Electronic Supplementary Material (ESI) for Dalton Transactions

Temperature-/Solvent-Dependent Low-dimensional Compounds Based on Quinoline-2,3-dicarboxylic Acid: Structures and Fluorescent Properties

Ming-Fang Wang,[a] Xu-Jia Hong,[a] Qing-Guang Zhan,[a] Yi-Ting Liu,[a] Hong-Guang Jin,[a] Zhi-Peng Zheng,[a] Shi-Hai Xu[b] and Yue-Peng Cai,*[a]

[a]*School of Chemistry and Environment, South China Normal University; Key Laboratory of the energy conversion and energy storage materials,, Guangzhou 510006, P. R. China. Fax: 86-020-39310; Tel: 86-020-39310383; E-mail: caiyp@scnu.edu.cn*

[b]*Department of Chemistry, Jinan University, Guangzhou 510632. E-mail: txush@jnu.edu.cn*

Contents

Table **S1**

	1	**2**	**3**	**4**
Chemical formula	$C_{22}H_{16}N_2O_{10}Co$	$C_{20}H_{12}N_2O_4Co$	$C_{26}H_{24}N_2O_{10}Co$	$C_{22}H_{16}N_2O_{10}Zn$
M	527.30	403.25	583.40	533.76
Crystal system	Triclinic	Monoclinic	Monoclinic	Triclinic
Space group	*P*-1	*C*2/*c*	*P*2(1)/*c*	*P*-1
a /Å	7.3968(14)	28.867(4)	13.090(5)	7.4062(17)
b /Å	9.1349(18)	8.0358(12)	7.694(3)	9.136(2)
c /Å	9.410(3)	15.211(2)	12.632(5)	9.415(3)
α /°	110.547(4)	90	90	110.466(4)
β /°	98.240(4)	114.151(2)	97.422(6)	98.320(4)
γ/°	111.630(2)	90	90	111.664(3)
V/Å^3	525.6(2)	3219.7(8)	1261.6(8)	526.6(2)
Z	1	8	2	1
T /*K*	298(2)	298(2)	298(2)	298(2)
F(000)	269	1640	602	272
D_{calcd} / g cm^{-3}	1.666	1.664	1.536	1.683
μ /mm^{-1}	0.882	1.097	0.743	1.232
λ /Å	0.71073	0.71073	0.71073	0.71073
R_{int}	0.0410	0.0436	0.0792	0.0250
data/restraint/parm	2735/0/161	2890 / 0 / 244	2270 / 0 / 183	1861 / 3 / 165
GOF	1.062	1.041	1.011	1.044
R_1 [$I = 2\sigma(I)$][a]	0.0645	0.0388	0.0571	0.0544
wR_2 [$I = 2\sigma(I)$][b]	0.1143	0.0827	0.0985	0.1362

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

	5	**6**	**8**	**9**
Chemical formula	$C_{20}H_{12}N_2O_4Zn$	$C_{26}H_{24}N_2O_{10}Zn$	$C_{20}H_{12}N_2O_4Cd$	$C_{12}H_8NO_4ClCd$
M	409.69	589.84	456.72	378.04
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*C*2/*c*	*P*2(1)/*c*	*C*2/*c*	*C*2/*c*
a /Å	29.004(9)	12.984(8)	28.777(8)	15.433(9)
b /Å	8.040(3)	7.731(5)	8.059(2)	18.004(10)
c /Å	15.251(5)	12.571(8)	15.281(4)	9.215(5)
α /°	90	90	90	90
β /°	114.337(4)	97.320(7)	114.007(4)	91.158(8)
γ/°	90	90	90	90
V/Å^3	3240.3(18)	1251.7(13)	3237.4(15)	2560(2)
Z	8	2	8	8
T /*K*	298 (2)	298(2)	298(2)	298(2)
F(000)	1664	608	1808	1472
D_{calcd} / g cm^{-3}	1.680	1.565	1.874	1.962
μ /mm^{-1}	1.547	1.045	1.381	1.922
λ /Å	0.71073	0.71073	0.71073	0.71073
R_{int}	0.0872	0.0705	0.0646	0.1551
data/restraint/parm	2921 / 0 / 244	2248 / 0 / 163	2918 / 24 / 244	2312 / 0 / 174
GOF	1.043	1.093	1.062	0.953
R_1 $[I = 2\sigma(I)]^a$	0.0555	0.0677	0.0657	0.0788
wR_2 $[I = 2\sigma(I)]^b$	0.1109	0.1368	0.1512	0.1047

