

## Supporting Information

### Syntheses and magnetic properties of a bis-bidentate nitronyl nitroxide radical based on triazolopyrimidine and its metal complexes

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## 1. X-ray crystallography and powder x-ray diffraction

**Table S1** Crystallographic data and structure refinement parameters for **NIT-2-TrzPm** radical.

Complex	<b>NIT-2-TrzPm</b>
Formula	C <sub>12</sub> H <sub>15</sub> N <sub>6</sub> O <sub>2</sub>
Formula weight	275.30
<i>T</i> /K	193
Crystal system	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>a</i> /Å	6.4642(15)
<i>b</i> /Å	10.078(2)
<i>c</i> /Å	20.367(4)
<i>α</i> /°	90
<i>β</i> /°	95.559(7)
<i>γ</i> /°	90
<i>V</i> /Å <sup>3</sup>	1320.6(5)
<i>Z</i>	4
<i>F</i> (000)	580.0
Collected refl.	9125
Unique refl.	2401
<i>R</i> <sub>int</sub>	0.0670
GOF	1.103
<i>R</i> <sub>1</sub> <sup>a</sup> , w <i>R</i> <sub>2</sub> <sup>b</sup> ( <i>I</i> > 2σ( <i>I</i> ))	0.0510, 0.1084

$R_1, wR_2$ (all data)	0.0742, 0.1193
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$${}^a R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|}, {}^b wR_2 = \left\{ \frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)]} \right\}^{1/2}.$$

**Table S2** Selected bond lengths [Å] and angles [°] for **NIT-2-TrzPm** radical.

N(4)-N(3)	1.359(3)	N(6)-C(9)	1.348(3)
N(4)-C(9)	1.377(3)	N(6)-C(10)	1.319(3)
N(4)-C(12)	1.358(3)	N(3)-C(8)	1.330(3)
O(1)-N(1)	1.272(2)	C(8)-C(7)	1.454(3)
O(2)-N(2)	1.279(2)	C(11)-C(12)	1.350(3)
N(1)-C(7)	1.347(3)	C(11)-C(10)	1.412(4)
N(5)-C(9)	1.332(3)	N(5)-C(8)	1.352(3)
N(2)-C(7)	1.338(3)	N(1)-C(7)-C(8)	123.8(2)
N(3)-N(4)-C(9)	110.08(19)	N(2)-C(7)-N(1)	109.8(2)
C(12)-N(4)-N(3)	127.1(2)	N(2)-C(7)-C(8)	126.4(2)
C(12)-N(4)-C(9)	122.8(2)	C(12)-C(11)-C(10)	119.3(2)
O(1)-N(1)-C(7)	125.7(2)	C(11)-C(12)-N(4)	116.0(2)
C(9)-N(5)-C(8)	102.02(19)	N(6)-C(10)-C(11)	125.0(2)
O(2)-N(2)-C(7)	125.9(2)	C(9)-N(6)-C(10)-C(11)	0.4(4)
C(10)-N(6)-C(9)	114.8(2)	C(8)-N(5)-C(9)-N(4)	0.2(2)
C(8)-N(3)-N(4)	101.00(19)	C(8)-N(5)-C(9)-N(6)	179.4(2)
N(5)-C(9)-N(4)	109.57(19)	C(12)-N(4)-C(9)-N(5)	177.6(2)
N(5)-C(9)-N(6)	128.3(2)	C(12)-N(4)-C(9)-N(6)	1.6(3)
N(6)-C(9)-N(4)	122.2(2)	C(12)-C(11)-C(10)-N(6)	0.0(4)
N(5)-C(8)-C(7)	121.4(2)	C(10)-N(6)-C(9)-N(4)	1.2(3)
N(3)-C(8)-N(5)	117.3(2)	C(10)-N(6)-C(9)-N(5)	177.9(2)
N(3)-C(8)-C(7)	121.2(2)	C(10)-C(11)-C(12)-N(4)	0.3(3)
N(4)-N(3)-C(8)-N(5)	0.4(3)	O(1)-N(1)-C(7)-N(2)	178.2(2)
N(4)-N(3)-C(8)-C(7)	177.0(2)	C(9)-N(4)-C(12)-C(11)	1.1(3)
O(1)-N(1)-C(7)-C(8)	1.7(4)	C(9)-N(5)-C(8)-N(3)	0.1(3)
O(2)-N(2)-C(7)-N(1)	179.2(2)	C(9)-N(5)-C(8)-C(7)	177.3(2)
O(2)-N(2)-C(7)-C(8)	0.9(4)	N(3)-N(4)-C(12)-C(11)	178.8(2)
N(5)-C(8)-C(7)-N(1)	50.6(3)	N(3)-C(8)-C(7)-N(1)	126.7(3)
N(5)-C(8)-C(7)-N(2)	129.6(3)	N(3)-C(8)-C(7)-N(2)	53.1(3)
N(3)-N(4)-C(9)-N(5)	0.4(3)	C(9)-N(4)-N(3)-C(8)	0.5(2)
N(3)-N(4)-C(9)-N(6)	179.7(2)		

**Table S3** Selected bond lengths [Å] and angles [°] for complex **1Mn**.

Mn1-O4	2.138(2)	N5-C8	1.353(3)
Mn1-O3	2.135(2)	N3-C8	1.327(3)
Mn1-O5	2.152(2)	N1-C7	1.332(3)
Mn1-O6	2.140(2)	N2-C7	1.343(4)
Mn1-O1	2.174(2)	N6-C9	1.338(3)
Mn1-N5	2.231(2)	N5-C9	1.330(3)

