Electronic Supplementary Information (ESI)

Structural diversity of 5-methylnicotinate coordination assemblies regulated by metal-ligating tendency and metal-dependent anion effect

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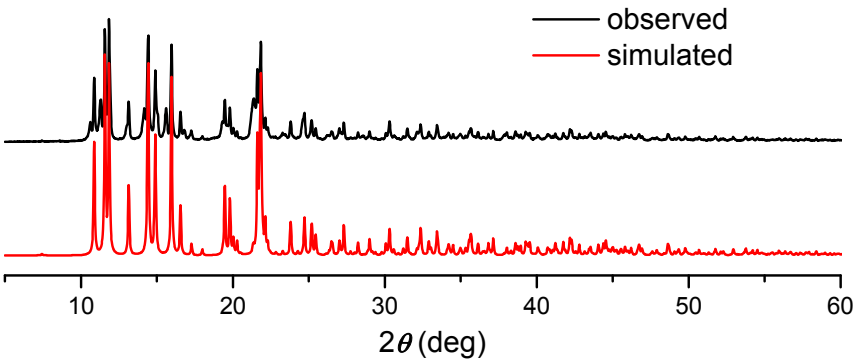
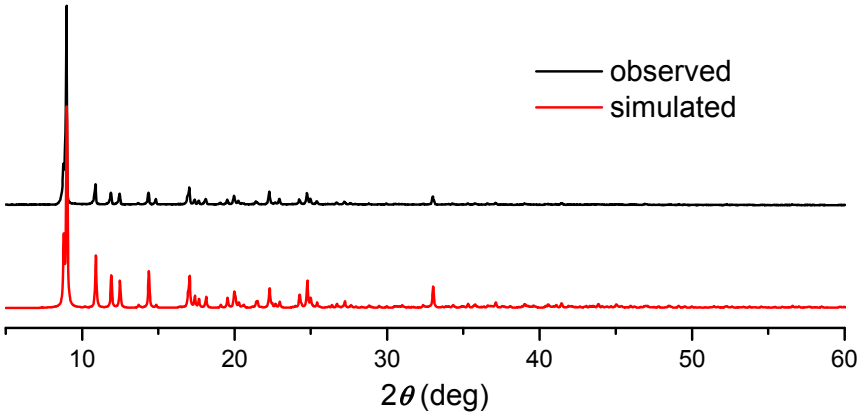

observed
simulated
10
20
30
40
50
60
2θ (deg)

(a)


observed
simulated
10
20
30
40
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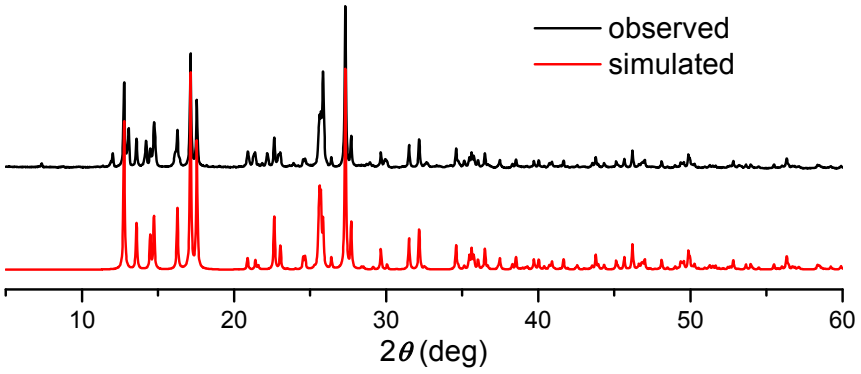
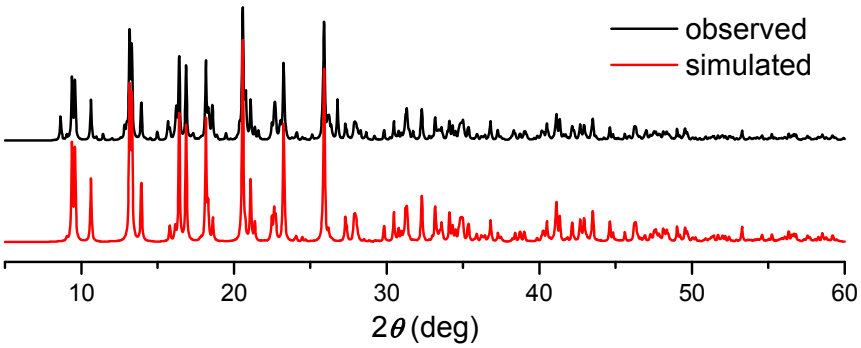
60
2θ (deg)

