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Magnetic Properties and Luminescence Sensing of Five Coordination Polymers Based on a Rigid Terphenyl-tetracarboxylic Acid

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Experimental section

1. Photoluminescent sensing experiments

1.1 Solvent molecules sensing experiments

The fine grinding sample of **3** (2 mg) was immersed in different organic solvents (2 mL). Then the sample was treated by ultrasonication for 30 min to form a uniform emulsion before the fluorescence study.

1.2 Nitrobenzene derivatives sensing experiments

The fine grinding sample of **3** (2 mg) was immersed in DMSO (2 mL), treated by ultrasonication for 30 min. Then equal volume of aromatic molecules was added into the above samples. Finally, the sample was treated by ultrasonication, which was then added to quartz cuvette. The fluorescence upon excitation at 280 nm was measured in-situ after incremental addition of freshly prepared nitrobenzene derivative solution (1 mmol/L). The emulsion was stirred at constant rate during experiment to maintain homogeneity.

Table S1. Selected bond length (Å) and angles (°) for complexes **1**-**5**.

Complex **1**

Ni1—O1	2.199 (3)	Ni1—O4^{ii}	2.036 (3)
Ni1—O2	2.115 (3)	Ni1—N1	2.054 (3)
Ni1—O3^{i}	2.058 (3)	Ni1—N4^{iii}	2.051 (4)
O3—Ni1^{i}	2.058 (3)	Ni1—C1	2.470 (4)
O4—Ni1^{iv}	2.036 (3)	N4—Ni1^{v}	2.051 (4)
O1—Ni1—C1	30.67 (11)	O3^{i}—Ni1—O2	94.42 (10)
O2—Ni1—O1	61.11 (10)	O3^{i}—Ni1—C1	124.69 (12)
O2—Ni1—C1	30.44 (11)	O4^{ii}—Ni1—O1	96.02 (10)
O3^{i}—Ni1—O1	155.11 (10)	O4^{ii}—Ni1—O2	157.10 (11)
O4^{ii}—Ni1—N1	93.05 (12)	O4^{ii}—Ni1—O3^{i}	108.26 (10)
O4^{ii}—Ni1—N4^{iii}	87.43 (12)	N4^{iii}—Ni1—N1	176.96 (14)
O4^{ii}—Ni1—C1	126.67 (12)	N4^{iii}—Ni1—C1	89.35 (13)
N1—Ni1—O1	94.02 (13)	C1—O1—Ni1	86.6 (2)
N1—Ni1—O2	89.90 (12)	C1—O2—Ni1	90.7 (2)
N1—Ni1—O3^{i}	90.10 (13)	C5—O3—Ni1^{i}	150.2 (3)
N1—Ni1—C1	92.77 (13)	C5—O4—Ni1^{iv}	126.1 (2)
N4^{iii}—Ni1—O1	88.91 (13)	C12—N1—Ni1	123.8 (3)
N4^{iii}—Ni1—O2	90.83 (12)	N4^{iii}—Ni1—O3^{i}	86.90 (13)

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

Complex **2**

Co1—O2^{i}	2.0641 (19)	Co1—N4^{ii}	2.112 (3)
Co1—O1	2.039 (2)	Co1—O3^{iii}	2.130 (2)
Co1—N1	2.114 (3)	Co1—O4^{iii}	2.291 (2)
O2—Co1^{i}	2.0641 (19)		
O2^{i}—Co1—N1	86.93 (9)	O1—Co1—O4^{iii}	151.67 (8)
O2^{i}—Co1—N4^{ii}	92.79 (9)	N1—Co1—O3^{iii}	91.86 (9)
O2^{i}—Co1—O3^{iii}	152.07 (8)	N1—Co1—O4^{iii}	86.85 (9)
O2^{i}—Co1—O4^{iii}	93.17 (7)	N4^{ii}—Co1—N1	178.18 (10)
O1—Co1—O2^{i}	114.44 (7)	N4^{ii}—Co1—O3^{iii}	89.23 (9)
O1—Co1—N1	88.39 (10)	N4^{ii}—Co1—O4^{iii}	94.95 (9)
O1—Co1—N4^{ii}	90.10 (9)	O3^{iii}—Co1—O4^{iii}	58.91 (7)
O1—Co1—O3^{iii}	93.39 (8)	C1—O2—Co1^{i}	123.79 (17)
C5—O4—Co1^{iii}	86.08 (17)	C5—O3—Co1^{iii}	93.79 (17)

