Electronic Supplementary Material (ESI) for CrystEngComm

Coordination Polymers of Tetrazole-yl Acylamide with Octahedrally Coordinated Divalent Transition Metal: the effects of metal-centers and side-groups on the structural topologies and symmetries

*Jian-Zhen Liao, Hua Ke, Jian-Jun Liu, Zuo-Yin Li, Mei-Jin Lin, Jun-Dong Wang, Chang-Cang Huang**

College of Chemistry and Chemical Engineering, Fuzhou University, Fuzhou, Fujian, 350108, P. R. China

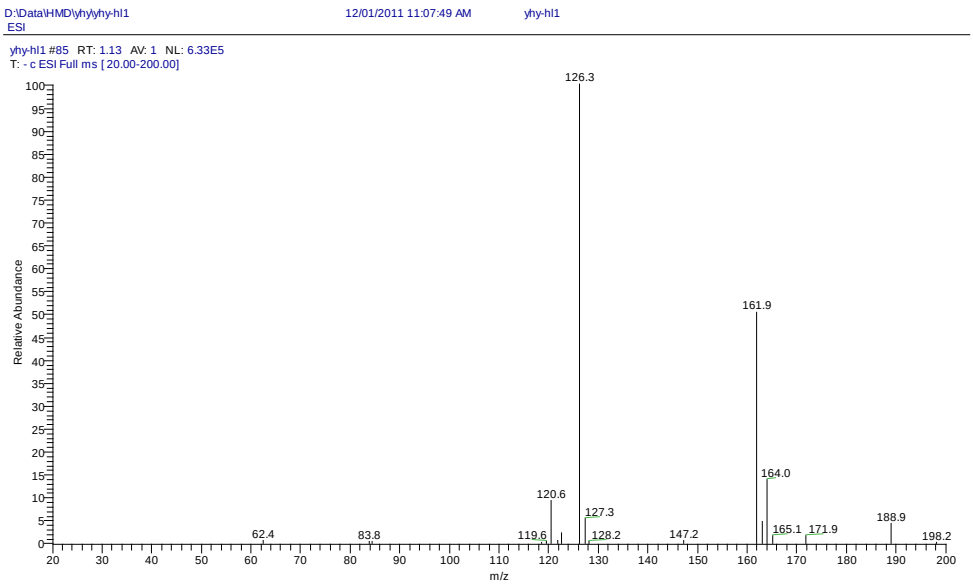

Figure S1. The MS of the H-NTAA.

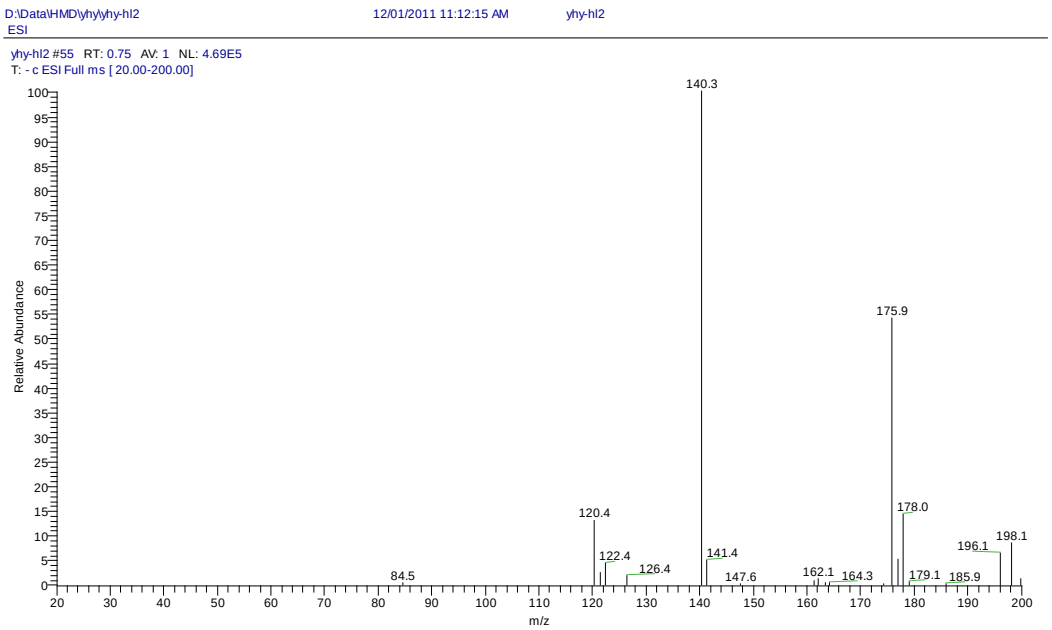

Figure S2. The MS of the H-NTPA.