O1-N1	1.299(3)	N4-C9	1.371(3)
O2-N2	1.263(3)	N6-C9-N4	123.2(2)
N4-N3	1.360(3)	N5-C9-N4	108.4(2)
O4-Mn1-O5	93.16(9)	N5-C9-N6	128.4(2)
O4-Mn1-O6	175.78(9)	N5-C8-C7	121.6(2)
O4-Mn1-O1	96.59(9)	N3-C8-N5	116.5(2)
O4-Mn1-N5	94.16(8)	C8-N3-N4	100.9(2)
O3-Mn1-O4	83.19(8)	O1-N1-C7	126.4(2)
O3-Mn1-O5	101.67(9)	O2-N2-C7	126.5(2)
O3-Mn1-O6	95.42(9)	N3-C8-C7	121.9(2)
O3-Mn1-O1	86.58(9)	N1-C7-N2	110.1(2)
O3-Mn1-N5	165.89(9)	N2-C7-C8	125.4(2)
O5-Mn1-O1	167.93(8)	N1-O1-Mn1	120.15(17)
O5-Mn1-N5	92.29(8)	N3-N4-C9	111.0(2)
O6-Mn1-O5	83.21(9)	C9-N5-Mn1	131.56(17)
O6-Mn1-O1	87.28(9)	C9-N5-C8	103.2(2)
O6-Mn1-N5	88.15(8)	C8-N5-Mn1	125.05(17)
O1-Mn1-N5	79.95(8)	N1-C7-C8	124.4(2)
N4-N3-C8-C7	179.6(2)	N4-N3-C8-N5	0.2(3)
N3-C8-C7-N1	157.5(3)	N3-C8-C7-N2	23.3(4)
Mn1-N5-C9-N4	175.57(17)	Mn1-O1-N1-C7	44.2(4)
Mn1-N5-C9-N6	4.1(4)	C9-N4-N3-C8	0.0(3)
Mn1-N5-C8-N3	176.01(18)	C9-N5-C8-N3	0.3(3)
Mn1-N5-C8-C7	3.8(4)	C9-N5-C8-C7	179.5(3)
O1-N1-C7-N2	178.5(3)	C8-N5-C9-N4	0.3(3)
O1-N1-C7-C8	0.8(5)	C8-N5-C9-N6	179.4(3)
O2-N2-C7-N1	176.8(3)	N5-C8-C7-N1	22.7(4)
O2-N2-C7-C8	2.5(5)	N5-C8-C7-N2	156.4(3)
N3-N4-C9-N5	0.2(3)		

**Table S4** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for complex **2co**.

Co1-O6	2.049(2)	C7-C8	1.452(4)
Co1-O3	2.055(2)	C9-N4-N3-C8	0.4(3)
Co1-O5	2.071(2)	N1-C7-C8-N3	154.1(3)
Co1-O1	2.093(2)	C9-N5-C8-N3	0.4(3)
Co1-O4	2.066(2)	C9-N5-C8-C7	179.5(3)
Co1-N5	2.103(2)	Co1-O1-N1-C7	42.4(4)
O1-N1	1.295(3)	Co1-N5-C9-N4	178.85(19)
O2-N2	1.264(3)	Co1-N5-C9-N6	1.3(5)
N5-C9	1.328(4)	Co1-N5-C8-N3	179.33(19)
N5-C8	1.355(4)	Co1-N5-C8-C7	1.6(4)
N4-N3	1.361(3)	C8-N5-C9-N4	0.1(3)

N4-C9	1.370(4)	C8-N5-C9-N6	179.9(3)
N3-C8	1.324(4)	O1-N1-C7-N2	177.1(3)
N6-C9	1.343(4)	O1-N1-C7-C8	1.7(5)
N2-C7	1.345(4)	O2-N2-C7-N1	177.1(3)
N1-C7	1.336(4)	O2-N2-C7-C8	1.7(5)
O6-Co1-O3	92.76(9)	N4-N3-C8-N5	0.5(3)
O6-Co1-O5	87.79(9)	N4-N3-C8-C7	179.6(3)
O6-Co1-O1	87.26(9)	N3-N4-C9-N5	0.2(3)
O6-Co1-O4	178.92(9)	N3-N4-C9-N6	179.6(3)
O6-Co1-N5	88.78(9)	N2-C7-C8-N5	153.8(3)
O3-Co1-O5	95.84(9)	N2-C7-C8-N3	27.3(5)
O3-Co1-O1	87.01(9)	C7-N2-C6	111.9(2)
O3-Co1-O4	87.03(9)	O1-N1-C7	126.3(2)
O3-Co1-N5	171.36(9)	N5-C9-N4	108.3(2)
O5-Co1-O1	174.39(8)	N5-C9-N6	128.4(3)
O5-Co1-N5	92.71(9)	N6-C9-N4	123.2(3)
O1-Co1-N5	84.57(9)	N2-C7-C8	125.7(3)
O4-Co1-O5	91.18(9)	N1-C7-N2	110.2(2)
O4-Co1-O1	93.79(9)	N1-C7-C8	124.1(3)
O4-Co1-N5	91.58(9)	N5-C8-C7	121.5(2)
N1-O1-Co1	117.44(17)	N3-C8-N5	116.5(2)
C9-N5-Co1	133.38(19)	N3-C8-C7	122.0(2)
C9-N5-C8	103.2(2)	N1-C7-C8-N5	24.9(4)
C8-N5-Co1	123.36(18)	O2-N2-C7	126.0(2)
N3-N4-C9	111.1(2)	O2-N2-C6	121.9(2)
C8-N3-N4	100.8(2)		

