Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary materials

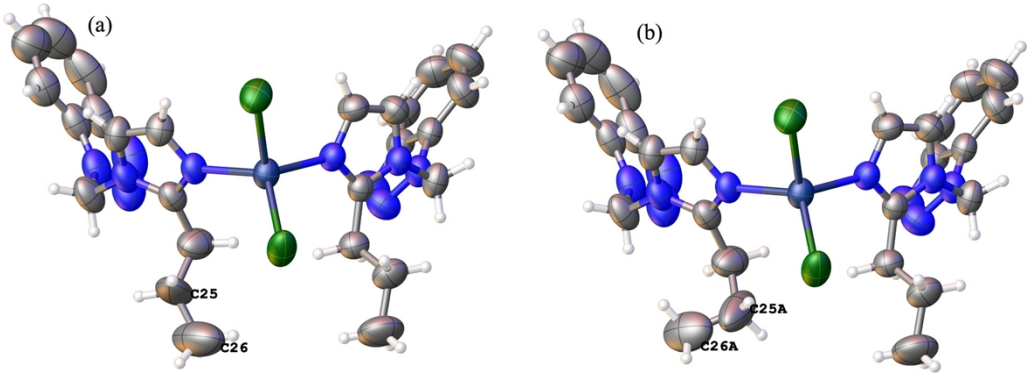


Fig. S1 Showing **1** exhibits the disorder in the terminal group of the bpmi ligand.

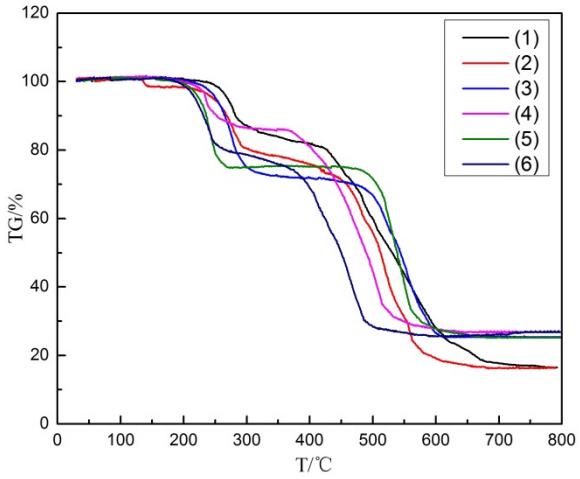


Fig. S2. The thermogravimetric analyses for complexes **1–6**.