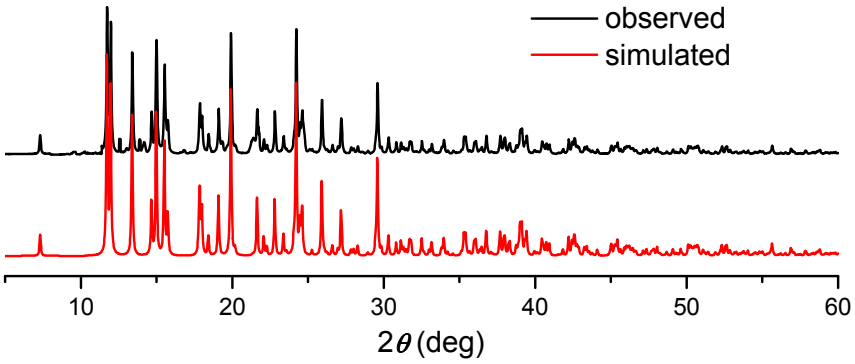
(b)


observed
simulated
10
20
30
40
50
60
2θ (deg)

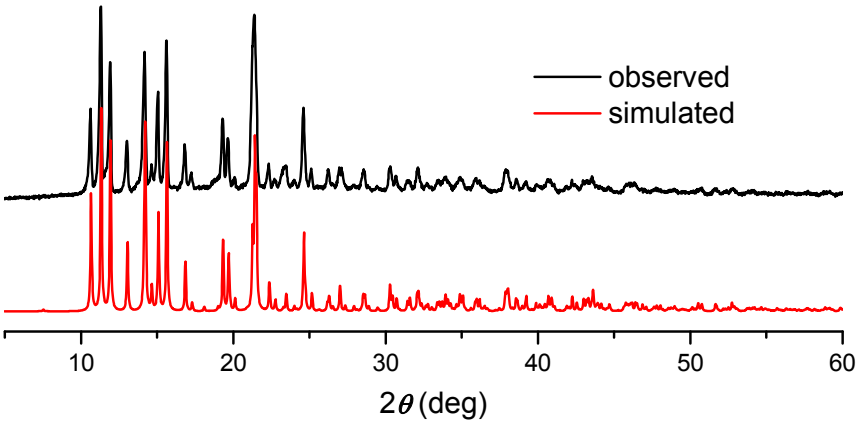
(c)


observed
simulated
10
20
30
40
50
60
2θ (deg)

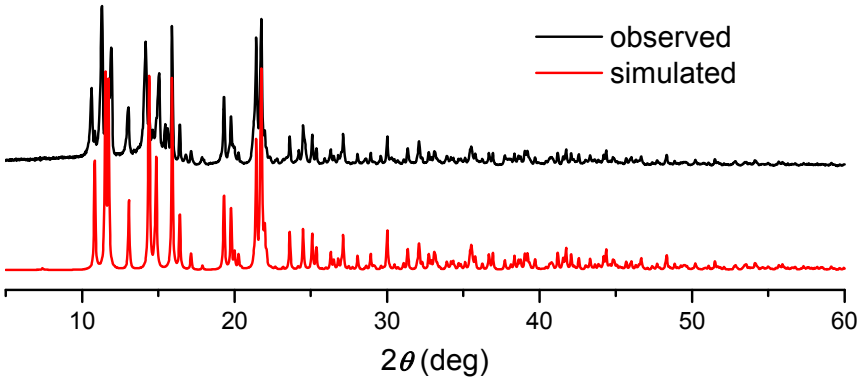
(d)


observed
simulated
10
20
30
40
50
60
2θ (deg)

