Electronic Supplementary Information (ESI) for

Hydrothermal Syntheses, Structural Characterizations, and Magnetic Properties of Five MOFs Assembled From C_2-Symmetric Ligand of 1,3-Di((2',4'-dicarboxylphenyl)benzene with Various Coordination Modes

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ESI

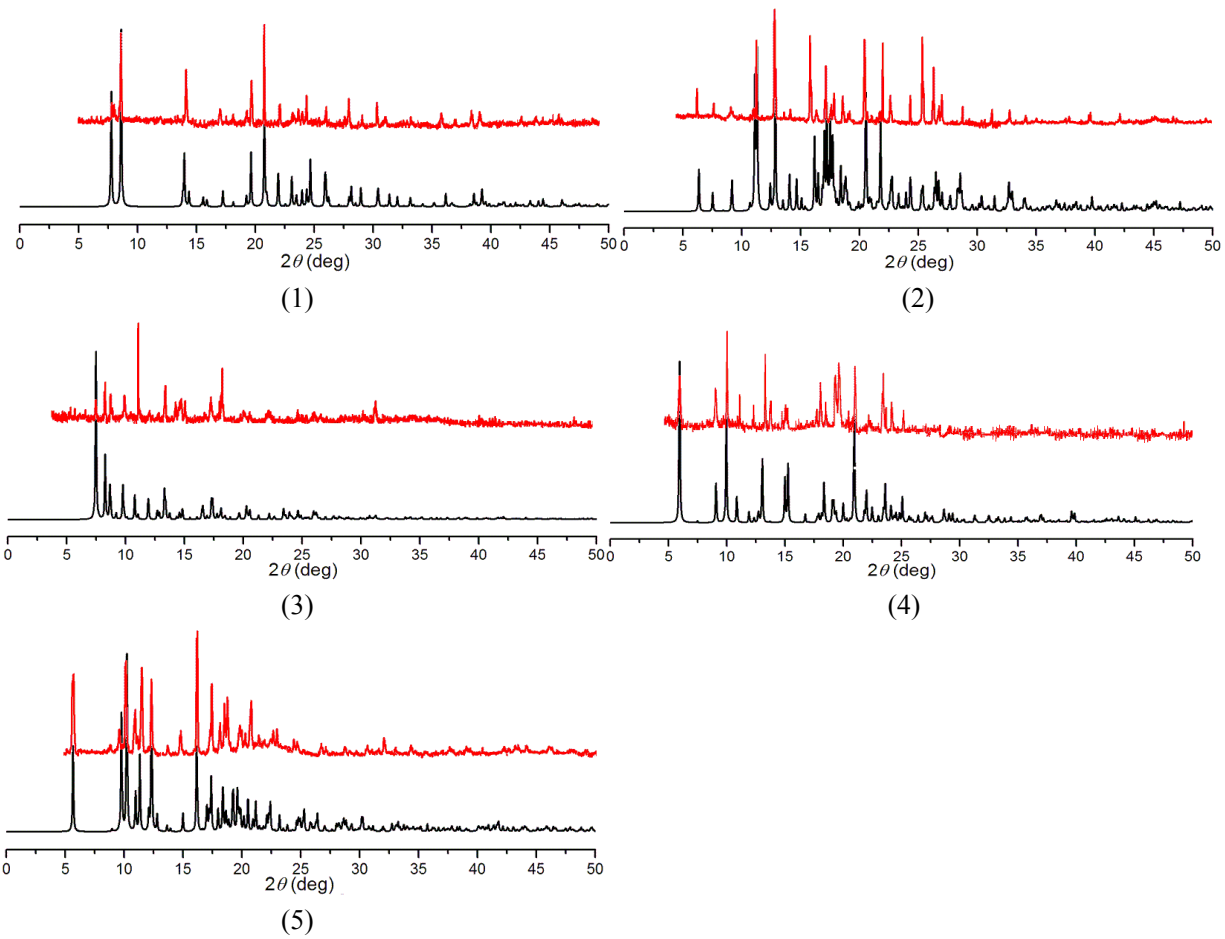
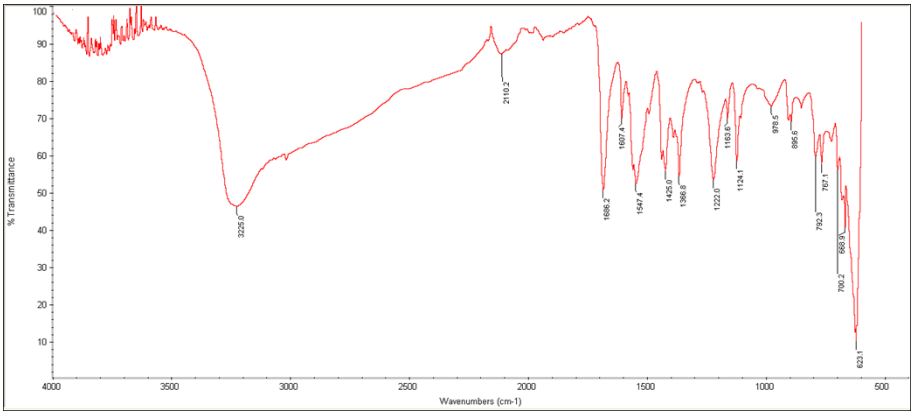


