Two Novel Nickel(II) and Cobalt(II) Metal-Organic Frameworks Based on a Rigid Aromatic Multicarboxylate Ligand: Syntheses, Structural Characterization and Magnetic Properties

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Table S1 Selected bond lengths/Å and bond angles/°for complexes (**1**) and (**2**)

Complex 1

Ni1—O6^{i}	2.008 (3)	Ni2—O1W	2.075 (3)
Ni1—O12^{ii}	2.014 (3)	Ni2—O2W	2.100 (3)
Ni1—O3W	2.051 (3)	Ni2—O13	2.106 (3)
Ni1—O9	2.060 (3)	Ni3—O2	2.016 (3)
Ni1—O7	2.138 (3)	Ni3—O11^{v}	2.036 (3)
Ni1—O8	2.156 (3)	Ni3—O5^{vi}	2.036 (3)
Ni1—C28	2.464 (4)	Ni3—O3W^{vii}	2.072 (3)
Ni2—O16^{iii}	2.028 (3)	Ni3—O2W	2.072 (3)
Ni2—O1	2.035 (3)	Ni3—O13	2.108 (3)
Ni2—O4^{iv}	2.052 (3)	O4—Ni2^{iv}	2.052 (3)
O11—Ni3^{ix}	2.036 (3)	O5—C27	1.266 (5)
O3W—Ni3^{vii}	2.072 (3)	O5—Ni3^{viii}	2.036 (3)
O12—Ni1^{ii}	2.014 (3)	O6—Ni1^{i}	2.008 (3)
O16—Ni2^{iii}	2.028 (3)		
O6^{i}—Ni1—O12^{ii}	91.80 (13)	O3W—Ni1—O9	90.16 (10)
O6^{i}—Ni1—O3W	88.70 (11)	O6^{i}—Ni1—O7	90.81 (11)
O12^{ii}—Ni1—O3W	105.70 (11)	O12^{ii}—Ni1—O7	94.60 (12)

O6^{i}—Ni1—O9	178.60 (11)	O3W—Ni1—O7	159.71 (12)
O12^{ii}—Ni1—O9	87.72 (12)	O9—Ni1—O7	90.53 (11)
O6^{i}—Ni1—O8	87.30 (12)	O9—Ni1—C28	93.81 (12)
O12^{ii}—Ni1—O8	155.77 (12)	O7—Ni1—C28	30.37 (13)
O3W—Ni1—O8	98.49 (11)	O8—Ni1—C28	30.92 (13)
O9—Ni1—O8	93.67 (12)	O16^{iii}—Ni2—O1	175.65 (12)
O7—Ni1—O8	61.23 (12)	O16^{iii}—Ni2—O4^{iv}	91.36 (12)
O6^{i}—Ni1—C28	87.54 (12)	O1—Ni2—O4^{iv}	86.09 (12)
O12^{ii}—Ni1—C28	124.86 (14)	O16^{iii}—Ni2—O1W	86.17 (13)
O3W—Ni1—C28	129.38 (14)	O1—Ni2—O1W	90.22 (13)
O4^{iv}—Ni2—O1W	88.27 (14)	O1W—Ni2—O13	98.85 (13)
O16^{iii}—Ni2—O2W	93.14 (11)	O2W—Ni2—O13	78.91 (10)
O1—Ni2—O2W	90.57 (11)	O2—Ni3—O11^{v}	86.37 (12)
O4^{iv}—Ni2—O2W	94.01 (12)	O2—Ni3—O5^{vi}	178.36 (12)
O1W—Ni2—O2W	177.63 (13)	O11^{v}—Ni3—O5^{vi}	95.12 (11)
O16^{iii}—Ni2—O13	92.78 (11)	O2—Ni3—O3W^{vii}	89.67 (11)
O1—Ni2—O13	90.18 (11)	O11^{v}—Ni3—O3W^{vii}	97.10 (11)
O4^{iv}—Ni2—O13	171.98 (12)	O5^{vi}—Ni3—O3W^{vii}	89.45 (11)
O2—Ni3—O2W	93.04 (11)	O2W—Ni3—O13	79.47 (11)
O11^{v}—Ni3—O2W	92.75 (11)	C1—O1—Ni2	129.1 (3)
O5^{vi}—Ni3—O2W	87.59 (11)	C1—O2—Ni3	129.6 (3)
O3W^{vii}—Ni3—O2W	169.93 (10)	C8—O4—Ni2^{iv}	127.3 (3)
O2—Ni3—O13	88.60 (11)	C27—O5—Ni3^{viii}	135.0 (3)
O11^{v}—Ni3—O13	170.50 (11)	C27—O6—Ni1^{i}	127.5 (3)
O5^{vi}—Ni3—O13	90.03 (11)	C28—O7—Ni1	89.4 (3)

