Supplementary Material (ESI) for CrystEngComm

Electronic Supplementary Information (ESI)

Structural diversity of Zn(II)/Cd(II) complexes based on bis(pyridyl) ligands with long flexible spacer: from zero-dimensional binuclear, one-dimensional chain, two-dimensional layer, to three-dimensional frameworks †

Zhao-Peng Deng, Li-Hua Huo, Hui-Ling Qi, Li-Na Zhu, Hui Zhao and Shan Gao*

PXRD Analysis. In order to check the bulk purity of the complexes, powder X-ray diffraction patterns have been measured at room temperature (Figure S1). The measured and simulated PXRD patterns for all the complexes are quite similar, confirming the homogeneity of the bulk samples.

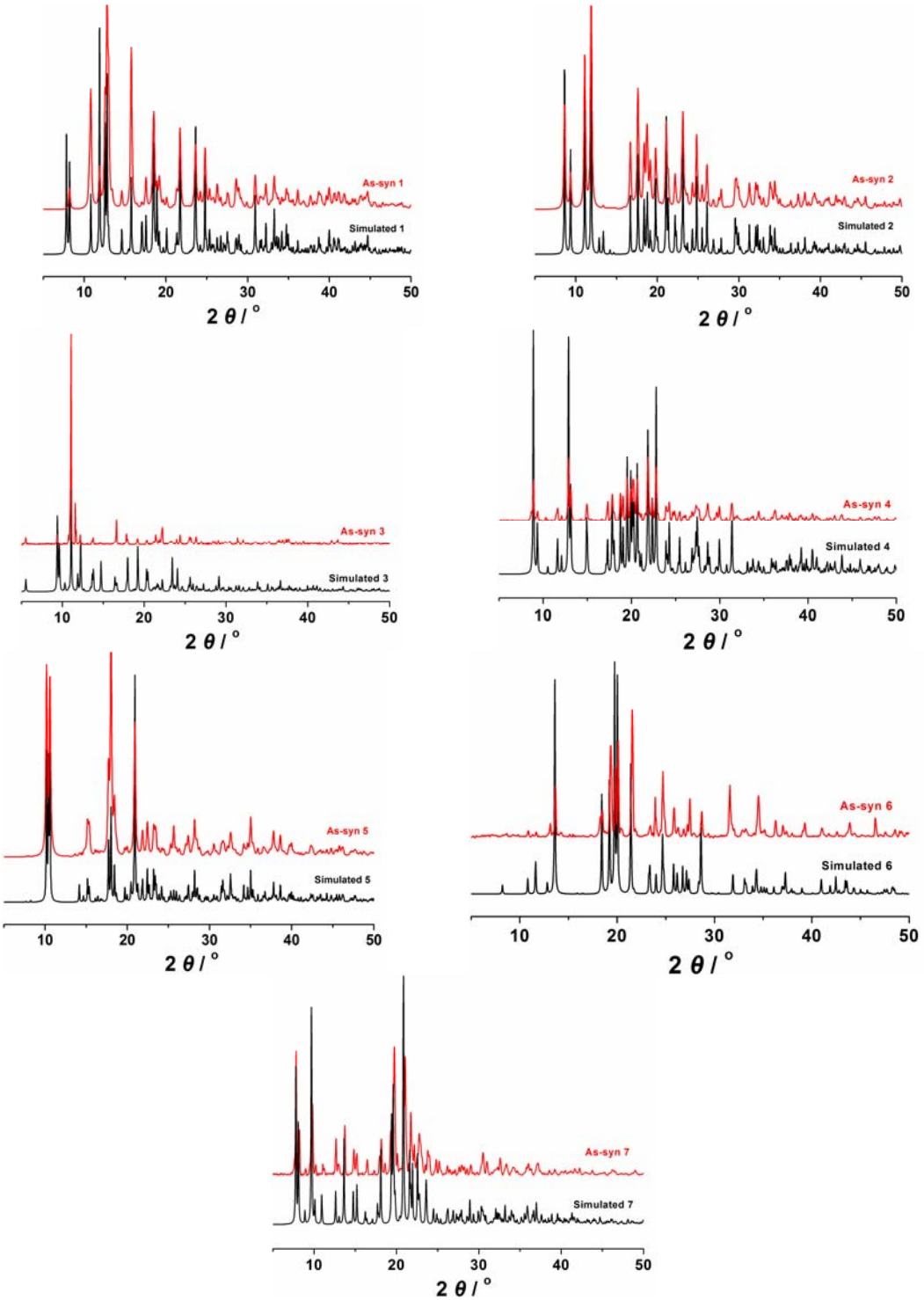

Figure S1. PXRD patterns for complexes **1**-**7**.