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

Complex **3**

Zn1—O1	1.924 (2)	Zn1—N2	2.007 (2)
Zn1—O3	1.955 (2)	Zn1—N1	2.017 (2)
N3—C12	1.341 (3)	C25—N1^{iv}	1.381 (4)
C5—C6	1.391 (4)	C7—C2	1.387 (4)
C5—C4	1.390 (4)	C11—O3^{v}	1.276 (3)
C21—C20	1.384 (4)	C2—C1	1.511 (4)
O1—Zn1—O3	117.00 (9)	C11^{i}—O3—Zn1	114.04 (18)
O1—Zn1—N2	115.15 (9)	C13—N2—Zn1	126.1 (2)
O1—Zn1—N1	100.39 (9)	C12—N2—Zn1	127.99 (19)
O3—Zn1—N2	102.05 (9)	C23^{ii}—N1—Zn1	130.3 (2)
O3—Zn1—N1	113.88 (9)	C23^{ii}—N1—C25^{ii}	104.6 (3)
N2—Zn1—N1	108.61 (10)	C25^{ii}—N1—Zn1	124.5 (2)
C1—O1—Zn1	119.1 (2)		

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

−*x*+3/2, *y*−1/2, −*z*+1/2; (v) −*x*−1/2, *y*−1/2, −*z*+1/2.

Complex 4

Co1-O1	2.027(4)	Co1-O4^{2}	2.125(4)	O2-Co1^{ii}	2.038(4)
Co1-O2^{ii}	2.038(4)	Co1-N1	2.090(5)	Co1-N4^{iii}	2.098(5)
Co1-O3^{i}	2.235(3)	O2^{ii}-Co1-O3^{i}	90.53(14)	O1-Co1-N4^{iii}	90.73(14)
O1-Co1-O2^{ii}	114.32(11)	O2^{ii}-Co1-O4^{i}	150.08(9)	N1-Co1-O3^{i}	88.03(16)
O1-Co1-O3^{i}	154.32(8)	O2^{ii}-Co1-N1	87.24(11)	N1-Co1-O4^{i}	92.87(12)
O1-Co1-O4^{i}	95.54(8)	O2^{ii}-Co1-N4^{iii}	93.59(10)	N1-Co1-N4^{iii}	177.62(9)
O1-Co1-N1	86.90(14)	O4^{i}-Co1-O3^{i}	59.60(9)	N4^{iii}-Co1-O3^{2}	94.18(15)
N4^{iii}-Co1-O4^{i}	87.53(12)				

Symmetry codes: ^{i}-X, 1-Y, 1-Z;^{ii}1-X, 1-Y, 1-Z; ^{iii}-1+X, +Y, -1+Z.