**Table S5** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for complex **3<sub>Mn</sub>**.

Mn(1)-O(3)	2.1288(18)	O(2)-N(2)	1.291(2)
Mn(1)-O(4)	2.1312(18)	N(6)-C(10)	1.321(3)
Mn(1)-O(5)	2.1227(18)	N(6)-C(9)	1.338(3)
Mn(1)-O(6)	2.1090(19)	N(4)-N(3)	1.358(3)
Mn(1)-O(1)	2.2010(18)	N(4)-C(9)	1.371(3)
Mn(1)-N(5)	2.2968(19)	N(4)-C(12)	1.361(3)
Mn(2)-O(7)	2.1451(17)	N(3)-C(8)	1.333(3)
Mn(2)-O(8)	2.106(2)	N(5)-C(9)	1.333(3)
Mn(2)-O(9)	2.149(2)	N(5)-C(8)	1.338(3)
Mn(2)-O(2)	2.1684(18)	N(1)-C(7)	1.339(3)
Mn(2)-O(10)	2.1326(17)	N(5)-C(8)-C(7)-N(1)	24.7(3)
Mn(2)-N(3)	2.286(2)	C(10)-N(6)-C(9)-N(4)	0.2(4)
N(2)-C(7)	1.330(3)	C(9)-N(5)-C(8)-N(3)	0.0(3)
C(11)-C(10)	1.410(4)	C(12)-N(4)-C(9)-N(6)	0.2(4)

C(11)-C(12)	1.352(4)	C(12)-N(4)-C(9)-N(5)	179.7(2)
C(8)-C(7)	1.451(3)	N(4)-N(3)-C(8)-N(5)	0.3(2)
O(1)-N(1)	1.281(3)	N(4)-N(3)-C(8)-C(7)	178.47(19)
O(3)-Mn(1)-O(4)	84.14(7)	N(3)-N(4)-C(9)-N(6)	179.3(2)
O(3)-Mn(1)-O(1)	84.58(7)	N(3)-N(4)-C(9)-N(5)	0.5(3)
O(3)-Mn(1)-N(5)	84.75(7)	N(3)-N(4)-C(12)-C(11)	179.0(2)
O(4)-Mn(1)-O(1)	166.74(7)	N(3)-C(8)-C(7)-N(1)	154.0(2)
O(4)-Mn(1)-N(5)	93.45(7)	N(3)-C(8)-C(7)-N(2)	25.6(3)
O(5)-Mn(1)-O(3)	174.95(7)	Mn(1)-O(1)-N(1)-C(7)	48.7(3)
O(5)-Mn(1)-O(4)	93.93(8)	N(5)-C(8)-C(7)-N(2)	155.7(2)
O(5)-Mn(1)-O(1)	96.72(8)	Mn(1)-N(5)-C(9)-N(6)	2.2(4)
O(5)-Mn(1)-N(5)	90.72(7)	Mn(1)-N(5)-C(9)-N(4)	178.03(15)
O(6)-Mn(1)-O(3)	101.18(8)	Mn(1)-N(5)-C(8)-N(3)	178.52(14)
O(6)-Mn(1)-O(4)	101.92(8)	Mn(1)-N(5)-C(8)-C(7)	0.2(3)
O(6)-Mn(1)-O(5)	83.78(7)	C(10)-N(6)-C(9)-N(5)	179.6(3)
O(6)-Mn(1)-O(1)	87.10(7)	C(10)-C(11)-C(12)-N(4)	0.0(4)
O(6)-Mn(1)-N(5)	163.97(8)	C(9)-N(6)-C(10)-C(11)	0.1(4)
O(1)-Mn(1)-N(5)	78.58(7)	C(9)-N(4)-N(3)-Mn(2)	175.04(15)
O(7)-Mn(2)-O(9)	82.69(8)	C(9)-N(4)-N(3)-C(8)	0.5(2)
O(7)-Mn(2)-O(2)	110.16(7)	C(9)-N(4)-C(12)-C(11)	0.0(4)
O(7)-Mn(2)-N(3)	83.51(7)	Mn(2)-O(2)-N(2)-C(7)	46.1(3)
O(8)-Mn(2)-O(7)	84.16(7)	C(9)-N(5)-C(8)-C(7)	178.7(2)
O(8)-Mn(2)-O(9)	94.03(8)	C(12)-N(4)-N(3)-Mn(2)	4.0(3)
O(8)-Mn(2)-O(2)	94.03(7)	C(12)-N(4)-N(3)-C(8)	179.5(2)
O(8)-Mn(2)-O(10)	105.40(8)	Mn(2)-N(3)-C(8)-N(5)	175.57(14)
O(8)-Mn(2)-N(3)	163.05(8)	Mn(2)-N(3)-C(8)-C(7)	5.7(3)
O(9)-Mn(2)-O(2)	165.47(7)	C(12)-C(11)-C(10)-N(6)	0.0(5)
O(9)-Mn(2)-N(3)	95.89(8)	C(8)-N(5)-C(9)-N(6)	179.5(2)
O(2)-Mn(2)-N(3)	79.40(7)	C(8)-N(5)-C(9)-N(4)	0.3(2)
O(10)-Mn(2)-O(7)	162.22(8)	O(1)-N(1)-C(7)-N(2)	177.9(2)
O(10)-Mn(2)-O(9)	81.73(7)	O(1)-N(1)-C(7)-C(8)	1.8(4)
O(10)-Mn(2)-O(2)	84.49(7)	O(2)-N(2)-C(7)-N(1)	178.6(2)
O(10)-Mn(2)-N(3)	89.63(7)	O(2)-N(2)-C(7)-C(8)	1.8(4)
N(1)-O(1)-Mn(1)	120.35(13)	O(2)-N(2)-C(7)	125.29(19)
N(2)-O(2)-Mn(2)	122.27(14)	O(2)-N(2)-C(6)	121.75(19)
C(10)-N(6)-C(9)	115.2(2)	C(7)-N(2)-C(6)	112.97(19)
N(3)-N(4)-C(9)	109.92(18)	C(12)-C(11)-C(10)	119.9(2)
N(3)-N(4)-C(12)	127.9(2)	N(6)-C(10)-C(11)	124.0(3)
C(12)-N(4)-C(9)	122.2(2)	N(6)-C(9)-N(4)	122.9(2)
N(4)-N(3)-Mn(2)	131.84(14)	N(5)-C(9)-N(6)	128.3(2)
C(8)-N(3)-Mn(2)	126.14(15)	N(5)-C(9)-N(4)	108.8(2)
C(8)-N(3)-N(4)	101.87(18)	C(11)-C(12)-N(4)	115.8(2)
C(9)-N(5)-Mn(1)	132.43(16)	N(3)-C(8)-N(5)	115.83(19)