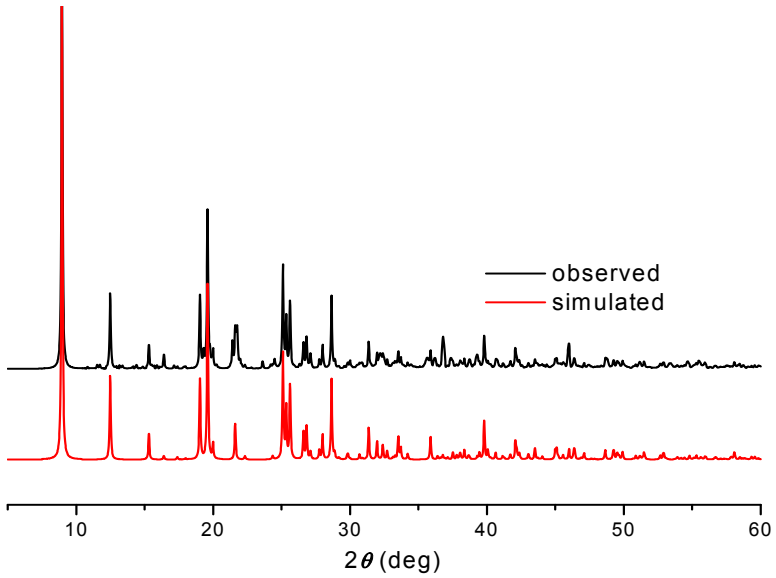
(e)


observed
simulated
10
20
30
40
50
60
2θ (deg)

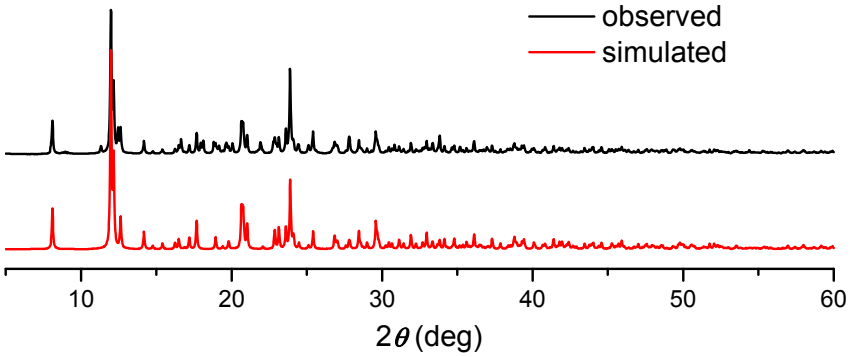
(f)



(g)



(h)



(i)

Fig. S1 Powder X-ray diffraction (PXRD) patterns for complexes **1**–**9** (**a**–**i**).

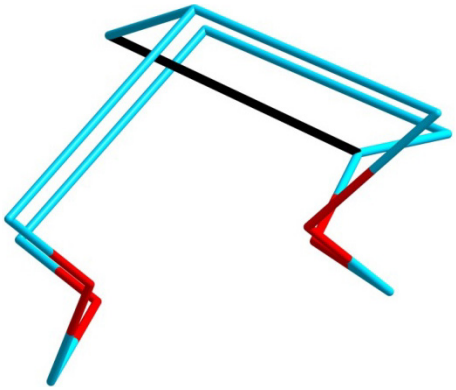


Fig. S2 View of the self-interpenetrating pattern in **2**.

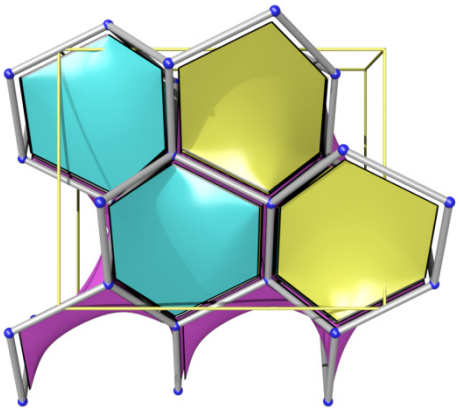


Fig. S3 Topological view of the **noz** network for **2** with $[Ni_2(H_2O)(COO)_2]$ units as the nodes.

