Syntheses, Characterization and Properties of Three Coordination Polymers with Interpenetrating Structures Comprising 4,4′-(1H-1,2,4-triazol-1-yl)methylene-bis(benzonic acid)

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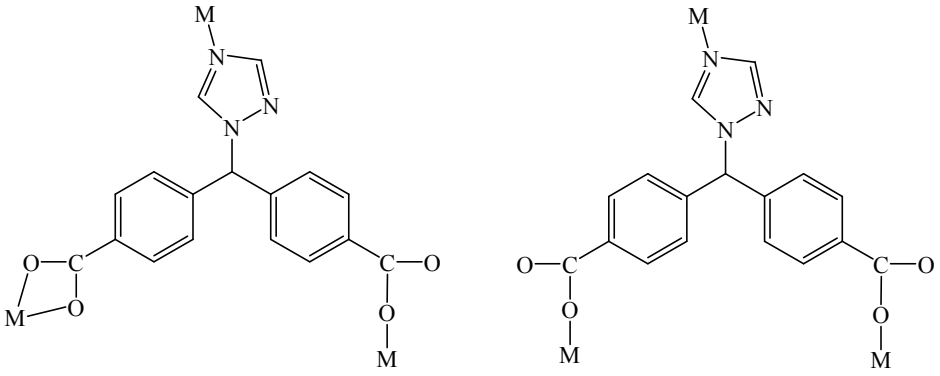
Table S1 Crystal and Structure Refinement Data for Compounds **1-3**

Compound	**1**	**2**	**3**
CCDC No.	1947245	1947250	1947261
Formula	$C_{17}H_{11}PbN_3O_5$	$C_{23}H_{15}ZnN_5O_4$	$C_{78}H_{69}N_{12}O_{21}Zn_3$
Fw	544.49	490.77	1706.56
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*C2/c*	$P2_1/c$	$P2_1/c$
a/Å	25.182(4)	10.8124(9)	11.3793(9)
b/Å	7.5625(11)	19.8774(17)	21.0931(17)
c/Å	21.189(3)	10.1244(9)	46.794(4)
α(°)	90.00	90.00	90.00
β(°)	114.029(2)	96.662(2)	92.07
γ(°)	90.00	90.00	90.00
V(Å^3)	3685.5(10)	2161.3(3)	11224.4(16)
Z	8	4	4
Dc(g cm^{-3})	1.963	1.508	1.010
μ/mm^{-1}	9.187	1.177	0.693
F(000)	2048.0	1000.0	3516.0
GOF on F^2	1.113	1.319	1.027
R_1/wR_2[$I>2\sigma(I)$]	0.0243, 0.0476	0.1078, 0.3175	0.1257, 0.3407
R_1/wR_2(all data)	0.0310, 0.0490	0.1427, 0.3415	0.2309, 0.3806