C(9)-N(5)-C(8)	103.61(19)	N(3)-C(8)-C(7)	120.9(2)
C(8)-N(5)-Mn(1)	123.94(14)	N(5)-C(8)-C(7)	123.2(2)
O(1)-N(1)-C(7)	125.73(19)	N(1)-C(7)-C(8)	124.0(2)
N(2)-C(7)-C(8)	125.7(2)	N(2)-C(7)-N(1)	110.3(2)

**Table S6** Selected bond lengths [Å] and angles [°] for complex **4co**.

Co(1)-O(4)	2.0550(19)	N(6)-C(9)	1.338(3)
Co(1)-O(3)	2.0236(18)	N(6)-C(10)	1.321(4)
Co(1)-O(6)	2.0335(17)	N(4)-N(3)	1.362(3)
Co(1)-O(5)	2.0479(19)	N(4)-C(9)	1.366(3)
Co(1)-O(1)	2.1362(19)	N(4)-C(12)	1.363(3)
Co(1)-N(5)	2.153(2)	N(3)-C(8)	1.333(3)
Co(2)-O(2)	2.1299(18)	N(5)-C(9)	1.341(3)
Co(2)-O(10)	2.0427(18)	N(5)-C(8)	1.341(3)
Co(2)-O(8)	2.062(2)	N(1)-C(7)	1.335(3)
Co(2)-O(7)	2.0398(18)	N(6)-C(9)-N(4)	123.2(2)
Co(2)-O(9)	2.0393(19)	N(6)-C(9)-N(5)	127.9(2)
Co(2)-N(3)	2.134(2)	N(5)-C(9)-N(4)	108.8(2)
N(2)-C(7)	1.337(3)	N(6)-C(10)-C(11)	124.0(3)
C(10)-C(11)	1.405(4)	C(12)-C(11)-C(10)	120.3(3)
C(11)-C(12)	1.354(4)	C(11)-C(12)-N(4)	115.3(2)
C(8)-C(7)	1.445(3)	N(3)-C(8)-N(5)	115.7(2)
O(1)-N(1)	1.285(3)	N(3)-C(8)-C(7)	120.9(2)
O(2)-N(2)	1.286(3)	N(3)-C(8)-C(7)-N(2)	26.8(4)
O(4)-Co(1)-O(1)	173.52(7)	N(5)-C(8)-C(7)-N(2)	153.4(2)
O(4)-Co(1)-N(5)	95.73(8)	N(3)-C(8)-C(7)-N(1)	153.3(2)
O(3)-Co(1)-O(4)	88.99(8)	Co(1)-O(1)-N(1)-C(7)	45.6(3)
O(3)-Co(1)-O(6)	175.64(8)	N(5)-C(8)-C(7)-N(1)	26.4(4)
O(3)-Co(1)-O(5)	96.11(8)	Co(1)-N(5)-C(9)-N(6)	3.4(4)
O(3)-Co(1)-O(1)	84.53(7)	Co(1)-N(5)-C(9)-N(4)	176.96(16)
O(3)-Co(1)-N(5)	86.95(8)	Co(1)-N(5)-C(8)-N(3)	177.47(15)
O(6)-Co(1)-O(4)	92.45(8)	Co(1)-N(5)-C(8)-C(7)	2.3(3)
O(6)-Co(1)-O(5)	87.87(8)	Co(2)-O(2)-N(2)-C(7)	43.1(3)
O(6)-Co(1)-O(1)	93.98(7)	Co(2)-N(3)-C(8)-N(5)	173.38(15)
O(6)-Co(1)-N(5)	88.81(7)	Co(2)-N(3)-C(8)-C(7)	6.9(3)
O(5)-Co(1)-O(4)	94.56(8)	C(9)-N(6)-C(10)-C(11)	0.3(4)
O(5)-Co(1)-O(1)	86.43(8)	C(9)-N(4)-N(3)-Co(2)	172.61(16)
O(5)-Co(1)-N(5)	169.31(8)	C(9)-N(4)-N(3)-C(8)	0.2(2)
O(1)-Co(1)-N(5)	83.67(7)	C(9)-N(4)-C(12)-C(11)	0.3(4)
O(2)-Co(2)-N(3)	83.17(7)	C(9)-N(5)-C(8)-N(3)	0.3(3)
O(10)-Co(2)-O(2)	83.78(7)	C(9)-N(5)-C(8)-C(7)	180.0(2)
O(10)-Co(2)-O(8)	86.51(8)	C(10)-N(6)-C(9)-N(4)	1.0(4)

