Supplementary Material (ESI) for CrystEngComm

Supporting Information for

Four Novel Metal Coordination Polymers Directed By 1, 1′-dibutyl-4, 4′-bipyridinium dibromide (BBP) and Their Framework Dependent Luminescent Properties

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Table S1. Selected bond distances(Å) and angles(°)for compound **1-4**

Compound **1**					
Ag(1)-I(1)	2.9093(4)	Ag(1) #1-I(1)	2.9263(4))	Ag(1)-I(2)	2.8111(4)
Ag(1)-I(3)	2.7837(4)				
I(1)-Ag(1)-I(1) #1	82.401(11)	I(3)-Ag(1)-I(2)	114.307(13)	I(3)-Ag(1)-I(1)	111.798(12)
I(2)-Ag(1)-I(1)	113.125(12)	I(3)-Ag(1)-I(1) #1	111.274(13)	I(2)-Ag(1)-I(1) #1	107.408(12)
I(1)-Ag(1)-I(1) #1	97.599(11)				
Compound **2**					
Pb(1)-I(3)	3.0463(13)	Pb(1)-I(2)	3.0639(12)	Pb(1)-I(1)	3.1714(12)
Pb(1)-I(6)	3.3524(12)	Pb(1)-I(5)	3.3525(14)	Pb(1)-I(4)	3.4043(12)
Pb(2)-I(8)	3.0016(14)	Pb(2)-I(6)	3.1017(12)	Pb(2)-I(7)	3.1456(12)
Pb(2)-I(10)#1	3.3140(12)	Pb(2)-I(9)	3.3292(12)	Pb(2)-I(5)	3.3726(13)
Pb(3)-I(11)	3.0903(12)	Pb(3)-I(5)	3.1491(13)	Pb(3)-I(4)	3.1635(11)
Pb(3)-I(9)#1	3.2115(12)	Pb(3)-I(10)	3.2733(13)	Pb(3)-I(9)	3.3054(12)
I(9)-Pb(3)#1	3.2113(12)	I(10)-Pb(2)#1	3.3141(12)	I(3)-Pb(1)-I(2)	94.80(4)
I(3)-Pb(1)-I(1)	90.27(4)	I(2)-Pb(1)-I(1)	101.28(4)	I(3)-Pb(1)-I(6)	87.35(3)
I(2)-Pb(1)-I(6)	90.42(3)	I(1)-Pb(1)-I(6)	168.22(3)	I(3)-Pb(1)-I(5)	96.81(4)

