Supporting Information for *Acta Phys. -Chim. Sin.* 2016, *32* (6): 1397－1403
doi: 10.3866/PKU.WHXB201603102

三个不同穿插的锌配合物的合成、结构和热动力学分析

何 甜[1] 岳可芬[1,*] 陈三平[1] 周春生[2,*] 晏 妮[1]

([1]西北大学化学与材料科学学院，教育部合成与天然功能分子化学重点实验室，西安 710069；
[2]商洛学院化工与现代材料科学学院，陕西省尾矿资源利用重点实验室，陕西 商洛 726000)

Synthesis, Structure and Thermodynamics/Kinetics Analysis of Three Different Interpenetrating Zinc(II) Coordination Architectures

HE Tian[1] YUE Ke-Fen[1,*] CHEN San-Ping[1] ZHOU Chun-Sheng[2,*] YAN Ni[1]

([1]*Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of the Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi'an 710069, P. R. China*; [2]*Shaanxi Key Laboratory of Comprehensive Utilization of Tailings Resources, College of Chemical Engineering and Modern Materials, Shangluo University, Shangluo 726000, Shaanxi Province, P. R. China*)

[*]Corresponding authors. YUE Ke-Fen, Email: ykflyy@nwu.edu.cn; Tel: +86-29-81535026.
ZHOU Chun-Sheng, Email: slzhoucs@126.com.cn.

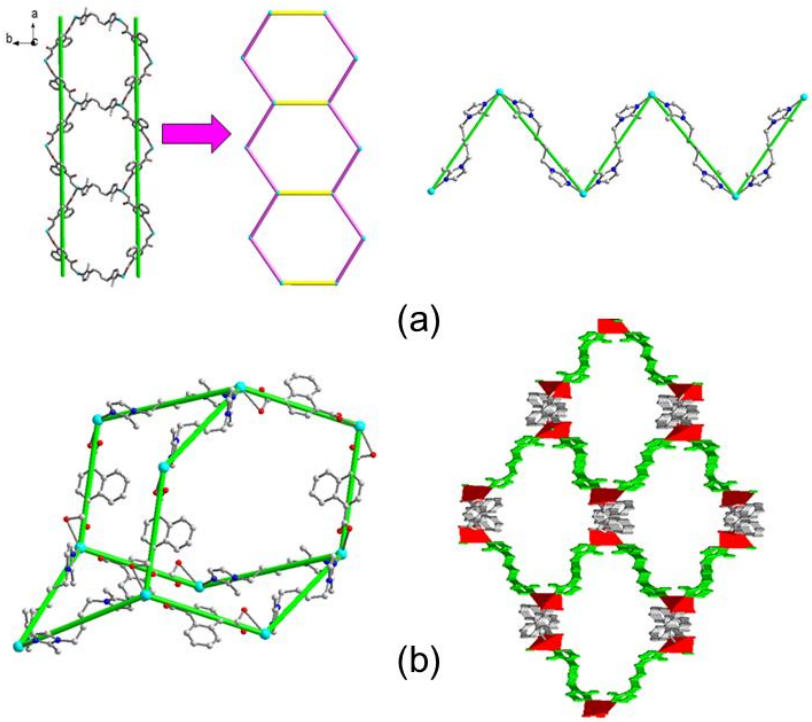


Fig.S1 (a) two kinds of $[Zn(1,4\text{-ndc})]_n$ zigzag chains and $[Zn(bib)]_n$ zigzag chain; (b) left: A single adamantanoid cage of 1, right: A single dia network

