Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Materials

Structure-directing roles of auxiliary carboxylate ligands in the formation of Zn(II) and Cd(II) coordination polymers based on a flexible *N,N'*-di(3-pyridyl)dodecanedioamide

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Table S1. Crystal data for complexes **1** – **5**

compound	**1**	**2**	**3**	**4**	**5**
formula	$C_{29}H_{35}N_5O_7Zn$	$C_{31}H_{38}N_4O_{10}Zn$	$C_{40}H_{48}N_7O_7Zn$	$C_{41}H_{49}CdN_6O_8$	$C_{42}H_{53}CdN_6O_{11}$
fw	630.99	692.02	804.22	866.26	930.30
crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic	Triclinic
space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$P\bar{1}$
a, Å	19.6517(17)	9.482(2)	7.7047(8)	11.9409(1)	9.7935(4)
b, Å	5.9639(5)	11.424(3)	8.9034(11)	8.7538(1)	12.1729(6)
c, Å	26.919(3)	15.607(4)	29.447(4)	38.6259(4)	18.9627(9)
α,°	90	89.33(2)	89.256(12)	90	78.802(3)
β,°	105.210(7)	81.068(13)	89.387(10)	95.216(1)	89.871(3)
γ,°	90	78.376(16)	71.385(10)	90	70.511(3)
V, Å^3	3044.4(5)	1635.5(7)	1914.1(4)	4020.78(7)	2085.76(17)
Z	4	2	2	4	2
D_{calc}, g/cm^3	1.377	1.405	1.395	1.431	1.481
F(000)	1320	724	846	1796	966
μ(Mo K_α), mm^{-1}	0.859	0.812	0.702	0.603	0.592
range(2θ) for data collection, deg	$4.30 \le 2\theta \le 50.00$	$5.28 \le 2\theta \le 58.20$	$4.16 \le 2\theta \le 50.00$	$3.50 \le 2\theta \le 56.58$	$3.62 \le 2\theta \le 56.68$
independent reflections	5321 [R(int) = 0.0787]	7509 [R(int) = 0.0355]	6701 [R(int) = 0.0357]	9987 [R(int) = 0.0963]	10282 [R(int) = 0.0547]
data / restraints / parameters	5321 / 0 / 396	7509/ 0 / 418	6701 / 0 / 496	9987 / 0 / 505	10282 / 0 / 561
quality–of–fit indicator [c]	1.051	1.013	1.044	1.002	1.050
final R indices [$I > 2\sigma(I)$] [a,b]	R1 = 0.0337, wR2 = 0.0815	R1 = 0.0405, wR2 = 0.0740	R1 = 0.0433, wR2 = 0.1110	R1 = 0.0529, wR2 = 0.0873	R1 = 0.0404, wR2 = 0.0783
R indices (all data)	R1 = 0.0480, wR2 = 0.0873	R1 = 0.0754, wR2 = 0.0773	R1 = 0.0533, wR2 = 0.1179	R1 = 0.1142, wR2 = 0.1027	R1 = 0.0599, wR2 = 0.0857

[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$. $w = 1 / [\sigma^2(F_o^2) + (ap)^2 + (bp)]$, $p = [\max(F_o^2 \text{ or } 0) + 2(F_c^2)] / 3$. a = 0.0393, b = 1.6958, **1**; a = 0.0255, b = 0.0000, **2**; a = 0.0577, b = 1.3771, **3**; a = 0.0359, b = 0.0000, **4**; a = 0.0346, b = 0.4081, **5**. [c] quality–of–fit = $[\Sigma w(|F_o^2| - |F_c^2|)^2 / (N_{observed} - N_{parameters})]^{1/2}$.

Table S2. Selected bond distances (Å) and angles (°) for **1 – 5**.