O(10)-Co(2)-N(3)	91.27(8)	C(10)-N(6)-C(9)-N(5)	178.6(2)
O(8)-Co(2)-O(2)	170.21(7)	C(10)-C(11)-C(12)-N(4)	0.9(4)
O(8)-Co(2)-N(3)	98.32(8)	C(12)-N(4)-N(3)-Co(2)	5.9(4)
O(7)-Co(2)-O(2)	105.22(8)	C(12)-N(4)-N(3)-C(8)	178.7(2)
O(7)-Co(2)-O(10)	169.76(8)	C(12)-N(4)-C(9)-N(6)	0.7(4)
O(7)-Co(2)-O(8)	84.56(8)	C(12)-N(4)-C(9)-N(5)	179.0(2)
O(7)-Co(2)-N(3)	85.08(8)	C(8)-N(5)-C(9)-N(6)	179.3(2)
O(9)-Co(2)-O(2)	89.09(7)	C(8)-N(5)-C(9)-N(4)	0.4(2)
O(9)-Co(2)-O(10)	96.56(8)	O(1)-N(1)-C(7)-N(2)	179.1(2)
O(9)-Co(2)-O(8)	90.79(8)	O(1)-N(1)-C(7)-C(8)	1.1(4)
O(9)-Co(2)-O(7)	88.58(8)	O(2)-N(2)-C(7)-N(1)	178.9(2)
O(9)-Co(2)-N(3)	168.34(8)	O(2)-N(2)-C(7)-C(8)	1.0(4)
N(5)-C(8)-C(7)	123.4(2)	C(9)-N(5)-Co(1)	134.26(16)
N(1)-C(7)-N(2)	110.6(2)	C(9)-N(5)-C(8)	103.49(19)
N(1)-C(7)-C(8)	124.4(2)	C(8)-N(5)-Co(1)	122.20(15)
N(2)-C(7)-C(8)	125.0(2)	O(1)-N(1)-C(7)	125.4(2)
N(1)-O(1)-Co(1)	117.51(14)	O(2)-N(2)-C(7)	125.3(2)
N(2)-O(2)-Co(2)	119.82(14)	N(6)-C(10)-C(11)-C(12)	0.6(5)
C(10)-N(6)-C(9)	115.0(2)	N(4)-N(3)-C(8)-N(5)	0.1(3)
N(3)-N(4)-C(9)	109.97(19)	N(4)-N(3)-C(8)-C(7)	179.8(2)
N(3)-N(4)-C(12)	127.8(2)	N(3)-N(4)-C(9)-N(6)	179.3(2)
C(12)-N(4)-C(9)	122.3(2)	N(3)-N(4)-C(9)-N(5)	0.4(3)
N(4)-N(3)-Co(2)	131.40(15)	N(3)-N(4)-C(12)-C(11)	178.1(2)
C(8)-N(3)-Co(2)	126.20(16)	C(8)-N(3)-N(4)	101.99(19)

**Table S7** Selected bond lengths [Å] and angles [°] for complex **5<sub>Mn</sub>**.

Mn(1)-O(1)	2.1280(16)	N(5)-C(9)	1.335(3)
Mn(1)-O(4)	2.1920(16)	N(4)-C(9)	1.376(3)
Mn(1)-O(3)	2.1353(17)	N(4)-C(12)	1.357(3)
Mn(1)-O(5)	2.1216(16)	N(6)-C(9)	1.337(3)
Mn(1)-N(11)	2.2391(18)	N(6)-C(10)	1.321(3)
Mn(1)-N(5)	2.2275(18)	C(7)-C(8)	1.449(3)
O(2)-N(2)	1.263(2)	C(10)-C(11)	1.414(3)
O(1)-N(1)	1.296(2)	C(11)-C(12)	1.357(3)
O(5)-N(7)	1.289(2)	C(22)-C(23)	1.415(3)
O(6)-N(8)	1.265(2)	C(23)-C(24)	1.354(3)
N(10)-N(9)	1.363(3)	C(20)-C(19)	1.449(3)
N(10)-C(24)	1.362(3)	N(1)-C(7)-N(2)	109.11(18)
N(10)-C(21)	1.375(3)	N(1)-C(7)-C(8)	124.73(19)
N(9)-C(20)	1.326(3)	N(2)-C(7)-C(8)	126.14(18)
N(11)-C(21)	1.335(3)	N(3)-C(8)-N(5)	116.22(19)
N(11)-C(20)	1.361(3)	N(3)-C(8)-C(7)	121.55(19)