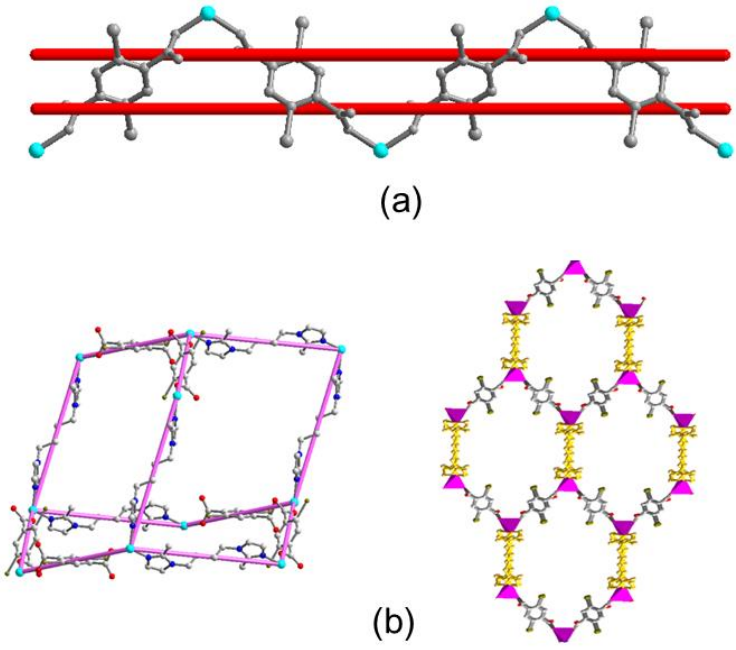


Fig.S2 (a) View of the *meso*-helical chain in 2; (b) left: A single adamantanoid cage of 2, right: A single 3D dia network

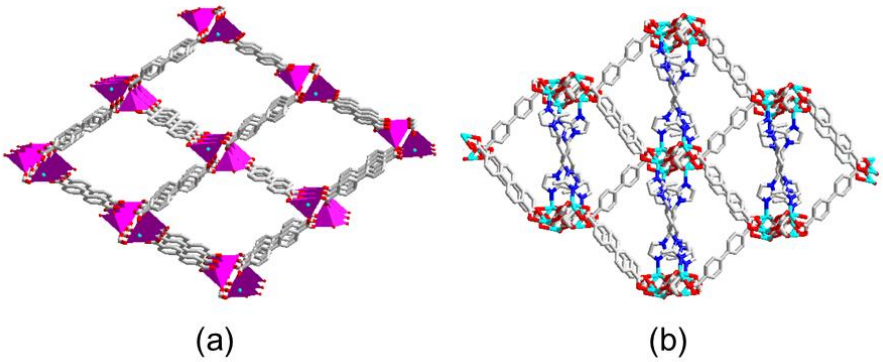
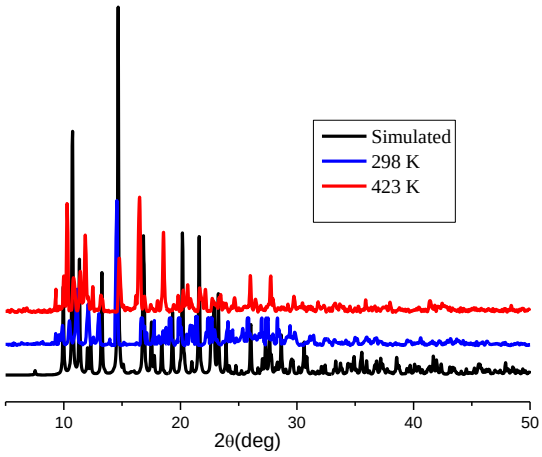
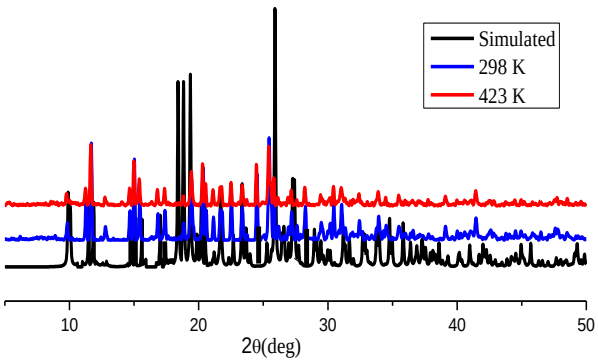