1			
Bond distances			
Zn-N(1)	2.150(2)	Zn-O(1)	2.154(2)
Zn-N(2)	2.102(2)	Zn-O(2A)	2.089(2)
Zn-N(5B)	2.165(2)	Zn-O(7)	2.136(2)
Bond angles			
N(1)-Zn-N(5B)	94.48(7)	N(1)-Zn-O(1)	76.16(6)
N(2)-Zn-N(1)	169.23(7)	N(2)-Zn-N(5B)	87.43(7)
N(2)-Zn-O(1)	93.12(6)	N(2)-Zn-O(7)	87.75(7)
O(1)-Zn-N(5B)	95.54(7)	O(2A)-Zn-N(1)	89.31(6)
O(2A)-Zn-N(2)	101.20(6)	O(2A)-Zn-N(5B)	92.60(8)
O(2A)-Zn-O(1)	163.83(6)	O(2A)-Zn-O(7)	85.22(7)
O(7)-Zn-N(1)	90.85(7)	O(7)-Zn-N(5B)	174.22(7)
O(7)-Zn-O(1)	87.90(7)		
2			
Bond distances			
Zn-N(1)	2.086(2)	Zn-O(3)	1.936(2)
Zn-N(4B)	2.036(2)	Zn-O(5A)	1.943(2)
Bond angles			
N(4B)-Zn-N(1)	95.53(9)	O(3)-Zn-N(1)	105.37(8)
O(3)-Zn-N(4B)	126.49(8)	O(3)-Zn-O(5A)	119.31(7)
O(5A)-Zn-N(1)	102.27(8)	O(5A)-Zn-N(4B)	102.73(7)
3			
Bond distances			
Zn-N(1)	2.042(2)	Zn-O(5B)	1.938(2)
Zn-N(7)	2.076(2)	Zn-O(6A)	1.924(2)
Bond angles			
N(1)-Zn-N(7)	96.73(9)	O(6A)-Zn-N(1)	101.71(9)
O(5B)-Zn-N(1)	121.43(11)	O(6A)-Zn-O(5B)	123.90(11)
O(5B)-Zn-N(7)	96.60(9)	O(6A)-Zn-N(7)	113.18(8)
4			
Bond distances			
Cd-N(1)	2.336(3)	Cd-N(4A)	2.300(3)
Cd-O(3)	2.336(2)	Cd-O(4)	2.523(2)
Cd-O(5B)	2.352(2)	Cd-O(6B)	2.455(2)
Cd-O(8)	2.383(2)		
Bond angles			

Table S2. Selected bond distances (Å) and angles (°) for **1 – 5**. (cont.)

N(1)-Cd-O(4)	88.92(9)	N(1)-Cd-O(5B)	90.27(9)
N(1)-Cd-O(6B)	90.94(10)	N(1)-Cd-O(8)	174.72(8)
N(4A)-Cd-N(1)	96.20(10)	N(4A)-Cd-O(3)	135.04(9)
N(4A)-Cd-O(4)	83.80(8)	N(4A)-Cd-O(5B)	138.01(8)
N(4A)-Cd-O(6B)	84.69(9)	N(4A)-Cd-O(8)	86.54(9)
O(3)-Cd-N(1)	96.04(9)	O(3)-Cd-O(4)	53.40(8)
O(3)-Cd-O(5B)	84.92(8)	O(3)-Cd-O(6B)	138.07(8)
O(3)-Cd-O(8)	78.88(8)	O(5B)-Cd-O(4)	137.93(7)
O(5B)-Cd-O(6B)	53.67(8)	O(5B)-Cd-O(8)	90.69(8)
O(6B)-Cd-O(4)	168.40(8)	O(8)-Cd-O(4)	86.89(8)
O(8)-Cd-O(6B)	93.81(9)		
5			
Bond distances			
Cd-N(1)	2.415(2)	Cd-N(5)	2.314(2)
Cd-O(4)	2.339(2)	Cd-O(5)	2.428(2)
Cd-O(5B)	2.479(2)	Cd-O(8A)	2.381(2)
Cd-O(9A)	2.359(2)		
Bond angles			
N(1)-Cd-O(5)	107.76(6)	N(1)-Cd-O(5B)	168.89(6)
N(5)-Cd-N(1)	85.60(7)	N(5)-Cd-O(4)	135.75(7)
N(5)-Cd-O(5)	89.00(7)	N(5)-Cd-O(5B)	83.89(6)
N(5)-Cd-O(8A)	143.14(7)	N(5)-Cd-O(9A)	91.21(7)
O(4)-Cd-N(1)	82.73(7)	O(4)-Cd-O(5)	55.08(6)
O(4)-Cd-O(5B)	107.39(6)	O(4)-Cd-O(8A)	81.11(6)
O(4)-Cd-O(9A)	128.66(6)	O(5)-Cd-O(5B)	75.68(6)
O(8A)-Cd-N(1)	102.86(7)	O(8A)-Cd-O(5)	120.93(6)
O(8A)-Cd-O(5B)	83.61(6)	O(9A)-Cd-N(1)	81.75(7)
O(9A)-Cd-O(5)	170.48(6)	O(9A)-Cd-O(5B)	94.88(6)
O(9A)-Cd-O(8A)	55.61(6)		