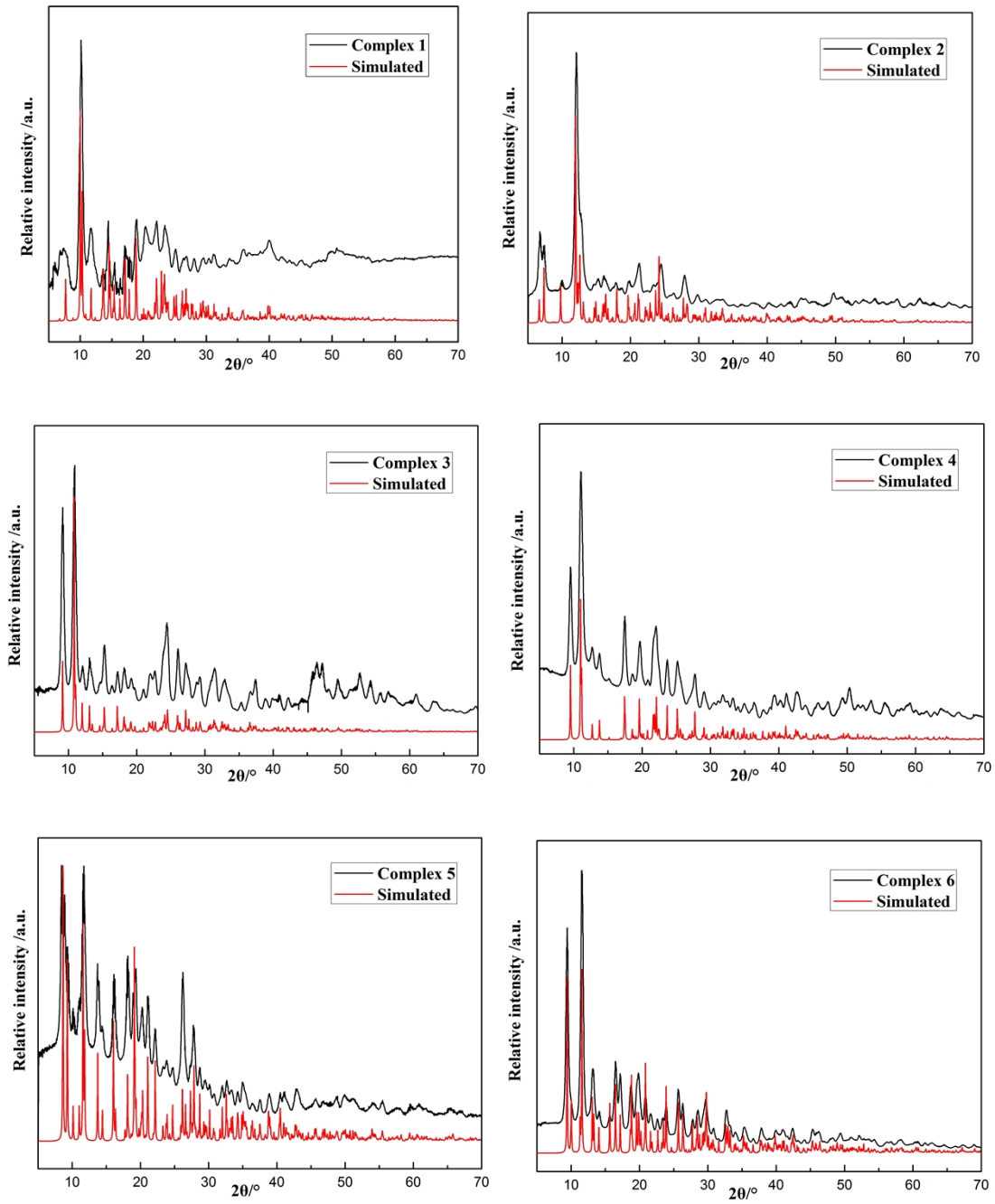
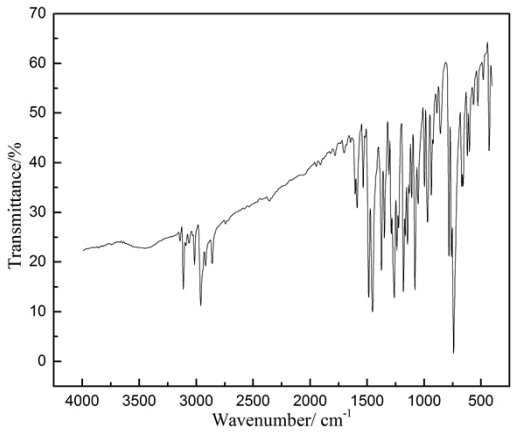
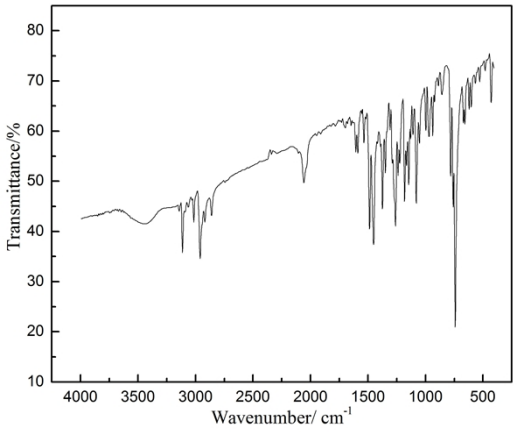


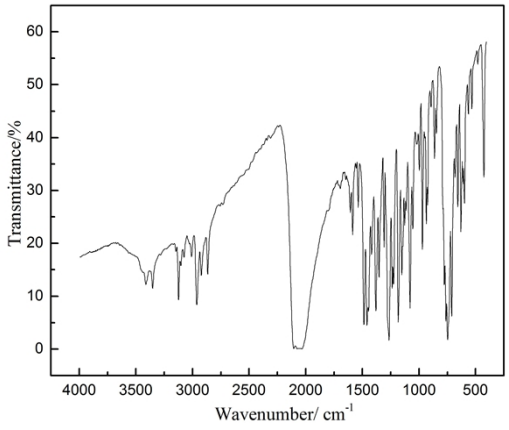
Fig. S3. Experimental (black) and simulative (red) powder x-ray diffraction patterns for complexes **1-6**.



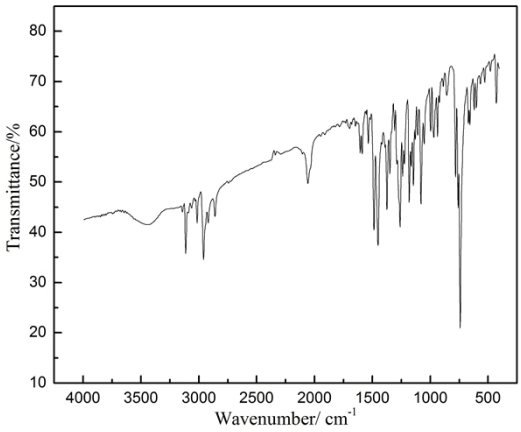
(**1**)