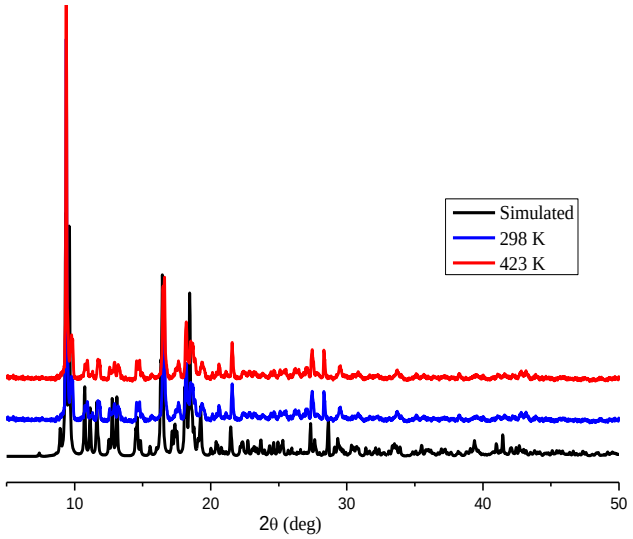
Fig.S3 (a) 3D framework formed by only Zn(II) and 4,4′-bpdc^{2-} in 3; (b) 3D framework of 3



(a)



(b)



(c)

Fig.S4 PXRD patterns for 1(a), 2(b) and 3(c) recorded N_2 atmosphere

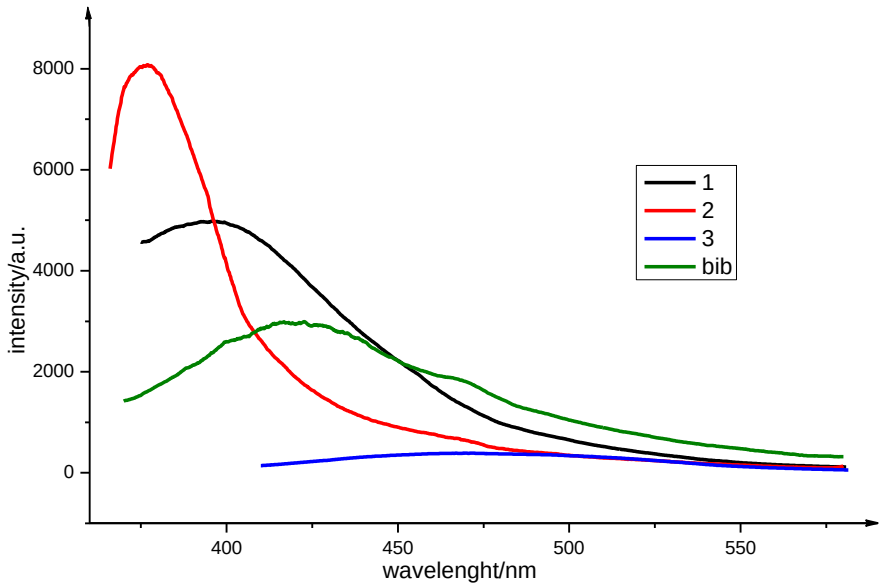


Fig.S5 Luminescences of free ligand bib and complexes 1–3

Table S1 Crystal data and structure refinements for 1–3

Complex	1	2	3
Empirical formula	$C_{48}H_{46}Zn_2N_8O_8$	$C_{20}H_{20}ZnBr_2N_4O_7$	$C_{40}H_{34}Zn_2N_4O_9$
Formula weight	993.71	653.59	845.45
Temperature/K	296(2)	296(2)	296(2)
Crystal system	Monoclinic	orthorhombic	Monoclinic
Space group	*C2/c*	*Pnna*	C2/c