Table S1. Selected Bond Lengths [Å] and Angles [°] for Complexes **1–7**[a]

Complex **1**			
Cd(1)-O(2W)	2.287(2)	Cd(1)-O(1)	2.333(2)
Cd(1)-N(4)^{i}	2.309(3)	Cd(1)-O(1W)	2.357(2)
Cd(1)-N(1)	2.314(3)	Cd(1)-O(3W)	2.362(2)
O(2W)-Cd(1)-N(4)^{i}	96.03(9)	N(1)-Cd(1)-O(1W)	176.62(9)
O(2W)-Cd(1)-N(1)	97.34(10)	O(1)-Cd(1)-O(1W)	80.97(8)
N(4)^{i}-Cd(1)-N(1)	92.10(10)	O(2W)-Cd(1)-O(3W)	79.78(9)
O(2W)-Cd(1)-O(1)	160.40(8)	N(4)^{i}-Cd(1)-O(3W)	175.28(8)
N(4)^{i}-Cd(1)-O(1)	98.09(9)	N(1)-Cd(1)-O(3W)	90.60(10)
N(1)-Cd(1)-O(1)	95.65(9)	O(1)-Cd(1)-O(3W)	85.48(8)
O(2W)-Cd(1)-O(1W)	85.90(9)	O(1W)-Cd(1)-O(3W)	89.03(9)
N(4)^{i}-Cd(1)-O(1W)	88.50(9)		
Complex **2**			
Zn(1)-O(1)	1.914(4)	Zn(1)-N(1)	1.995(5)
Zn(1)-O(4)^{i}	1.926(5)	Zn(1)-N(4)^{ii}	2.027(5)
O(1)-Zn(1)-O(4)^{i}	103.7(2)	O(1)-Zn(1)-N(4)^{ii}	110.52(19)
O(1)-Zn(1)-N(1)	114.9(2)	O(4)^{i}-Zn(1)-N(4)^{ii}	104.99(19)
O(4)^{i}-Zn(1)-N(1)	113.6(2)	N(1)-Zn(1)-N(4)^{ii}	108.65(19)
Complex **3**			
Cd(1)-N(5)	2.327(3)	Cd(1)-O(1)	2.423(3)
Cd(1)-N(1)	2.356(3)	Cd(1)-O(2)	2.476(3)
Cd(1)-N(4)^{i}	2.374(3)	Cd(1)-O(5)	2.554(4)
Cd(1)-O(4)	2.384(3)		
N(5)-Cd(1)-N(1)	87.26(10)	N(1)-Cd(1)-O(2)	88.83(12)
N(5)-Cd(1)-N(4)^{i}	90.04(11)	N(4)^{i}-Cd(1)-O(2)	91.77(11)
N(1)-Cd(1)-N(4)^{i}	177.22(11)	O(4)-Cd(1)-O(2)	126.79(11)
N(5)-Cd(1)-O(4)	144.74(12)	O(1)-Cd(1)-O(2)	51.33(11)
N(1)-Cd(1)-O(4)	88.86(12)	N(5)-Cd(1)-O(5)	93.95(10)
N(4)^{i}-Cd(1)-O(4)	92.96(12)	N(1)-Cd(1)-O(5)	89.13(12)

N(5)-Cd(1)-O(1)	139.23(12)	N(4)^{i}-Cd(1)-O(5)	90.37(11)
N(1)-Cd(1)-O(1)	95.28(12)	O(4)-Cd(1)-O(5)	50.94(10)
N(4)^{i}-Cd(1)-O(1)	87.21(12)	O(1)-Cd(1)-O(5)	126.71(11)
O(4)-Cd(1)-O(1)	76.03(13)	O(2)-Cd(1)-O(5)	176.99(9)
N(5)-Cd(1)-O(2)	88.17(10)		

Complex **4**

Zn(1)-O(1)	1.968(6)	Zn(1)-O(2)	2.551(6)
Zn(1)-N(3)	1.986(6)	Zn(1)-O(4)	2.049(6)
Zn(1)-N(1)	2.007(6)	Zn(1)-O(5)	2.766(6)
O(1)-Zn(1)-N(3)	126.5(3)	O(1)-Zn(1)-O(4)	95.0(2)
O(1)-Zn(1)-N(1)	116.0(3)	N(3)-Zn(1)-O(4)	113.8(2)
N(3)-Zn(1)-N(1)	106.9(2)	N(1)-Zn(1)-O(4)	92.7(2)
O(1)-Zn(1)-O(2)	53.9(2)	O(2)-Zn(1)-O(5)	120.7(2)
O(2)-Zn(1)-O(4)	147.5(2)	O(2)-Zn(1)-N(1)	93.4(2)
O(2)-Zn(1)-N(3)	94.8(2)	O(5)-Zn(1)-N(1)	142.3(2)
O(5)-Zn(1)-N(3)	87.2(2)	O(5)-Zn(1)-O(1)	78.1(2)
O(5)-Zn(1)-O(4)	50.1(2)		