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I(2)-Pb(1)-I(5)	165.37(4)	I(1)-Pb(1)-I(5)	87.55(3)	I(6)-Pb(1)-I(5)	81.28(3)
I(3)-Pb(1)-I(4)	176.53(4)	I(2)-Pb(1)-I(4)	85.76(3)	I(1)-Pb(1)-I(4)	92.98(3)
I(6)-Pb(1)-I(4)	89.22(3)	I(5)-Pb(1)-I(4)	82.13(3)	I(8)-Pb(2)-I(6)	96.09(4)
I(8)-Pb(2)-I(7)	95.51(4)	I(6)-Pb(2)-I(7)	96.31(3)	I(8)-Pb(2)-I(10)#1	92.22(4)
I(6)-Pb(2)-I(10)#1	167.06(3)	I(7)-Pb(2)-I(10)#1	92.74(3)	I(8)-Pb(2)-I(9)	91.26(3)
I(6)-Pb(2)-I(9)	86.14(3)	I(7)-Pb(2)-I(9)	172.51(3)	I(10)#1-Pb(2)-I(9)	83.78(3)
I(8)-Pb(2)-I(5)	168.23(4)	I(6)-Pb(2)-I(5)	84.72(3)	I(7)-Pb(2)-I(5)	96.08(3)
I(10)#1-Pb(2)-I(5)	85.13(3)	I(9)-Pb(2)-I(5)	77.06(3)	I(11)-Pb(3)-I(5)	90.95(3)
I(11)-Pb(3)-I(4)	99.86(3)	I(5)-Pb(3)-I(4)	89.36(3)	I(11)-Pb(3)-I(9)#1	87.40(3)
I(5)-Pb(3)-I(9)#1	95.67(3)	I(4)-Pb(3)-I(9)#1	171.12(3)	I(11)-Pb(3)-I(10)	98.56(4)
I(5)-Pb(3)-I(10)	170.37(4)	I(4)-Pb(3)-I(10)	87.54(3)	I(9)#1-Pb(3)-I(10)	86.31(3)
I(11)-Pb(3)-I(9)	168.44(3)	I(5)-Pb(3)-I(9)	80.56(3)	I(4)-Pb(3)-I(9)	87.96(3)
I(9)#1-Pb(3)-I(9)	85.67(3)	I(10)-Pb(3)-I(9)	90.21(3)		
		Compound **3**			
Cu(1)-N(2)	1.990(2)	Cu(1)-N(1)	1.997(2)	Cu(1)-S(2)#1	2.3786(8)
Cu(1)-S(1)#2	2.4206(9)				