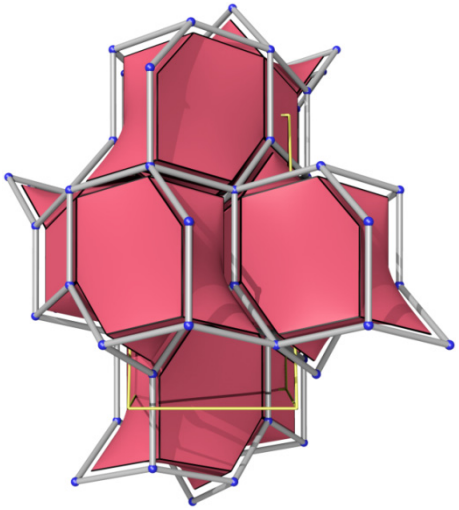
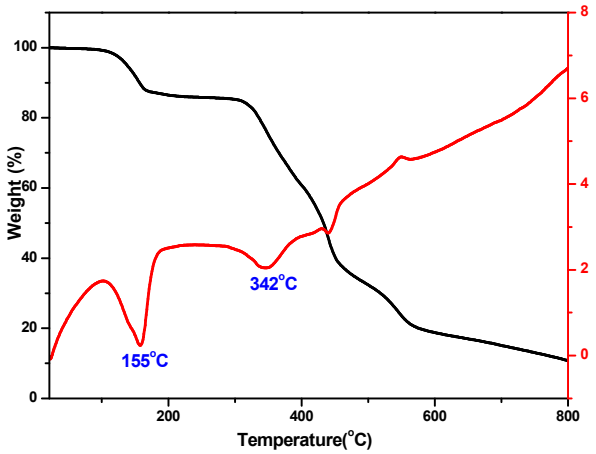
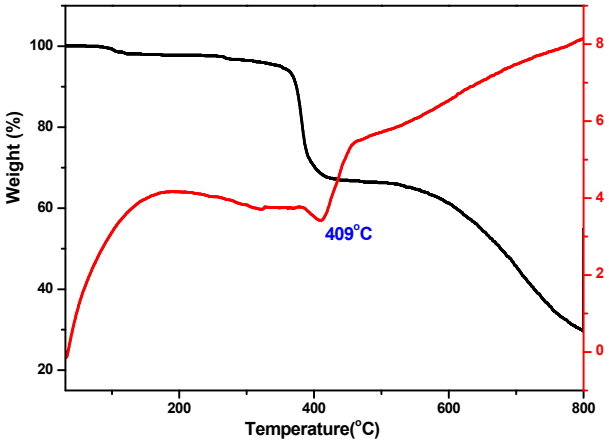


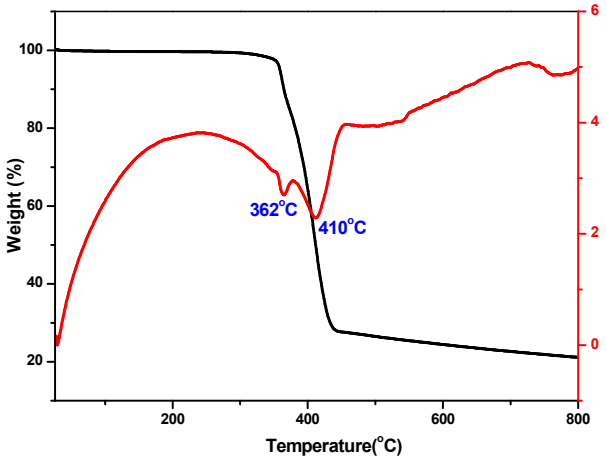
Fig. S4 Topological view the (3,5)-connected $(4.6^2)(4.6^7.8^2)$ network for **9**.


Weight (%)
Temperature(°C)
155°C
342°C

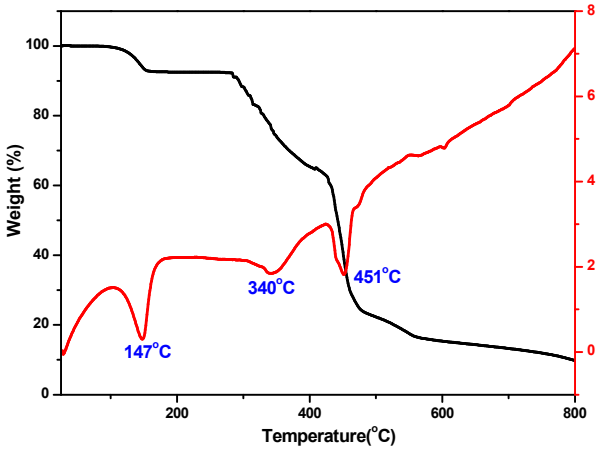
(a)


