Electronic Supplementary Material (ESI) for CrystEngComm.

Three Novel Metal-Organic Frameworks Based on an Unsymmetrical Rigid Carboxylate Ligand for Luminescence Sensing of Nitrobenzene Derivatives and Magnetic Properties

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Table S1. Selected bond lengths (Å) and angles (°) for complexes **1** -**3**.

Co1—O3	1.956 (3)	O6—Co1^{ii}	1.954 (3)
Co1—O6^{i}	1.954 (3)	C11—C12	1.504 (6)
Co1—N2	2.017 (4)	C12—C13	1.383 (5)
Co1—N5	2.005 (4)	C13—H13	0.9300
C7—C31^{iv}	1.335 (7)	C15—H15	0.9300
N5—C31	1.332 (6)	C15—C16	1.345 (6)
N5—C2^{iii}	1.312 (5)	C11—C12	1.504 (6)
O3—Co1—N2	115.26 (14)	O5—C14—C9	119.7 (4)
O3—Co1—N5	114.47 (14)	O6—C14—C9	115.6 (4)
O6^{i}—Co1—O3	111.97 (12)	N2—C15—H15	125.4
O6^{i}—Co1—N2	96.31 (14)	C16—C15—N2	109.2 (4)
O6^{i}—Co1—N5	109.00 (14)	C16—C15—H15	125.4
N5—Co1—N2	108.27 (15)	N3—C16—H16	126.3
C11—O3—Co1	108.4 (3)	C15—C16—H16	126.3
C14—O6—Co1^{ii}	117.5 (3)	N2—C17—N3	112.3 (4)

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

Cd1—O4	2.314 (6)	Cd2—O5^{iv}	2.568 (6)
Cd1—O3	2.597 (8)	Cd2—O5^{i}	2.568 (6)
Cd1—O2	2.251 (9)	Cd2—O6^{iv}	2.298 (7)
Cd1—O5^{i}	2.544 (7)	Cd2—O6^{i}	2.298 (7)
Cd1—N1	2.220 (8)	O5—Cd1^{v}	2.544 (7)
Cd1—C18^{ii}	2.355 (9)	O5—Cd2^{v}	2.568 (6)
Cd2—O4^{iii}	2.373 (7)	O6—Cd2^{v}	2.298 (7)
Cd2—O4	2.373 (7)	C31—C30^{vi}	1.342 (17)
C3—C2	1.335 (12)	C7—C10	1.504 (16)
O4—Cd1—O3	53.3 (2)	N1—Cd1—O4	134.8 (3)
O4—Cd1—O5^{i}	76.7 (2)	N1—Cd1—O3	85.5 (3)
O4—Cd1—C18^{ii}	99.3 (3)	N1—Cd1—O2	138.6 (3)
O2—Cd1—O4	85.2 (3)	N1—Cd1—O5^{i}	87.4 (3)
O2—Cd1—O3	135.8 (3)	N1—Cd1—C18^{ii}	92.3 (3)
O2—Cd1—O5^{i}	94.0 (3)	C18^{ii}—Cd1—O3	83.2 (3)
O2—Cd1—C18^{ii}	90.3 (3)	C18^{ii}—Cd1—O5^{i}	173.8 (3)
O5^{i}—Cd1—O3	90.6 (2)	O4—Cd2—O4^{iii}	163.8 (3)
O4—Cd2—O5^{i}	75.2 (2)	O6^{iv}—Cd2—O4^{iii}	90.5 (2)
O4—Cd2—O5^{iv}	103.3 (2)	O6^{i}—Cd2—O4^{iii}	101.7 (2)
O4^{iii}—Cd2—O5^{i}	103.3 (2)	O6^{i}—Cd2—O5^{i}	54.2 (2)
O4^{iii}—Cd2—O5^{iv}	75.2 (2)	O6^{i}—Cd2—O5^{iv}	136.1 (2)
O5^{iv}—Cd2—O5^{i}	169.6 (3)	O6^{iv}—Cd2—O5^{iv}	54.2 (2)
O6^{i}—Cd2—O4	90.5 (2)	O6^{iv}—Cd2—O5^{i}	136.1 (2)
O6^{iv}—Cd2—O4	101.7 (2)	O6^{i}—Cd2—O6^{iv}	82.5 (4)

