Novel Amine Templated Three-Dimensional Zinc-Organophosphonates with Variable Pore-Openings

Avijit Kumar Paul,*[a] Rajendiran Kanagaraj,[a] Ajay Jana,[b] and Pradip K. Maji[c]

ELECTRONIC SUPPORTING INFORMATION

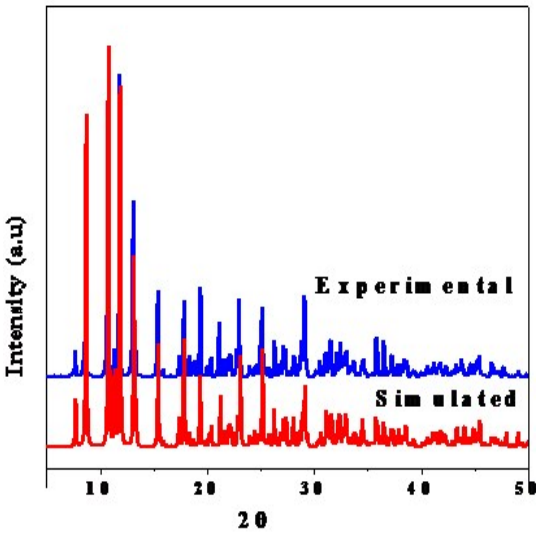
[a] Department of Chemistry, National Institute of Technology Kurukshetra, Kurukshetra-136119, Haryana, India; E-mail: apaul@nitkkr.ac.in

[b] Solid State & Structural Chemistry Unit, Indian Institute of Science, Bangalore-560012, India

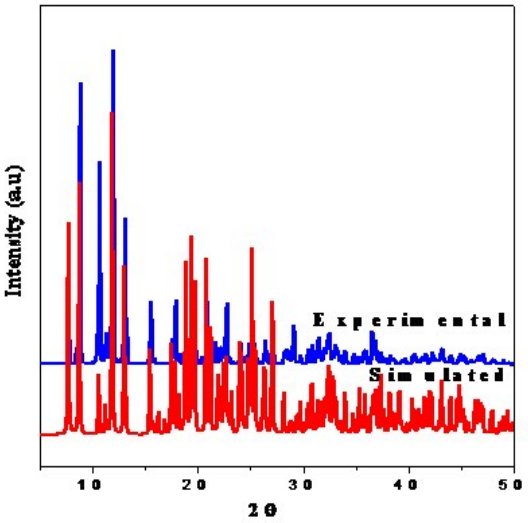
[c] Department of Polymer and Process Engineering, Indian Institute of Technology Roorkee, Saharanpur-247001, India.

Table S1: Selected bond angles observed in $[C_2N_2H_{10}][Zn_3(hedp)_2].H_2O$, **I**; $[C_4N_3H_{15}][Zn_3(hedp)_2]$, **II**; $[C_3N_2H_{12}][Zn_3(hedp)_2]$, **III**; $[C_3N_2H_{12}][Zn_3(hedp)_2]$, **IV** and $[C_6N_2H_{14}][Zn_3(hedp)_2]$, **V**.