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

Table **S2**. Bond lengths (Å) and angles (°) for complexes **1**-**6** and **8**-**9**

Complex **1**			
Co(1)-O(2)#1	2.027(3)	Co(1)-O(3)#1	2.093(3)
Co(1)-O(2)	2.027(3)	Co(1)-N(1)#1	2.228(4)
Co(1)-O(3)	2.093(3)	Co(1)-N(1)	2.228(4)
O(2)#1-Co(1)-O(2)	180.00(14)	O(3)-Co(1)-N(1)#1	88.96(14)
O(2)#1-Co(1)-O(3)	90.32(14)	O(3)#1-Co(1)-N(1)#1	91.04(14)
O(2)-Co(1)-O(3)	89.68(14)	O(2)#1-Co(1)-N(1)	105.35(14)
O(2)#1-Co(1)-O(3)#1	89.68(14)	O(2)-Co(1)-N(1)	74.65(14)
O(2)-Co(1)-O(3)#1	90.32(14)	O(3)-Co(1)-N(1)	91.04(14)
O(2)#1-Co(1)-N(1)#1	74.65(14)	O(3)#1-Co(1)-N(1)	88.96(14)
O(2)-Co(1)-N(1)#1	105.35(14)		
Complex **2**			
Co(1)-O(3)	1.936(2)	O(3)-Co(1)-N(1)	101.08(10)
Co(1)-O(2)#2	1.977(2)	O(2)#2-Co(1)-N(1)	100.07(9)
Co(1)-N(1)	2.085(2)	O(3)-Co(1)-N(2)#3	108.68(10)
Co(1)-N(2)#3	2.103(2)	O(2)#2-Co(1)-N(2)#3	100.19(9)
O(3)-Co(1)-O(2)#2	139.90(10)	N(1)-Co(1)-N(2)#3	100.91(9)
Complex **3**			
Co(1)-O(1)#4	2.008(3)	Co(1)-O(3)	2.125(4)
Co(1)-O(1)	2.008(3)	Co(1)-N(1)	2.218(4)
Co(1)-O(3)#4	2.125(4)	Co(1)-N(1)#4	2.218(4)
O(1)#4-Co(1)-O(1)	180.0	O(3)#4-Co(1)-N(1)	91.62(14)
O(1)#4-Co(1)-O(3)#4	89.00(16)	O(3)-Co(1)-N(1)	88.38(14)
O(1)-Co(1)-O(3)#4	91.00(16)	O(1)#4-Co(1)-N(1)#4	79.01(13)
O(1)#4-Co(1)-O(3)	91.00(16)	O(1)-Co(1)-N(1)#4	100.99(13)
O(1)-Co(1)-O(3)	89.00(16)	O(3)#4-Co(1)-N(1)#4	88.38(14)
O(1)#4-Co(1)-N(1)	100.99(13)	O(3)-Co(1)-N(1)#4	91.62(14)
O(1)-Co(1)-N(1)	79.01(13)	O(3)#4-Co(1)-N(1)	91.62(14)
Complex **4**			
Zn(1)-O(2)#1	2.031(3)	Zn(1)-O(3)	2.093(3)