Table S2.Selected Bond Lengths (Å) and Angles (deg) for Compounds **1**-**3**

Compound (**1**)			
Pb(1)-O(1)#1	2.355(3)	Pb(1)-N(3)	2.568(3)
Pb(1)-O(3)#2	2.498(2)	O(1)-Pb(1)#1	2.355(2)
Pb(1)-O(4)#2	2.553(2)	O(4)-Pb(1)#3	2.553(2)
O(3)-Pb(1)#3	2.498(2)		
O(1)#1-Pb(1)-O(3)#2	79.04(9)	O(1)#1-Pb(1)-O(4)#2	81.14(10)
O(3)#2-Pb(1)-O(4)#2	51.75(8)	O(1)#1-Pb(1)-N(3)	75.38(9)
O(3)#2-Pb(1)-N(3)	78.33(9)	O(4)#2-Pb(1)-N(3)	128.01(9)
C(10)-N(3)-Pb(1)	127.4(2)	C(9)-N(3)-Pb(1)	125.2(2)
C(1)-O(1)-Pb(1)#1	102.3(2)	C(17)-O(4)-Pb(1)#3	91.9(2)
C(17)-O(3)-Pb(1)#3	94.3(2)		
Symmetry codes: #1 -x+1,-y,-z+1 #2 x,-y+1,z-1/2 #3 x,-y+1,z+1/2			
Compound (**2**)			
Zn(1)-O(2)#1	1.948(7)	Zn(1)-O(4)	1.984(9)
Zn(1)-N(4)	2.005(6)	Zn(1)-N(3)#2	2.029(7)
N(3)-Zn(1)#4	2.029(7)	O(2)-Zn(1)#1	1.948(7)
O(2)#1-Zn(1)-O(4)	106.8(3)	O(2)#1-Zn(1)-N(4)	102.5(3)
O(4)-Zn(1)-N(4)	119.5(3)	O(2)#1-Zn(1)-N(3)#2	115.8(4)
O(4)-Zn(1)-N(3)#2	106.6(4)	N(4)-Zn(1)-N(3)#2	106.1(3)
Symmetry codes: #1 -x,-y+1,-z #2 -x+1,y-1/2,-z+1/2 #3 -x,-y+1,-z+2 #4 -x+1,y+1/2,-z+1/2			
Compound (**3**)			
Zn(2)-O(5)	1.959(9)	Zn(2)-O(2)#1	1.970(10)
Zn(2)-N(4)	2.003(12)	Zn(2)-N(3)#2	2.026(12)
Zn(1)-O(10)	1.903(10)	Zn(1)-O(12)#3	1.951(10)
Zn(1)-N(12)#4	2.027(14)	Zn(1)-N(1)	2.060(13)
Zn(3)-O(8)#4	1.924(10)	Zn(3)-O(4)#5	1.928(9)
Zn(3)-N(9)	1.977(12)	Zn(3)-N(2)	2.011(11)
O(2)-Zn(2)#4	1.970(10)	O(12)-Zn(1)#6	1.951(10)
O(4)-Zn(3)#7	1.928(9)	N(3)-Zn(2)#8	2.026(12)
O(8)-Zn(3)#1	1.924(10)	N(12)-Zn(1)#1	2.027(14)
O(5)-Zn(2)-O(2)#1	105.5(4)	O(5)-Zn(2)-N(4)	110.5(5)
O(2)#1-Zn(2)-N(4)	122.0(4)	O(5)-Zn(2)-N(3)#2	100.3(5)
O(2)#1-Zn(2)-N(3)#2	106.6(5)	N(4)-Zn(2)-N(3)#2	109.6(5)
O(10)-Zn(1)-O(12)#3	103.9(4)	O(10)-Zn(1)-N(12)#4	115.8(4)
O(12)#3-Zn(1)-N(12)#4	120.7(6)	O(10)-Zn(1)-N(1)	105.9(5)
O(12)#3-Zn(1)-N(1)	102.9(5)	N(12)#4-Zn(1)-N(1)	106.0(5)
O(8)#4-Zn(03)-O(4)#5	108.4(4)	O(8)#4-Zn(03)-N(9)	112.7(4)
O(4)#5-Zn(03)-N(9)	115.4(5)	O(8)#4-Zn(03)-N(2)	114.2(5)
O(4)#5-Zn(03)-N(2)	96.6(5)	N(9)-Zn(03)-N(2)	108.7(5)

Symmetry codes:	#1 #1 x+1,y,z	#2 x,-y+1/2,z-1/2	#3 -x-1,y-1/2,-z+3/2
	#4 x-1,y,z	#5 x,y-1,z	#6 -x-1,y+1/2,-z+3/2
	#7 x,y+1,z	#8 x,-y+1/2,z+1/2	#9 -x-2,-y,-z+1



Scheme 1 Coordination pattern diagram of carboxylic acid ligand

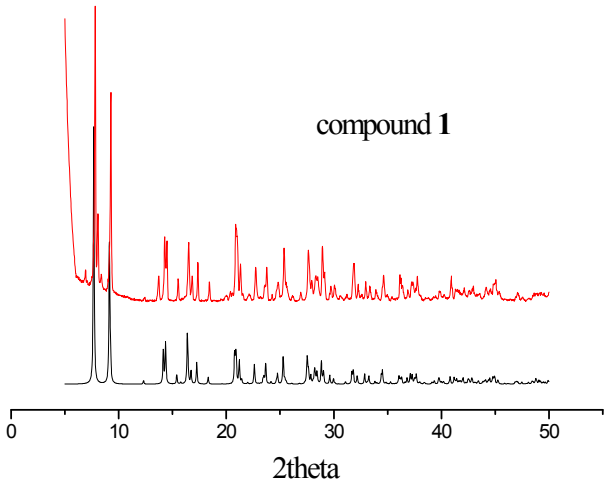


Figure S1. Simulated (a) and as-synthesized (b) powder X-ray diffraction patterns of **1**.