N(2)-Cu(1)-N(1)	115.09(10)	N(2)-Cu(1)-S(2)#1	117.85(7)	N(1)-Cu(1)-S(2)#1	102.37(7)
N(2)-Cu(1)-S(1)#2	101.01(6)	N(1)-Cu(1)-S(1)#2	112.14(8)	S(2)#1-Cu(1)-S(1)#2	108.57(3)
		Compound **4**			
Cu(1)-N(3)	1.9337(16)	Cu(1)-N(2)	1.9738(15)	Cu(1)-S(1)	2.4068(5)
Cu(1)-S(3)	2.4803(5)	Cu(1)-Cu(2)	2.9565(3)	Cu(2)-N(4)	2.0041(15)
Cu(2)-S(2)	2.3251(5)	Cu(2)-S(3)	2.3735(5)	Cu(2)-S(1)	2.4543(5)
N(3)-Cu(1)- N(2)	124.40(7)	N(3)-Cu(1)-S(1)	114.32(5)	N(2)-Cu(1)-S(1)	102.39(5)
N(3)-Cu(1)-S(3)	106.53(5)	N(2)-Cu(1)-S(3)	102.93(5)	S(1)-Cu(1) –S(3)	104.125(17)
N(3)-Cu(1)-Cu(2)	124.35(5)	N(2)-Cu(1)-Cu(2)	110.90(5)	S(1)-Cu(1)-Cu(2)	53.275(13)
S(3)-Cu(1)-Cu(2)	50.850(12)	N(4)-Cu(2)-S(2)	112.38(5)	N(4)-Cu(2)-S(3)	103.95(5)
S(2)-Cu(2)-S(3)	122.050(18)	N(4)-Cu(2)-S(1)	104.60(5)	S(2)-Cu(2)-S(1)	106.524(17)
S(3)-Cu(2)-S(1)	105.950(17)	N(4)-Cu(2)-Cu(1)	114.19(4)	S(2)-Cu(2)-Cu(1)	132.320(15)
S(3)-Cu(2)-Cu(1)	54.135(13)	S(1)-Cu(2)-Cu(1)	51.815(12)	C(10)-S(1)-Cu(1)	97.07(6)
C(10)-S(1)-Cu(2)	94.69(6)	Cu(1)-S(1)-Cu(2)	74.911(15)	C(11)-S(2)-Cu(2)	93.23(6)
C(12)-S(3)-Cu(2)	95.39(6)	C(12)-S(3)-Cu(1)	95.48(6)	Cu(2)-S(3)-Cu(1)	75.015(15)

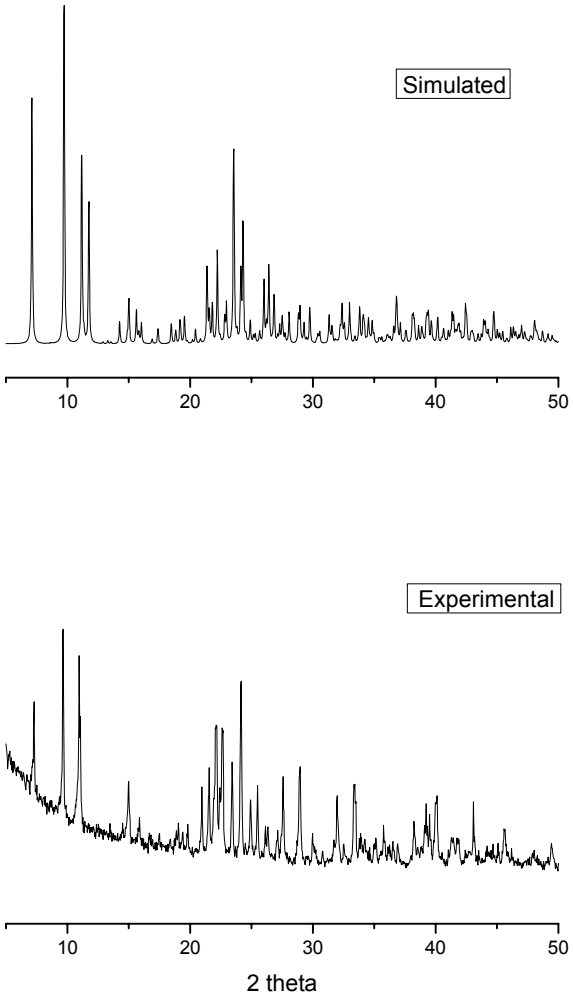
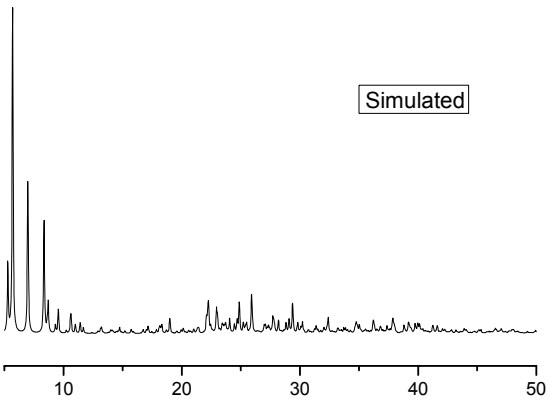