Zn(1)-O(2)	2.031(3)	Zn(1)-N(1)#1	2.221(3)
Zn(1)-O(3)#1	2.093(3)	Zn(1)-N(1)	2.221(3)
O(2)#1-Zn(1)-O(3)#1	89.76(14)	O(3)#1-Zn(1)-N(1)#1	90.74(13)
O(2)-Zn(1)-O(3)#1	90.24(14)	O(3)-Zn(1)-N(1)#1	89.26(13)
O(2)#1-Zn(1)-O(3)	90.24(14)	O(2)#1-Zn(1)-N(1)	104.76(13)
O(2)-Zn(1)-O(3)	89.76(14)	O(2)-Zn(1)-N(1)	75.24(13)
O(3)#1-Zn(1)-O(3)	180.00(9)	O(3)#1-Zn(1)-N(1)	89.26(13)
O(2)#1-Zn(1)-N(1)#1	75.24(13)	O(3)-Zn(1)-N(1)	90.74(13)
O(2)-Zn(1)-N(1)#1	104.76(13)		
Complex **5**			
Zn(1)-O(2)#2	1.920(4)	Zn(1)-N(2)	2.101(4)
Zn(1)-O(4)#3	1.958(4)	Zn(1)-N(1)	2.103(4)
O(2)#2-Zn(1)-O(4)#3	138.55(18)	O(2)#2-Zn(1)-N(1)	110.13(17)
O(2)#2-Zn(1)-N(2)	100.16(17)	O(4)#3-Zn(1)-N(1)	100.53(17)
O(4)#3-Zn(1)-N(2)	100.54(17)	N(2)-Zn(1)-N(1)	101.11(18)
Complex **6**			
N(1)-Zn(1)	2.171(2)	Zn(1)-O(3)#4	2.101(3)
Zn(1)-O(1)#4	2.000(3)	Zn(1)-O(3)	2.101(3)
Zn(1)-O(1)	2.000(3)	Zn(1)-N(1)#4	2.171(2)
O(1)#4-Zn(1)-N(1)	99.69(9)	O(3)#4-Zn(1)-N(1)	91.72(10)
O(1)-Zn(1)-N(1)	80.31(9)	O(3)-Zn(1)-N(1)	88.28(10)
O(1)-Zn(1)-O(3)#4	91.74(13)	O(1)-Zn(1)-N(1)#4	99.69(16)
O(1)#4-Zn(1)-O(3)	91.74(13)	O(3)#4-Zn(1)-N(1)#4	88.28(19)
O(1)-Zn(1)-O(3)	88.26(13)	O(3)-Zn(1)-N(1)#4	91.72(19)
Complex **8**			
Cd(1)-O(4)#2	1.939(7)	N(2)-Cd(1)-O(2)#3	91.1(3)
Cd(1)-O(1)#3	1.992(7)	N(1)-Cd(1)-O(2)#3	153.9(3)
Cd(1)-N(2)	2.136(7)	O(4)#2-Cd(1)-C(3)#3	122.6(3)
Cd(1)-N(1)	2.153(7)	O(1)#3-Cd(1)-C(3)#3	29.0(3)
Cd(1)-O(2)#3	2.582(7)	N(2)-Cd(1)-C(3)#3	94.9(3)
N(2)-Cd(1)-N(1)	99.4(3)	N(1)-Cd(1)-C(13)#2	95.8(3)

O(4)#2-Cd(1)-O(2)#3	99.4(3)	O(2)#3-Cd(1)-C(13)#2	94.0(3)
O(1)#3-Cd(1)-O(2)#3	56.1(3)	N(2)-Cd(1)-O(2)#3	91.1(3)
		Complex **9**	
Cd(1)-O(4)	2.300(11)	Cd(1)-O(4)#5	2.472(11)
Cd(1)-O(3)#5	2.373(11)	Cd(1)-Cl(1)	2.519(4)
Cd(1)-N(1)	2.395(8)	Cd(1)-Cl(1)#6	2.581(4)
O(4)-Cd(1)-O(3)#5	98.8(4)	O(3)#5-Cd(1)-Cl(1)#6	88.9(3)
O(4)-Cd(1)-N(1)	72.2(4)	N(1)-Cd(1)-Cl(1)#6	164.3(4)
O(3)#5-Cd(1)-N(1)	87.6(3)	O(4)#5-Cd(1)-Cl(1)#6	96.0(3)
O(4)-Cd(1)-O(4)#5	151.2(5)	Cl(1)-Cd(1)-Cl(1)#6	91.08(14)
O(3)#5-Cd(1)-O(4)#5	54.2(4)	O(4)-Cd(1)-C(7)#5	126.0(5)
N(1)-Cd(1)-O(4)#5	94.4(4)	O(3)#5-Cd(1)-C(7)#5	27.7(4)
O(4)-Cd(1)-Cl(1)	106.0(3)	N(1)-Cd(1)-C(7)#5	91.5(4)
O(3)#5-Cd(1)-Cl(1)	155.1(3)	O(4)#5-Cd(1)-C(7)#5	26.5(4)
N(1)-Cd(1)-Cl(1)	98.5(2)	Cl(1)-Cd(1)-C(7)#5	127.5(5)
O(4)#5-Cd(1)-Cl(1)	101.1(3)	Cl(1)#6-Cd(1)-C(7)#5	92.6(4)
O(4)-Cd(1)-Cl(1)#6	93.3(3)		

*Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1; #2 x,-y+1,z+1/2; #3 x,y-1,z; #4 -x+1,-y+1,-z+1; #5 x,-y,z-1/2; #6 -x,-y,-z+1.

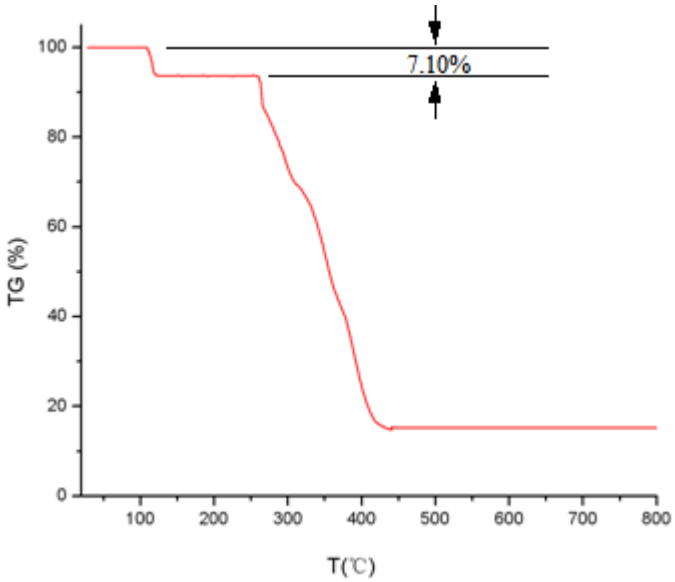
Table **S3** Distances (Å) and angles (°) of hydrogen bonds for compounds **1**-**6** and **8**-**9**.

D-H···A	d(H···A)	d(D···A)	∠D-H···A
		1	
O3-H3B···O4#1	1.871	2.777(5)	164.7(5)
O3-H3B···O5#2	2.032	2.735(5)	131.2(4)
O4-H4···O1	1.564	2.383(5)	175.4(6)
C10-H10···O2	2.274	3.071(5)	143.5(5)
		3	
O3-H3···O2#3	2.041(6)	2.708(5)	168.1(7)
C11-H11···O1	2.254(5)	3.115(6)	153.7(6)
		4	
O3-H3B···O4#1	1.868	2.773(5)	164.7(5)
O3-H3B···O5#2	2.030	2.732(5)	131.2(4)
O4-H4···O1	1.548	2.380(5)	175.4(6)
C10-H10···O2	2.269	3.063(5)	143.0(5)
		6	
O3-H3···O2#3	1.982(5)	2.710(4)	134.4(5)
C11-H11···O1	2.189(5)	3.041(5)	151.9(5)

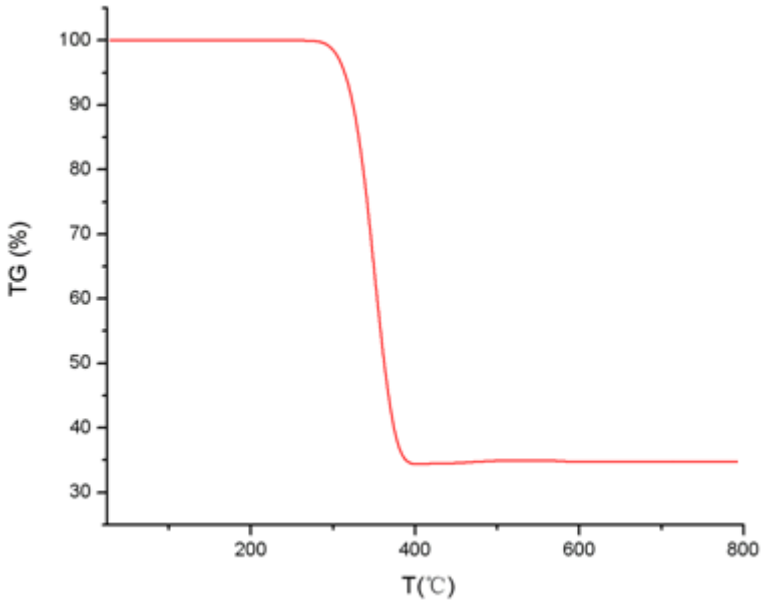
*Symmetry transformation used to generate equivalent atoms: #1 –x+1,-y+1,-z+1; #2 x-1,y-1,z; #3 -x+1,y+1/2,-z+1/2.