Weight (%)
Temperature(°C)
409°C

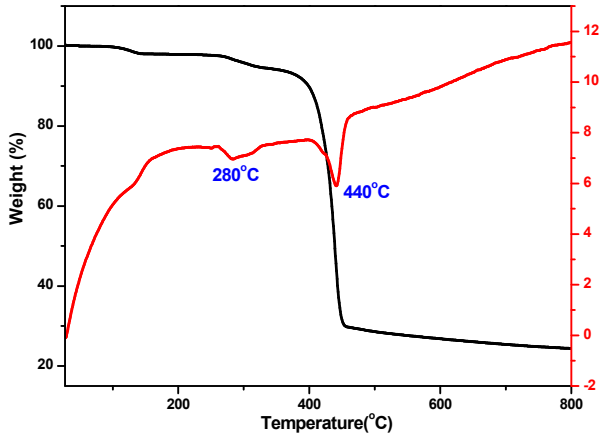
(b)


Weight (%)
Temperature(°C)
362°C
410°C

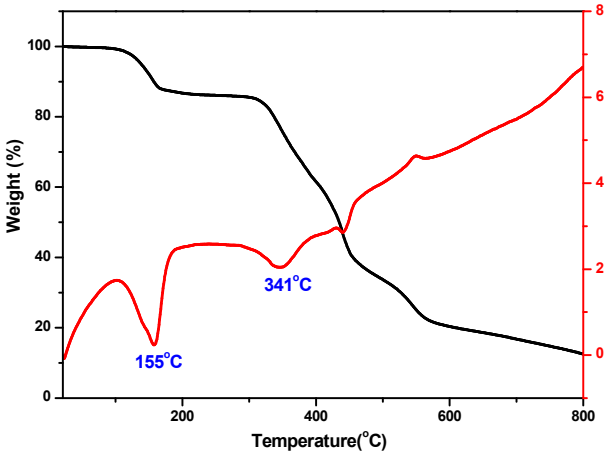
(c)


Weight (%)
Temperature(°C)
147°C
340°C
451°C

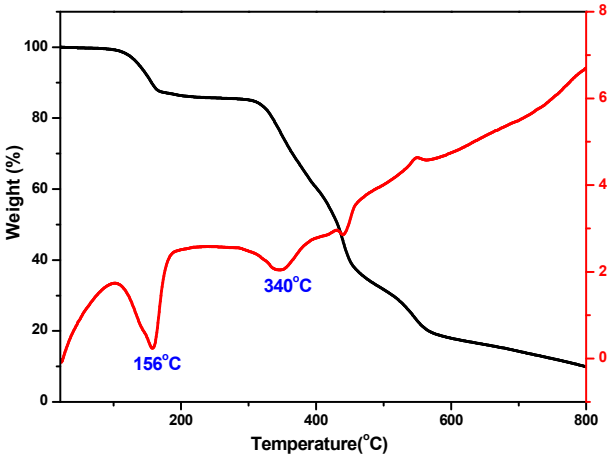
(d)


Weight (%)
Temperature(°C)
280°C
440°C

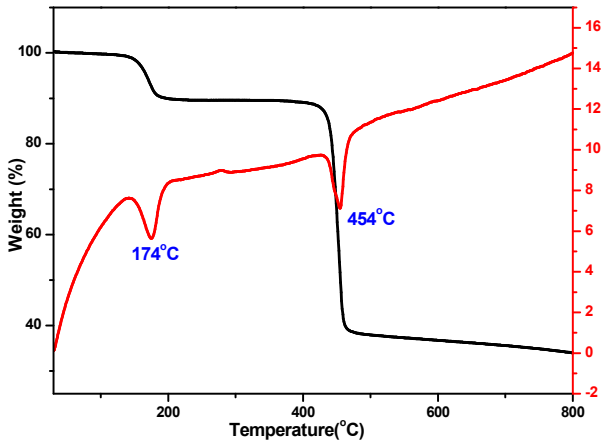
(e)


