Construction of a series of Metal–Organic Frameworks with one neutral tetradentate ligand and rigid carboxylate co-ligand

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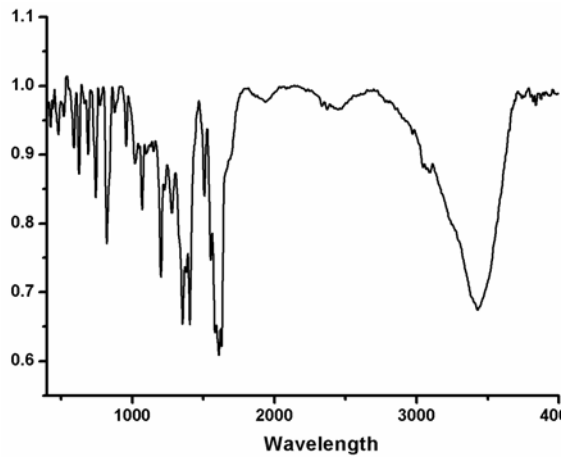

Figure S1. IR spectra of complex **1**

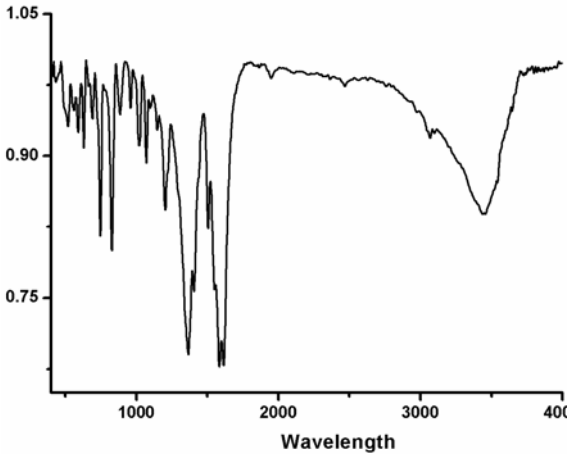

Figure S2. IR spectra of complex **2**

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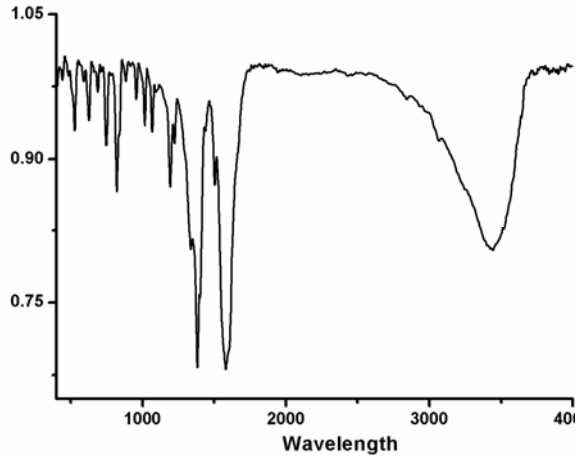