Complex **5**

Cd(1)-N(4)^{i}	2.321(2)	Cd(1)-N(5)	2.379(2)
Cd(1)-N(1)	2.347(2)	Cd(1)-O(1)	2.5197(19)
Cd(1)-N(8)^{ii}	2.362(2)	Cd(1)-O(4)	2.546(3)
N(4)^{i}-Cd(1)-N(1)	174.86(7)	N(8)^{ii}-Cd(1)-O(1)	86.69(6)
N(4)^{i}-Cd(1)-N(8)^{ii}	89.98(7)	N(5)-Cd(1)-O(1)	78.13(6)
N(1)-Cd(1)-N(8)^{ii}	86.42(7)	N(4)^{i}-Cd(1)-O(4)	85.59(8)
N(4)^{i}-Cd(1)-N(5)	97.70(8)	N(1)-Cd(1)-O(4)	92.94(8)
N(1)-Cd(1)-N(5)	86.72(8)	N(8)^{ii}-Cd(1)-O(4)	118.95(8)
N(8)^{ii}-Cd(1)-N(5)	163.61(7)	N(5)-Cd(1)-O(4)	76.26(8)
N(4)^{i}-Cd(1)-O(1)	96.24(7)	O(1)-Cd(1)-O(4)	154.34(8)
N(1)-Cd(1)-O(1)	87.23(7)		

Complex **6**

Zn(1)-N(1)	2.002(5)		
N(1)-Zn(1)-N(1)^{i}	111.15(14)	N(1)-Zn(1)-N(1)^{iii}	106.2(3)

Complex **7**			
Cd(1)-N(3)	2.405(5)	Cd(1)-N(5)	2.409(4)
Cd(1)-N(3)^{i}	2.405(5)	Cd(1)-N(1)^{i}	2.420(5)
Cd(1)-N(5)^{i}	2.409(4)	Cd(1)-N(1)	2.420(5)
N(3)-Cd(1)-N(3)^{i}	180.000(1)	N(5)^{i}-Cd(1)-N(1)^{i}	88.44(17)
N(3)-Cd(1)-N(5)^{i}	89.72(17)	N(5)-Cd(1)-N(1)^{i}	91.56(17)
N(3)^{i}-Cd(1)-N(5)^{i}	90.28(17)	N(3)-Cd(1)-N(1)	89.91(18)
N(3)-Cd(1)-N(5)	90.28(17)	N(3)^{i}-Cd(1)-N(1)	90.09(18)
N(3)^{i}-Cd(1)-N(5)	89.72(17)	N(5)^{i}-Cd(1)-N(1)	91.56(17)
N(5)^{i}-Cd(1)-N(5)	180.0(2)	N(5)-Cd(1)-N(1)	88.44(17)
N(3)-Cd(1)-N(1)^{i}	90.09(18)	N(1)^{i}-Cd(1)-N(1)	180.000(1)
N(3)^{i}-Cd(1)-N(1)^{i}	89.91(18)		

[a] Symmetry transformations used to generate equivalent atoms: (i) -x+1,-y+1,-z+1 for **1**; (i) -x+3/2,y+1/2,-z+1/2; (ii) -x+1/2,y+1/2,-z+1/2 for **2**; (i) x,-y+1,z+1/2 for **3**; (i) x-1/2,-y+1/2,z; (ii) x,y,z-1 for **5**; (i) x,-y+2,-z+2; (iii) -x+2,-y+2,z for **6**; (i) -x,-y+1,-z+1 for **7**.

Table S2. Selected Hydrogen Bond Parameters for Complexes **1**, **5** and **6**[a]

D-H...A	d(H...A)	d(D...A)	<(DHA)
Complex **1**			
O(1W)-H(1W1)...O(2)^{ii}	1.89(3)	2.737(3)	175(3)
O(1W)-H(1W2)...O(4)	1.995(12)	2.838(4)	170(4)
O(1W)-H(1W2)...S(1)	2.80(3)	3.493(3)	140(3)
O(2W)-H(2W1)...O(3)^{iii}	1.835(13)	2.678(4)	169(5)
O(2W)-H(2W2)...O(4)^{ii}	1.89(3)	2.744(3)	172(4)
O(3W)-H(3W1)...O(4)^{ii}	2.096(15)	2.893(3)	157(3)
O(3W)-H(3W1)...S(1)^{ii}	2.885(17)	3.700(3)	162(4)
O(3W)-H(3W2)...O(2)	1.959(16)	2.764(3)	160(4)
O(3W)-H(3W2)...S(1)	2.79(3)	3.418(3)	133(4)
N(2)-H(5)...O(1)	2.15	2.944(4)	153.8
N(3)-H(14)...O(1)^{i}	2.16	2.989(3)	162.9
Complex **5**			
N(2)-H(2N)...O(2)^{v}	2.24	2.887(3)	132.2
N(3)-H(3N)...O(3)^{vi}	2.21	3.045(4)	162.8

N(7)-H(7N)...O(3)[v]	2.54	3.183(4)	132.2
Complex **6**			
N(2)-H(2N)...O(2')	2.54	3.12(3)	125.6

[a] Symmetry transformations used to generate equivalent atoms: (i) -x+1,-y+1,-z+1; (ii) -x,y+1/2,-z+3/2; (iii) x,y+1,z for **1**; (v) -x+1/2,y-1/2,z+1/2; (vi) -x+1/2,y-1/2,z-1/2 for **5**.