Weight (%)
Temperature(°C)
155°C
341°C

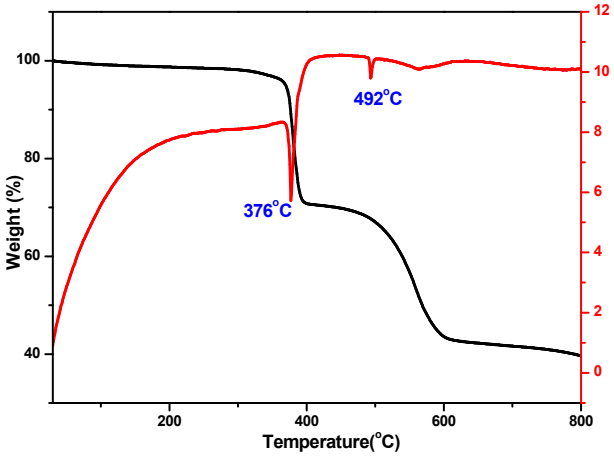
(f)



(g)



(h)



(i)

Fig. S4 TG-DTA curves for complexes **1**–**9**.

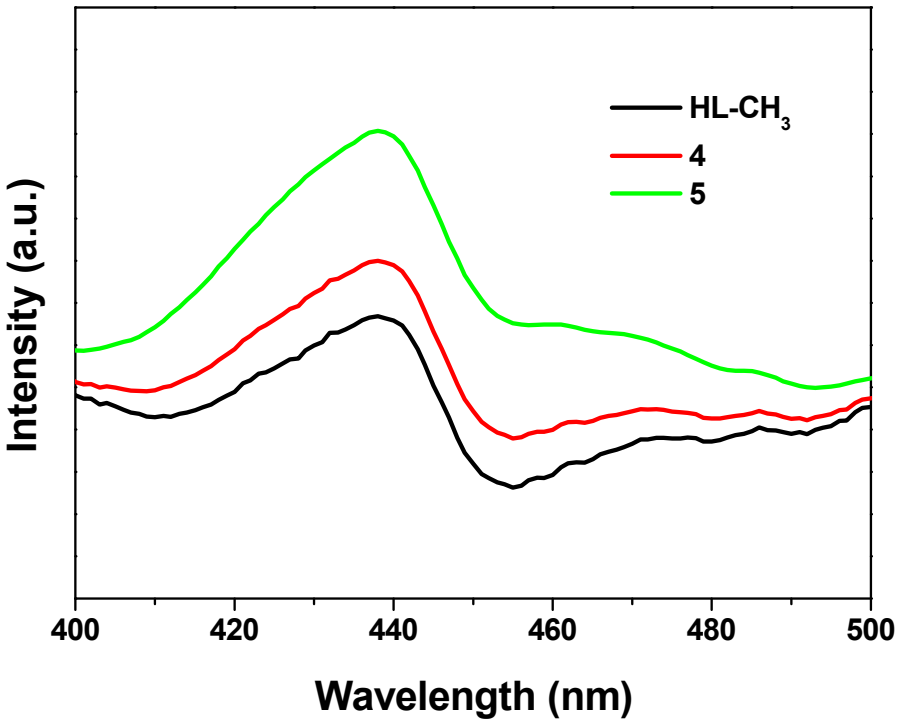


Fig. S6 Solid-state emission spectra for HL-CH_3 ligand and complexes **4** and **5**.