Figure S3. IR spectra of complex **3**

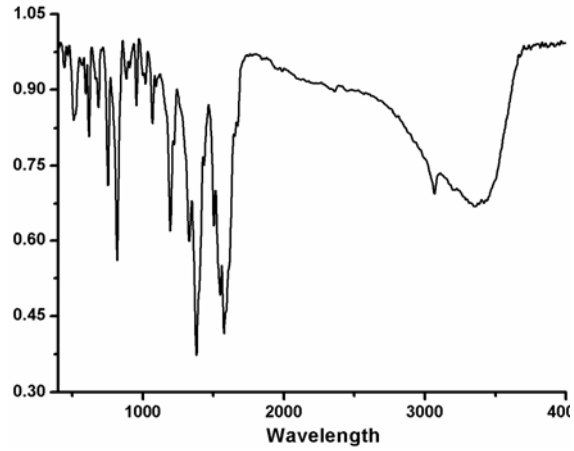


Figure S4. IR spectra of complex **4**

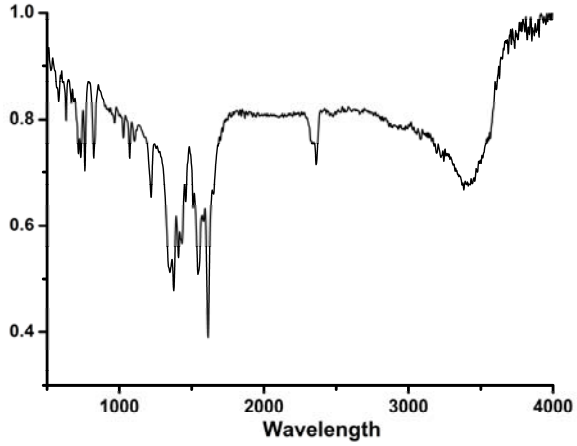


Figure S5. IR spectra of complex **5**

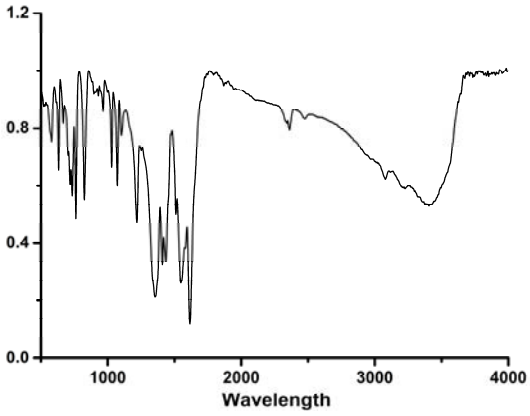


Figure S6. IR spectra of complex **6**

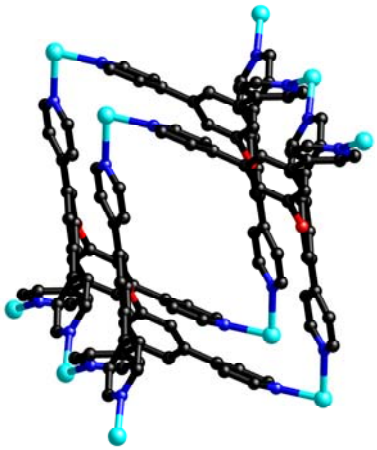
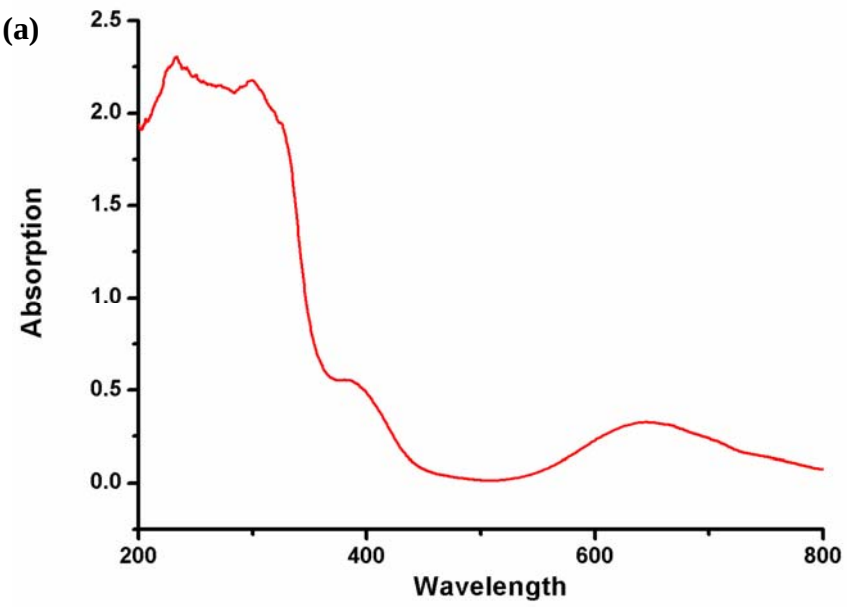


Figure S7 Views of the 1D chain by L ligands and Zn ions.



