Supplementary Material

Different Dimensional and Structural Variations in Coordination Compounds of Cadmium, Manganese and Nickel Constructed from the Ligand 2,2'-Bipyidine-3,3',6,6'-tetracarboxylic Acid (H_4bptc)

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Table S1. Crystallographic data and structure refinement summary for compounds **1-4**

Complex	**1**	**2**	**3**	**4**
Formula	$C_{14}H_{14}CdN_2O_{12}$	$C_{14}H_{16}CdN_2O_{13}$	$C_{14}H_7CdN_2NaO_9$	$C_{14}H_8MnN_2O_9$
Formula weight	514.67	532.69	482.61	403.16
T (K)	293 (2)	293 (2)	293 (2)	293 (2)
Wavelength (Å)	0.71	0.71	0.71	0.71
Crystal system	triclinic	monoclinic	orthorhombic	orthorhombic
space group	P-1	*Pc*	$Pca2_1$	$Pca2_1$
a (Å)	6.8419 (5)	9.2153(4)	6.8586 (9)	6.9352 (6)
b (Å)	9.6045 (6)	14.2539(8)	11.3063 (7)	11.1495 (7)
c (Å)	13.7158 (12)	6.8239(5)	17.9222 (12)	17.8220 (17)
α (°)	79.586 (6)	/	/	/
β (°)	79.214 (6)	96.446(5)	/	/
γ (°)	84.058 (6)	/	/	/
Volume (Å^3)	868.53 (11)	890.68(9)	1389.8 (2)	1378.1 (2)
Z	2	2	4	4
$D_{calc.}$ (mg·m^{-3})	1.968	1.986	2.307	1.943
μ (mm^{-1})	1.33	1.31	1.67	1.02
F(000)	512	532	944	812
Goodness-of-fit on F^2	1.02	1.00	1.14	1.08
R_1 ($I > 2\sigma(I)$)	0.042	0.0380	0.0852	0.0663
wR_2 ($I > 2\sigma(I)$)	0.073	0.0743	0.1620	0.1301
R_1 (all data)	0.058	0.0421	0.1095	0.0968
wR_2 (all data)	0.083	0.0777	0.1738	0.1480

Table S2. Selected bond parameters (Å, º) for **1** and **2**

1			
Cd1–O6	2.295 (4)	Cd1–N1	2.363 (4)
Cd1–O7	2.296 (4)	Cd1–N2	2.408 (4)
Cd1–O5	2.347 (4)	Cd1–O2	2.431 (3)
Cd1–O3	2.349 (3)		
O6–Cd1–O7	96.60 (18)	O7–Cd1–N2	90.94 (15)
O6–Cd1–O5	83.76 (18)	O5–Cd1–N2	80.87 (15)
O7–Cd1–O5	164.74 (16)	O3–Cd1–N2	136.96 (12)
O6–Cd1–O3	75.37 (15)	N1–Cd1–N2	67.59 (12)
O7–Cd1–O3	90.98 (15)	O6–Cd1–O2	81.42 (14)
O5–Cd1–O3	103.81 (16)	O7–Cd1–O2	83.47 (13)
O6–Cd1–N1	143.94 (15)	O5–Cd1–O2	81.50 (15)
O7–Cd1–N1	91.46 (14)	O3–Cd1–O2	155.35 (12)
O5–Cd1–N1	97.20 (14)	N1–Cd1–O2	134.53 (12)
O3–Cd1–N1	69.39 (13)	N2–Cd1–O2	67.35 (11)
O6–Cd1–N2	146.81 (15)		
2			
Cd1–O5	2.315 (6)	Cd1–O7^{i}	2.372 (6)
Cd1–O6	2.335 (6)	Cd1–N2	2.405 (6)
Cd1–O3	2.349 (5)		
O2–Cd1–O5	92.8 (2)	O5–Cd1–O7^{i}	83.5 (2)
O2–Cd1–O6	86.4 (2)	O6–Cd1–O7^{i}	83.2 (2)
O5–Cd1–O6	166.5 (2)	O3–Cd1–O7^{i}	76.1 (2)
O2–Cd1–O3	153.55 (18)	N1–Cd1–O7^{i}	148.5 (2)
O5–Cd1–O3	90.5 (2)	O2–Cd1–N2	137.5 (2)
O6–Cd1–O3	84.4 (2)	O5–Cd1–N2	87.0 (2)
O2–Cd1–N1	70.7 (2)	O6–Cd1–N2	102.7 (2)
O5–Cd1–N1	93.0 (2)	O3–Cd1–N2	68.85 (19)
O6–Cd1–N1	99.4 (2)	N1–Cd1–N2	66.9 (2)
O3–Cd1–N1	135.3 (2)	O7i–Cd1–N2	143.6 (2)
O2–Cd1–O7^{i}	78.2 (2)		