Figure S1. PXRD patterns of **1-5**. Dark: calculated from the X-ray single-crystal data; Red: observed for the as-synthesized solids.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Wavenumbers (cm-1)
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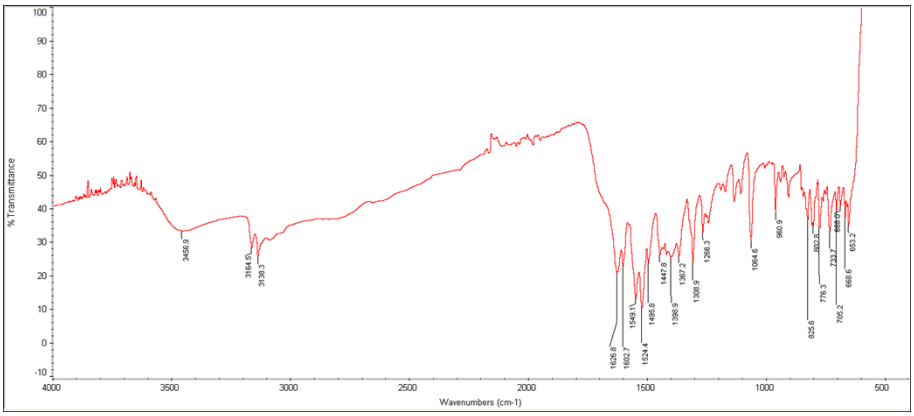
2119.2
1686.2
1607.4
1547.4
1425.0
1386.8
1222.0
1163.6
1124.1
978.5
895.6
792.3
761.1
700.2
688.9
623.1

(1)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Wavenumbers (cm-1)
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3139.3
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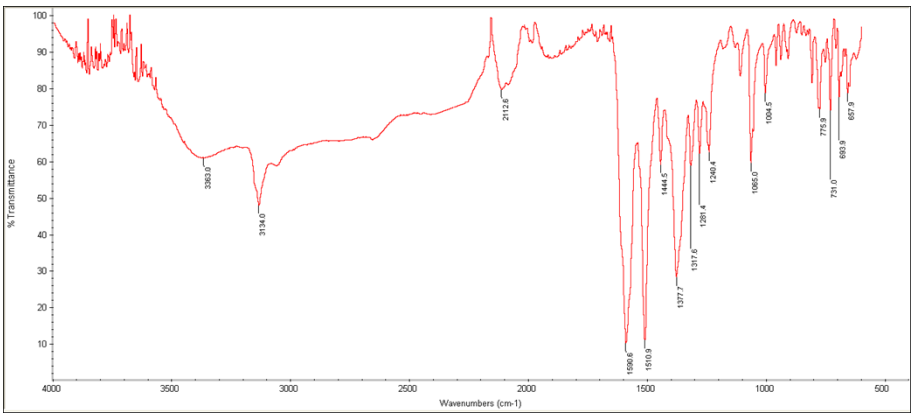
1495.6
1447.8
1398.9
1367.2
1308.9
1266.3
1094.6
980.9
825.6
802.6
776.3
733.2
705.2
668.6
653.2

(2)