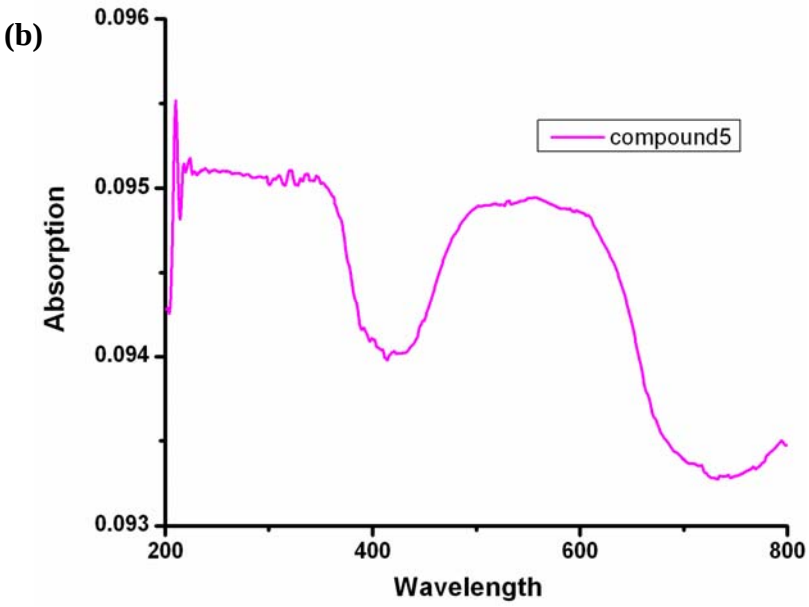


Figure S8. UV-vis absorbance spectra of **4 (a)** and **5** (b) at room temperature.

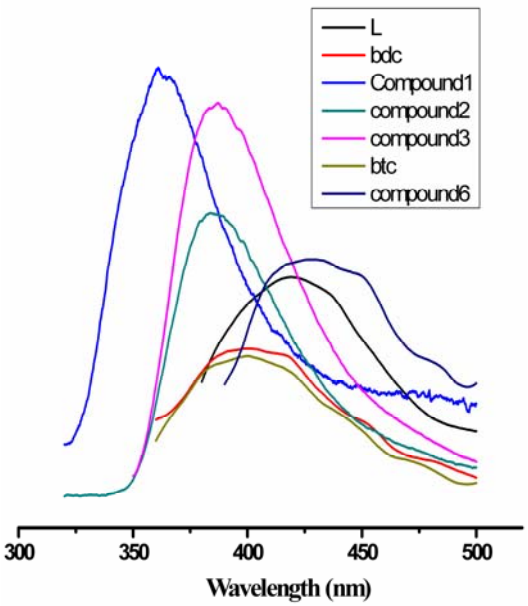


Figure S9. Solid-state photoluminescent spectra of **1-3**, **6**, and corresponding ligands at room temperature.

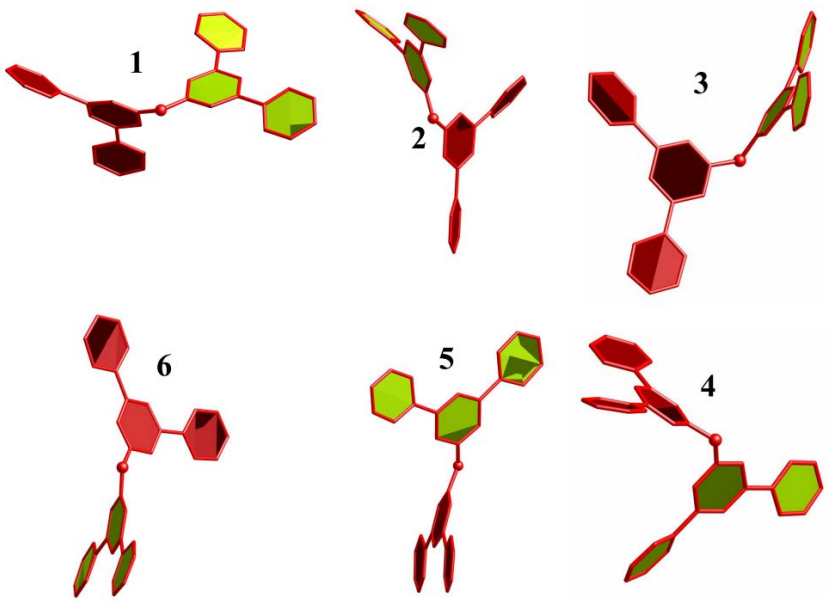


Figure S10. The conjugation degree of benzene ring and pyridine ring in the neutral tetradentate N-containing ligand.