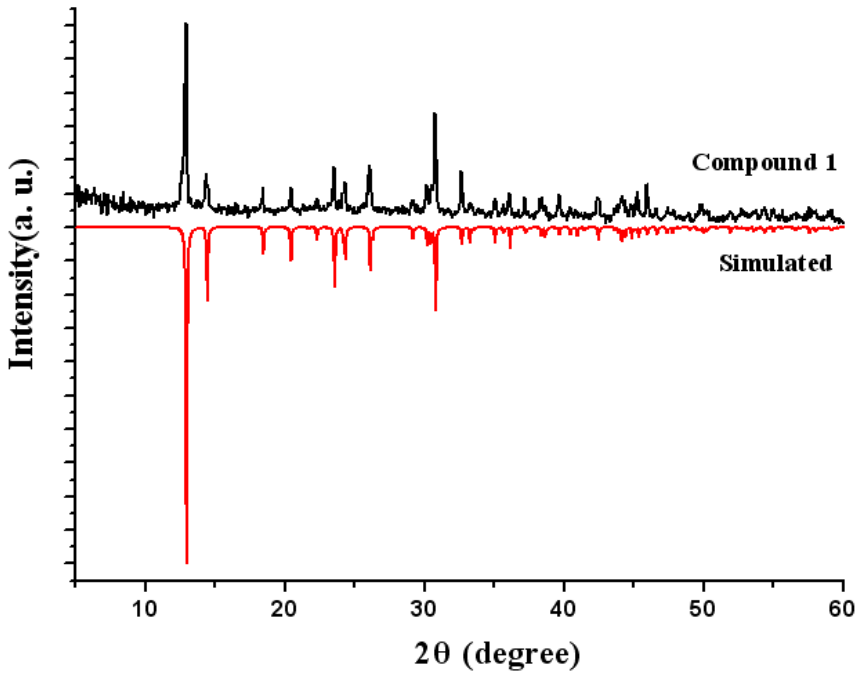

Figure S3. XRD patterns of **1** and the simulated pattern based on the single crystal **1**.

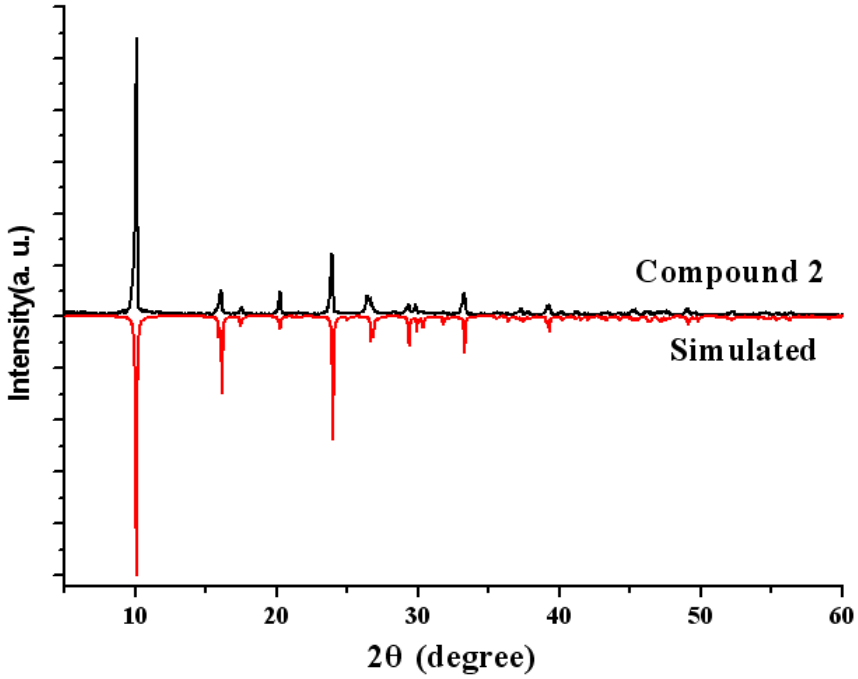

Figure S4. XRD patterns of **2** and the simulated pattern based on the single crystal **2**.