Moiety	Bond Angle (˚)	Moiety	Bond Angle(˚)
Compound **I**			
O(1)-Zn(1)-O(2)	116.7(3)	O(9)-Zn(3)-O(12)	102.7(3)
O(1)-Zn(1)-O(3)	119.3(2)	O(10)-Zn(3)-O(12)	105.4(3)
O(2)-Zn(1)-O(3)	108.1(3)	O(11)-Zn(3)-O(12)	113.1(3)
O(1)-Zn(1)-O(4)	97.5(2)	O(4)-P(1)-O(12)	111.6(4)
O(2)-Zn(1)-O(4)	100.9(2)	O(4)-P(1)-O(3)	110.5(3)
O(3)-Zn(1)-O(4)	112.2(2)	O(12)-P(1)-O(3)	112.3(4)
O(5)-Zn(2)-O(6)	120.9(3)	O(9)-P(2)-O(2)	111.2(4)
O(5)-Zn(2)-O(7)	109.7(2)	O(9)-P(2)-O(6)	114.4(5)
O(6)-Zn(2)-O(7)	107.9(3)	O(2)-P(2)-O(6)	109.1(4)
O(5)-Zn(2)-O(8)	104.9(3)	O(7)-P(3)-O(11)	113.8(4)
O(6)-Zn(2)-O(8)	107.9(3)	O(7)-P(3)-O(1)	109.3(3)
O(7)-Zn(2)-O(8)	104.3(3)	O(11)-P(3)-O(1)	110.6(3)
O(9)-Zn(3)-O(10)	122.2(3)	O(10)-P(4)-O(5)	110.3(4)
O(9)-Zn(3)-O(11)	110.6(3)	O(10)-P(4)-O(8)	113.8(4)
O(10)-Zn(3)-O(11)	103.0(3)	O(5)-P(4)-O(8)	108.1(3)
Compound **II**			
O(1)-Zn(1)-O(3)	117.22(15)	O(10)-Zn(3)-O(12)	103.00(14)
O(1)-Zn(1)-O(2)	114.93(14)	O(9)-Zn(3)-O(12)	101.86(13)
O(3)-Zn(1)-O(2)	106.08(15)	O(11)-Zn(3)-O(12)	108.96(13)
O(1)-Zn(1)-O(4)	105.56(14)	O(1)-P(1)-O(10)	112.0(2)
O(3)-Zn(1)-O(4)	107.55(14)	O(1)-P(1)-O(4)	108.95(18)
O(2)-Zn(1)-O(4)	104.58(13)	O(10)-P(1)-O(4)	111.7(2)
O(5)-Zn(2)-O(7)	121.32(14)	O(2)-P(2)-O(5)	110.00(18)
O(5)-Zn(2)-O(6)	116.53(14)	O(2)-P(2)-O(11)	113.66(19)
O(7)-Zn(2)-O(6)	108.41(14)	O(5)-P(2)-O(11)	110.15(18)
O(5)-Zn(2)-O(8)	98.66(13)	O(8)-P(3)-O(7)	111.01(17)
O(7)-Zn(2)-O(8)	108.72(12)	O(8)-P(3)-O(12)	111.64(19)
O(6)-Zn(2)-O(8)	100.14(13)	O(7)-P(3)-O(12)	112.53(18)
O(10)-Zn(3)-O(9)	127.18(16)	O(9)-P(4)-O(3)	112.87(19)
O(10)-Zn(3)-O(11)	101.59(14)	O(9)-P(4)-O(6)	111.6(2)
O(9)-Zn(3)-O(11)	113.05(14)	O(3)-P(4)-O(6)	110.5(2)
Compound **III**			
O(1)-Zn(1)-O(2)	115.86(18)	O(5)-Zn(2)-O(6)	104.08(16)
O(1)-Zn(1)-O(3)	113.04(18)	O(5)-Zn(2)-O(6)	106.92(18)
O(2)-Zn(1)-O(3)	109.39(18)	O(6)-Zn(2)-O(6)	117.7(3)
O(1)-Zn(1)-O(4)	110.53(18)	O(1)-P(1)-O(5)	108.8(2)
O(2)-Zn(1)-O(4)	101.57(16)	O(1)-P(1)-O(3)	111.8(2)
O(3)-Zn(1)-O(4)	105.36(17)	O(5)-P(1)-O(3)	112.9(2)
O(5)-Zn(2)-O(5)	117.9(3)	O(2)-P(2)-O(6)	109.4(2)
O(5)-Zn(2)-O(6)	106.92(18)	O(2)-P(2)-O(4)	112.1(2)
O(5)-Zn(2)-O(6)	104.08(16)	O(6)-P(2)-O(4)	111.1(2)
Compound **IV**			
O(1)-Zn(1)-O(2)	117.81(12)	O(5)-Zn(2)-O(6)	104.48(11)
O(1)-Zn(1)-O(3)	109.07(12)	O(5)-Zn(2)-O(6)	103.44(11)
O(2)-Zn(1)-O(3)	109.69(12)	O(6)-Zn(2)-O(6)	125.30(17)
O(1)-Zn(1)-O(4)	108.65(12)	O(2)-P(1)-O(4)	112.25(16)
O(2)-Zn(1)-O(4)	107.67(11)	O(2)-P(1)-O(6)	109.70(15)
O(3)-Zn(1)-O(4)	102.90(11)	O(4)-P(1)-O(6)	110.70(17)
O(5)-Zn(2)-O(5)	116.66(16)	O(1)-P(2)-O(5)	109.37(15)
O(5)-Zn(2)-O(6)	103.44(11)	O(1)-P(2)-O(3)	111.76(17)
O(5)-Zn(2)-O(6)	104.48(11)	O(5)-P(2)-O(3)	110.68(16)
Compound **V**			
O(1)-Zn(1)-O(2)	107.73(15)	O(6)-Zn(2)-O(7)	118.76(15)
O(1)-Zn(1)-O(3)	122.17(14)	O(6)-Zn(2)-O(7)	104.23(14)
O(2)-Zn(1)-O(3)	108.57(16)	O(7)-Zn(2)-O(7)	101.5(2)
O(1)-Zn(1)-O(4)	109.81(15)	O(2)-P(1)-O(7)	109.6(2)
O(2)-Zn(1)-O(4)	105.45(15)	O(2)-P(1)-O(4)	112.9(2)
O(3)-Zn(1)-O(4)	101.91(15)	O(7)-P(1)-O(4)	109.7(2)
O(6)-Zn(2)-O(6)	109.9(2)	O(1)-P(2)-O(6)	109.01(18)
O(6)-Zn(2)-O(7)	104.23(14)	O(1)-P(2)-O(3)	112.4(2)
O(6)-Zn(2)-O(7)	118.76(15)	O(6)-P(2)-O(3)	112.2(2)