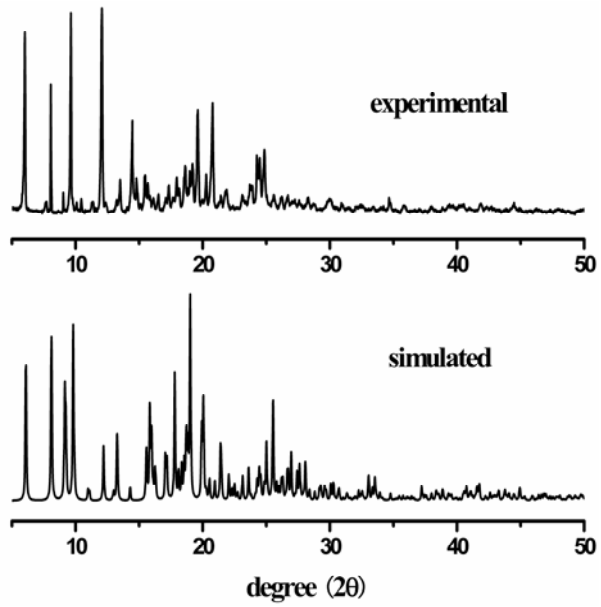


Figure S11. Powder X-ray diffraction patterns of complex **1**

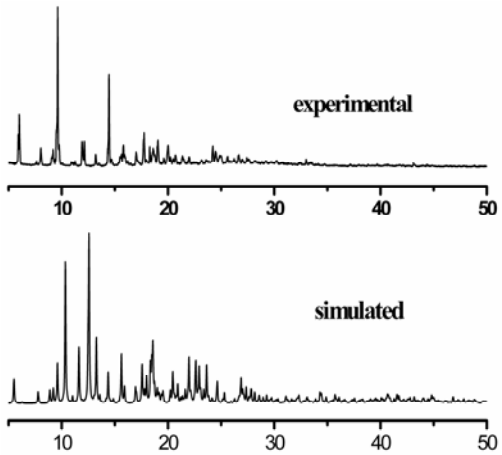


Figure S12. Powder X-ray diffraction patterns of complex **2**

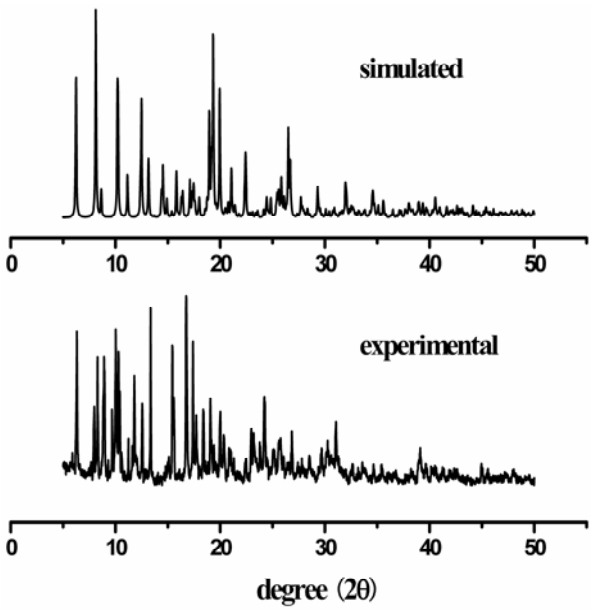


Figure S13. Powder X-ray diffraction patterns of complex **3**

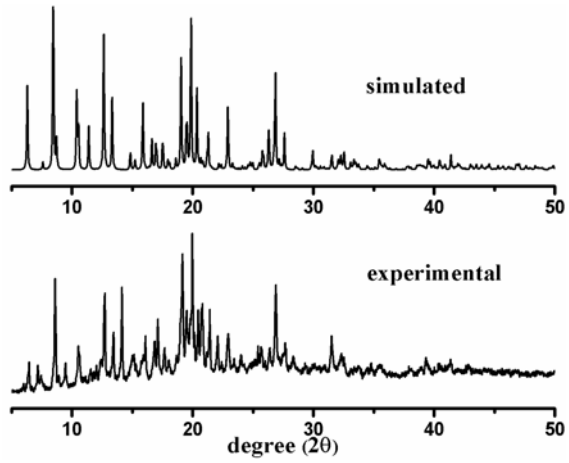


Figure S14. Powder X-ray diffraction patterns of complex **4**