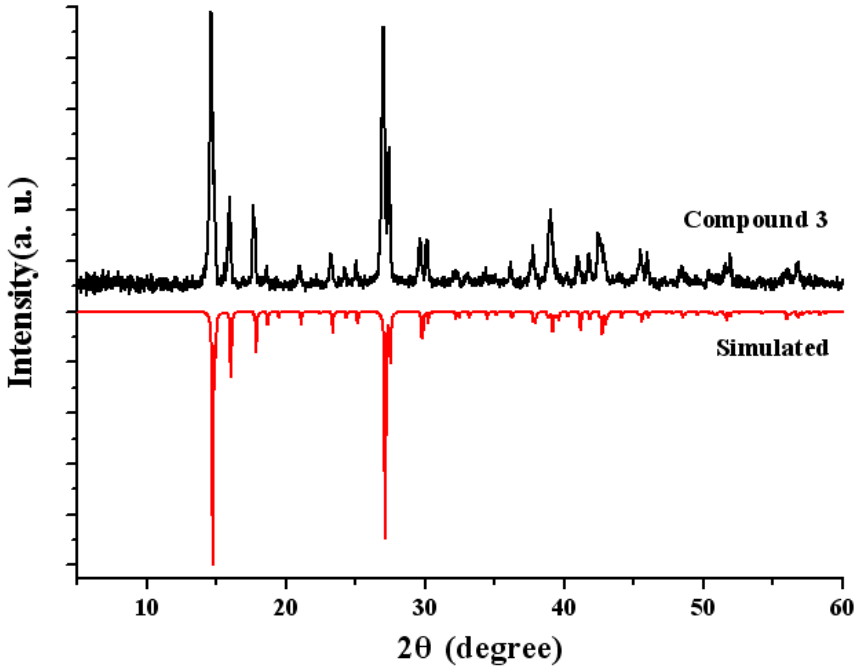

Figure S5. XRD patterns of **3** and the simulated pattern based on the single crystal **3**.

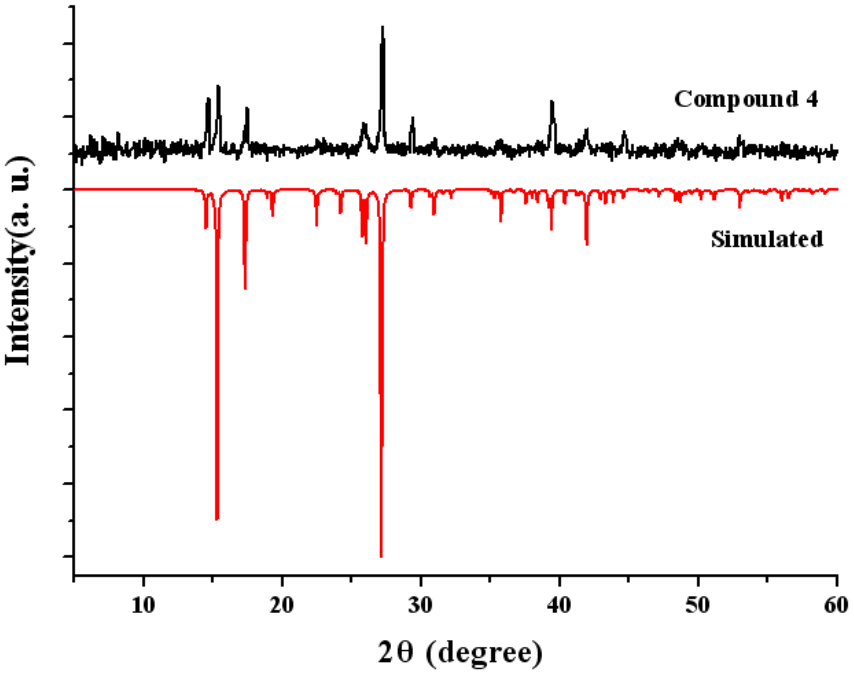

Figure S6. XRD patterns of **4** and the simulated pattern based on the single crystal **4**.

