829
Matrix
m/z: 1411