Symmetry codes: (i) x–1, y, z

Table S3. Hydrogen-bond geometry (Å, °) for **1**

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O10–H58···O12	0.64 (7)	1.98 (7)	2.546 (7)	150 (10)
O6–H56···O12^{i}	0.76 (7)	2.50 (7)	3.199 (9)	152 (7)
O7–H55···O4^{ii}	0.72 (7)	2.00 (7)	2.687 (6)	162 (8)
O12–H52···O11^{iii}	0.63 (6)	2.34 (7)	2.915 (7)	154 (9)
O6–H57···O9^{iv}	0.98 (8)	1.70 (8)	2.670 (5)	172 (7)
O12–H53···O3^{v}	0.92 (10)	1.85 (10)	2.752 (8)	163 (9)
O7–H54···O11^{iv}	1.00 (7)	1.81 (8)	2.805 (6)	178 (6)
O5–H51···O8^{vi}	0.78 (5)	2.66 (5)	3.179 (6)	126 (5)
O5–H51···O1^{vii}	0.78 (5)	2.20 (5)	2.916 (5)	153 (6)
O5–H50···O1^{viii}	0.74 (6)	1.96 (7)	2.679 (6)	167 (8)
O8–H8···O2^{ix}	0.82	1.72	2.534 (4)	171

Symmetry codes: (i) *x*+1, *y*-1, *z*; (ii) *x*-1, *y*, *z*; (iii) -*x*+1, -*y*+2, -*z*; (iv) *x*, *y*-1, *z*; (v) *x*-1, *y*+1, *z*; (vi) -*x*+1, -*y*+1, -*z*+1; (vii) -*x*+1, -*y*, -*z*+1; (viii) *x*+1, *y*, *z*; (ix) *x*, *y*+1, *z*.

Table S4. Hydrogen-bond geometry (Å, °) for **2**

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O13–H13A···O2^{ii}	0.85	2.11	2.898 (8)	155
O13–H13D···O2^{iii}	0.85	2.06	2.909 (8)	176
O12–H12B···O9	0.85	2.10	2.907 (9)	158
O12–H12D···O13^{iv}	0.85	1.99	2.797 (10)	158
O11–H11B···O1^{iv}	0.85	2.47	3.218 (15)	148
O11–H11D···O12	0.85	2.45	3.276 (15)	165
O10–H10···O4^{v}	0.82	1.77	2.578 (7)	168
O8–H7···O3^{iii}	0.82	1.87	2.659 (7)	162
O6–H6B···O1^{vi}	0.85	1.95	2.653 (8)	140
O6–H6A···O12^{vii}	0.85	2.26	2.821 (10)	123
O5–H5C···O11	0.85	2.35	3.191 (15)	172
O5–H5B···O4^{viii}	0.85	1.88	2.728 (8)	174

Symmetry codes: (ii) *x*+1, -*y*+1, *z*-1/2; (iii) *x*+1, *y*, *z*; (iv) *x*, -*y*+1, *z*+1/2; (v) *x*+1, -*y*, *z*+1/2; (vi) *x*, -*y*+1, *z*-1/2; (vii) *x*-1, *y*, *z*-1; (viii) *x*, -*y*, *z*+1/2.