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

Mn2—O4	2.143 (3)	Mn1—O1W^{i}	2.323 (3)
Mn2—O2W	2.332 (3)	Mn1—O1W	2.323 (3)

Mn2—O3	2.180 (3)	Mn1—O1	2.155 (3)
Mn2—O2	2.110 (3)	Mn1—O1^{i}	2.155 (3)
Mn2—N6	2.244 (3)	Mn1—N5^{i}	2.165 (3)
Mn2—N3	2.217 (3)	Mn1—N5	2.165 (3)
O4—Mn2—O2W	82.25 (10)	N5—Mn1—O1W	86.53 (11)
O4—Mn2—O3	88.25 (10)	N5^{i}—Mn1—N5	180.0
O4—Mn2—N6	81.70 (11)	Mn1—O1W—H1WA	120.0
O4—Mn2—N3	98.15 (11)	Mn1—O1W—H1WB	120.0
O3—Mn2—O2W	84.51 (11)	H1WA—O1W—H1WB	120.0
O3—Mn2—N6	90.23 (12)	C21—O1—Mn1	161.0 (2)
O3—Mn2—N3	171.23 (11)	C31—O4—Mn2	133.1 (2)
O2—Mn2—O4	168.96 (9)	Mn2—O2W—H2WA	96 (3)
O2—Mn2—O2W	103.39 (10)	Mn2—O2W—H2WB	92 (3)
O2—Mn2—O3	82.93 (10)	H2WA—O2W—H2WB	111 (3)
O2—Mn2—N6	91.68 (10)	C43^{ii}—O3—Mn2	124.4 (2)
O2—Mn2—N3	91.35 (11)	C21—O2—Mn2	132.2 (2)
N6—Mn2—O2W	163.24 (10)	C24—N5—Mn1	123.2 (3)
N3—Mn2—O2W	90.40 (12)	C22—N5—Mn1	131.9 (3)
N3—Mn2—N6	96.59 (13)	C1^{iv}—N6—Mn2	139.4 (3)
O1W^{i}—Mn1—O1W	180.0	C3^{iv}—N6—Mn2	114.6 (3)
O1^{i}—Mn1—O1W	79.09 (9)	C18—N3—Mn2	116.3 (4)
O1^{i}—Mn1—O1W^{i}	100.91 (9)	C17—N3—Mn2	123.9 (4)
O1—Mn1—O1W	100.92 (9)	C16—N3—Mn2	131.8 (3)
O1—Mn1—O1W^{i}	79.08 (9)	O1—Mn1—N5	87.66 (12)
O1—Mn1—O1^{i}	180.0	N5^{i}—Mn1—O1W^{i}	86.53 (11)
O1—Mn1—N5^{i}	92.35 (12)	N5^{i}—Mn1—O1W	93.47 (11)
O1^{i}—Mn1—N5^{i}	87.66 (13)	N5—Mn1—O1W^{i}	93.47 (11)
O1^{i}—Mn1—N5	92.34 (12)		

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

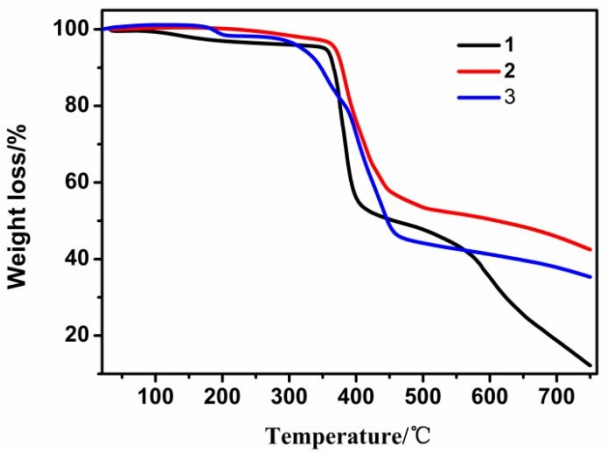

Fig. S1 The TGA curves of complexes **1**-**3**.