Figure S1. The thermal analyses (N2) of the crystalline **1-3** and **9** (TG curves).

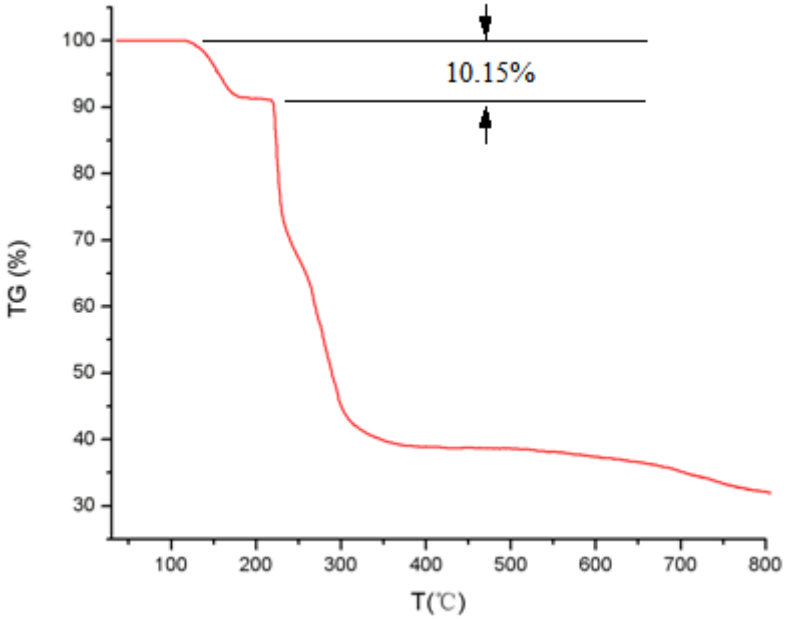
(a) Complex **1**



(b) Complex **2**



(c) Complex **3**



(d) Complex **9**

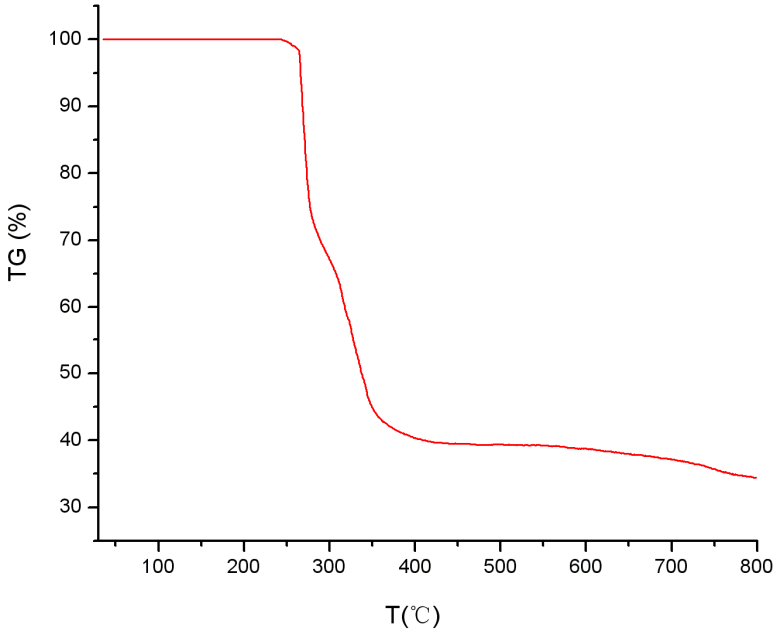