% Transmittance
Wavenumbers (cm-1)
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1596.6
1510.9
1444.5
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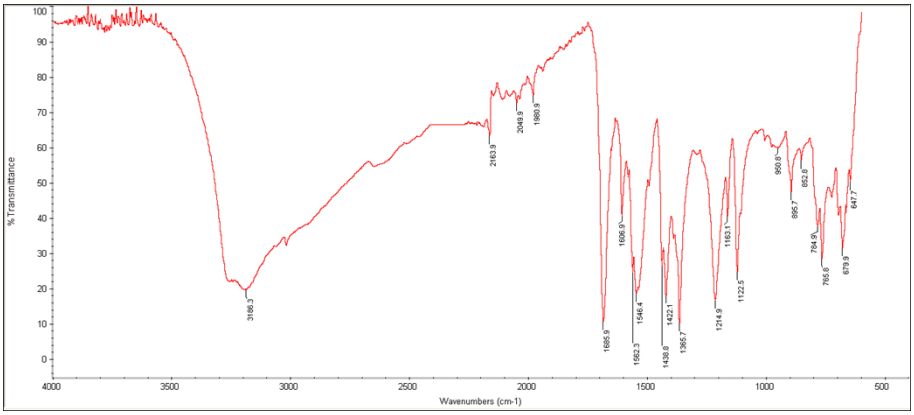
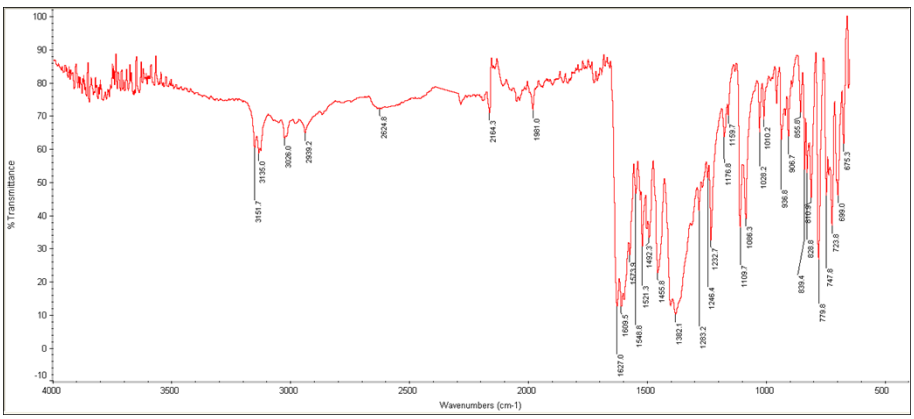
1085.0
1004.5
776.9
731.0
693.9
667.9

(3)



(4)



(5)

Figure S2. The IR spectra of complexes **1**-**5**.

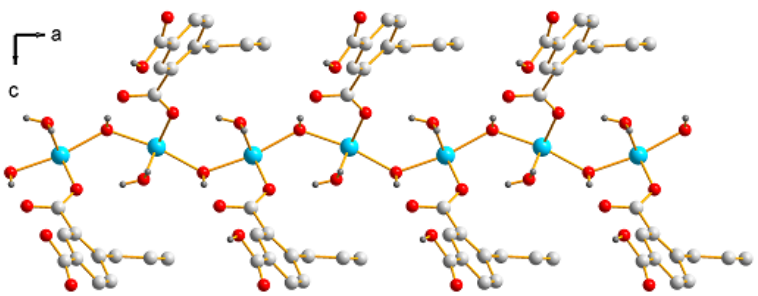


Figure S3. The 1D infinite $[Ni(H_2DDB)(H_2O)_2(\mu_2\text{-}H_2O)]_n$ chain in **1** view along *b* axis.

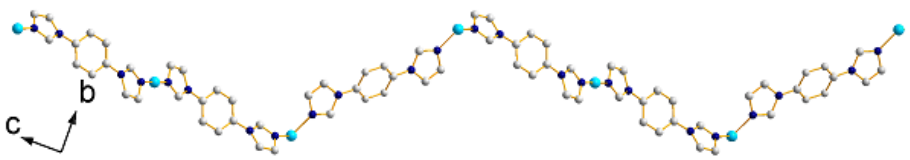


Figure S4. The 1D $[Ni(1,4\text{-bib})]_n$ zigzag chain in **2** view along *a* axis.