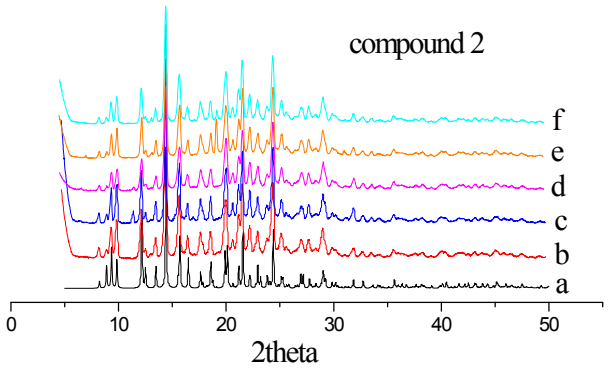


Figure S2. Simulated (a), as-synthesized (b), immersed in water after 2 days (c), immersed in PBS solution (0.1M, PH=11) after 2days (d), immersed in Fe^{3+} (0.01M) after 2 day (e) and after releasing test for MB (f) powder X-ray diffraction patterns of **2.**

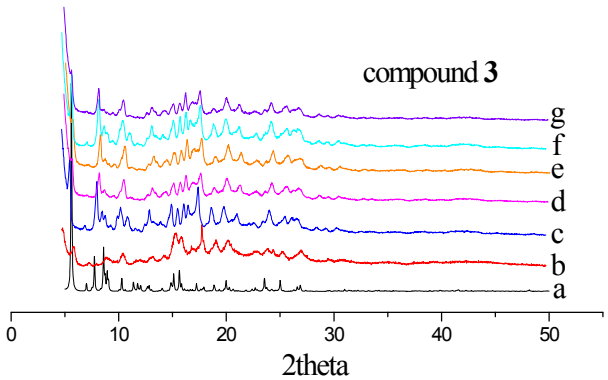


Figure S3. Simulated (a), as-synthesized (b), immersed in water after 2 days (c), immersed in PBS solution (0.1M, PH=11) after 2 days (d), immersed in Fe^{3+} (0.01M) after 2 day (e), after releasing test for MO (f) and vacuuming at 80°C for 6 hours (g) powder X-ray diffraction patterns of **3.**

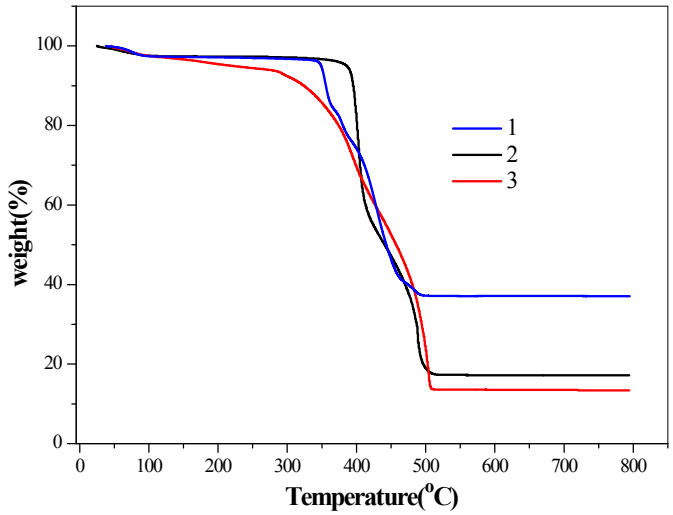


Figure S4 The TGA diagrams of compounds **1-3**.