Complex 5

Co2-O5	2.008(4)	Co2-O4^{i}	2.094(4)	Co1-O1	2.003(4)
Co2-O2^{ii}	2.039(4)	Co2-O6	2.165(4)	Co1-O8^{3}	2.112(4)
Co2-O3^{i}	2.294(4)	Co2-N1	2.091(5)	Co1-O7^{4}	2.003(4)
Co1-O9^{3}	2.211(4)	Co1-O10	2.126(5)	Co1-N4^{3}	2.094(6)
O5-Co2-O2^{ii}	112.60(13)	O2^{ii}-Co2-N1	97.54(16)	O10-Co1-O9^{3}	90.03(17)
O5-Co2-O3^{i}	154.81(13)	O4^{i}-Co2-O3^{i}	59.29(12)	N4^{3}-Co1-O8^{3}	91.13(18)
O5-Co2-O4^{i}	96.46(12)	O4^{i}-Co2-O6	89.07(14)	N4^{3}-Co1-O9^{3}	88.89(17)
O5-Co2-O6	85.96(13)	O6-Co2-O3^{i}	86.85(12)	N4^{3}-Co1-O10	178.80(17)
O8^{3}-Co1-O10	87.89(19)	N1-Co2-O3^{i}	93.15(14)	O5-Co2-N1	92.99(15)
O7^{4}-Co1-O8^{3}	154.47(14)	N1-Co2-O4^{i}	88.75(15)	O2^{ii}-Co2-O3^{i}	90.75(13)
O7^{4}-Co1-O9^{3}	94.44(15)	N1-Co2-O6	177.46(15)	O2^{ii}-Co2-O4^{i}	149.76(13)
O7^{4}-Co1-O10	91.20(19)	O1-Co1-O8^{3}	95.21(13)	O2^{ii}-Co2-O6	85.00(14)
O7^{4}-Co1-N4^{3}	89.39(18)	O1-Co1-O7^{4}	110.25(14)	O1-Co1-O9^{3}	155.24(14)
O8^{3}-Co1-O9^{3}	60.06(13)	O1-Co1-N4^{3}	93.07(18)	O1-Co1-O10	87.70(18)

Symmetry codes: ^{i}+*X*, +*Y*,- 1+*Z*; ^{ii}1+*X*, +*Y*, -1+*Z*; ^{3}+*X*, +*Y*, 1+*Z*; ^{4}-1+*X*,+*Y*, 1+*Z*.

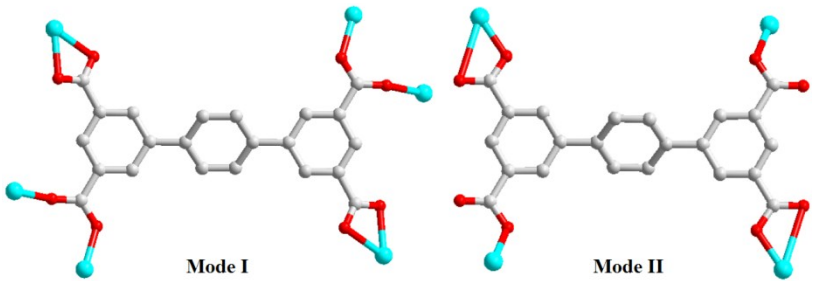


Fig. S1 The coordinated modes of H_4tptc in complexes **1, 2, 4, 5** (Mode I) and **3** (Mode II).