Fig. S1 Simulated and experimental PXRD pattern of compound **1.**



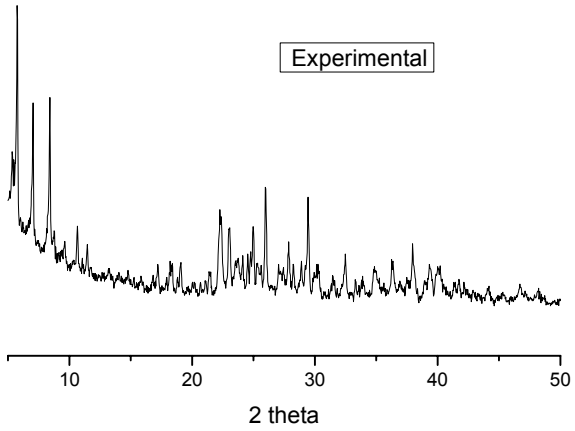


Fig. S2 Simulated and experimental PXRD pattern of compound **2.**

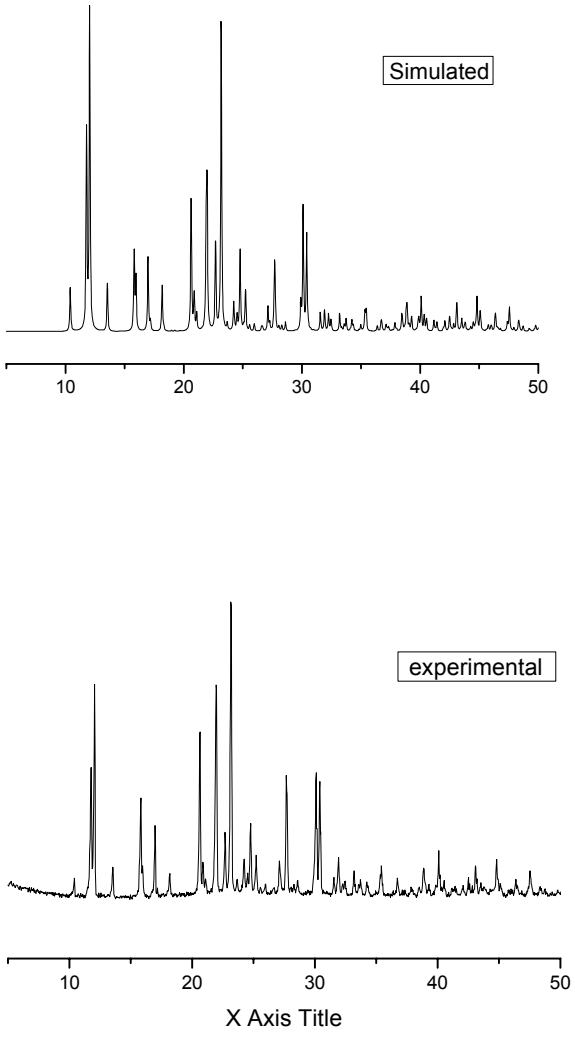


Fig. S3 Simulated and experimental PXRD pattern of compound **3**

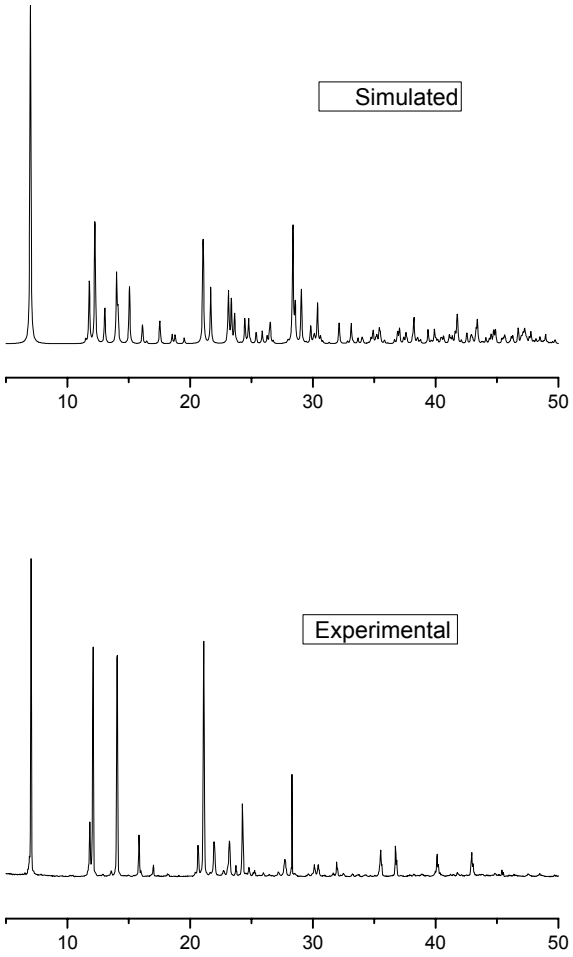


Fig. S4 Simulated and experimental PXRD pattern of compound **4.**

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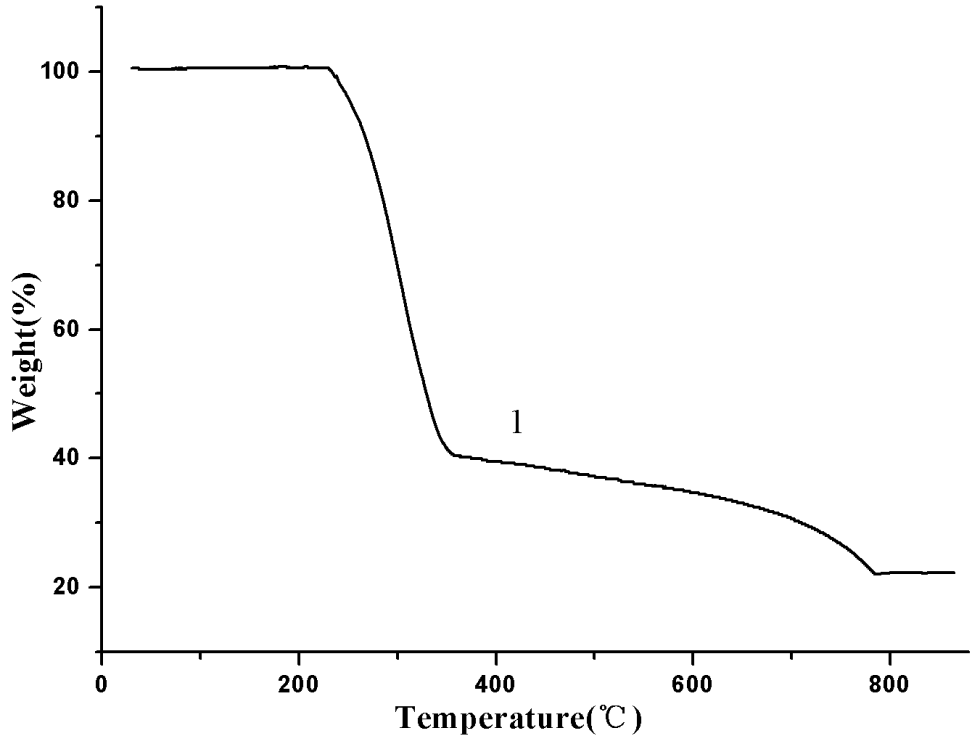