Table S1 Selective bond lengths (Å) and angles (º) for complexes **1–9**

		1	
Ni1–O4	2.0343(13)	Ni1–O5	2.0787(14)
Ni1–N1	2.1101(17)	Ni2–O1A	2.0126(13)
Ni2–N2	2.0852(16)	Ni2–O6	2.1035(14)
O4–Ni1–O5	91.10(6)	O4–Ni1–N1	89.19(6)
O5–Ni1–N1	90.49(6)	O1A–Ni2–N2	90.04(6)
O1A–Ni2–O6	92.03(6)	N2–Ni2–O6	88.64(6)
		2	
Ni1–O3A	2.047(2)	Ni1–N2	2.087(2)
Ni1–O8	2.088(2)	Ni1–N1	2.100(3)
Ni1–O6B	2.113(2)	Ni1–O9	2.134(2)
Ni2–O4A	2.055(2)	Ni2–O7	2.067(2)
Ni2–N4	2.096(3)	Ni2–N3A	2.097(3)
Ni2–O9	2.103(2)	Ni2–O2C	2.114(2)
O3A–Ni1–N2	93.76(9)	O3A–Ni1–O8	97.30(8)
N2–Ni1–O8	84.31(9)	O3A–Ni1–N1	90.55(9)
N2–Ni1–N1	89.75(10)	O8–Ni1–N1	170.43(9)
O3A–Ni1–O6B	174.84(9)	N2–Ni1–O6B	91.39(9)
O8–Ni1–O6B	82.92(9)	N1–Ni1–O6B	89.75(9)
O3A–Ni1–O9	86.15(8)	N2–Ni1–O9	175.28(9)
O8–Ni1–O9	91.02(8)	N1–Ni1–O9	94.97(9)
O6B–Ni1–O9	88.69(8)	O4A–Ni2–O7	96.39(8)
O4A–Ni2–N4	173.83(9)	O7–Ni2–N4	89.25(9)
O4A–Ni2–N3A	85.62(9)	O7–Ni2–N3A	92.51(9)
N4–Ni2–N3A	91.66(10)	O4A–Ni2–O9	89.11(8)

O7–Ni2–O9	88.59(8)	N4–Ni2–O9	93.53(9)
N3A–Ni2–O9	174.71(9)	O4A–Ni2–O2C	83.15(8)
O7–Ni2–O2C	177.75(8)	N4–Ni2–O2C	91.30(9)
N3A–Ni2–O2C	89.65(9)	O9–Ni2–O2C	89.20(8)

3

Ni1–O1	1.9724(18)	Ni1–Cl1	2.2326(8)
Ni1–O1A	1.9724(18)	Ni1–Cl1A	2.2326(8)
O1–Ni1–O1A	88.62(11)	O1–Ni1–Cl1A	116.47(7)
O1A–Ni1–Cl1A	112.38(6)	O1–Ni1–Cl1	112.38(6)
O1A–Ni1–Cl1	116.47(7)	Cl1A–Ni1–Cl1	109.46(5)

4

Cd1–O8	2.276(7)	Cd1–O5	2.282(6)
Cd1–O6	2.298(6)	Cd1–N2	2.308(8)
Cd1–N1	2.309(8)	Cd1–O7	2.316(6)
Cd2–O11	2.230(7)	Cd2–O9	2.251(6)
Cd2–O10	2.268(7)	Cd2–O4A	2.275(6)
Cd2–O2	2.275(6)	Cd2–O1	2.671(1)
Cd2–O3A	2.655(1)		
O8–Cd1–O5	90.8(2)	O8–Cd1–O6	175.92(19)
O5–Cd1–O6	90.5(2)	O8–Cd1–N2	87.3(2)
O5–Cd1–N2	92.3(2)	O6–Cd1–N2	88.7(2)
O8–Cd1–N1	92.5(2)	O5–Cd1–N1	87.8(2)
O6–Cd1–N1	91.5(2)	N2–Cd1–N1	179.78(19)
O8–Cd1–O7	89.2(2)	O5–Cd1–O7	176.4(2)
O6–Cd1–O7	89.8(2)	N2–Cd1–O7	91.3(2)
N1–Cd1–O7	88.6(2)	O11–Cd2–O9	87.3(2)
O11–Cd2–O10	173.7(3)	O9–Cd2–O10	87.4(2)

O11–Cd2–O4A	98.9(3)	O9–Cd2–O4A	135.5(2)
O10–Cd2–O4A	87.3(3)	O11–Cd2–O2	90.8(3)
O9–Cd2–O2	136.8(2)	O10–Cd2–O2	90.7(3)
O4A–Cd2–O2	87.4(3)	O3A–Cd2–O11	95.8(3)
O3A–Cd2–O9	83.5(2)	O3A–Cd2–O10	87.0(3)
O3A–Cd2–O4A	52.1(2)	O3A–Cd2–O2	139.5(2)
O3A–Cd2–O1	168.3(2)	O1–Cd2–O11	85.2(3)
O1–Cd2–O9	84.9(2)	O1–Cd2–O10	90.9(3)
O1–Cd2–O4A	139.3(2)	O1–Cd2–O2	51.9(2)