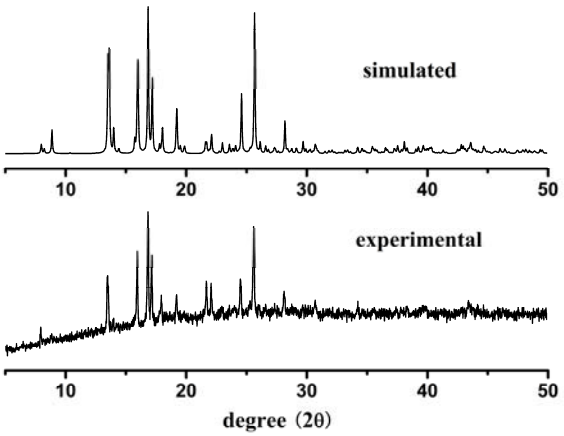


Figure S15. Powder X-ray diffraction patterns of complex **5**

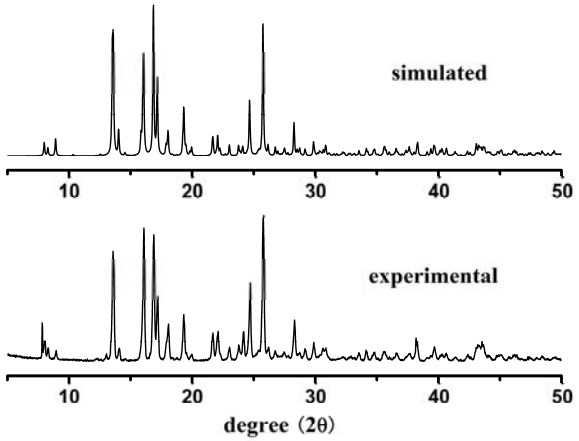


Figure S16. Powder X-ray diffraction patterns of complex **6**

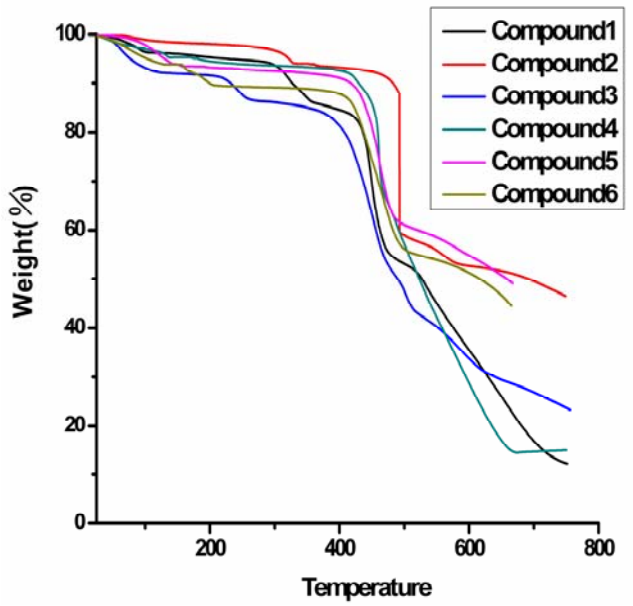


Figure S17. The TGA diagrams of complexes 1- 6.

Table S1. Selected Bond Lengths (Å) and Angles (deg) for Complexes **1**-**6**.