Table S5. Selected bond lengths (Å) and angles (º) for complexes **3** and **4**

3			
Cd1–O1	2.300 (11)	Cd1–O8^{ii}	2.401 (11)
Cd1–O9	2.309 (16)	Cd1–N1	2.405 (12)
Cd1–O6^{i}	2.323 (12)	Cd1–N2	2.419 (13)
Cd1–O5	2.337 (9)		
O1–Cd1–O9	83.1 (5)	O9–Cd1–N1	102.1 (5)
O1–Cd1–O6^{i}	99.3 (5)	O6^{i}–Cd1–N1	84.2 (4)
O9–Cd1–O6^{i}	173.7 (5)	O5–Cd1–N1	134.5 (5)
O1–Cd1–O5	154.9 (5)	O8^{ii}–Cd1–N1	144.4 (4)
O9–Cd1–O5	83.9 (5)	O1–Cd1–N2	134.9 (4)
O6^{i}–Cd1–O5	91.7 (4)	O9–Cd1–N2	97.8 (5)
O1–Cd1–O8^{ii}	77.6 (4)	O6^{i}–Cd1–N2	84.7 (4)
O9–Cd1–O8^{ii}	86.8 (5)	O5–Cd1–N2	68.2 (5)
O6^{i}–Cd1–O8^{ii}	88.0 (4)	O8^{ii}–Cd1–N2	147.4 (4)
O5–Cd1–O8^{ii}	80.3 (5)	N1–Cd1–N2	66.2 (4)
O1–Cd1–N1	69.6 (5)		

Symmetry codes: (i) x-1/2, -y+2, z; (ii) -x+1/2, y, z-1/2; (iii) -x+3/2, y, z-1/2; (iv) x+1/2, -y+1, z; (v) -x+1, -y+1, z-1/2.

4			
Mn1–O6^{i}	2.175 (6)	Mn1–O8^{ii}	2.335 (6)
Mn1–O9	2.192 (7)	Mn1–N1	2.366 (7)
Mn1–O2	2.220 (6)	Mn1–N2	2.375 (8)
Mn1–O5	2.246 (5)		
O6^{i}–Mn1–O9	175.8 (3)	O6i–Mn1–N1	85.6 (2)
O6^{i}–Mn1–O2	97.7 (2)	O9–Mn1–N1	98.2 (3)
O9–Mn1–O2	81.8 (2)	O2–Mn1–N1	70.1 (2)
O6^{i}–Mn1–O5	94.0 (2)	O5–Mn1–N1	135.4 (3)
O9–Mn1–O5	84.7 (2)	O8^{ii}–Mn1–N1	146.8 (2)
O2–Mn1–O5	152.9 (3)	O6^{i}–Mn1–N2	87.3 (2)
O6^{i}–Mn1–O8^{ii}	87.9 (3)	O9–Mn1–N2	96.0 (2)
O9–Mn1–O8^{ii}	87.9 (3)	O2–Mn1–N2	134.7 (2)
O2–Mn1–O8^{ii}	78.6 (2)	O5–Mn1–N2	69.9 (3)
O5–Mn1–O8^{ii}	77.5 (3)	O8^{ii}–Mn1–N2	146.7 (2)

Symmetry codes: (i) x-1/2, -y+2, z; (ii) -x+1/2, y, z-1/2.

Table S6. Hydrogen-bond geometry (Å, °) for **3**

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O9–H9A···O5^{vi}	0.850 (9)	1.91 (7)	2.726 (19)	161 (20)
O3–H10···O2^{vii}	0.851 (9)	2.13 (7)	2.696 (18)	123 (7)

Symmetry codes: (vi) *x*+1/2, -*y*+2, *z*; (vii) -*x*+1, -*y*+1, *z*+1/2.

Table S7. Hydrogen-bond geometry (Å, °) for **4**

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O9–H9D···O1^{i}	0.85	2.12	2.965 (9)	176
O7–H7···O2^{ii}	0.82	1.86	2.602 (9)	150
O3–H3···O1^{iii}	0.82	1.80	2.595 (9)	163

Symmetry codes: (i) *x*+1/2, -*y*+1, *z*; (ii) -*x*+1/2, *y*, *z*+1/2; (iii) -*x*+1, -*y*+1, *z*+1/2.