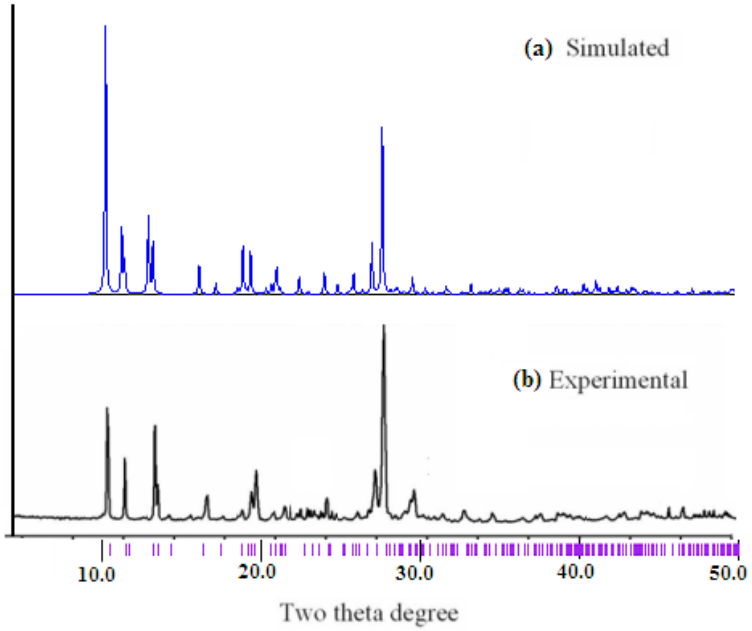
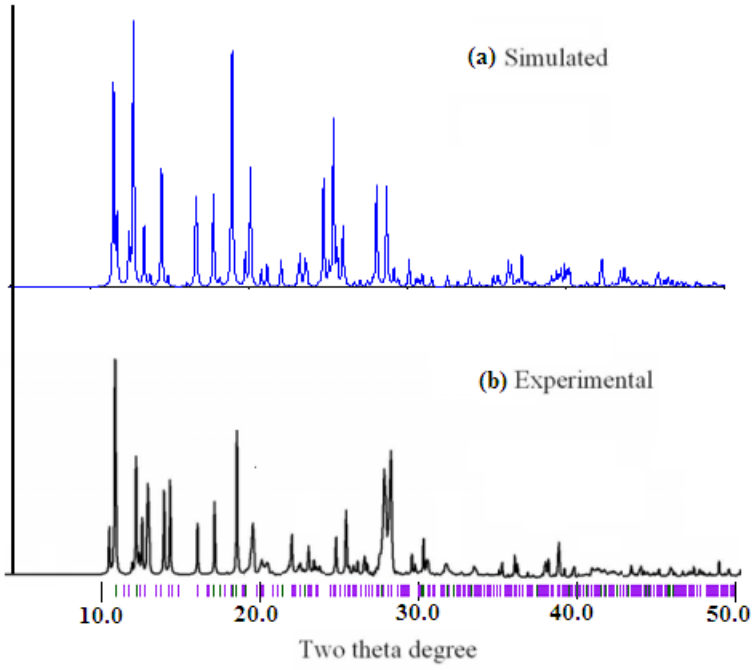


Figure **S2** X-ray powder diffraction patterns of simulated (***a***) and as prepared complex (***b***) for compounds **1**, **2**, **3** and **9**.