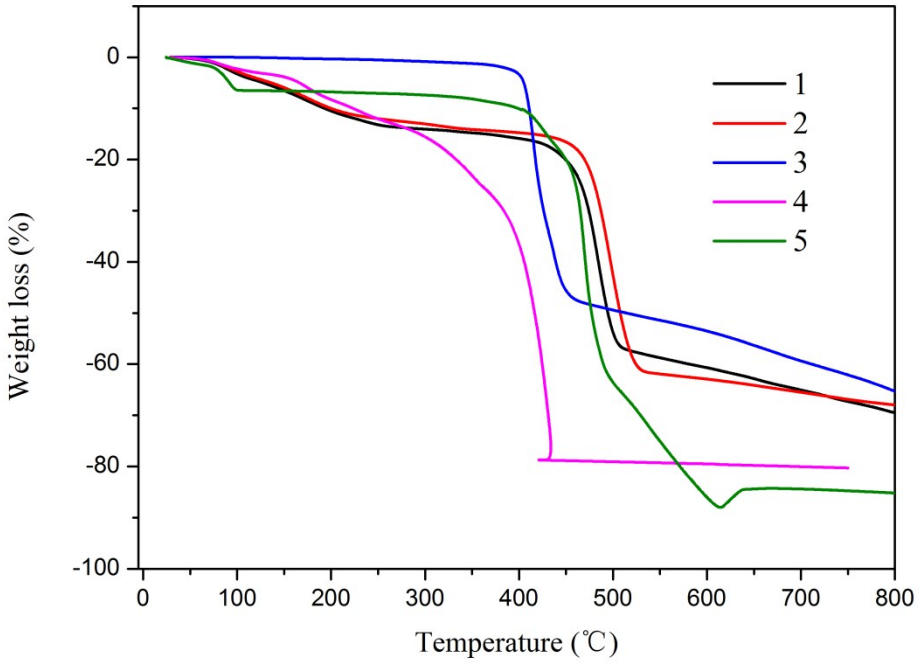
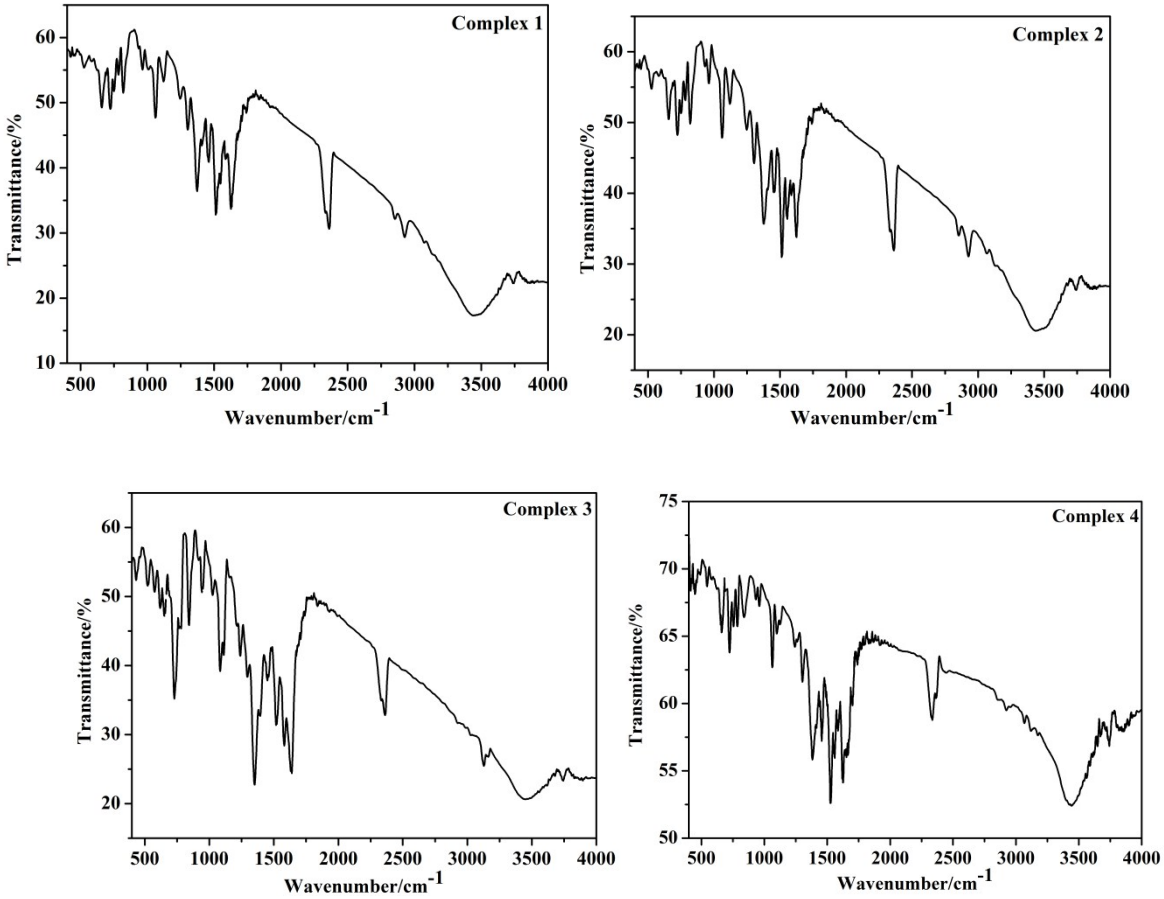


Fig. S2 The TGA of complexes 1-5.