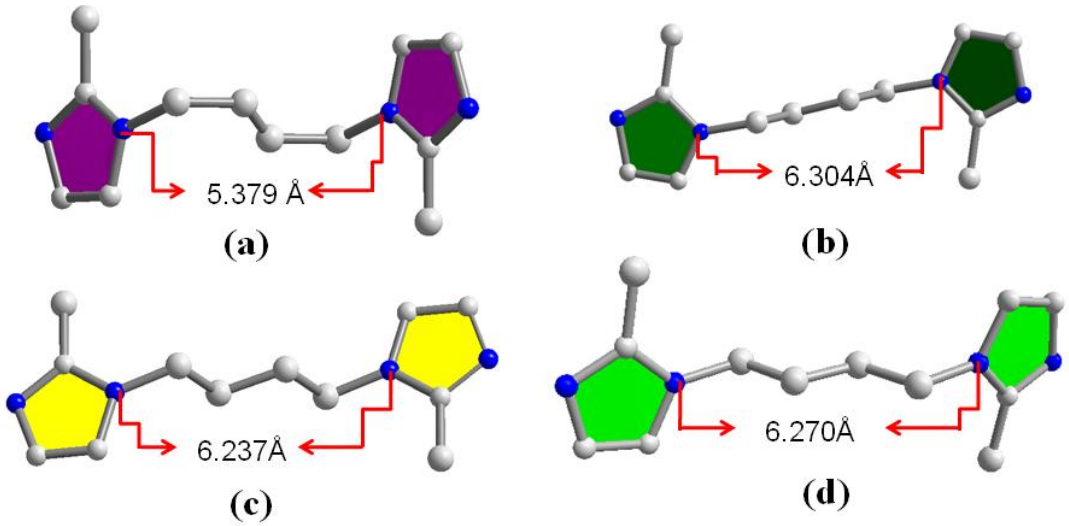
a/Å	20.273(5)	17.862(4)	24.242(4)
b/Å	17.762(5)	13.888(3)	15.713(2)
c/Å	16.121(5)	10.086(2)	10.7475(16)
α/(°)	90	90	90
β/(°)	125.668(5)	90	101.581(3)
γ/(°)	90	90	90
V/Å^3	4716(6)	2502.1(9)	4010.6(10)
Z	4	4	4
Calculated density (mg m^{-3})	1.467	1.735	1.400
R_{int}	0.1136	0.1041	0.0664
GOF on F^2	1.267	0.676	1.012
R_1[a][$I>2\sigma(I)$]	0.1396	0.0832	0.0575
wR_2[b][$I>2\sigma(I)$]	0.3580	0.1869	0.1599

[a] $R_1 = \sum(|F_o| - |F_c|)/\sum|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S2 Selected bond distances (Å) and angles (°) for 1–3.

Complex **1**			
Zn(1)-O(5)	1.916(8)	Zn(1)-O(2)	2.002(7)
Zn(1)-N(4)	2.024(9)	Zn(1)-N(2)	2.039(8)
O(5)-Zn(1)-O(2)	98.6(3)	O(5)-Zn(1)-N(4)	117.4(4)
O(2)-Zn(1)-N(4)	120.4(3)	O(5)-Zn(1)-N(2)	113.4(4)
O(2)-Zn(1)-N(2)	99.4(3)	N(4)-Zn(1)-N(2)	106.5(4)
Complex **2**			
Zn(1)-O(2)#1	1.928(7)	Zn(1)-O(2)	1.928(6)
Zn(1)-N(1)	2.011(7)	Zn(1)-N(1)#1	2.011(7)
O(2)#1-Zn(1)-O(2)	114.3(5)	O(2)#1-Zn(1)-N(1)	104.4(3)
O(2)#1-Zn(1)-N(1)#1	112.1(3)	O(2)-Zn(1)-N(1)	112.1(3)
O(2)-Zn(1)-N(1)#1	104.4(3)	N(1)-Zn(1)-N(1)#1	109.7(5)
Complex **3**			
Zn(1)-O(2)	1.945(4)	Zn(1)-O(4)	1.958(4)
Zn(1)-N(2)	1.991(4)	Zn(1)-O(3)	2.002(3)
O(2)-Zn(1)-O(4)	105.62(19)	O(2)-Zn(1)-N(2)	137.22(19)
O(4)-Zn(1)-N(2)	98.41(19)	O(2)-Zn(1)-O(3)	103.30(18)
O(4)-Zn(1)-O(3)	113.74(16)	N(2)-Zn(1)-O(3)	98.46(16)

Symmetry transformations used to generate equivalent atoms: **For 1**, #1 x+1/2,-y+1/2,z+1/2 #2 -x+1/2,-y-1/2,-z+2 #3 -x+1/2,-y-1/2,-z+1 #4 x-1/2,-y+1/2,z-1/2 ; **For 2**, #1 x,-y+1/2,-z+1/2 #2 -x+1,-y,-z #3 -x,-y+1,-z; **For 3**, #1 -x+1/2,-y+1/2,-z+1#2 -x+1,y,-z+1/2#3 -x,-y+1,-z #4 -x+1/2,-y-1/2,-z+1



Scheme S1 A variety of spatial configuration of bib in 1–3