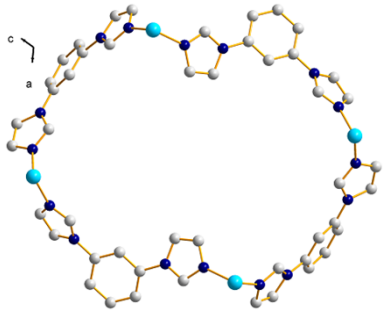


Figure S5. The interestingly $[Ni_4(1,3\text{-bib})_4]$ loop in **3**.

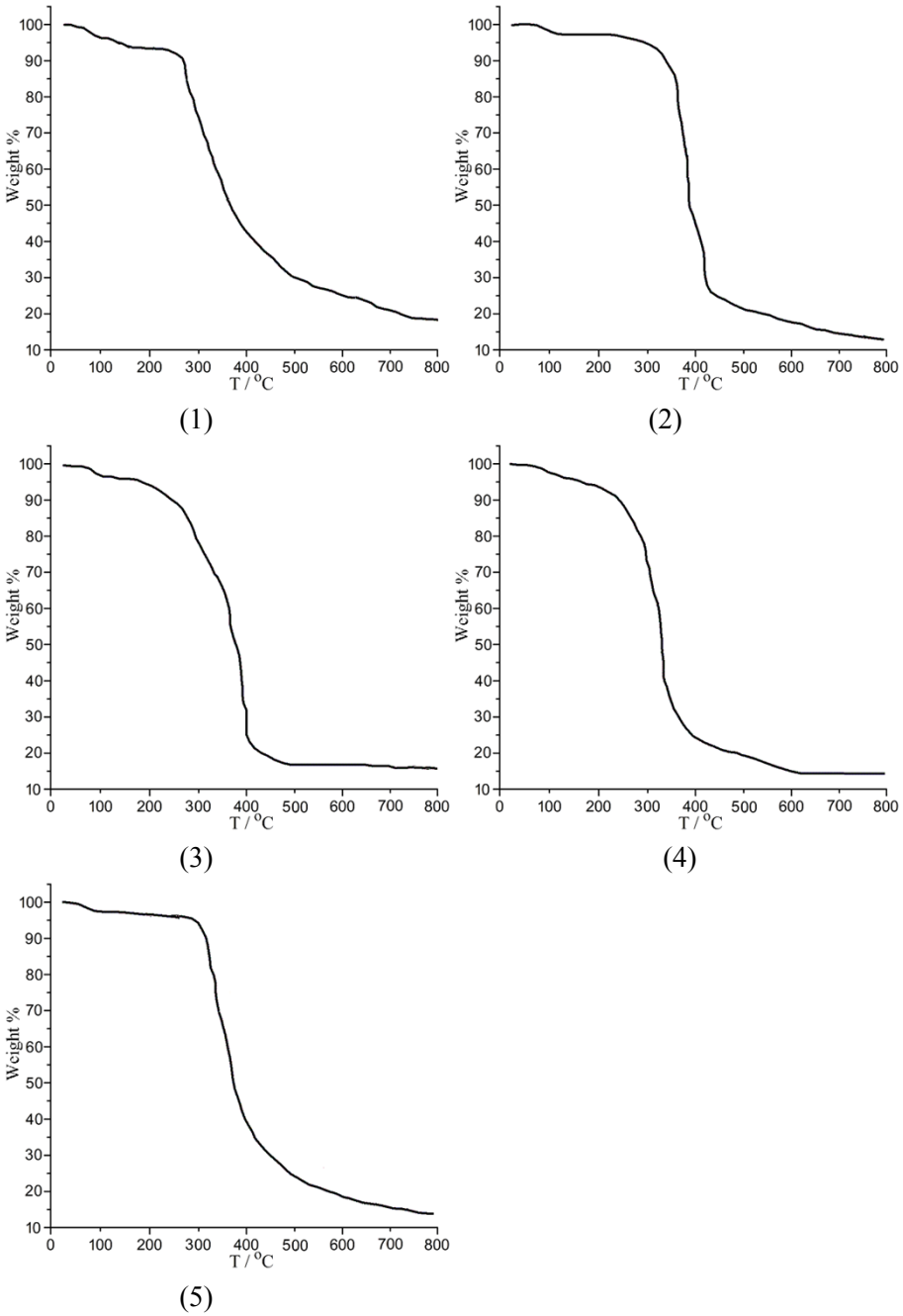


Figure S6. TG curves of **1**-**5**.