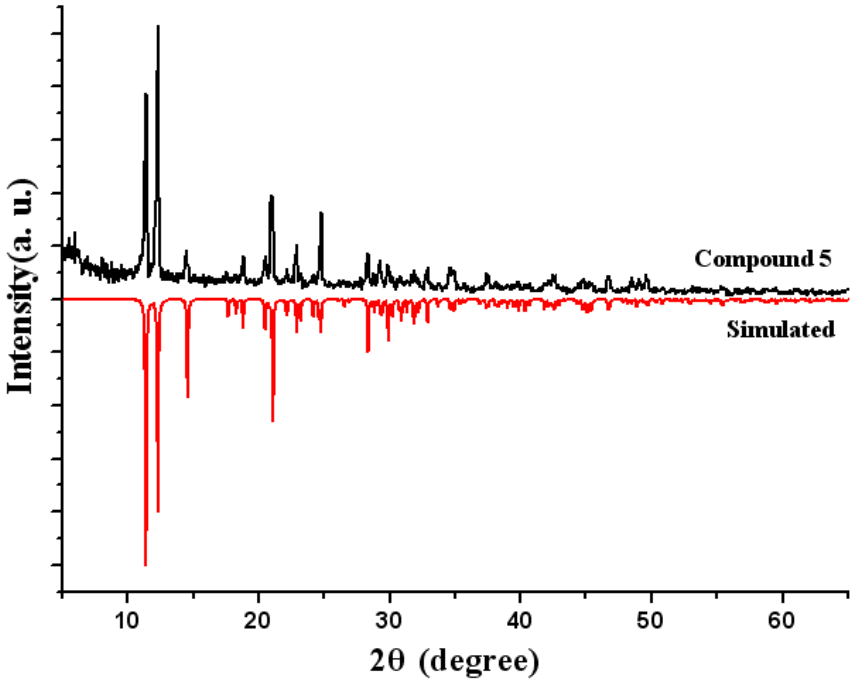

Figure S7. XRD patterns of **5** and the simulated pattern based on the single crystal **5**.

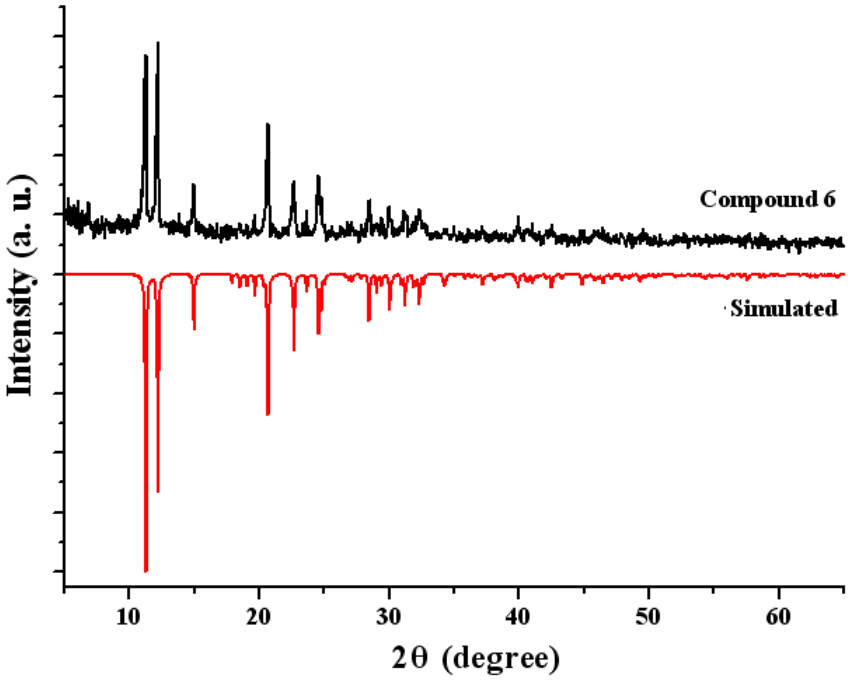

Figure S8. XRD patterns of **6** and the simulated pattern based on the single crystal **6**.