Fig. S5 TGA curves of **1**

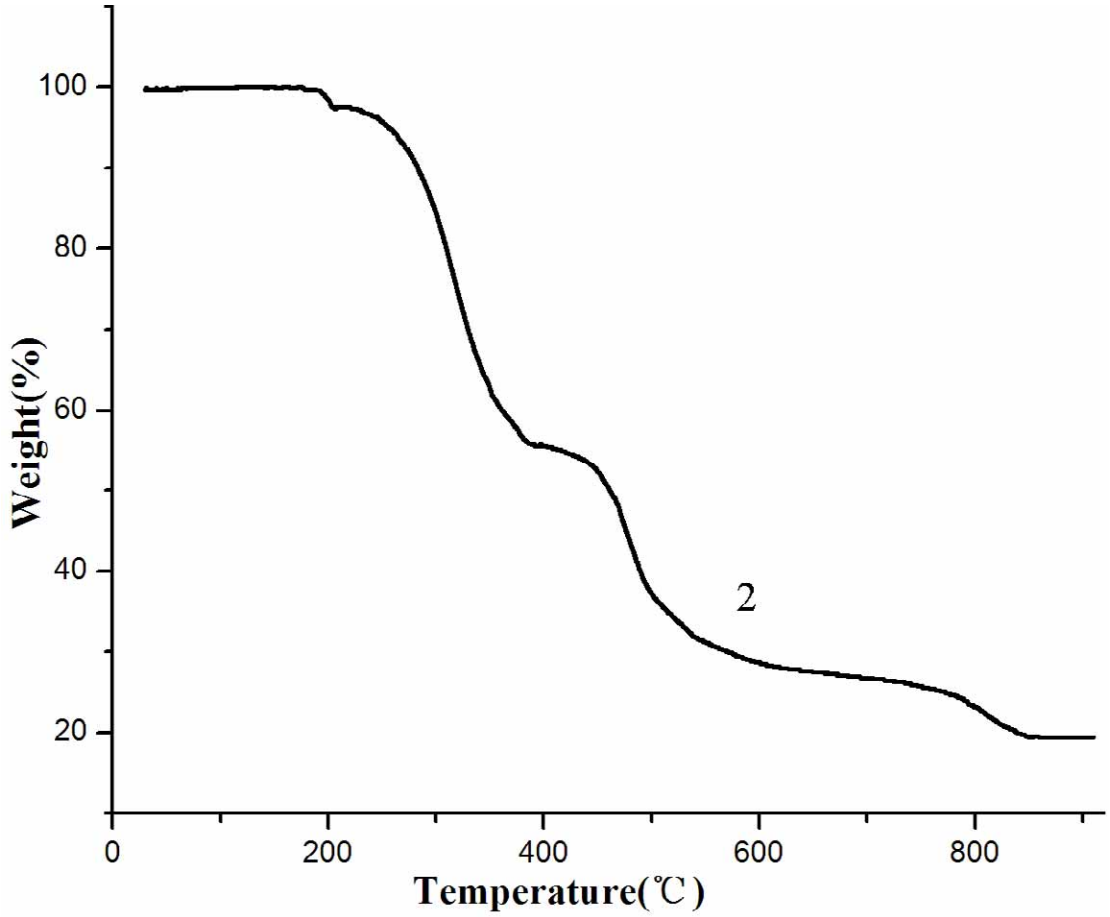

Fig. S6 TGA curves of **2**