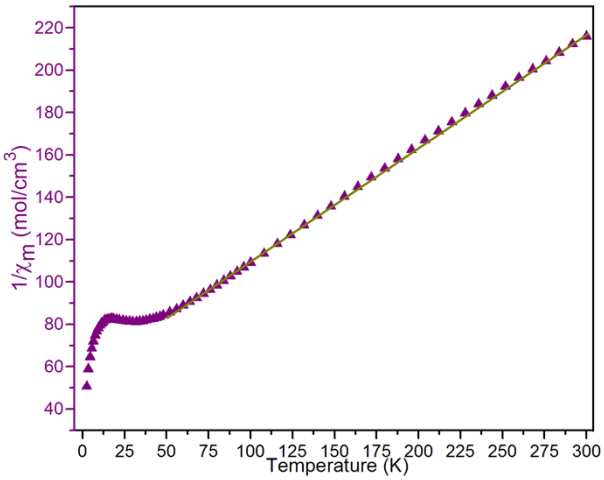


Figure S7. The χ_M^{-1}-T of **1** under a static field of 1000 Oe.

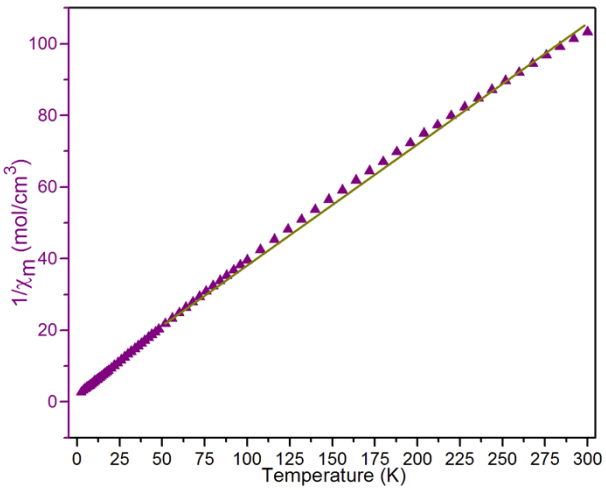


Figure S8. The χ_M^{-1}-T of **3** under a static field of 1000 Oe.

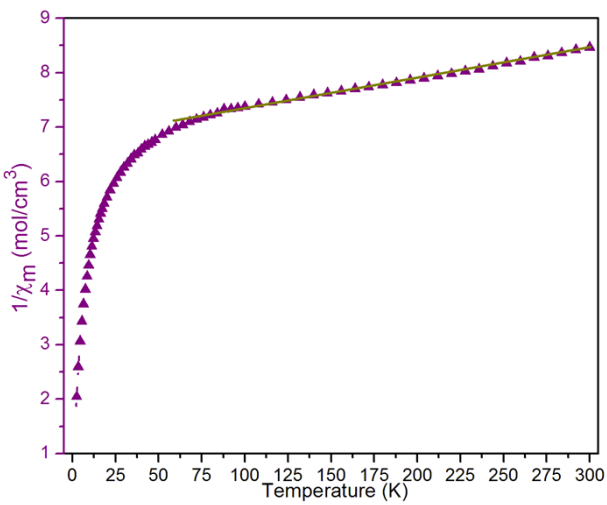


Figure S9. The χ_M^{-1}-T of **5** under a static field of 1000 Oe.

Table S1 Selected bond lengths (Å) and angles (°) for **1 – 5**.

