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Electronic supplementary information (ESI)

Sorption and sensing properties of coordination polymers with mixed 1,3,5-tri(1-imidazolyl)benzene and 2,6-naphthalenedicarboxylate ligands

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Table S1 Selected bond lengths (Å) and angles (deg) for complexes **1**-**5**.

Compound **1**			
Cd(1)-N(1)	2.2854(17)	Cd(1)-O(1)	2.411(4)
Cd(1)-N(3)#2	2.2872(18)	Cd(1)-O(2)	2.431(3)
Cd(1)-N(5)#1	2.3017(17)	Cd(1)-O(3)	2.275(2)
O(1)-Cd(1)-O(2)	54.42(14)	O(2)-Cd(1)-N(3)#2	164.78(11)
O(1)-Cd(1)-O(3)	148.02(14)	O(3)-Cd(1)-N(1)	88.43(7)
O(1)-Cd(1)-N(1)	93.1(2)	O(3)-Cd(1)-N(3)#2	101.23(7)
O(1)-Cd(1)-N(5)#1	86.1(2)	O(3)-Cd(1)-N(5)#1	87.69(7)
O(1)-Cd(1)-N(3)#2	110.36(13)	N(1)-Cd(1)-N(3)#2	95.79(7)
O(2)-Cd(1)-O(3)	93.94(12)	N(1)-Cd(1)-N(5)#1	171.21(7)
O(2)-Cd(1)-N(1)	85.71(11)	N(5)#1-Cd(1)-N(3)#2	92.70(6)
O(2)-Cd(1)-N(5)#1	86.69(11)		

Symmetry transformations used to generate equivalent atoms:

#1 -1/2+x,-1/2+y,z #2 1-x,y,3/2-z.

Compound **2**			
Co(1)-N(1)	2.107(3)	Co(1)-O(1)	2.227(3)
Co(1)-N(3)#2	2.139(3)	Co(1)-O(2)	2.170(3)
Co(1)-N(5)#1	2.133(3)	Co(1)-O(3)	2.076(3)
O(1)-Co(1)-O(2)	59.36(12)	O(2)-Co(1)-N(3)#2	87.12(10)
O(1)-Co(1)-O(3)	157.33(12)	O(3)-Co(1)-N(1)	98.94(12)
O(1)-Co(1)-N(1)	103.89(12)	O(3)-Co(1)-N(5)#1	89.27(12)
O(1)-Co(1)-N(5)#1	91.97(11)	O(3)-Co(1)-N(3)#2	88.63(11)
O(1)-Co(1)-N(3)#2	87.67(11)	N(1)-Co(1)-N(5)#1	93.44(11)
O(2)-Co(1)-O(3)	98.12(12)	N(1)-Co(1)-N(3)#2	92.79(11)
O(2)-Co(1)-N(1)	162.93(12)	N(5)#1-Co(1)-N(3)#2	173.67(12)
O(2)-Co(1)-N(5)#1	87.26(11)		

Symmetry transformations used to generate equivalent atoms:

#1 1-x,y,3/2-z #2 -1/2+x,-1/2+y,z.

Compound **3**			
Ni(1)-N(2)	2.091(2)	Ni(1)-O(1)	2.052(2)
Ni(1)-N(4)#2	2.062(2)	Ni(1)-O(2)	2.173(2)
Ni(1)-N(6)#1	2.100(2)	Ni (1)-O(3)	2.144(2)
O(1)-Ni(1)-O(2)	158.71(9)	O(2)-Ni(1)-N(4)#2	101.98(9)
O(1)-Ni(1)-O(3)	98.05(9)	O(3)-Ni(1)-N(2)	87.81(8)
O(1)-Ni(1)-N(2)	88.69(9)	O(3)-Ni(1)-N(6)#1	87.24(8)
O(1)-Ni(1)-N(6)#1	89.21(9)	O(3)-Ni(1)-N(4)#2	162.67(9)
O(1)-Ni(1)-N(4)#2	99.27(9)	N(2)-Ni(1)-N(6)#1	174.30(9)
O(2)-Ni(1)-O(3)	60.69(9)	N(2)-Ni(1)-N(4)#2	92.96(9)
O(2)-Ni(1)-N(2)	91.47(9)	N(6)#1-Ni(1)-N(4)#2	92.60(9)
O(2)-Ni(1)-N(6)#1	88.56(9)		

Symmetry transformations used to generate equivalent atoms:

#1 1/2+x,1/2-y,1/2+z #2 1-x,y,-1/2-z.