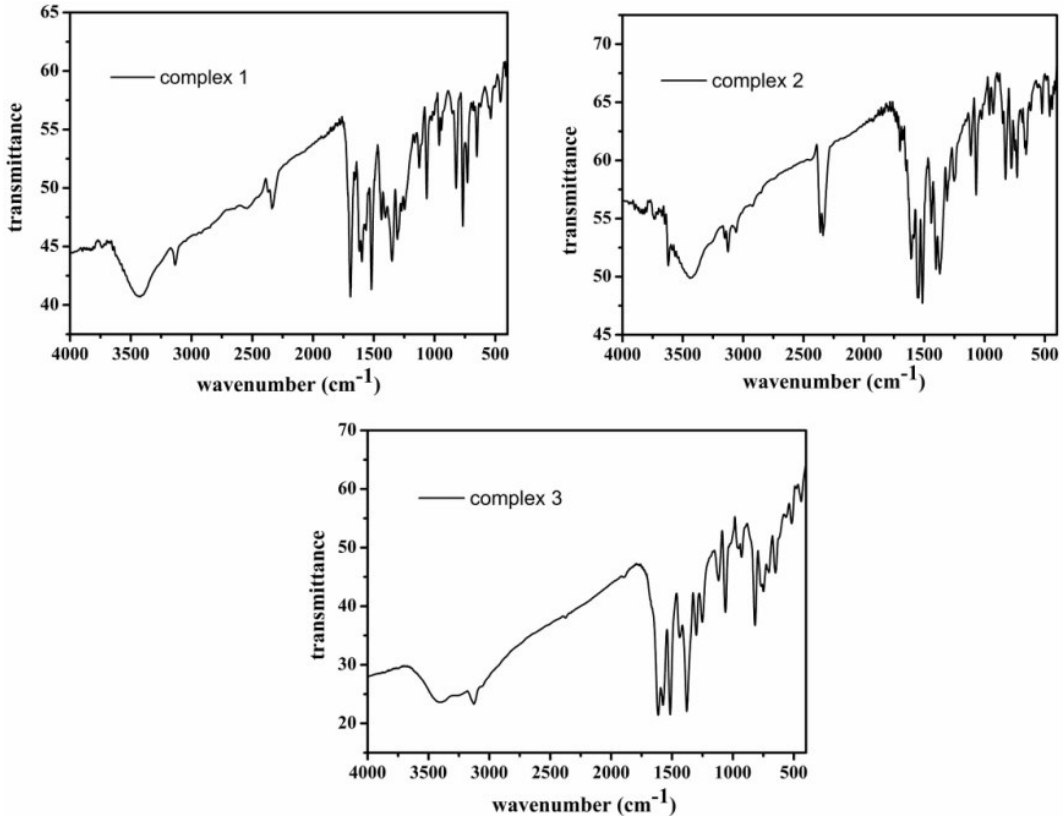

Fig. S2 The IR of complexes **1**-**3**.

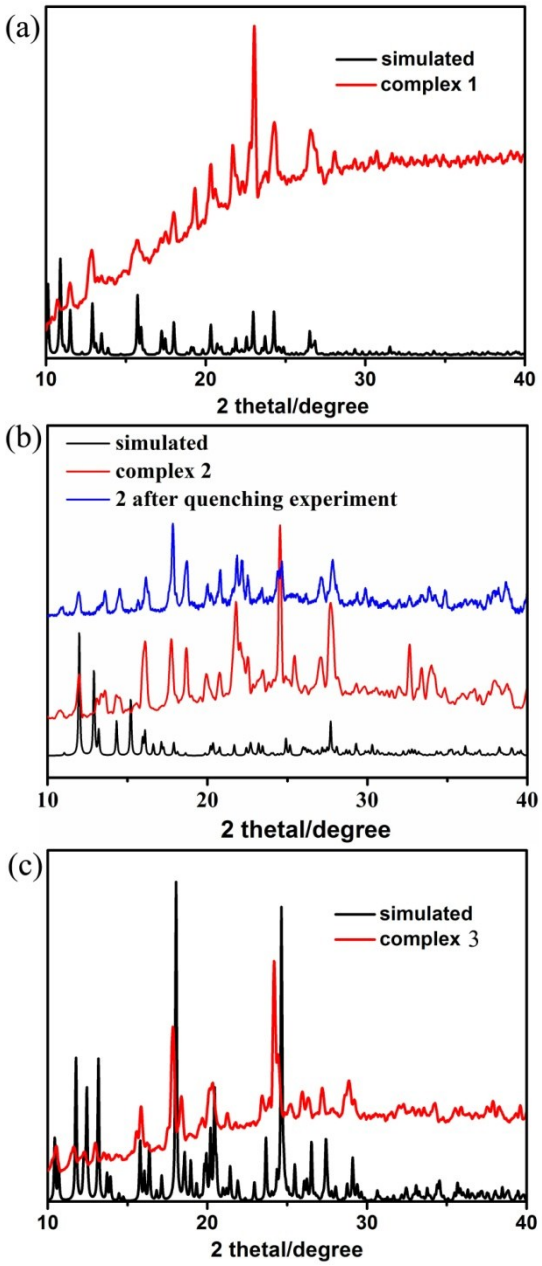

Fig. S3 The XRD of complexes **1**-**3** and complex **2** after quenching experiment.