Symmetry transformations used to generate equivalent atoms:

(A) x,y-1,z; (B) -x+7/2,y-5/2,-z+5/2 for **1**; (A) x-1,y,z; (B) x-2,y,z for **2**; (A) -x+1,-y+1,-z; (B) x-1,y,z for **3**; (A) -x+2,-y-3,-z; (B) -x+1/2,y-1/2,-z+1/2 for **4**; (A) x-1,y,z; (B) -x+2,-y+1,-z-1 for **5**.

Table S3. Ligand conformations and corresponding angles for complexes **1** – **5**.

pound	Torsion angle (°)	Conformation	Dihedral angle (°)
1	175.8, 173.6, 178.5, 176.4, 176.9, 177.5, 175.8, 175.9, 174.4	AAAAAAAAA trans	76.1
2	-174.0, 170.9, -170.6, 171.0, 76.4, -175.0, -170.1, -167.3, -163.1	AAAAGAAAA trans	86.4
3	-177.1, -177.8, 179.3, -179.8, 179.6, -179.2, 179.2, -177.4, -179.2	AAAAAAAAA trans	14.2
	178.8, 176.9, 179.5, 179.2, -180.0, -179.2, 179.5, -176.9, -178.8	AAAAAAAAA trans	0
4	178.4, 177.7, -178.8, -177.2, 178.7, -176.4, -177.7, 176.0, 176.3	AAAAAAAAA trans	63.1
	-178.5, 177.0, 178.4, 179.5, 180.0, -179.5, -178.4, -177.0, 178.5	AAAAAAAAA trans	0
5	176.6, 176.4, 178.8, 176.9, -179.1, -178.6, -168.7, -65.1, -173.5	AAAAAAAGA trans	77.1
	166.8, 179.4, -172.9, -60.3, -180.0, 60.3, 172.9, -179.4, -166.8	AAAGAGAAA trans	0

Figure S1. TGA curves for complexes **1** – **5**.