Compound **4**			
Cd(1)-N(1)	2.292(8)	Cd(2)-N(3)	2.268(9)
Cd(1)-N(7)	2.307(9)	Cd(2)-N(9)	2.267(9)

Cd(1)-N(11)#1	2.287(9)	Cd(2)-N(5)#2	2.314(9)
Cd(1)-O(1)	2.356(8)	Cd(2)-O(6)	2.445(8)
Cd(1)-O(2)	2.481(8)	Cd(2)-O(7)	2.374(9)
Cd(1)-O(3)	2.457(8)	Cd(2)-O(8)	2.433(8)
Cd(1)-O(4)	2.504(8)	Cd(2)-O(9)	2.478(8)
O(1)-Cd(1)-O(2)	53.8(3)	O(6)-Cd(2)-O(7)	53.7(3)
O(1)-Cd(1)-O(3)	133.0(3)	O(6)-Cd(2)-O(8)	136.1(3)
O(1)-Cd(1)-O(4)	80.7(3)	O(6)-Cd(2)-O(9)	172.0(3)
O(1)-Cd(1)-N(1)	137.5(3)	O(6)-Cd(2)-N(3)	88.7(4)
O(1)-Cd(1)-N(7)	87.7(3)	O(6)-Cd(2)-N(9)	84.4(3)
O(1)-Cd(1)-N(11)#1	90.6(3)	O(6)-Cd(2)-N(5)#2	93.1(3)
O(2)-Cd(1)-O(3)	173.1(3)	O(7)-Cd(2)-O(8)	83.1(3)
O(2)-Cd(1)-O(4)	133.8(3)	O(7)-Cd(2)-O(9)	133.9(3)
O(2)-Cd(1)-N(1)	83.9(3)	O(7)-Cd(2)-N(3)	90.9(3)
O(2)-Cd(1)-N(7)	93.9(3)	O(7)-Cd(2)-N(9)	137.8(3)
O(2)-Cd(1)-N(11)#1	88.8(3)	O(7)-Cd(2)-N(5)#2	86.7(3)
O(3)-Cd(1)-O(4)	53.1(3)	O(8)-Cd(2)-O(9)	51.8(3)
O(3)-Cd(1)-N(1)	89.3(3)	O(8)-Cd(2)-N(3)	84.5(3)
O(3)-Cd(1)-N(7)	85.5(3)	O(8)-Cd(2)-N(9)	139.1(3)
O(3)-Cd(1)-N(11)#1	92.2(3)	O(8)-Cd(2)-N(5)#2	91.2(3)
O(4)-Cd(1)-N(1)	141.8(3)	O(9)-Cd(2)-N(3)	93.2(3)
O(4)-Cd(1)-N(7)	91.4(3)	O(9)-Cd(2)-N(9)	87.8(3)
O(4)-Cd(1)-N(11)#1	83.7(3)	O(9)-Cd(2)-N(5)#2	85.6(3)
N(1)-Cd(1)-N(7)	91.9(3)	N(3)-Cd(2)-N(9)	93.0(3)
N(1)-Cd(1)-N(11)#1	92.5(3)	N(3)-Cd(2)-N(5)#2	175.2(3)
N(7)-Cd(1)-N(11)#1	175.0(3)	N(9)-Cd(2)-N(5)#2	91.6(3)

Symmetry transformations used to generate equivalent atoms:

#1 -1+x,y,z #2 1+x,y,z.

Compound **5**

Zn(1)-O(1)	1.958(3)	Zn(1)-N(3)	2.071(2)
Zn(1)-N(1)	1.988(2)	Zn(1)-O(4)#1	2.014(5)
N(1)-Zn(1)-O(1)	127.91(12)	N(1)-Zn(1)-N(3)	108.69(10)
O(1)-Zn(1)-N(3)	98.18(14)	N(1)-Zn(1)-O(4)#1	109.7(4)