Complex **1**							
Ni(1)-O(6)	2.0208(13)	Ni(1)-O(1)	2.0483(12)	Ni(1)-O(5)	2.1032(18)	O(6)$^{\#1}$-Ni(1)-O(6)	93.93(8)
O(6)-Ni(1)-O(1)$^{\#1}$	175.21(6)	O(1)$^{\#1}$-Ni(1)-O(1)	85.71(7)	O(1)-Ni(1)-O(5)	94.82(5)	O(1)$^{\#1}$-Ni(1)-O(5)$^{\#2}$	92.14(5)
O(6)-Ni(1)-O(1)$^{\#1}$	90.13(5)	O(6)-Ni(1)-O(5)	87.87(5)	O(6)-Ni(1)-O(5)$^{\#2}$	85.64(5)	O(1)-Ni(1)-O(5)$^{\#2}$	92.14(5)
O(6)$^{\#1}$-Ni(1)-O(1)	90.13(5)	O(6)$^{\#1}$-Ni(1)-O(5)	87.87(5)	O(6)$^{\#1}$-Ni(1)-O(5)$^{\#2}$	85.64(5)	O(5)-Ni(1)-O(5)$^{\#2}$	170.49(4)
O(6)-Ni(1)-O(1)	175.21(6)	O(1)$^{\#1}$-Ni(1)-O(5)	94.82(5)				
Symmetry codes: #1 *x*, -*y*+3/2, *z*; #2 *x*+1/2, *y*, -*z*+1/2.							
Complex **2**							
N(1)-Ni(1)	2.0398(16)	Ni(1)-O(8)$^{\#2}$	2.1059(14)	Ni(2)-O(9)	2.0693(15)	Ni(2)-O(4)	2.1028(13)
N(6)-Ni(2)	2.0787(13)	Ni(1)-O(8)$^{\#3}$	2.1059(14)	Ni(2)-N(4)$^{\#4}$	2.0717(15)	Ni(2)-O(3)	2.1671(13)
Ni(1)-O(2)	2.0787(13)	Ni(2)-N(6)	2.0536(17)	Ni(2)-O(5)	2.0745(14)	N(1)$^{\#1}$-Ni(1)-N(1)	180.0
N(1)$^{\#1}$-Ni(1)-O(2)$^{\#1}$	89.33(6)	O(2)$^{\#1}$-Ni(1)-O(8)$^{\#2}$	94.85(6)	N(6)-Ni(2)-O(9)	98.83(7)	O(9)-Ni(2)-O(4)	99.51(6)
N(1)-Ni(1)-O(2)$^{\#1}$	90.67(6)	O(2)-Ni(1)-O(8)$^{\#2}$	85.15(6)	N(6)-Ni(2)-N(4)$^{\#4}$	99.39(7)	N(4)$^{\#4}$-Ni(2)-O(4)	88.24(6)
N(1)$^{\#1}$-Ni(1)-O(2)	90.67(6)	N(1)$^{\#1}$-Ni(1)-O(8)$^{\#3}$	93.28(6)	O(9)-Ni(2)-N(4)$^{\#4}$	93.00(6)	O(5)-Ni(2)-O(4)	83.51(6)
N(1)-Ni(1)-O(2)	89.33(6)	N(1)-Ni(1)-O(8)$^{\#3}$	86.72(6)	N(6)-Ni(2)-O(5)	88.03(6)	N(6)-Ni(2)-O(3)	99.31(6)
O(2)$^{\#1}$-Ni(1)-O(2)	180.0	O(2)$^{\#1}$-Ni(1)-O(8)$^{\#3}$	85.15(6)	O(9)-Ni(2)-O(5)	89.61(6)	O(9)-Ni(2)-O(3)	160.89(6)
N(1)$^{\#1}$-Ni(1)-O(8)$^{\#2}$	86.72(6)	O(2)-Ni(1)-O(8)$^{\#3}$	94.85(6)	N(4)$^{\#4}$-Ni(2)-O(5)	171.66(6)	N(4)$^{\#4}$-Ni(2)-O(3)	89.97(6)
N(1)-Ni(1)-O(8)$^{\#2}$	93.28(6)	O(8)$^{\#2}$-Ni(1)-O(8)$^{\#3}$	180.000(1)	N(6)-Ni(2)-O(4)	159.71(6)	O(5)-Ni(2)-O(3)	85.03(5)
O(4)-Ni(2)-O(3)	61.68(5)						
Symmetry codes: #1 -*x*+2, -*y*+1, -*z*+1; #2 -*x*+3/2, *y*+1/2, -*z*+1/2; #3 *x*+1/2, -*y*+1/2, *z*+1/2; #4 *x*+1, *y*, *z*.							
Complex **3**							
N(1)-Ni(2)	2.069(3)	O(9)-Ni(1)	2.063(2)	Ni(1)-N(4)$^{\#1}$	2.070(3)	Ni(2)-O(5)$^{\#1}$	2.059(2)
N(7)-Ni(1)	2.072(3)	O(9)-Ni(2)	2.098(2)	Ni(1)-O(4)$^{\#1}$	2.188(2)	Ni(2)-O(7)$^{\#6}$	2.068(2)
O(1)-Ni(1)	2.056(2)	Ni(1)-O(6)$^{\#1}$	2.050(2)	Ni(2)-N(5)$^{\#5}$	2.057(3)	Ni(2)-O(4)$^{\#1}$	2.179(2)
O(6)$^{\#1}$-Ni(1)-O(1)	176.48(9)	O(9)-Ni(1)-N(7)	88.87(10)	N(5)$^{\#5}$-Ni(2)-O(7)$^{\#6}$	89.41(10)	O(7)$^{\#6}$-Ni(2)-O(9)	89.84(8)