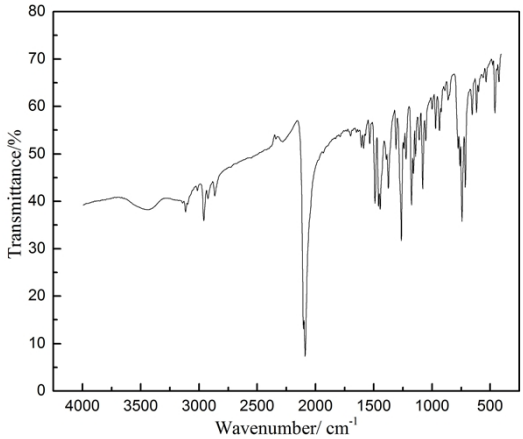
(**2**)



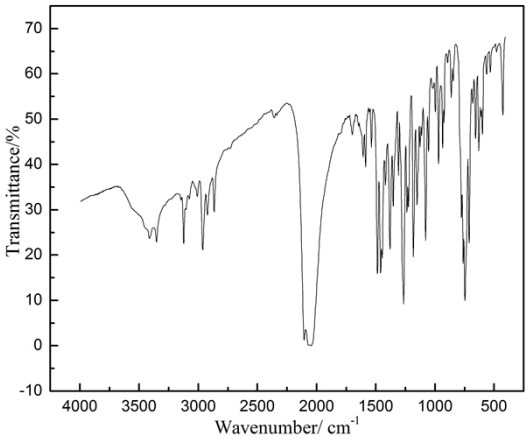
(**3**)



(**4**)



(**5**)



(**6**)

Fig. S4. The IR spectrum for complexes (**1**)-(**6**)

Table S1. Selected Bond Lengths [Å] and Angles [°] for Complexes (**1**)–(**6**)

(**1**)	Cd–N5	2.2234(1)	Cd–N10	2.2321(1)
	Cd–Cl1	2.4319(1)	Cd–Cl2	2.4013(1)
	N5– Cd–N10	107.668(2)	N5– Cd– Cl1	105.406(3)
	N10– Cd– Cl1	99.335(2)	N10– Cd– Cl2	119.692(2)
	Cl1– Cd– Cl2	111.197(2)		
(**2**)	Cd–O1	2.4994(1)	Cd –O3	2.4235(1)
	Cd –O4	2.4453(1)	Cd –O5	2.5248(1)
	Cd1–N7^{i}	2.2971(1)	Cd –N3	2.3427(1)
	Cd –N8	2.2800(1)		
	O1– Cd –O3	51.751(1)	O1– Cd –O4	130.418(1)
	O1– Cd –O5	170.303(2)	O1– Cd –N3	84.292(1)
	O1– Cd –N8	89.072(1)	O1– Cd –N7^{i}	91.012(1)
	O3– Cd –O4	79.546(1)	O3– Cd –O5	129.995(2)
	O3– Cd –N3	88.344(1)	O3– Cd –N8	140.752(2)
	O3– Cd –N7^{i}	81.685(1)	O4– Cd –O5	50.497(1)
	O4– Cd –N3	85.786(1)	O4– Cd –N8	139.414(2)
	O4– Cd –N7^{i}	90.459(1)	O5– Cd –N3	86.215(1)
	O5– Cd –N8	88.967(1)	O5– Cd –N7^{i}	98.674(1)
	N3– Cd –N8	90.086(2)	N3– Cd –N7^{i}	169.839(2)
	N8– Cd –N7^{i}	98.863(1)		
	Symmetry transformation used to generate equivalent atoms: (i) x, 2–y, 0.5+z			
(**3**)	Cd1–N11	2.3731(0)	Cd1–N14	2.3478(0)
	Cd1–O^{i}	2.4607(0)	Cd1–Cl4^{i}	2.5112(0)
	Cd2–N1	2.3542(0)	Cd2–N10	2.2953(0)
	Cd2–N11	2.3554(0)	Cd2–N14	2.3500(0)
	Cd2–O2	2.4281(0)	Cd2–Cl1	2.5586(0)
	O1^{i}–Cd1–Cl4^{i}	168.987(0)	O1^{i}–Cd1–N11	80.873(0)
	O1^{i}–Cd1–N14	79.112(0)	N11– Cd1–N14	78.791(0)
	N11– Cd1–Cl4	89.178(0)	N14–Cd1–Cl4	94.402(0)
	O2–Cd2–Cl1	168.566(0)	O2–Cd2–N1	90.200(0)
	O2–Cd2–N10	88.061(0)	O2–Cd2–N11	79.750(0)
	O2–Cd2–N14	81.117(0)	N1–Cd2– Cl1	97.054(0)
	N1–Cd2–N10	93.466(0)	N1–Cd2–N11	166.618(0)
	N1–Cd2–N14	90.702(0)	N10–Cd2– Cl1	100.255(0)
	N10–Cd2– N11	94.988(0)	N10–Cd2– N14	168.418(0)
	N11– Cd2–Cl1	91.631(0)	N11– Cd2–N14	79.104(0)
	N14– Cd2–Cl1	89.935(0)		