O3W^{vii}—Ni3—O13	90.91 (11)	C28—O8—Ni1	88.1 (3)
C29—O9—Ni1	126.1 (3)	Ni3^{vii}—O3W—H3WB	109.8
C36—O11—Ni3^{ix}	130.5 (3)	Ni3^{vii}—O3W—H3WA	109.6
C36—O12—Ni1^{ii}	128.7 (3)	Ni1—O3W—H3WB	109.8
C55—O13—Ni2	137.3 (3)	Ni3—O2W—Ni2	97.70 (12)
C55—O13—Ni3	125.3 (3)	Ni3—O2W—H2WA	112.1
Ni2—O13—Ni3	96.38 (11)	Ni2—O2W—H2WA	112.2
C56—O16—Ni2^{iii}	125.9 (3)	Ni3—O2W—H2WB	112.2
Ni2—O1W—H1WA	108 (4)	Ni2—O2W—H2WB	112.3

Symmetry codes: (i) −*x*+3, −*y*+3, −*z*; (ii) −*x*+3, −*y*+2, −*z*; (iii) −*x*+1, −*y*+2, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*−1, *y*−1, *z*; (vi) *x*−1, *y*, *z*; (vii) −*x*+2, −*y*+2, −*z*; (viii) *x*+1, *y*+1, *z*; (ix) *x*+1, *y*, *z*.

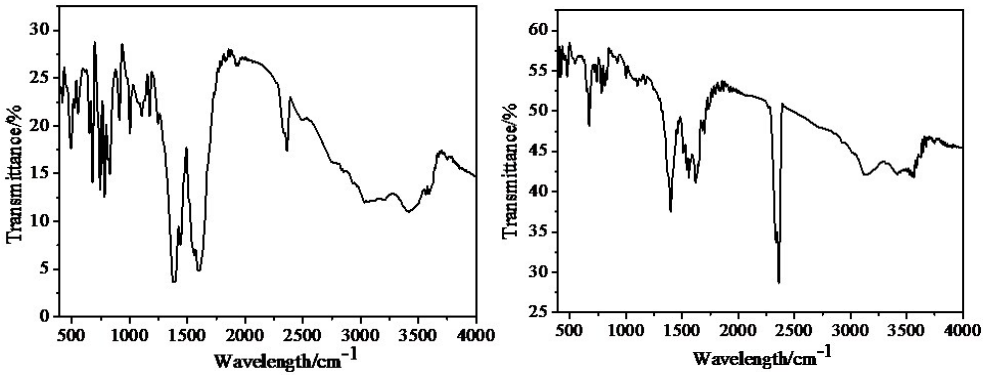
Complex 2

Co1—O1	2.014 (3)	Co2—O2^{iv}	2.045 (3)
Co1—O7^{i}	2.077 (3)	Co2—O2	2.045 (3)
Co1—O5^{ii}	2.096 (3)	Co2—O6^{ii}	2.128 (3)
Co1—O4^{iii}	2.100 (3)	Co2—O6^{v}	2.128 (3)
Co1—O1W	2.148 (4)	Co2—O2W	2.134 (3)
Co1—O2W	2.163 (3)	Co2—O2W^{iv}	2.134 (3)
O4—Co1^{vi}	2.100 (3)	C3—C4	1.386 (7)
O6—Co2^{ii}	2.128 (3)	O7—Co1^{vii}	2.077 (3)
O5—Co1^{ii}	2.096 (3)		

O1—Co1—O7^{i}	85.86 (14)	O1—Co1—O1W	89.43 (15)
O1—Co1—O5^{ii}	92.98 (14)	O7^{i}—Co1—O1W	90.26 (14)
O7^{i}—Co1—O5^{ii}	173.64 (13)	O5^{ii}—Co1—O1W	83.47 (14)
O1—Co1—O4^{iii}	173.53 (14)	O4^{iii}—Co1—O1W	84.29 (14)
O7^{i}—Co1—O4^{iii}	92.58 (13)	O1—Co1—O2W	98.34 (13)
O5^{ii}—Co1—O4^{iii}	87.88 (13)	O7^{i}—Co1—O2W	94.62 (11)
O5^{ii}—Co1—O2W	91.73 (12)	O2^{iv}—Co2—O6^{v}	94.53 (13)
O4^{iii}—Co1—O2W	88.04 (12)	O2—Co2—O6^{v}	168.42 (12)
O1W—Co1—O2W	171.09 (15)	O6^{ii}—Co2—O6^{v}	84.28 (18)