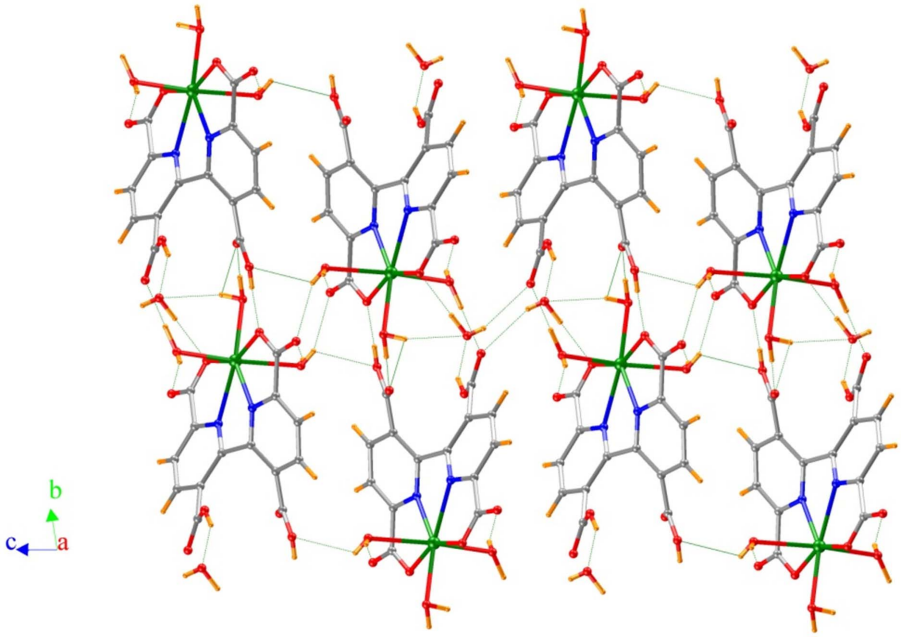

Figure S1. Perspective view showing the H-bonding interactions in **1**.

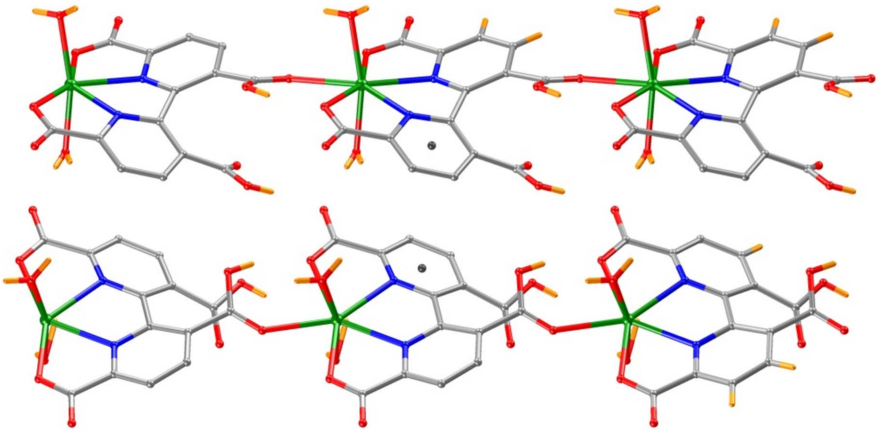

Figure S2. The π-π stacking interactions between the adjacent chains in packing diagram of **2**.

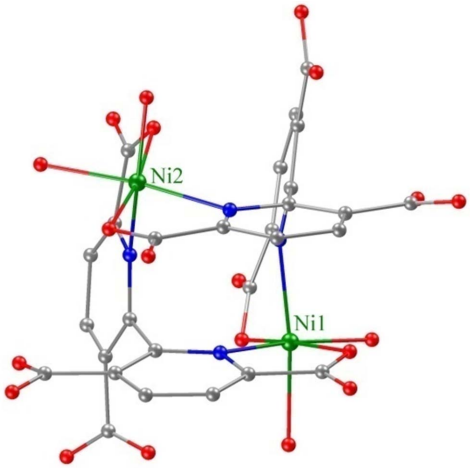

Figure S3. Perspective view showing structure of dinuclear compound **5**.

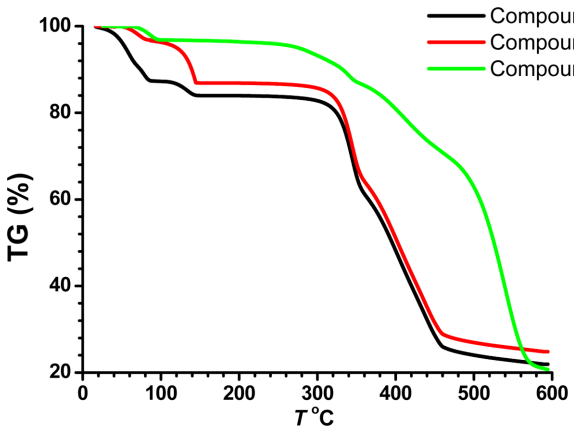

Figure S4. TG curves of complexes **1-3**.