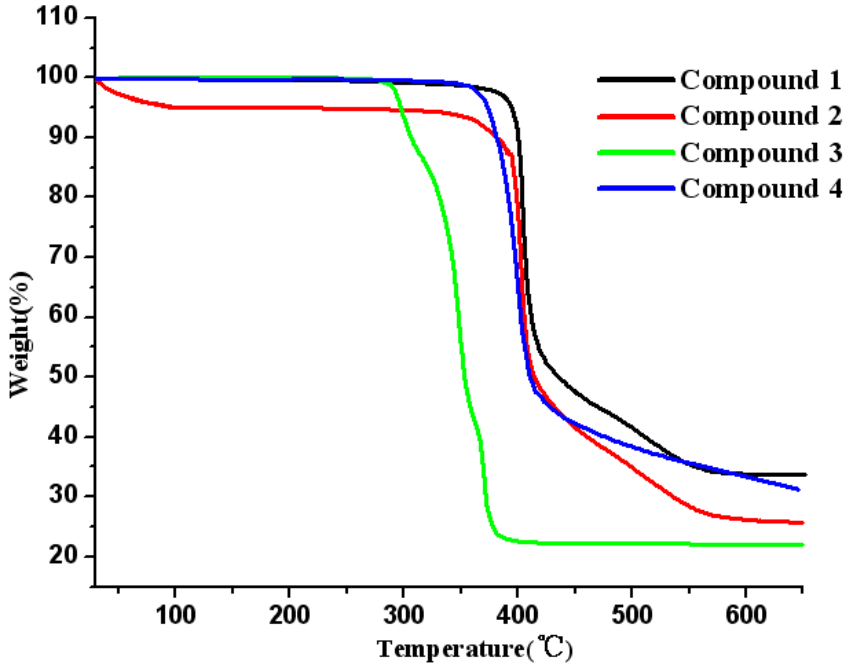

Figure S9. TGA diagrams of compounds **1-4**.

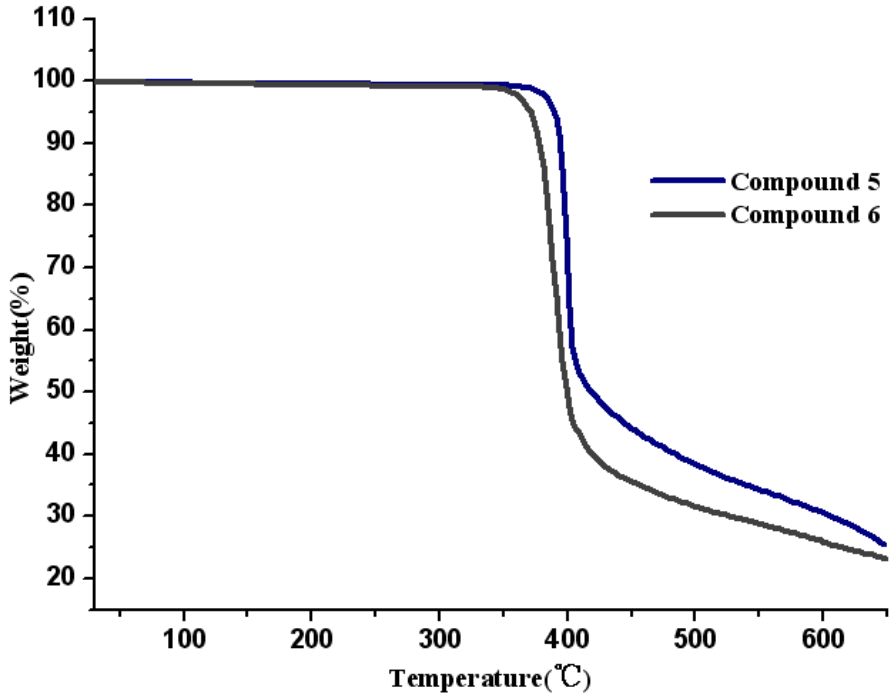

Figure S10. TGA diagrams of compounds **5-6**.