O(6)$^{\#1}$-Ni(1)-O(9)	88.41(9)	N(4)$^{\#1}$-Ni(1)-N(7)	91.40(11)	O(5)$^{\#1}$-Ni(2)-O(7)$^{\#6}$	89.13(9)	N(1)-Ni(2)-O(9)	86.32(10)
O(1)-Ni(1)-O(9)	95.11(9)	O(6)$^{\#1}$-Ni(1)-O(4)$^{\#1}$	91.18(8)	N(5)$^{\#5}$-Ni(2)-N(1)	91.23(12)	N(5)$^{\#5}$-Ni(2)-O(4)$^{\#1}$	106.88(9)
O(6)$^{\#1}$-Ni(1)-N(4)$^{\#1}$	85.97(10)	O(1)-Ni(1)-O(4)$^{\#1}$	89.71(9)	O(5)$^{\#1}$-Ni(2)-N(1)	174.84(10)	O(5)$^{\#1}$-Ni(2)-O(4)$^{\#1}$	83.34(9)
O(1)-Ni(1)-N(4)$^{\#1}$	90.51(9)	O(9)-Ni(1)-O(4)$^{\#1}$	74.78(8)	O(7)$^{\#6}$-Ni(2)-N(1)	89.76(10)	O(7)$^{\#6}$-Ni(2)-O(4)$^{\#1}$	161.09(9)
O(9)-Ni(1)-N(4)$^{\#1}$	174.37(9)	N(4)$^{\#1}$-Ni(1)-O(4)$^{\#1}$	104.98(9)	N(5)$^{\#5}$-Ni(2)-O(9)	177.45(10)	N(1)-Ni(2)-O(4)$^{\#1}$	99.20(9)
O(6)$^{\#1}$-Ni(1)-N(7)	89.30(10)	N(7)-Ni(1)-O(4)$^{\#1}$	163.62(10)	O(5)$^{\#1}$-Ni(2)-O(9)	98.72(9)	O(9)-Ni(2)-O(4)$^{\#1}$	74.28(8)
O(1)-Ni(1)-N(7)	90.81(10)	N(5)$^{\#5}$-Ni(2)-O(5)$^{\#1}$	83.71(10)				
Symmetry codes: #1 -*x*+2, -*y*+1, -*z*-1; #5 *x*, -*y*+1, *z*-1/2; #6 *x*+1/2, -*y*+1/2, *z*+1/2.							
Complex **4**							
Cu(1)-O(4)$^{\#1}$	2.030(3)	Cu(1)-O(3)	2.032(3)	Cu(1)-O(6)$^{\#1}$	2.046(3)	Cu(1)-O(5)	2.051(3)
Cu(1)-N(1)	2.029(3)	O(4)$^{\#1}$-Cu(1)-N(1)	94.65(12)	O(4)$^{\#1}$-Cu(1)-O(3)	164.10(11)	N(1)-Cu(1)-O(3)	101.24(12)
O(4)$^{\#1}$-Cu(1)-O(6)$^{\#1}$	87.54(11)	O(3)-Cu(1)-O(6)$^{\#1}$	89.18(11)	N(1)-Cu(1)-O(5)	95.64(13)	O(6)$^{\#1}$-Cu(1)-O(5)	164.67(12)
N(1)-Cu(1)-O(6)$^{\#1}$	99.68(13)	O(4)$^{\#1}$-Cu(1)-O(5)	90.73(12)	O(3)-Cu(1)-O(5)	88.33(12)		
Symmetry code: #1 -*x*+1, -*y*+2, -*z*+1.							
Complex **5**							
O(2)-Cu(1)	1.995(2)	Cu(1)-O(5)$^{\#1}$	1.957(3)	Cu(1)-N(1)$^{\#2}$	2.123(3)	Cu(2)-N(3)$^{\#3}$	1.963(3)
O(6)-Cu(1)	1.953(2)	Cu(1)-O(1)$^{\#1}$	1.978(3)	Cu(2)-N(3)	1.963(3)	Cu(2)-O(8)$^{\#3}$	1.997(3)
O(8)-Cu(2)	1.997(3)	O(5)$^{\#1}$-Cu(1)-O(2)	90.05(11)	O(1)$^{\#1}$-Cu(1)-N(1)$^{\#2}$	98.67(12)	N(3)$^{\#3}$-Cu(2)-O(8)	92.29(13)
O(6)-Cu(1)-O(5)$^{\#1}$	166.73(11)	O(1)$^{\#1}$-Cu(1)-O(2)	167.00(11)	O(2)-Cu(1)-N(1)$^{\#2}$	94.33(12)	N(3)-Cu(2)-O(8)$^{\#3}$	92.29(13)
O(6)-Cu(1)-O(1)$^{\#1}$	89.73(10)	O(6)-Cu(1)-N(1)$^{\#2}$	96.27(12)	N(3)-Cu(2)-N(3)$^{\#3}$	180.00(15)	N(3)$^{\#3}$-Cu(2)-O(8)$^{\#3}$	87.71(13)
O(5)$^{\#1}$-Cu(1)-O(1)$^{\#1}$	88.55(11)	O(5)$^{\#1}$-Cu(1)-N(1)$^{\#2}$	97.00(13)	N(3)-Cu(2)-O(8)	87.71(13)	O(8)-Cu(2)-O(8)$^{\#3}$	180.00(12)
O(6)-Cu(1)-O(2)	88.67(10)						
Symmetry codes: #1 -*x*+1, -*y*+1, -*z*+2; #2 -*x*+1/2, *y*+1/2, -*z*+3/2; #3 -*x*+1, -*y*+1, -*z*+1.							