Complex **1**

Zn1-N1	2.053(3)	Zn1- N2^{a}	2.050(3)
Zn1-O2	1.924(2)	Zn1-O4	1.932(2)
N1- Zn1- N2^{a}	102.70(11)	N1- Zn1-O2	120.23(11)
N1- Zn1-O4	110.85(11)	N2^{a} - Zn1- O2	111.28(12)
N2^{a} - Zn1-O4	113.59(12)	O2- Zn1-O4	98.70(11)

Complex **2**

Zn1-N1	2.018(8)	Zn1-N3^{a}	2.041(8)
Zn1-O4	1.935(6)	Zn1-O7	1.919(6)
Zn2- N2^{b}	2.107(6)	Zn2- N4^{c}	2.263(7)
Zn2- O2	2.022(6)	Zn2- O6	1.981(7)
Zn2- O1w	2.202(6)	N1 -Zn1- N3^{a}	106.0(3)
N1 -Zn1- O4	104.0(3)	N1 -Zn1- O7	124.5(4)
N3^{a} -Zn1- O4	96.8(3)	N3^{a} -Zn1- O7	106.6(3)
O4 -Zn1- O7	115.1(3)	N2^{b} –Zn2- N4^{c}	87.6(2)
N2^{b} –Zn2- O2	148.7(3)	N2^{b} –Zn2- O6	109.7(3)
N2^{b} –Zn2- O1w	90.6(2)	N4^{c} –Zn2- O2	92.2(2)
N4^{c} –Zn2- O6	90.2(3)	N4^{c} –Zn2- O1w	177.2(3)
O2 –Zn2- O6	101.6(3)	O2 –Zn2- O1w	88.2(2)
O6 –Zn2- O1w	92.4(3)		

Complex **3**

Cd1-N1	2.362(4)	Cd1-N4^{a}	2.322(4)
Cd1-O1	2.330(3)	Cd1-O3^{c}	2.214(3)
Cd1-O4^{b}	2.291(3)	Cd1-O1w	2.313(3)
N1-Cd1- N4^{a}	168.08(16)	N1-Cd1- O1	83.24(12)
N1-Cd1- O3^{c}	87.68(15)	N1-Cd1- O4^{b}	81.74(13)
N1-Cd1- O1w	94.64(13)	N4^{a}-Cd1- O1	89.85(13)
N4^{a} -Cd1- O3^{c}	101.69(15)	N4^{a} -Cd1- O4^{b}	88.56(15)
N4^{a} -Cd1- O1w	93.86(15)	O1-Cd1- O3^{c}	160.63(11)
O1-Cd1- O4^{b}	89.80(11)	O1 -Cd1- O1w	81.10(11)
O3^{c} -Cd1- O4^{b}	105.83(13)	O3^{c} -Cd1- O1w	82.62(13)
O4^{b} -Cd1- O1w	170.57(11)		

Complex **4**

Ni1-N1	2.117(3)	Ni1-N3^{a}	2.093(3)

Ni1-O2	2.100(2)	Ni1-O4^{b}	2.024(2)
Ni1-O5^{c}	2.060(2)	Ni1-O6	2.066(2)
N1- Ni1- N3^{a}	173.68(11)	N1- Ni1- O2	86.32(10)
N1- Ni1- O4^{b}	88.67(11)	N1- Ni1- O5^{c}	85.71(11)
N1- Ni1- O6	93.76(11)	N3^{a}- Ni1- O2	89.98(10)
N3^{a} - Ni1- O4^{b}	95.67(11)	N3^{a} - Ni1- O5^{c}	89.22(11)
N3^{a} - Ni1- O6	91.12(11)	O2- Ni1- O4^{b}	170.68(9)
O2- Ni1- O5^{c}	90.79(9)	O2 - Ni1- O6	86.38(9)
O4^{b} - Ni1- O5^{c}	96.67(10)	O4^{b} - Ni1- O6	86.11(10)
O5^{c} - Ni1- O6	177.14(9)		