O2^{iv}—Co2—O2	88.9 (2)	O2^{iv}—Co2—O2W	81.39 (12)
O2^{iv}—Co2—O6^{ii}	168.42 (12)	O2—Co2—O2W	95.49 (12)
O2—Co2—O6^{ii}	94.53 (13)	O6^{ii}—Co2—O2W	87.28 (12)
O6^{v}—Co2—O2W	95.95 (11)	O2—Co2—O2W^{iv}	81.38 (12)
O2^{iv}—Co2—O2W^{iv}	95.49 (12)	O6^{ii}—Co2—O2W^{iv}	95.95 (11)

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



(a) The IR spectra for **1**. (b) The IR spectra for **2**.

Fig. S1. The IR spectra of the MOFs.

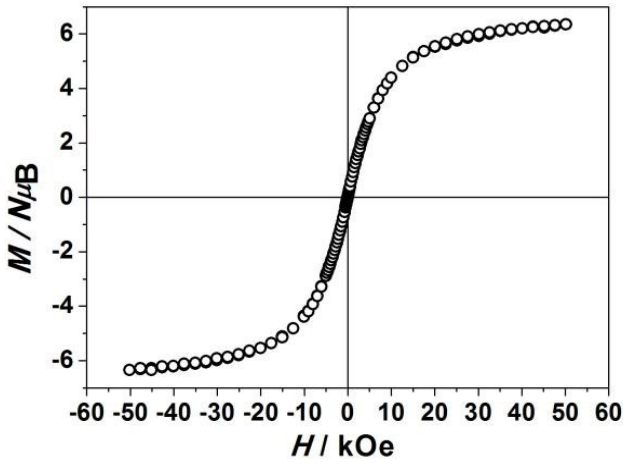


Fig. S2 The hysteresis loop for **1**.

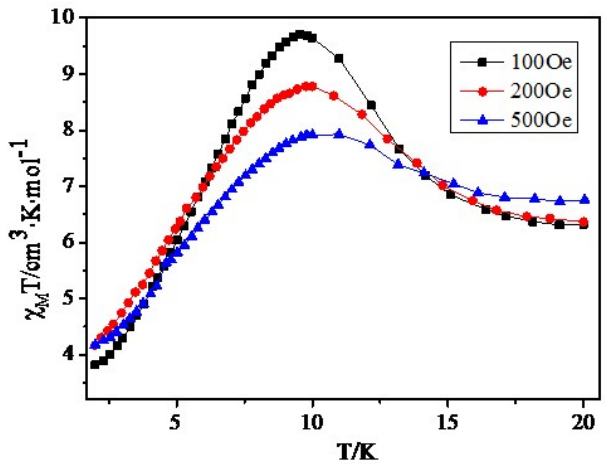


Fig. S3 The χ_MT vs. T plots of **2** at the indicated field.

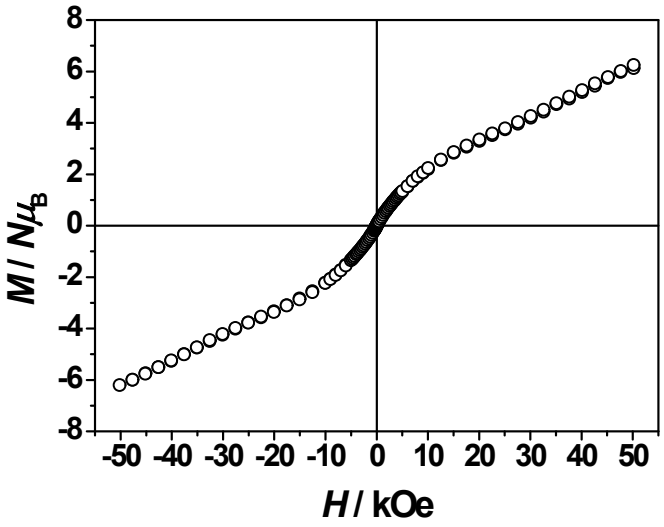


Fig. S4 The hysteresis loop for **2**.