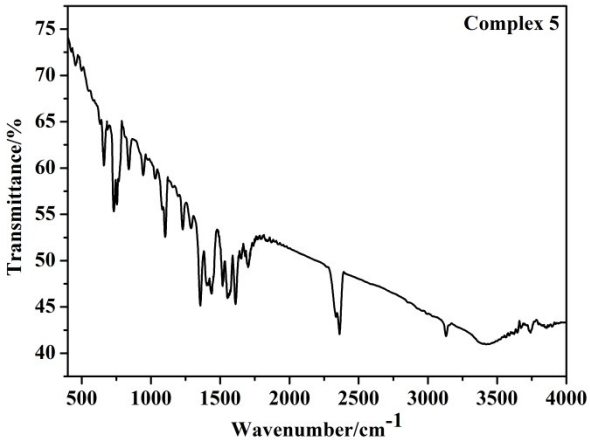


Fig. S3 The IR of complexes 1-5.

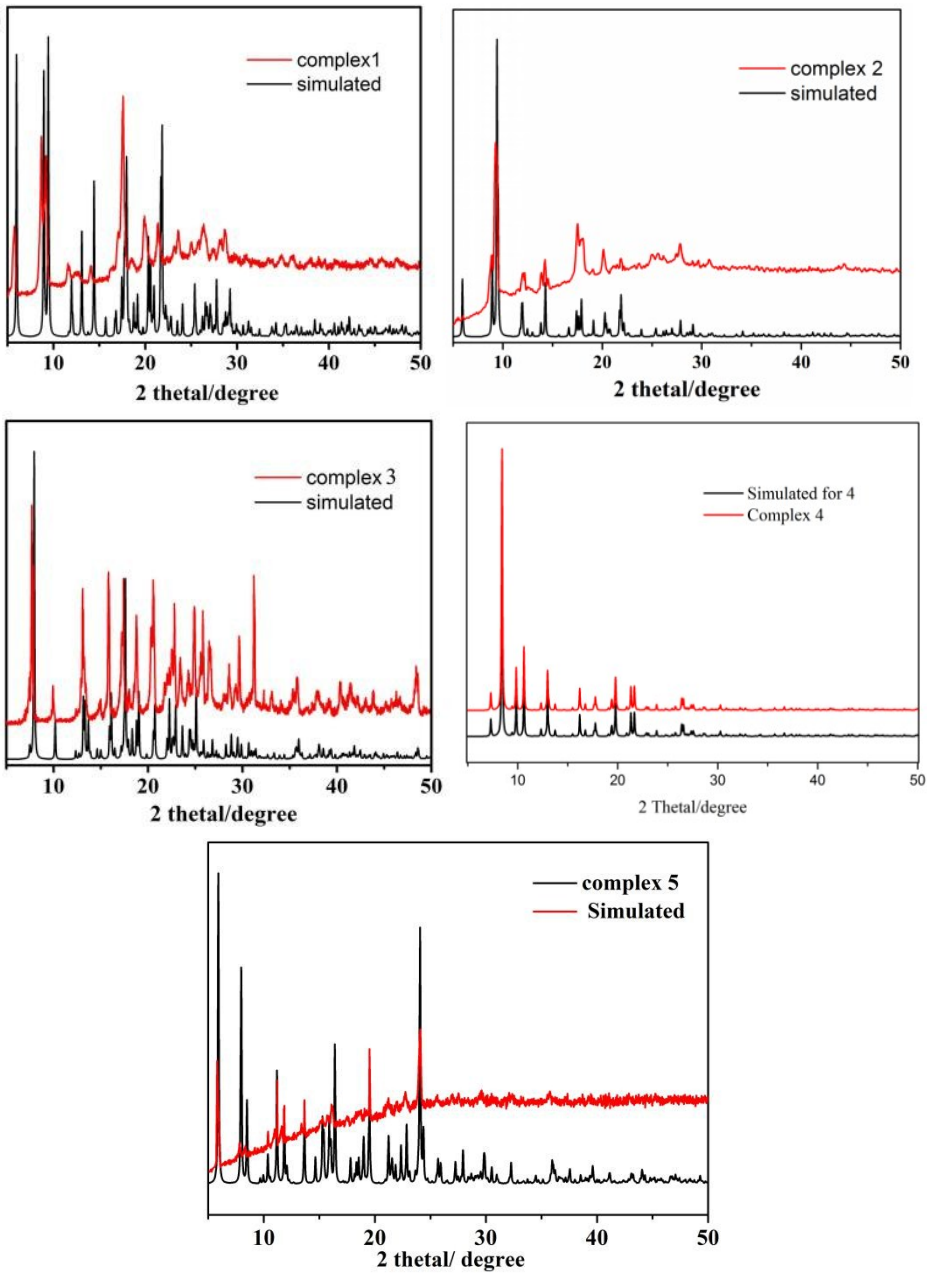


Fig. S4 The XRD of complexes **1**-**5**.

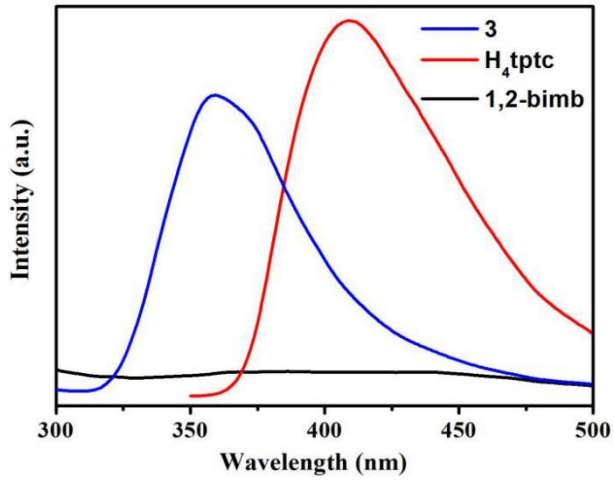


Fig. S5 The room-temperature emission spectra for free ligands and complex **3**.