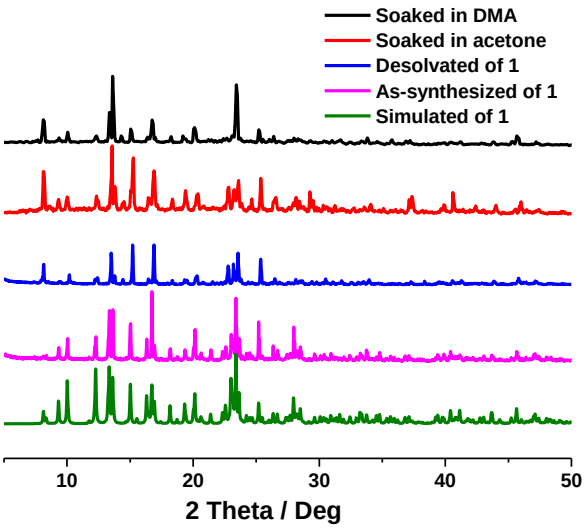
O(1)-Zn(1)-O(4)#1	104.7(3)	N(3)-Zn(1)-O(4)#1	105.4(3)

Symmetry transformations used to generate equivalent atoms:

#1 1-y,x-y,-1+z.

Table S2. Parameters of hydrogen bonds for **4**.

Complex **4**				
D-H---*A*	*D*-H	H---*A*	*D*---*A*	*D*-H---*A*
C(7)-H(7)---O(2)	0.9300	2.5300	3.107(13)	120
C(28)-H(28)---O(8)#1	0.9300	2.5500	3.317(18)	140
Symmetry codes:				
#1 x,-1+y,z.				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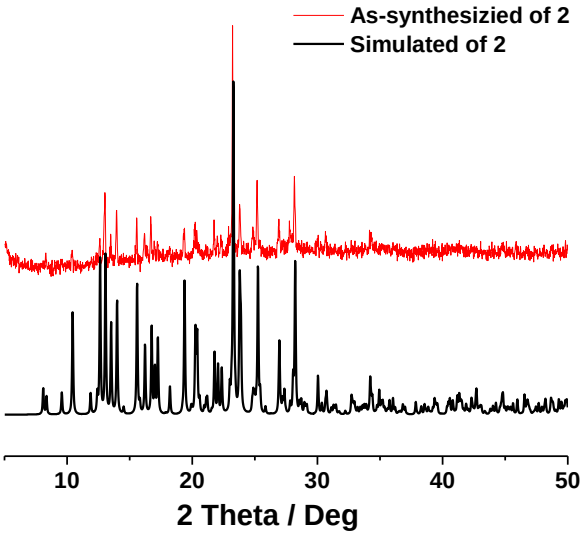
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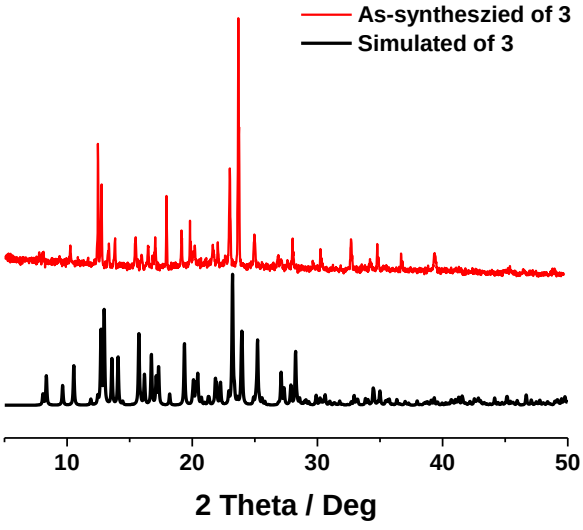
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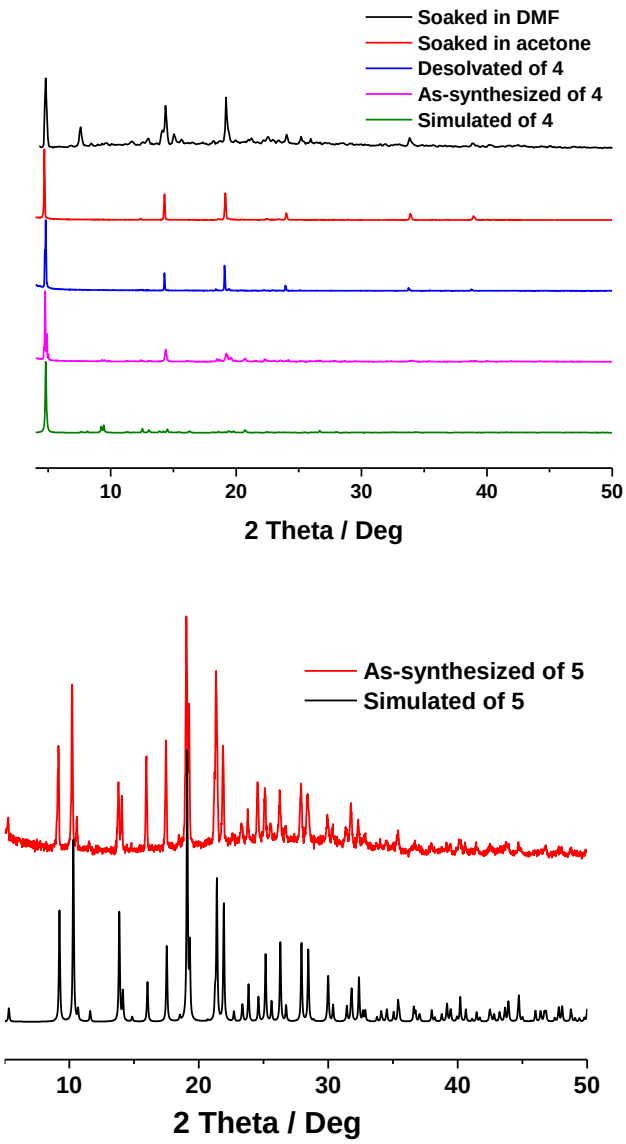