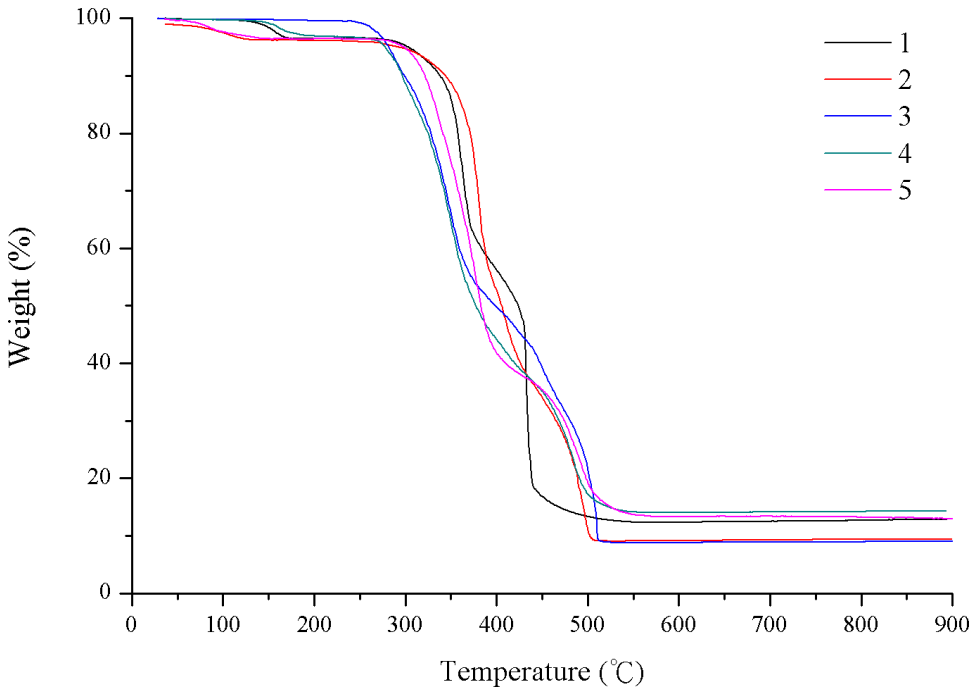

Figure S2. The PXRD patterns of (a) simulated single-crystal X-ray data of compound **1**, (b) bulk materials as synthesized for compound **1**.