Symmetry transformation used to generate equivalent atoms: (i) 1+x, y, z

(**4**)	Cd –N1	2.3817(1)	Cd –N5^{i}	2.2857(1)
	Cd –Cl1	2.4751(1)	Cd –Cl2	2.5711(1)
	Cd –Cl2^{ii}	2.6146(1)		
	N1– Cd – N5^{i}	164.951(1)	N1– Cd – Cl1	90.579(1)
	N1– Cd – Cl2	87.975(1)	N1– Cd – Cl2^{ii}	79.361(1)
	N5^{i}– Cd – Cl1	103.626(1)	N5^{i}– Cd – Cl2	92.175(1)
	N5^{i}– Cd – Cl2^{ii}	88.902(1)	Cl1– Cd – Cl2	108.236(1)
	Cl1– Cd – Cl2^{ii}	121.158(1)	Cl2– Cd – Cl2^{ii}	128.796(1)

Symmetry transformation used to generate equivalent atoms: (i) 1+x,1.5–y,0.5+z; (ii) x, 1.5–y, –0.5+z;

(**5**)	Cd –N1	2.3492(1)	Cd –N5^{i}	2.3761(1)
	Cd –N6^{ii}	2.2915(1)	Cd –N7^{iii}	2.2804(1)
	Cd –S1	2.7174(1)	Cd –S2	2.7863(1)
	N1– Cd –N5^{i}	90.112(2)	N1– Cd –N6^{ii}	86.074(2)
	N1– Cd –N7 ^{iii}	97.740(2)	N1– Cd –S1	91.213(2)
	N1– Cd –S2	171.466(1)	N5^{i}– Cd –N6^{ii}	174.947(3)
	N5^{i}– Cd –N7 ^{iii}	90.664(3)	N5^{i}– Cd –S1	83.400(2)
	N5^{i}– Cd –S2	91.392(1)	N6^{ii}– Cd –N7 ^{iii}	93.132(3)
	N6^{ii}– Cd –S1	93.356(3)	N6^{ii}– Cd –S2	91.900(2)
	N7 ^{iii} – Cd –S1	169.279(3)	N7 ^{iii} – Cd –S2	90.643(2)
	S1– Cd –S2	80.621(1)		

Symmetry transformation used to generate equivalent atoms: (i) 2–x, 1–y,1–z; (ii) 1–x, 1–y, –z; (iii) 1–x, –y, –z

(**6**)	Cd –N1^{i}	2.3499(3)	Cd –N5	2.3705(2)
	Cd –N6	2.3784(3)	Cd –N8^{ii}	2.3733(4)
	Cd –N9	2.3175(3)	Cd –N11	2.3359(2)
	N1^{i}– Cd – N5	93.307(6)	N1^{i}– Cd – N6	86.384(5)
	N1^{i}– Cd – N8^{ii}	170.415(7)	N1^{i}– Cd – N9	98.804(7)
	N1^{i}– Cd – N11	89.000(6)	N5– Cd – N6	95.510(6)
	N5– Cd – N8^{ii}	88.845(6)	N5– Cd – N9	86.446(6)
	N5– Cd – N11	174.685(7)	N6– Cd – N8^{ii}	84.112(6)
	N6– Cd – N9	174.359(7)	N6– Cd – N11	89.410(6)
	N8^{ii}– Cd – N9	90.647(5)	N8^{ii}– Cd – N11	89.663(5)
	N9– Cd – N11	88.471(6)		

Symmetry transformation used to generate equivalent atoms: (i) 1–x,1–y, 1–z; (ii) –x, –

Table S2. Selected hydrogen bonds lengths [Å] and angles [°] for compounds (**1**) and (**3**).

(**1**)	D–H···A	*d*(D–H)/Å	*d*(H···A)/Å	*d*(D···A)/Å	∠DHA
	C7–H7A···Cl1	0.97001(1)	2.4246(1)	3.3248(2)	129.292(3)
	C21–H21···Cl2	0.93001(1)	2.8505(1)	3.6402(1)	143.477(4)
(**3**)	C7–H7A···Cl^{i}	0.9701(0)	2.5456(0)	3.4951(0)	166.141(1)
	C7–H7B··· Cl4^{ii}	0.9700(0)	2.6259(0)	3.4438(0)	142.175(1)
		(ii)2-x, 0.5+y, 1.5-z; (iii) 1-x, 1-y, 1-z.			