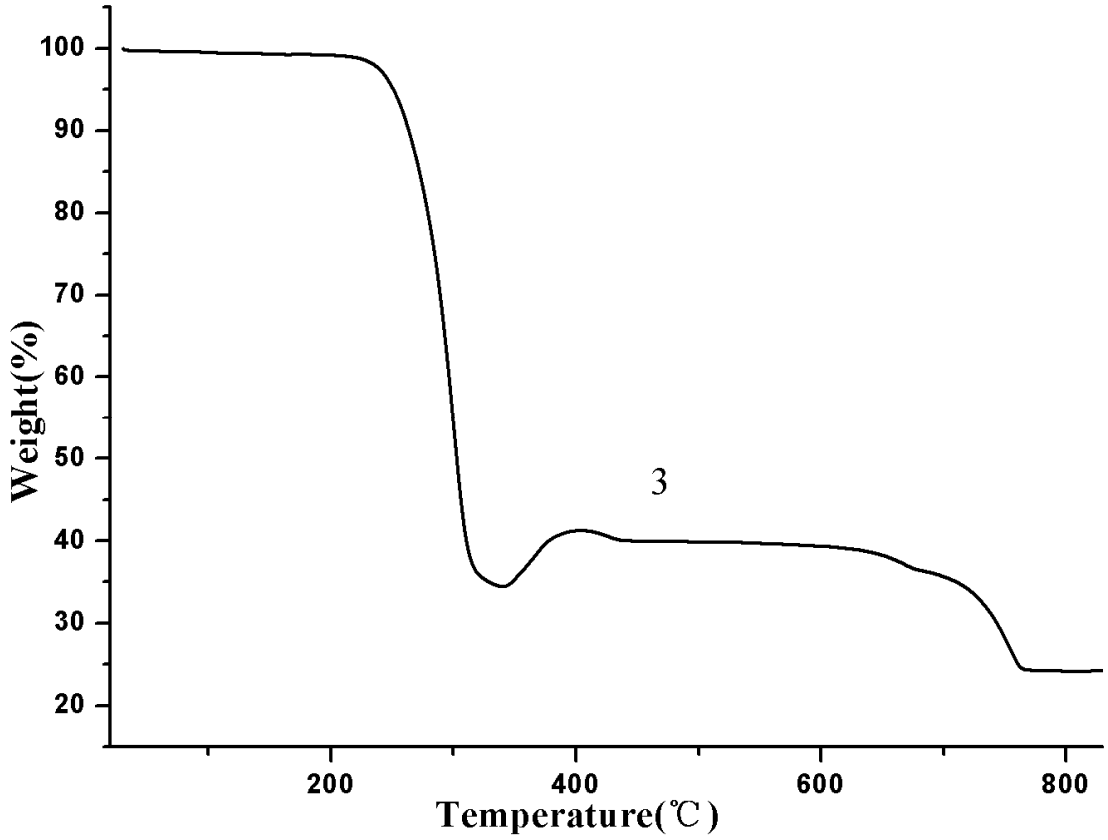

Fig. S7 TGA curves of **3**

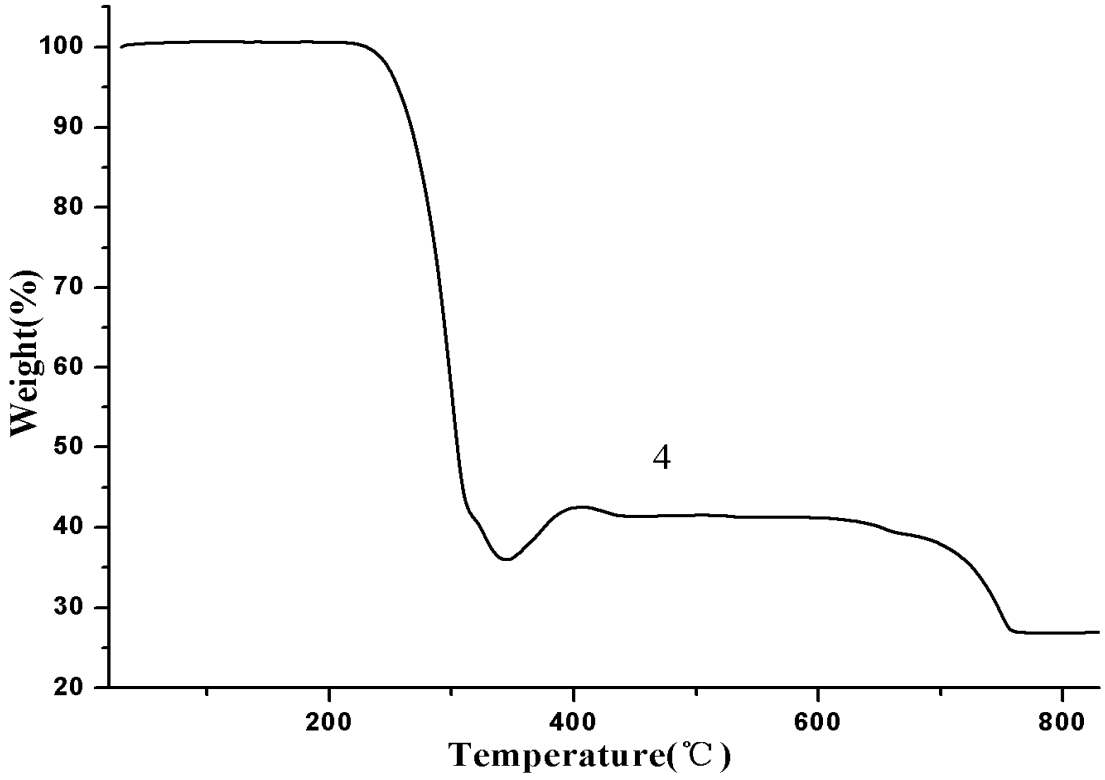

Fig. S8 TGA curves of **4**