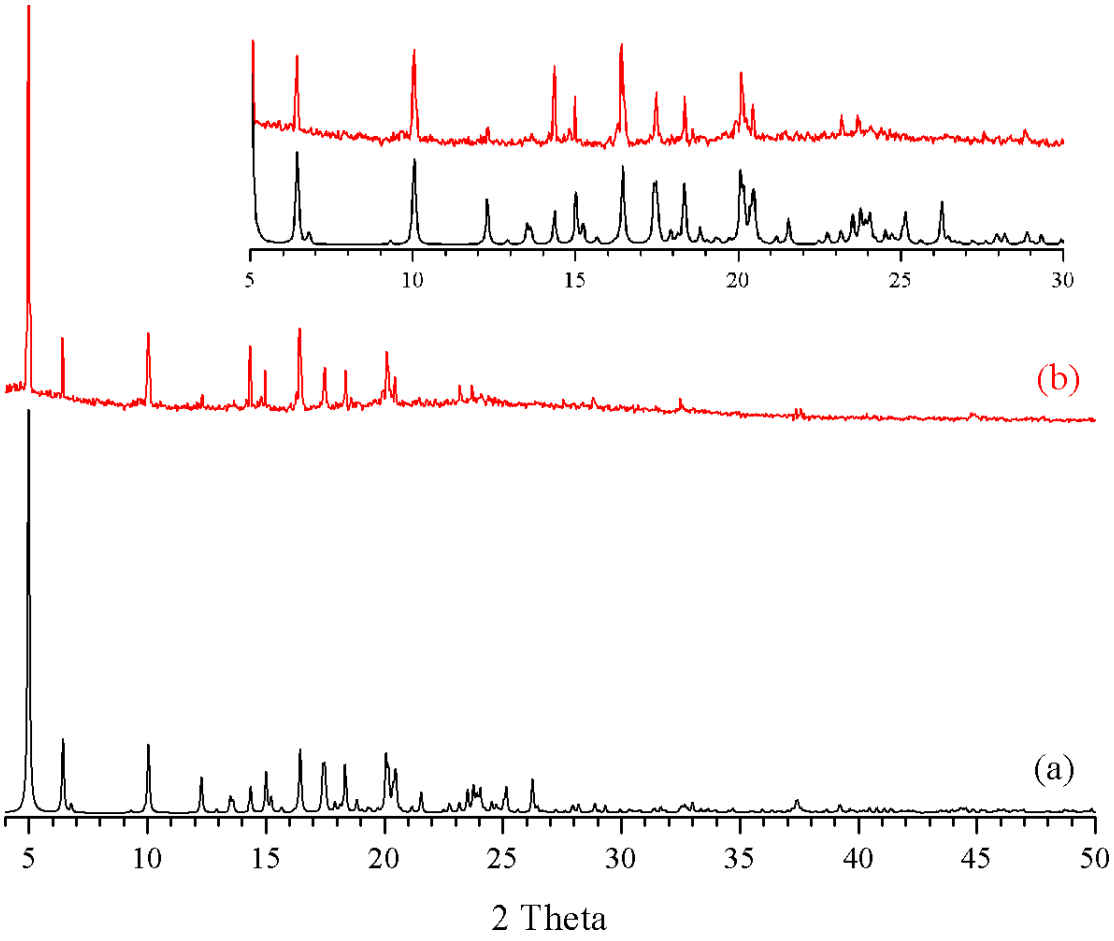

Figure S3. The PXRD patterns of (a) simulated single-crystal X-ray data of compound **2**, (b) bulk materials as synthesized for compound **2**.