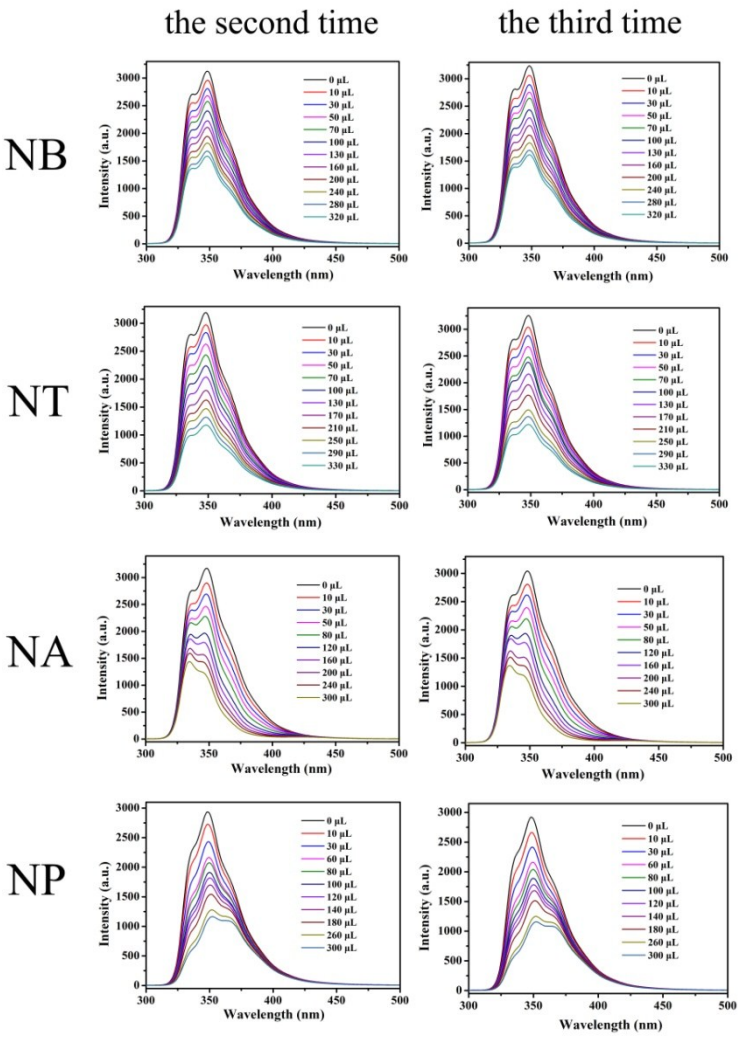

Fig. S4 Effect on the emission spectra of **2** dispersed in DMSO with increasing addition of a nitrobenzene derivative solution for the second and third time.