(S1)



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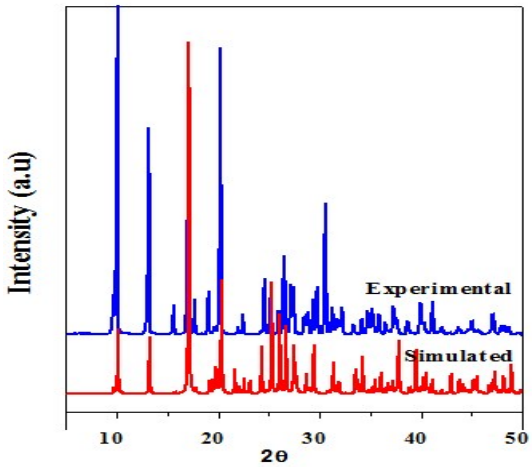

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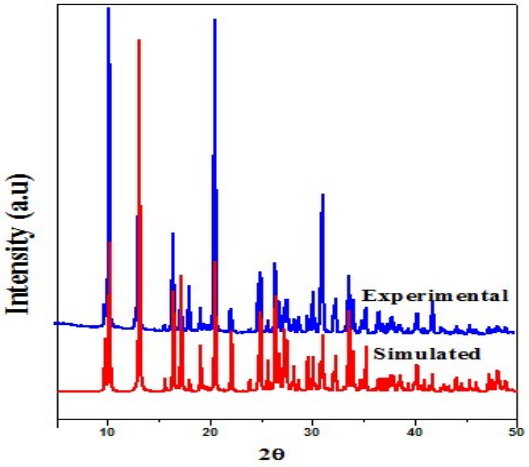

(S4)

(S5)

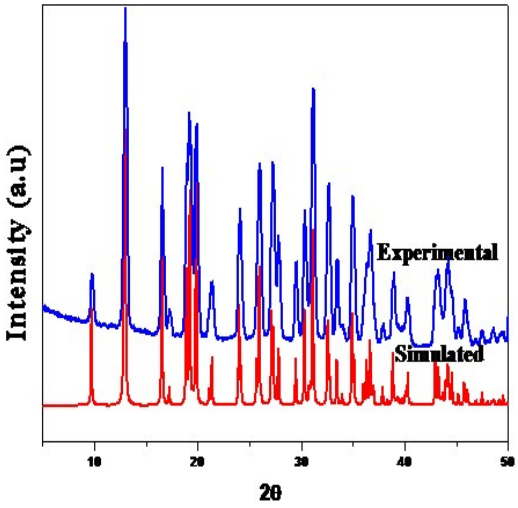

Fig. S1-S5: The simulated and experimental Powder XRD (CuKα) patterns for compound **1-V.**