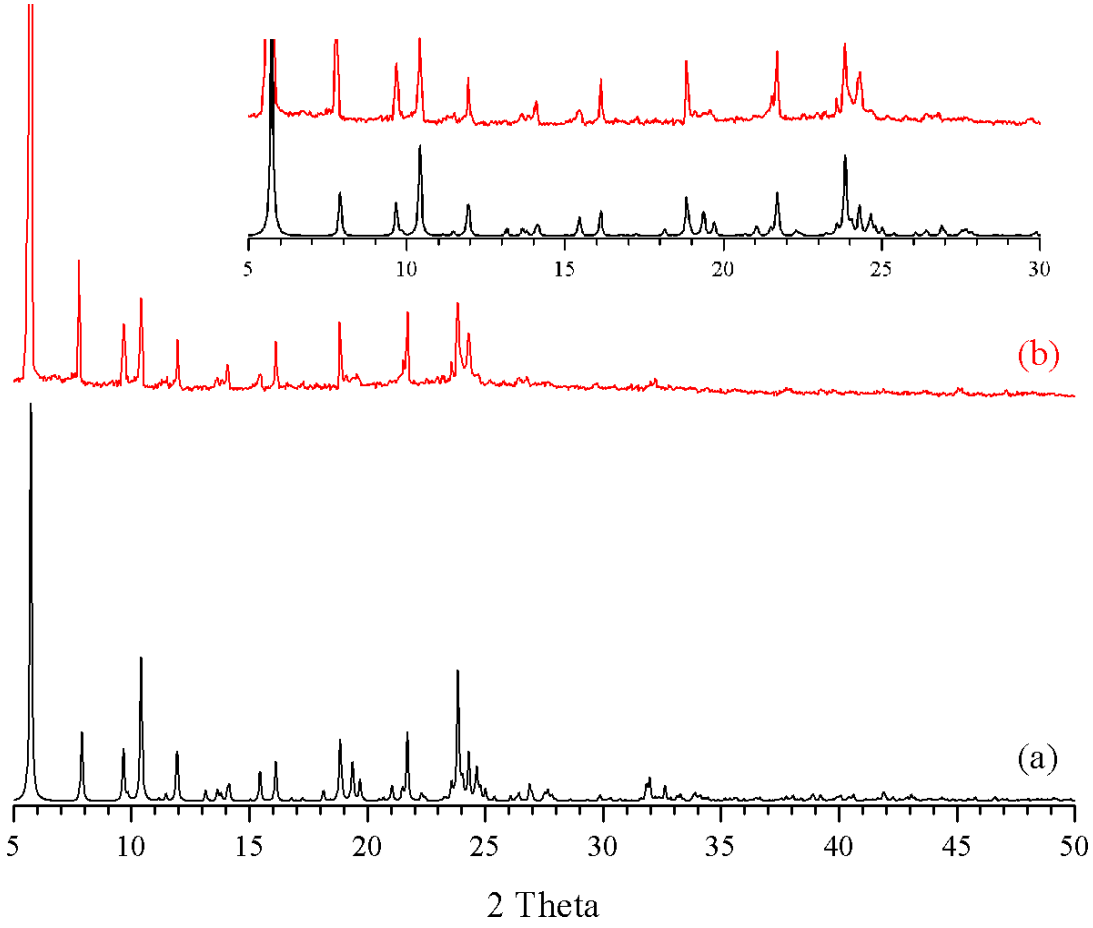

Figure S4. The PXRD patterns of (a) simulated single-crystal X-ray data of compound **3**, (b) bulk materials as synthesized for compound **3**.

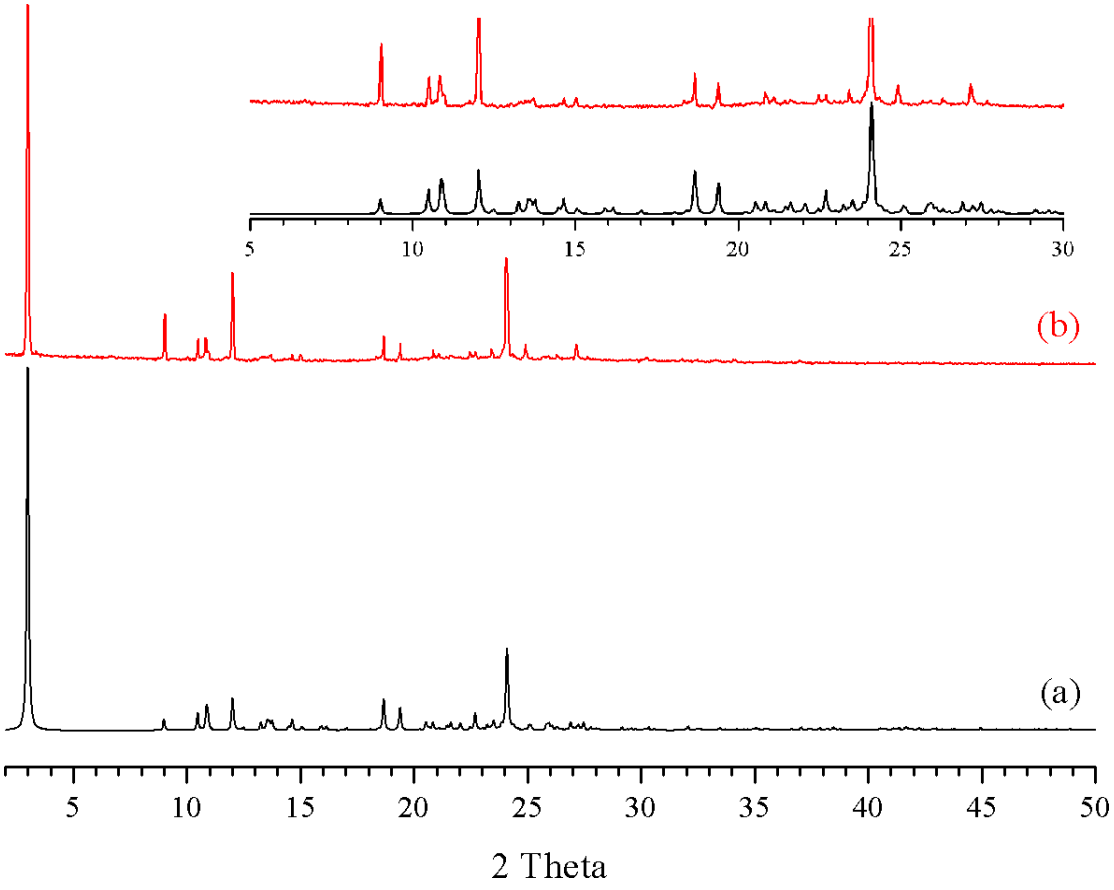

Figure S5. The PXRD patterns of (a) simulated single-crystal X-ray data of compound **4**, (b) bulk materials as synthesized for compound **4**.