N(12)-C(22)	1.326(3)	N(5)-C(8)-C(7)	122.23(18)
N(12)-C(21)	1.336(3)	N(5)-C(9)-N(4)	108.35(19)
N(8)-C(19)	1.354(3)	N(5)-C(9)-N(6)	128.7(2)
N(7)-C(19)	1.342(3)	N(6)-C(9)-N(4)	122.96(19)
N(1)-C(7)	1.341(3)	N(6)-C(10)-C(11)	124.5(2)
N(2)-C(7)	1.351(3)	C(12)-C(11)-C(10)	119.5(2)
N(3)-N(4)	1.364(3)	C(24)-C(23)-C(22)	119.5(2)
N(3)-C(8)	1.329(3)	C(23)-C(24)-N(10)	115.7(2)
N(5)-C(8)	1.363(3)	N(11)-C(21)-N(10)	108.49(18)
O(1)-Mn(1)-O(4)	89.45(6)	N(11)-C(21)-N(12)	129.0(2)
O(1)-Mn(1)-O(3)	95.32(7)	N(12)-C(21)-N(10)	122.51(19)
O(1)-Mn(1)-N(11)	90.52(6)	N(9)-C(20)-N(11)	116.39(19)
O(1)-Mn(1)-N(5)	81.92(6)	N(9)-C(20)-C(19)	121.26(19)
O(4)-Mn(1)-N(11)	86.24(7)	N(11)-C(20)-C(19)	122.29(18)
O(4)-Mn(1)-N(5)	90.52(6)	N(8)-C(19)-C(20)	125.34(19)
O(3)-Mn(1)-O(4)	174.51(7)	N(7)-C(19)-N(8)	109.06(19)
O(3)-Mn(1)-N(11)	96.40(7)	C(8)-N(3)-N(4)-C(9)	0.4(2)
O(3)-Mn(1)-N(5)	87.47(7)	C(9)-N(5)-C(8)-N(3)	0.8(3)
O(5)-Mn(1)-O(1)	170.86(6)	C(9)-N(5)-C(8)-C(7)	179.8(2)
O(5)-Mn(1)-O(4)	85.63(6)	C(9)-N(4)-C(12)-C(11)	1.5(3)
O(5)-Mn(1)-O(3)	90.00(7)	C(9)-N(6)-C(10)-C(11)	0.4(4)
O(5)-Mn(1)-N(11)	81.49(6)	C(12)-N(4)-C(9)-N(5)	178.1(2)
O(5)-Mn(1)-N(5)	105.78(6)	C(12)-N(4)-C(9)-N(6)	1.6(3)
N(5)-Mn(1)-N(11)	171.82(7)	C(24)-N(10)-N(9)-C(20)	177.3(2)
N(1)-O(1)-Mn(1)	123.46(12)	C(24)-N(10)-C(21)-N(11)	178.2(2)
C(11)-C(12)-N(4)	115.7(2)	C(24)-N(10)-C(21)-N(12)	1.3(3)
N(12)-C(22)-C(23)	124.3(2)	C(21)-N(10)-N(9)-C(20)	1.2(2)
N(7)-O(5)-Mn(1)	120.84(12)	C(21)-N(10)-C(24)-C(23)	2.6(3)
N(9)-N(10)-C(21)	110.87(17)	C(21)-N(11)-C(20)-N(9)	1.6(3)
C(24)-N(10)-N(9)	126.43(19)	C(21)-N(11)-C(20)-C(19)	175.6(2)
C(24)-N(10)-C(21)	122.69(19)	C(21)-N(12)-C(22)-C(23)	1.0(4)
C(20)-N(9)-N(10)	101.18(17)	C(20)-N(11)-C(21)-N(10)	0.6(2)
C(21)-N(11)-Mn(1)	134.24(15)	C(20)-N(11)-C(21)-N(12)	178.8(2)
C(21)-N(11)-C(20)	103.04(17)	Mn(1)-N(5)-C(9)-N(6)	4.3(3)
C(20)-N(11)-Mn(1)	121.84(14)	O(2)-N(2)-C(7)-N(1)	176.3(2)
C(22)-N(12)-C(21)	115.3(2)	O(2)-N(2)-C(7)-C(8)	2.4(4)
O(6)-N(8)-C(19)	126.33(19)	C(8)-N(3)-N(4)-C(12)	178.5(2)
N(7)-C(19)-C(20)	125.42(19)	C(8)-N(5)-C(9)-N(4)	0.9(2)
O(5)-N(7)-C(19)	126.91(18)	C(8)-N(5)-C(9)-N(6)	179.4(2)
O(1)-N(1)-C(7)	126.49(18)	O(1)-N(1)-C(7)-N(2)	176.53(19)
O(2)-N(2)-C(7)	126.20(18)	O(1)-N(1)-C(7)-C(8)	4.8(3)
C(8)-N(3)-N(4)	101.20(17)	O(5)-N(7)-C(19)-N(8)	177.3(2)
C(8)-N(5)-Mn(1)	125.72(14)	O(5)-N(7)-C(19)-C(20)	2.0(4)