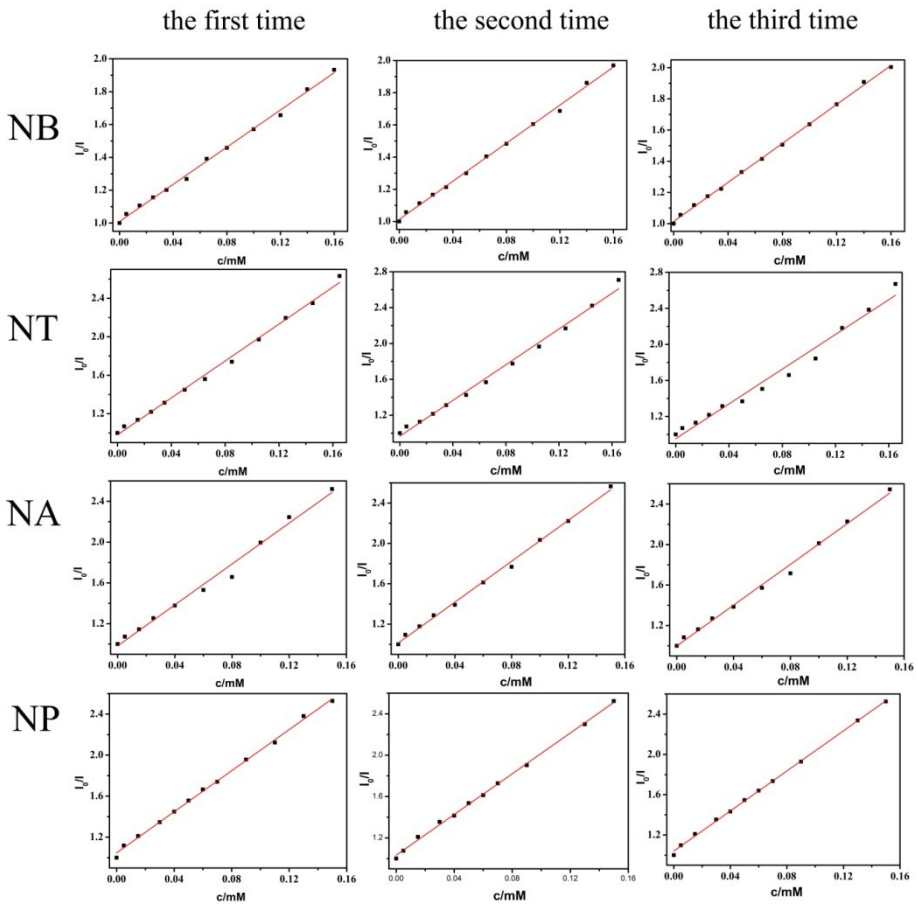

Fig. S5 The I_0/I versus the nitrobenzene derivatives for complex **2**: NB; NT; NA; NP.

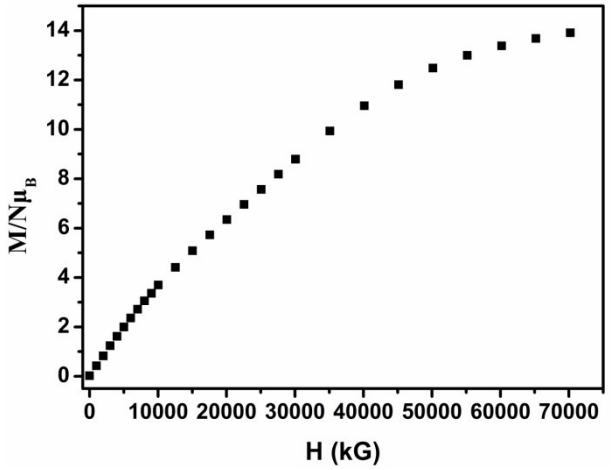

Fig. S6 M-H curve for complex **3** in the 1-7 T magnetic field ranges.

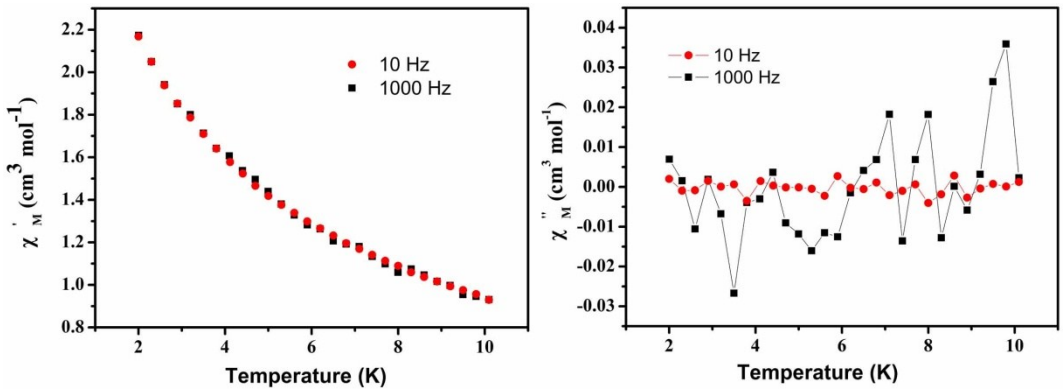

Fig. S7 Plots of the in phase (χ'_M) signal and out-of-phase (χ''_M) signal for complex **3** in ac susceptibility studies *vs*. T in a 2 Oe field with a zero dc field.