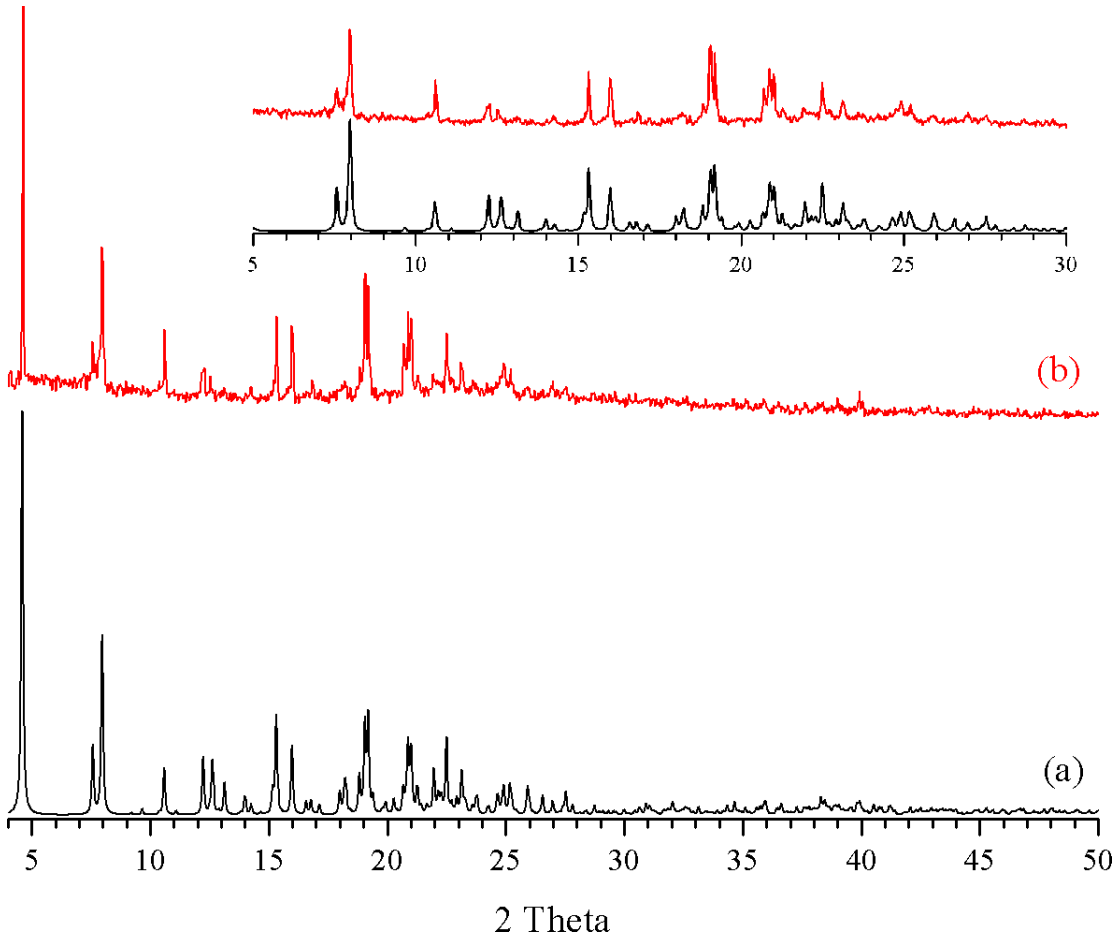

Figure S6. The PXRD patterns of (a) simulated single-crystal X-ray data of compound **5**, (b) bulk materials as synthesized for compound **5**.