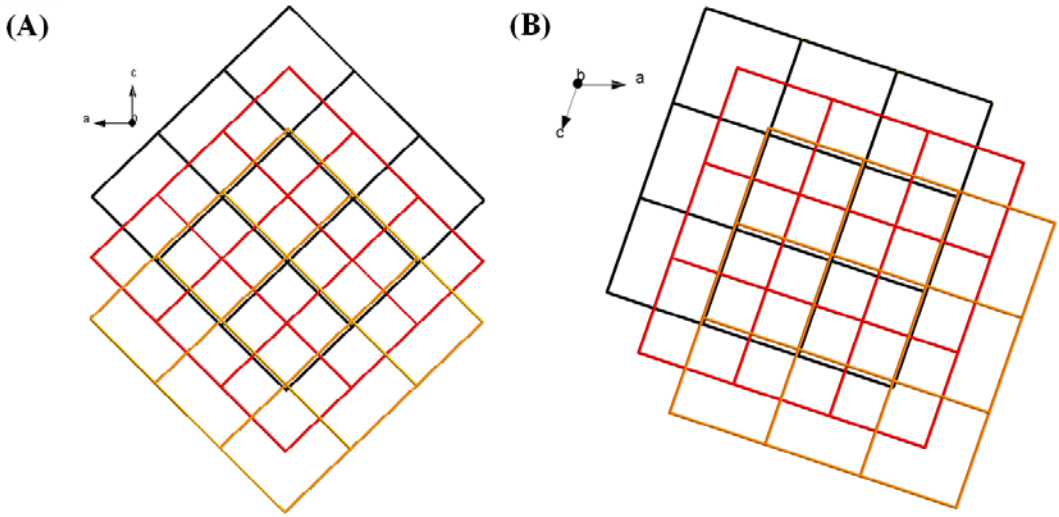

Figure S11. Schematic Representation of the Difference between the *Aba2*(a) and *Cc*(b) nets.

Table S1. Selected bond lengths (Å) and angles (°) for compounds **1**-**6**.[#]

Compound **1**			
Cd1—N1a	2.239 (2)	Cd1—N4c	2.330 (3)
Cd1—N1	2.239 (2)	Cd1—O1a	2.403 (2)
Cd1—N4b	2.330 (3)	Cd1—O1	2.403 (2)
N1a—Cd1—N1	162.57 (115)	N1a—Cd1—O1	92.54 (9)
N1a—Cd1—N4b	93.10 (9)	N1—Cd1—O1	75.33 (8)
N1—Cd1—N4b	97.02 (9)	N4b—Cd1—O1	169.12 (10)
N1a—Cd1—N4c	97.02 (9)	N4c—Cd1—O1	79.67 (10)
N1—Cd1—N4c	93.10 (9)	N1a—Cd1—O1a	75.33 (8)
N4b—Cd1—N4c	108.83 (14)	N1—Cd1—O1a	92.54 (9)
N4b—Cd1—O1a	79.67 (10)	O1a—Cd1—O1	92.78 (14)
N4c—Cd1—O1a	169.12 (10)		
Compound **2**			
Zn1—N1	2.0718 (17)	Zn1—N2^{c}	2.1497 (17)
Zn1—N2^{a}	2.1497 (17)	Zn1—O1^{b}	2.1856 (15)
Zn1—N1^{b}	2.0718 (17)	Zn1—O1	2.1853 (16)
N1—Zn1—N1^{b}	165.76 (9)	N2^{c}—Zn1—O1^{b}	174.89 (6)
N1—Zn1—N2^{c}	89.21 (6)	N2^{a}—Zn1—O1^{b}	89.13 (7)
N1^{b}—Zn1—N2^{c}	100.45 (6)	N1—Zn1—O1	82.80 (6)
N1—Zn1—N2^{a}	100.45 (6)	N1^{b}—Zn1—O1	86.89 (6)
N1^{b}—Zn1—N2^{a}	89.21 (6)	N2^{c}—Zn1—O1	89.13 (7)
N2^{c}—Zn1—N2^{a}	94.83 (10)	N2^{a}—Zn1—O1	174.89 (6)
N1—Zn1—O1^{b}	86.89 (6)	O1^{b}—Zn1—O1	87.10 (9)
N1^{b}—Zn1—O1^{b}	82.80 (6)		
Compound **3**			