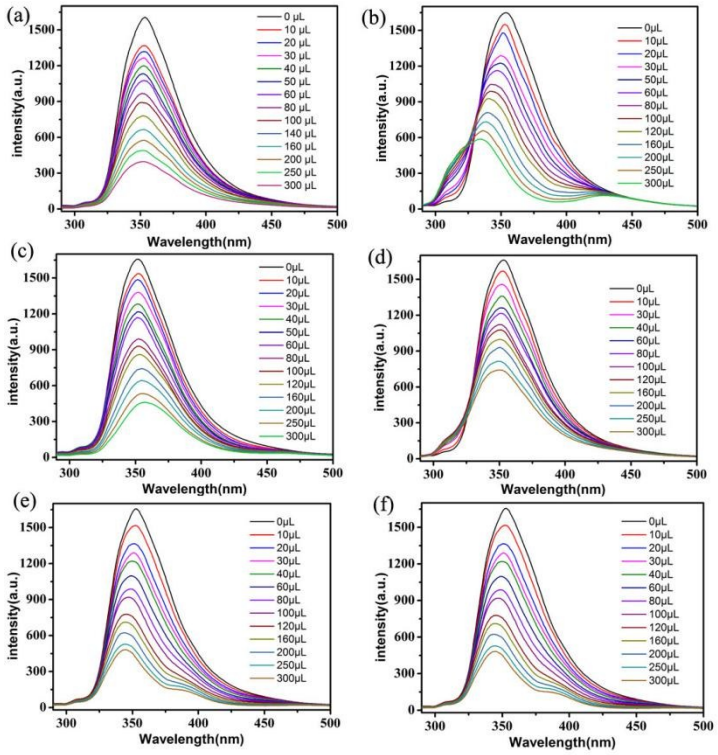


Fig. S6 Effect on the emission spectra of **3** dispersed in DMSO with increasing addition of a nitrobenzene derivative solution (a. NT; b. NA; c. NP; d. 1,3-DNB; e. 2,4-DNT; f. PA).