Fig. S1. PXRD of complexes **1**-**5**.

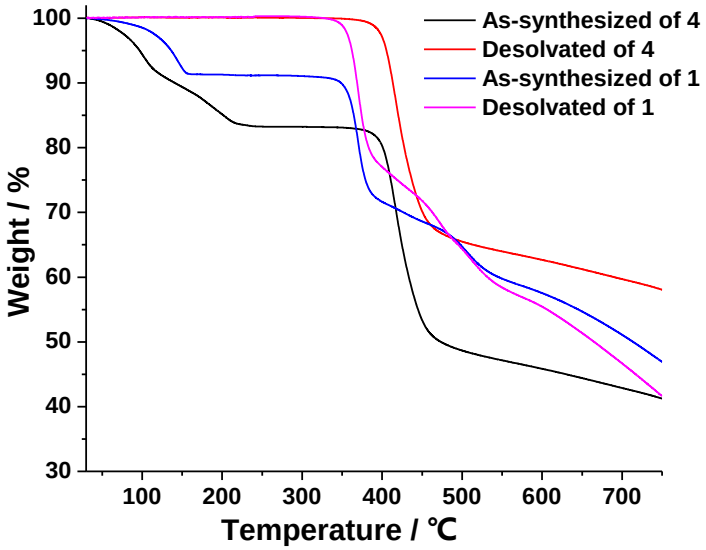

Fig. S2. TG curves of as-synthesized and desolvated of **1** and **4**.

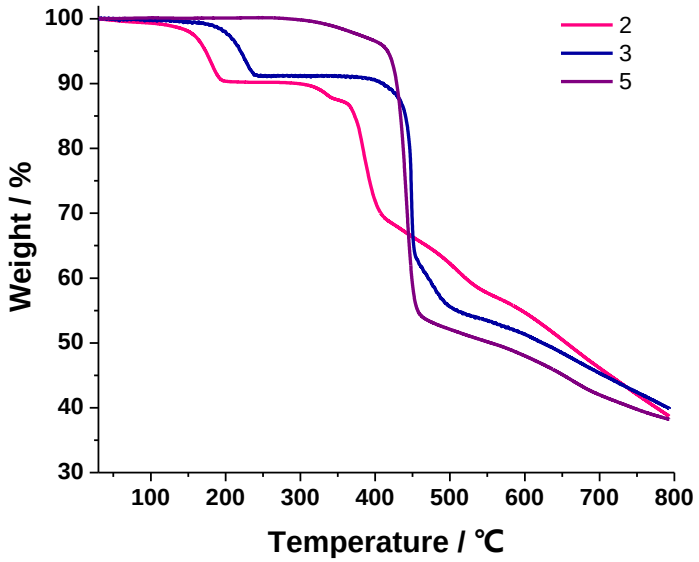

Fig. S3. TG curves of as-synthesized **2**, **3** and **5**.