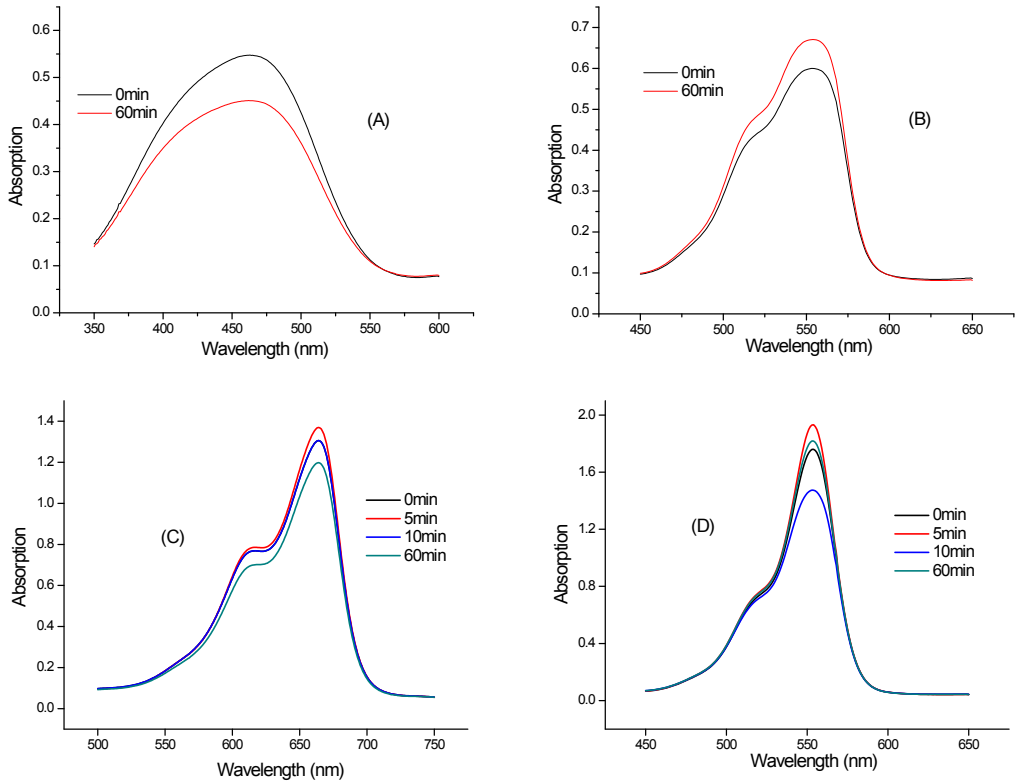


Figure S5 time-dependent UV-Vis spectra of MO (A) and RhB (B) in water solution in the presence of **2;** time-dependent UV-Vis spectra of MB (C) and RhB (D) in water solution in the presence of **3**

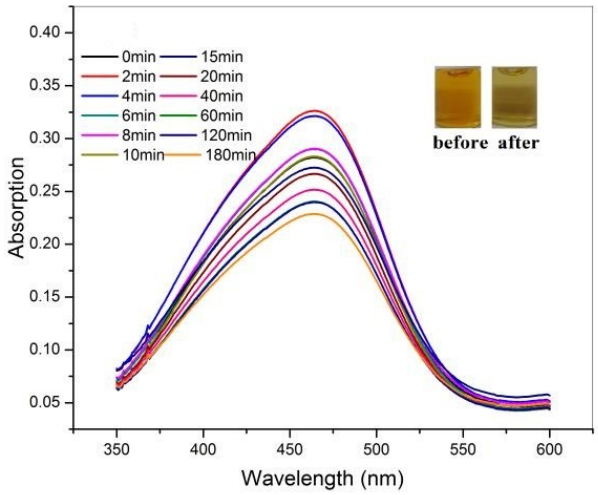


Figure S6 time-dependent UV-Vis spectra of MO in water solution in the presence of **3** (the inserted photographs show the color change before and after the dye degradation).

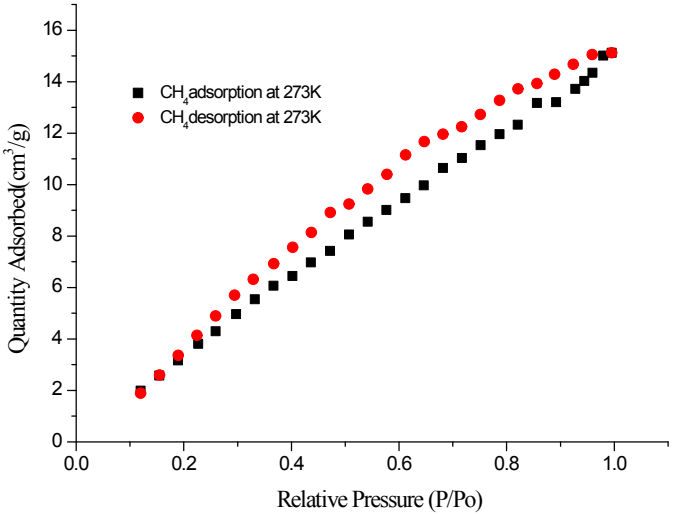


Figure S7 Adsorption isotherms for CH_4 at 273K of **3**.