5

Cd1–O1	2.237(2)	Cd1–N2A	2.311(2)
Cd1–O5	2.320(2)	Cd1–N1B	2.343(3)
Cd1–O3	2.368(2)	Cd1–O4	2.417(2)
O1–Cd1–N2A	97.76(9)	O1–Cd1–O5	81.92(8)
N2A–Cd1–O5	93.71(8)	O1–Cd1–N1B	87.76(8)
N2A–Cd1–N1B	93.69(9)	O5–Cd1–N1B	168.02(8)
O1–Cd1–O3	115.68(9)	N2A–Cd1–O3	146.53(8)
O5–Cd1–O3	89.94(8)	N1B–Cd1–O3	89.08(8)
O1–Cd1–O4	163.90(8)	N2A–Cd1–O4	92.37(8)
O5–Cd1–O4	84.99(8)	N1B–Cd1–O4	104.10(8)
O3–Cd1–O4	54.80(7)		

6

Cu1–O1	1.9641(19)	Cu1–N2	2.036(2)
Cu1–O5	2.395(3)	Cu2–O3	1.963(2)
Cu2–N1A	2.023(2)	Cu2–O6	2.400(2)
O1–Cu1–N2	89.78(9)	N2–Cu1–O5	91.80(10)

O1–Cu1–O5	92.39(9)	O3–Cu2–O6	95.21(8)
O3–Cu2–N1A	90.35(9)	N1A–Cu2–O6	88.80(9)

7

Co1–O3	2.0556(12)	Co1–O5	2.1188(13)
Co1–N1	2.1666(15)	Co2–O1A	2.0276(12)
Co2–N2	2.1397(15)	Co2–O6	2.1444(12)
O3–Co1–O5	90.22(5)	O3–Co1–N1	89.15(5)
O5–Co1–N1	89.58(6)	N2–Co2–O6	88.61(5)
O1A–Co2–O6	88.93(5)	O1A–Co2–N2	90.11(6)

8

Mn1–O2A	2.1669(11)	Mn1–O3	2.1963(11)
Mn1–N1	2.2762(13)		
O2A–Mn1–O3	88.57(4)	O2A–Mn1–N1	91.49(4)
O3–Mn1–N1	85.39(5)		

9

Pb1–O2	2.375(4)	Pb1–O3	2.423(4)
Pb1–N2	2.587(5)	Pb1–O1	2.710(6)
Pb1–N1A	2.734(6)	Pb1–O4	2.850(5)
Pb1–O4B	2.782(6)		
O2–Pb1–O3	88.34(15)	O2–Pb1–N2	81.43(18)
O3–Pb1–N2	90.15(17)	O2–Pb1–O1	51.37(15)
O3–Pb1–O1	139.70(14)	N2–Pb1–O1	83.50(17)
O2–Pb1–N1A	81.98(18)	O3–Pb1–N1A	79.09(17)
N2–Pb1–N1A	160.45(19)	O1–Pb1–N1A	94.13(18)
O4–Pb1–O2	132.04(18)	O4–Pb1–O3	48.53(15)

O4–Pb1–N2	79.24(19)	O4–Pb1–O1	161.13(18)
O4–Pb1–N1A	104.69(22)	O4–Pb1–O4B	82.70(21)
O4B–Pb1–O2	131.89(19)	O4B–Pb1–O3	130.94(18)
O4B–Pb1–N2	73.33(22)	O4B–Pb1–O1	85.08(18)
O4B–Pb1–N1A	125.93(25)		

Symmetry codes: A = $x + 1/2, -y + 3/2, z + 1/2$ for **1**; A = $-x + 1/2, y - 1/2, z$; B = $-x + 1, -y + 2, -z + 1$; C = $-x + 1, y - 1/2, -z + 1/2$ for **2**; A = $-x + 1, y, -z + 3/2$ for **3**; A = $x - 1, -y + 1/2, z - 1/2$ for **4**; A = $x, y - 1, z$; B = $-x + 2, -y, -z + 1$ for **5**; A = $-x + 2, y, -z + 1/2$ for **6**; A = $x - 1/2, -y + 1/2, z - 1/2$ for **7**; A = $x, -y + 3/2, z - 1/2$ for **8**; A = $-x + 1, y - 1/2, -z + 3/2$; B = $-x, -y + 1, -z + 1$ for **9**.