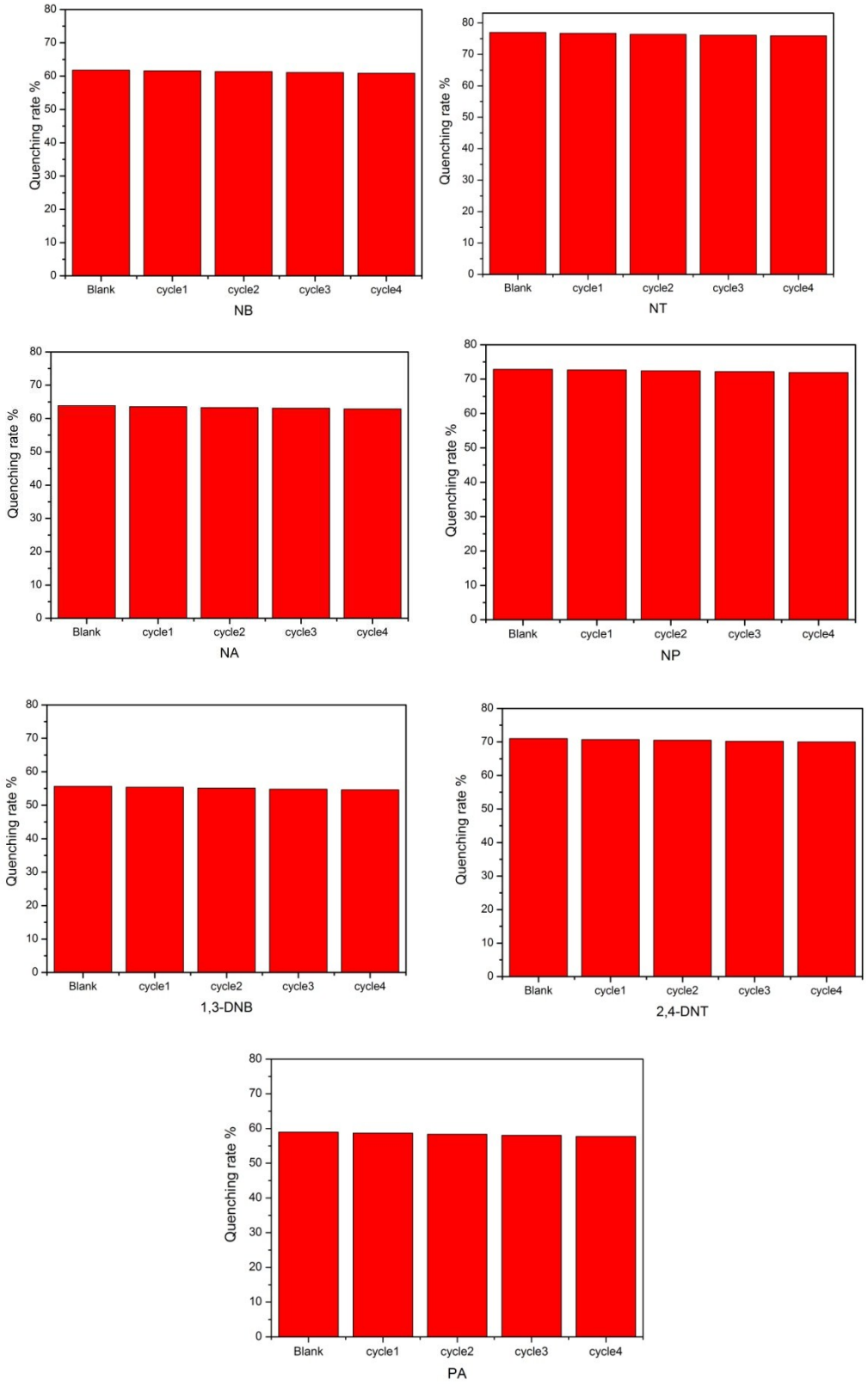


Fig. S7 The recycle performance of complex **3** as sensor to sensing nitrobenzene derivatives.