C(9)-N(5)-Mn(1)	130.87(15)	C(10)-N(6)-C(9)-N(5)	179.1(2)
C(9)-N(5)-C(8)	103.23(17)	C(10)-N(6)-C(9)-N(4)	0.5(3)
N(3)-N(4)-C(9)	110.99(17)	C(10)-C(11)-C(12)-N(4)	0.6(4)
C(12)-N(4)-N(3)	126.58(19)	O(6)-N(8)-C(19)-N(7)	176.5(2)
C(12)-N(4)-C(9)	122.42(19)	O(6)-N(8)-C(19)-C(20)	8.2(4)
C(10)-N(6)-C(9)	114.9(2)	C(22)-N(12)-C(21)-N(10)	0.6(3)
Mn(1)-O(1)-N(1)-C(7)	42.5(3)	C(22)-N(12)-C(21)-N(11)	180.0(2)
Mn(1)-O(5)-N(7)-C(19)	39.6(3)	C(22)-C(23)-C(24)-N(10)	2.1(3)
Mn(1)-N(11)-C(21)-N(10)	168.31(15)	N(10)-N(9)-C(20)-N(11)	1.8(3)
Mn(1)-N(11)-C(21)-N(12)	12.3(4)	N(10)-N(9)-C(20)-C(19)	175.4(2)
Mn(1)-N(11)-C(20)-N(9)	169.11(15)	N(9)-N(10)-C(24)-C(23)	179.0(2)
Mn(1)-N(11)-C(20)-C(19)	13.8(3)	N(9)-N(10)-C(21)-N(11)	0.4(3)
Mn(1)-N(5)-C(8)-N(3)	176.21(14)	N(9)-N(10)-C(21)-N(12)	179.9(2)
Mn(1)-N(5)-C(8)-C(7)	4.8(3)	N(9)-C(20)-C(19)-N(8)	12.8(3)
Mn(1)-N(5)-C(9)-N(4)	176.04(14)	N(9)-C(20)-C(19)-N(7)	161.8(2)
N(2)-C(7)-C(8)-N(3)	20.7(3)	N(11)-C(20)-C(19)-N(8)	170.2(2)
N(2)-C(7)-C(8)-N(5)	158.3(2)	N(11)-C(20)-C(19)-N(7)	15.2(4)
N(3)-N(4)-C(9)-N(5)	0.9(2)	N(12)-C(22)-C(23)-C(24)	0.3(4)
N(3)-N(4)-C(9)-N(6)	179.5(2)	N(1)-C(7)-C(8)-N(3)	160.9(2)
N(3)-N(4)-C(12)-C(11)	179.7(2)	N(1)-C(7)-C(8)-N(5)	20.1(3)
N(4)-N(3)-C(8)-N(5)	0.2(2)	N(6)-C(10)-C(11)-C(12)	0.4(4)
N(4)-N(3)-C(8)-C(7)	179.29(19)		

**Table S8** Selected bond lengths [Å] and angles [°] for complex **6c<sub>o</sub>**.

Co(1)-O(1)	2.0072(15)	O(2)-N(2)	1.259(2)
O(9)-N(7)	1.260(2)	N(9)-C(23)	1.373(3)
N(9)-N(8)	1.354(3)	N(7)-C(21)	1.354(3)
Co(1)-O(3)	2.1295(17)	N(2)-C(7)	1.350(3)
N(9)-C(26)	1.356(3)	N(6)-C(9)	1.333(3)
Co(1)-N(5)	2.1054(16)	C(10)-C(11)	1.404(3)
Co(2)-O(10)	2.0425(15)	C(26)-C(25)	1.358(3)
N(3)-C(8)	1.325(3)	C(24)-C(25)	1.403(3)
Co(2)-O(11)	2.0787(17)	O(8)-C(14)	1.35(4)
N(8)-C(22)	1.321(3)	N(8)-N(9)-C(23)	111.04(17)
Co(2)-N(11)	2.1465(17)	N(8)-N(9)-C(26)	126.11(18)
N(6)-C(10)	1.323(3)	O(9)-N(7)-C(21)	126.82(19)
N(10)-C(23)	1.337(3)	C(8)-N(3)-N(4)	101.17(16)
N(10)-C(24)	1.322(3)	O(2)-N(2)-C(7)	126.42(19)
C(7)-C(8)	1.449(3)	N(1)-C(7)-N(2)	108.87(18)
C(22)-C(21)	1.443(3)	N(5)-C(8)-C(7)	121.55(17)
C(12)-C(11)	1.355(3)	N(8)-C(22)-N(11)	116.23(19)
C(17)-C(16)	1.526(3)	C(11)-C(12)-N(4)	116.20(19)