Cu1—N2	1.954 (2)	Cu1—O1^{b}	1.9873 (19)
Cu1—N4^{a}	2.583 (7)	Cu1—O1	1.9873 (19)
Cu1—N2^{b}	1.954 (2)	Cu1—N4^{c}	2.583 (7)
N2—Cu1—N2^{b}	180.000 (1)	N2—Cu1—O1	87.99 (8)
N2—Cu1—O1^{b}	92.01 (8)	N2^{b}—Cu1—O1	92.01 (8)
N2^{b}—Cu1—O1^{b}	87.99 (8)	O1^{b}—Cu1—O1	180.0
N4^{a}—Cu1—N4^{c}	180.0		
Compound **4**			
Mn1—O1^{a}	2.136 (5)	Mn1—N3^{c}	2.264 (8)
Mn1—O1^{b}	2.136 (5)	Mn1—N5^{a}	2.259(8)
Mn1—N3	2.264 (8)	Mn1—N5^{b}	2.259 (8)
O1^{a}—Mn1—O1^{b}	179.9 (8)	N3—Mn1—N5^{a}	177.5 (4)
O1^{a}—Mn1—N3	94.6 (4)	N3^{c}—Mn1—N5^{a}	87.95 (17)
O1^{b}—Mn1—N3	85.5 (4)	O1^{a}—Mn1—N5^{b}	96.1 (4)
O1^{a}—Mn1—N3^{c}	85.5 (4)	O1^{b}—Mn1—N5^{b}	83.8 (4)
O1^{b}—Mn1—N3^{c}	94.6 (4)	N3—Mn1—N5^{b}	87.95 (17)
N3—Mn1—N3^{c}	93.9 (4)	N3^{c}—Mn1—N5^{b}	177.5 (4)
O1^{a}—Mn1—N5^{a}	83.8 (4)	N5^{a}—Mn1—N5^{b}	90.2(4)
O1^{b}—Mn1—N5^{a}	96.1 (4)		
Compound **5**			
Cd1—N10^{a}	2.250 (3)	Cd1—N7	2.341 (3)
Cd1—N2	2.254 (3)	Cd1—O1	2.388 (3)
Cd1—N5^{b}	2.308 (3)	Cd1—O2^{a}	2.414 (3)
N10^{a}—Cd1—N2	158.52 (13)	N5^{b}—Cd1—O1	82.67 (12)
N10^{a}—Cd1—N5^{b}	98.11 (12)	N7—Cd1—O1	169.70 (12)
N2—Cd1—N5^{b}	96.81 (12)	N10^{a}—Cd1—O2^{a}	74.63 (11)
N10^{a}—Cd1—N7	92.68 (12)	N2—Cd1—O2^{a}	89.01 (12)

N2—Cd1—N7	97.86 (12)	N5^{b}—Cd1—O2^{a}	171.33 (12)
N5^{b}—Cd1—N7	106.36 (13)	N7—Cd1—O2^{a}	79.07 (13)
N10^{a}—Cd1—O1	90.89 (11)	O1—Cd1—O2^{a}	92.59 (13)
N2—Cd1—O1	75.77 (11)		
Compound **6**			
Mn1—N1	2.199 (6)	Mn1—O2	2.238 (6)
Mn1—N6	2.218 (6)	Mn1—N4^{a}	2.245 (6)
Mn1—O1	2.227 (5)	Mn1—N9^{b}	2.274 (6)
N1—Mn1—N6	162.3 (2)	O1—Mn1—N4^{a}	84.8 (2)
N1—Mn1—O1	78.4 (2)	O2—Mn1—N4^{a}	174.0 (2)
N6—Mn1—O1	91.7 (2)	N1—Mn1—N9^{b}	96.5 (2)
N1—Mn1—O2	88.0 (2)	N6—Mn1—N9^{b}	92.0 (2)
N6—Mn1—O2	77.8 (2)	O1—Mn1—N9^{b}	172.9 (2)
O1—Mn1—O2	93.0 (3)	O2—Mn1—N9^{b}	81.8 (3)
N1—Mn1—N4^{a}	97.0 (2)	N4^{a}—Mn1—N9^{b}	101.0 (2)
N6—Mn1—N4^{a}	96.7 (2)		

$^{\#}$Symmetry Code: **1**) (a) –x+1/2, −y+3/2, z; (b) −x+1/4, y−1/4, z−1/4; (c) x+1/4, −y+7/4, z−1/4. **2**) (a) −x, −y+1, −z; (b) −x, y, −z+1/2; (c) x, −y+1, z+1/2. **3**) (a) x-1/2, -y+5/2, z-1/2; (b) -x, 2-y, 1-z; (c) –x+1/2, y-1/2, -z+1/2. **4**) (a) *x*−1/2, −*y*, *z*−1/2; (b) −*x*+1/2, *y*, *z*−1/2; (c) −*x*, −*y*, *z*. **5**) (a) *x*, −*y*+1, *z*−1/2; (b) *x*−1/2, −*y*+1/2, *z*−1/2. **6**) (a) *x*+1/2, −*y*−1/2, *z*+1/2; (b) *x*, −*y*−1, *z*−1/2.