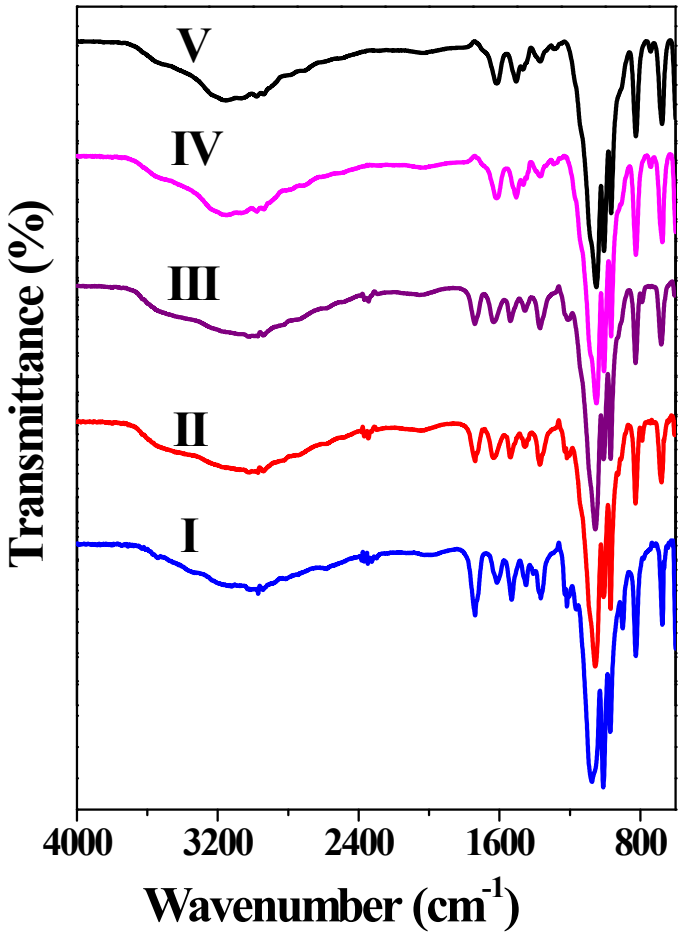

Fig. S6: Infrared (IR) spectra of compounds **I– V**

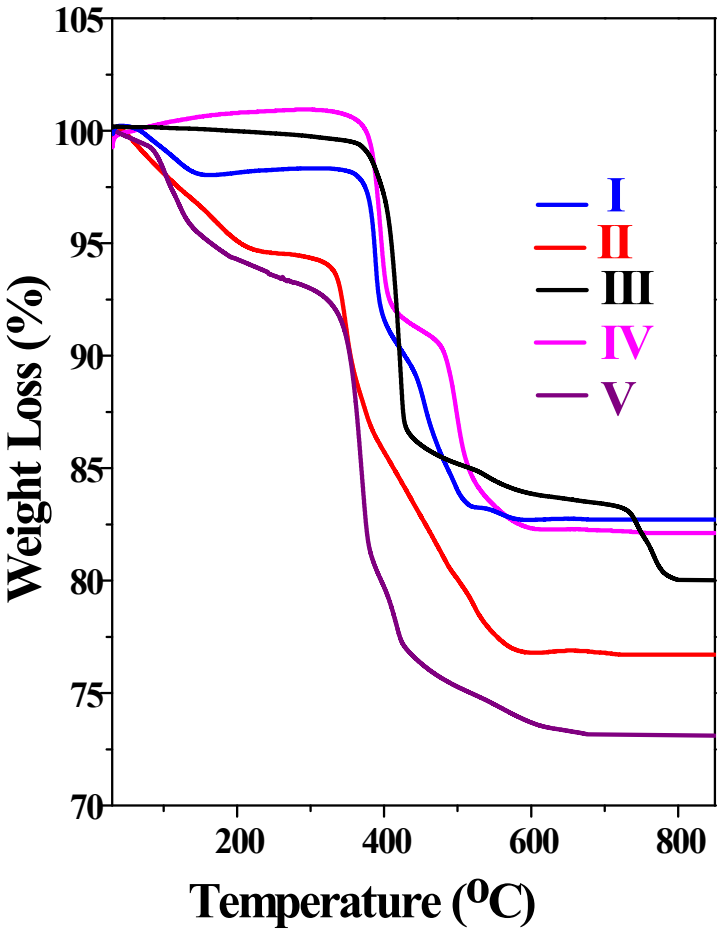

Fig. S7: TGA studies (in oxygen atmosphere) of compounds **I– V.**

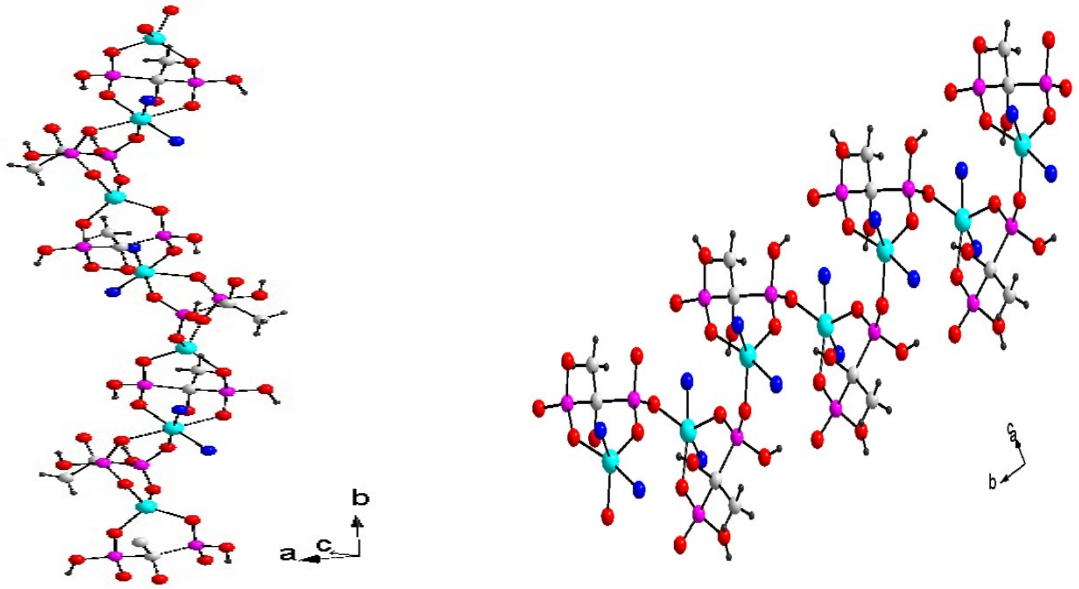

Fig. S8: One-dimensional chain observed in compounds $[Zn_2(1,10\text{-phen})(hedpH_2)_2].H_2O$ and $[Zn_2(1,10\text{-phen})(hedpH_2)_2]$.* Blue atoms are nitrogen from phenanothroline ligand.