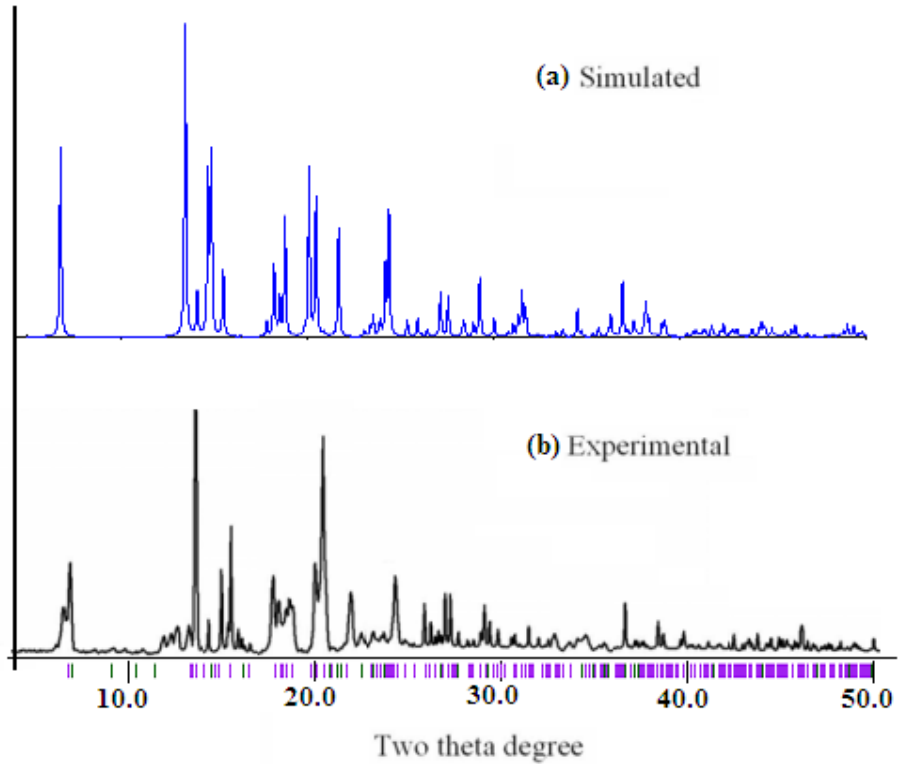
(1) for **1**.



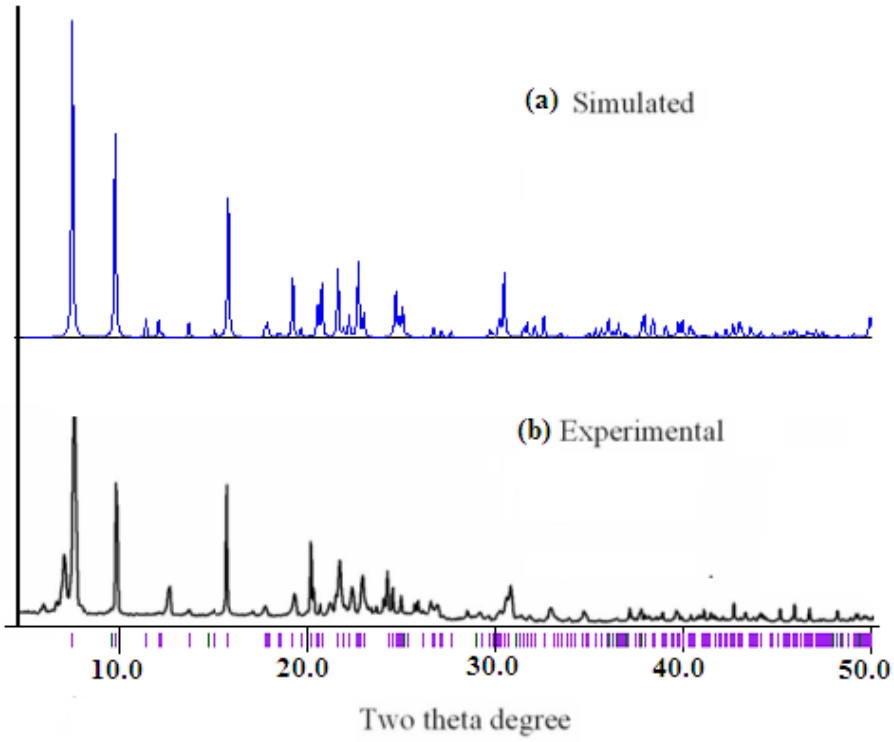
(2) for **2**



(3) for **3**


(a) Simulated
(b) Experimental
10.0
20.0
30.0
40.0
50.0
Two theta degree

(4) for **9**


(a) Simulated
(b) Experimental
10.0
20.0
30.0
40.0
50.0
Two theta degree