Complex **5**

Co1-N1	2.018(2)	Co1-N1^{a}	2.018(2)
Co1-O1	1.914(2)	Co1-O1^{a}	1.914(2)
Co2- N2^{c}	2.105(3)	Co2- O5^{b}	2.114(2)
Co2- O6^{b}	2.188(2)	Co2- O4	2.060(2)
Co2- O1w	2.158(3)	Co2- O2w	2.135(2)
N1 -Co1- N1^{a}	103.97(15)	N1 -Co1- O1	121.61(11)
N1 -Co1- O1^{a}	98.48(10)	N1^{a} -Co1- O1	98.48(10)
N1^{a} -Co1- O1^{a}	121.61(11)	O1 -Co1- O1^{a}	113.91(15)
N2^{c} –Co2- O5^{b}	158.54(9)	N2^{c} –Co2- O6^{b}	98.09(9)
N2^{c} –Co2- O4	100.54(9)	N2^{c} –Co2- O1w	90.21(10)
N2^{c} –Co2- O2w	90.00(10)	O5^{b} –Co2- O6^{b}	60.48(8)
O5^{b} –Co2- O4	100.92(9)	O5^{b} –Co2- O1w	91.26(10)
O5^{b} –Co2- O2w	90.13(10)	O6^{b} –Co2- O4	161.16(9)
O6^{b} –Co2- O1w	97.07(10)	O6^{b} –Co2- O2w	87.20(9)
O4 –Co2- O1w	85.66(9)	O4 –Co2- O2w	90.03(9)
O1w –Co2- O2w	175.65(9)		

Complex **6**

Zn1-N1	2.026(3)	Zn1-N1[a]	2.026(3)
Zn1-O2	1.906(3)	Zn1-O2[a]	1.906(3)
Zn2- N2[b]	2.066(4)	Zn2- O4	2.041(3)
Zn2- O5	2.334(3)	Zn2- O7[c]	2.002(3)
Zn2- O8	2.183(3)	Zn2- O9	2.208(3)
N1 -Zn1- N1[a]	104.5(2)	N1 -Zn1- O2	121.37(14)
N1 -Zn1- O2[a]	98.76(14)	N1[a] -Zn1- O2	98.76(14)
N1[a] -Zn1- O2[a]	121.37(14)	O2 -Zn1- O2[a]	113.3(2)
N2[b] –Zn2- O5	93.59(13)	N2[b] –Zn2- O4	152.41(14)
N2[b] –Zn2- O7[c]	104.56(13)	N2[b] –Zn2- O8	90.30(13)
N2[b] –Zn2- O9	89.18(13)	O4 –Zn2- O5	58.84(12)
O4 –Zn2- O7[c]	102.94(13)	O4 –Zn2- O8	92.81(14)
O4 –Zn2- O9	88.22(13)	O5 –Zn2- O7[c]	160.78(13)
O5 –Zn2- O8	98.32(12)	O5 –Zn2- O9	82.95(12)
O7[c] –Zn2- O8	85.66(9)	O7[c] –Zn2- O9	90.91(12)
O8 –Zn2- O9	178.66(11)		

Symmetry codes: for **1:** a = *x*, 2 - *y*, 1/2 + *z*. for **2:** a = -1 + *x*, -1 + *y*, *z*; b = *x*, -1 + *y*, -1 + *z*; c = 1 - *x*, - *y*, - *z*.; for **3:** a = -1 + *x*, *y*, 1 + *z*; b = *x*, -1/2 - *y*, 1/2 + *z*; c = 1 - *x*, 1/2 + *y*, 5/2 - *z*.; for **4:** a = -1 + *x*, *y*, 1 + *z*; b = 1 - *x*, -1/2 + *y*, 3/2 - *z*; c = *x*, 1/2 - *y*, 1/2 + *z*. for **5**: a = 1 - *x*, *y*, 0.5 - *z*; b = *x*, - *y*, -0.5 + *z*; c = 0.5 - *x*, 1.5 - *y*, - *z*. for **6:** a = 1 - *x*, *y*, 1.5 - *z*; b = 1.5 - *x*, -1.5 + *y*, 1.5 - *z*; c = *x*, - *y*, -0.5 + *z*.