Table S2 The hydrogen bonds in complex **1**.

Donor--H···Acceptor	d(D---A) (Å)	d(D---H) (Å)	d(H·····A) (Å)	∠DHA (°)
O(5)--H(1w)···O(2)$^{\#1}$	2.623	0.820	1.832	161.61
O(3)--H(3)···O(2)$^{\#2}$	2.751	0.820	1.960	161.74
O(6)--H(3w)···O(1)$^{\#3}$	2.716	0.858	1.862	172.67
O(3)--H(4w)···O(4)$^{\#4}$	2.699	0.840	1.868	161.81
C(8)--H(8)···O(3)$^{\#2}$	3.223	0.930	2.504	134.36
Symmetry codes: #1 *x*, -*y*+3/2, *z*; #2 -*x*, -*y*+1, -*z*+1; #3 *x*-1/2, *y*, -*z*+1/2; #4 -*x*+1/2, -*y*+1, *z*-1/2.				

Table S3 The hydrogen bonds in complex **4**.

Donor--H···Acceptor	d(D---A) (Å)	d(D---H) (Å)	d(H·····A) (Å)	∠DHA (°)
O(2)--H(2)···O(8)$^{\#1}$	2.636	0.820	1.834	165.54
O(7)--H(7A)···N(4)$^{\#2}$	2.558	0.820	1.758	165.54
C(27)--H(27)···O(4)$^{\#3}$	3.433	0.930	2.602	149.24
C(32) --H(32)···O(1)$^{\#3}$	3.074	0.930	2.472	122.55
C(4)$^{\#4}$--H(4)$^{\#4}$···O(3)	3.172	0.930	2.524	127.06
Symmetry codes: #1 -*x*+3/2, -*y*+2, *z*+1/2; #2 *x*, -*y*+1/2, *z*-1/2; #3 *x*, *y*-1, *z*; #4 -*x*+3/2, *y*-1/2, *z*.				