* 34. W.-N. Wang, Z.-G. Sun, Y.-Y. Zhu, D.-P. Dong, J. Li, F. Tong, C.-Y. Huang, K. Chen, C. Li, C.-Q. Jiao, C.-L. Wang, *CrystEngComm*, 2011, **13**, 6099.

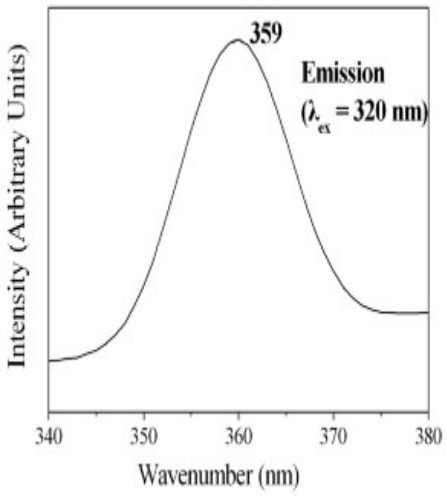

Fig. S9: The room-temperature luminescent emission spectrum of hedpH4 solution.*

* 34. W.-N. Wang, Z.-G. Sun, Y.-Y. Zhu, D.-P. Dong, J. Li, F. Tong, C.-Y. Huang, K. Chen, C. Li, C.-Q. Jiao, C.-L. Wang, *CrystEngComm*, 2011, **13**, 6099.
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