O(10)-N(12)	1.298(2)	N(6)-C(10)-C(11)	124.7(2)
O(1)-N(1)	1.288(2)	N(9)-C(26)-C(25)	115.5(2)
N(1)-C(7)	1.337(3)	C(12)-C(11)-C(10)	119.1(2)
N(5)-C(8)	1.357(3)	N(10)-C(24)-C(25)	124.8(2)
N(5)-C(9)	1.343(3)	C(26)-C(25)-C(24)	119.5(2)
N(11)-C(22)	1.366(3)	N(6)-C(10)-C(11)-C(12)	0.7(4)
N(11)-C(23)	1.341(3)	C(8)-N(5)-C(9)-N(4)	1.5(2)
N(12)-C(21)	1.330(3)	C(8)-N(5)-C(9)-N(6)	176.8(2)
N(12)-C(17)	1.504(3)	C(9)-N(5)-C(8)-N(3)	1.5(3)
N(4)-N(3)	1.356(3)	C(9)-N(5)-C(8)-C(7)	175.1(2)
N(4)-C(9)	1.371(3)	C(9)-N(4)-N(3)-C(8)	0.3(2)
N(4)-C(12)	1.360(3)	C(9)-N(4)-C(12)-C(11)	0.0(3)
O(1)-Co(1)-O(1 <sup>#1</sup> )	180.00(8)	C(9)-N(6)-C(10)-C(11)	0.5(4)
O(1 <sup>#1</sup> )-Co(1)-O(3)	89.23(7)	C(22)-N(11)-C(23)-N(9)	0.7(2)
C(26)-N(9)-C(23)	122.85(19)	C(22)-N(11)-C(23)-N(10)	179.2(2)
O(1)-Co(1)-O(3)	90.77(7)	C(23)-N(11)-C(22)-N(8)	0.3(3)
O(1 <sup>#1</sup> )-Co(1)-N(5)	93.42(6)	C(23)-N(11)-C(22)-C(21)	178.8(2)
O(1)-Co(1)-N(5)	86.58(6)	C(12)-N(4)-N(3)-C(8)	177.6(2)
O(3 <sup>#1</sup> )-Co(1)-O3	180.0	C(12)-N(4)-C(9)-N(5)	178.6(2)
C(22)-N(8)-N(9)	101.66(17)	C(12)-N(4)-C(9)-N(6)	0.2(3)
C(10)-N(6)-C(9)	114.93(19)	C(17)-N(12)-C(21)-N(7)	8.9(3)
C(24)-N(10)-C(23)	114.91(19)	C(17)-N(12)-C(21)-C(22)	171.0(2)
N(5)-Co(1)-O(3 <sup>#1</sup> )	93.43(7)	C(26)-N(9)-C(23)-N(11)	178.7(2)
N(5)-Co(1)-O(3)	86.57(7)	C(26)-N(9)-C(23)-N(10)	1.4(4)
N(5 <sup>#1</sup> )-Co(1)-N5	180.0	C(24)-N(10)-C(23)-N(11)	179.1(2)
N(1)-C(7)-C(8)	125.42(18)	C(24)-N(10)-C(23)-N(9)	0.8(3)
N(2)-C(7)-C(8)	125.61(18)	N(4)-N(3)-C(8)-N(5)	0.8(3)
O(10)-Co(2)-O(10 <sup>#2</sup> )	180.0	N(4)-N(3)-C(8)-C(7)	175.8(2)
O(10)-Co(2)-O(11)	90.55(7)	N(4)-C(12)-C(11)-C(10)	0.4(4)
O(10 <sup>#2</sup> )-Co(2)-O11	89.45(7)	O(2)-N(2)-C(7)-N(1)	176.2(2)
O(10 <sup>#2</sup> )-Co(2)-N(11)	93.96(6)	O(2)-N(2)-C(7)-C(8)	7.3(4)
N(3)-C(8)-N(5)	116.41(18)	O(9)-N(7)-C(21)-N(12)	176.0(2)
N(3)-C(8)-C(7)	121.94(18)	O(9)-N(7)-C(21)-C(22)	3.9(4)
N(5)-C(9)-N(4)	107.93(18)	C(10)-N(6)-C(9)-N(5)	178.0(2)
N(6)-C(9)-N(5)	129.00(19)	C(10)-N(6)-C(9)-N(4)	0.0(3)
N(6)-C(9)-N(4)	123.05(18)	C(26)-N(9)-N(8)-C(22)	178.9(2)
N(11)-C(22)-C(21)	122.36(18)	N(9)-N(8)-C(22)-N(11)	0.2(3)
O(10)-Co(2)-N(11)	86.04(6)	N(9)-N(8)-C(22)-C(21)	179.3(2)
O(11)-Co(2)-O(11 <sup>#2</sup> )	180.0	N(9)-C(26)-C(25)-C(24)	1.3(4)
O(11 <sup>#2</sup> )-Co(2)-N(11)	85.86(7)	N(3)-N(4)-C(9)-N(5)	1.2(3)
N(11 <sup>#2</sup> )-Co(2)-N(11)	180.00(9)	N(3)-N(4)-C(9)-N(6)	177.2(2)
O(11)-Co(2)-N(11 <sup>#2</sup> )	85.86(7)	N(3)-N(4)-C(12)-C(11)	177.0(2)
O(11)-Co(2)-N(11)	94.14(7)	N(2)-C(7)-C(8)-N(5)	173.4(2)

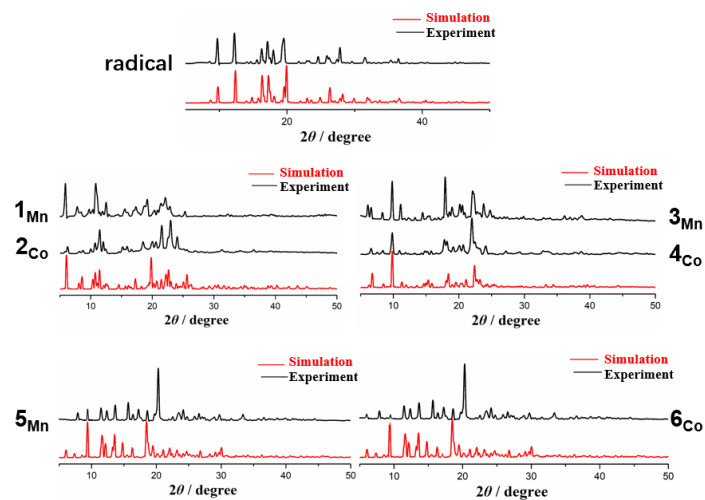
N(8)-C(22)-C(21)	121.40(19)	N(2)-C(7)-C(8)-N(3)	10.2(3)
N(11)-C(23)-N(9)	108.37(18)	N(8)-N(9)-C(23)-N(11)	0.9(3)
N(10)-C(23)-N(11)	129.18(19)	N(8)-N(9)-C(23)-N(10)	179.1(2)
N(10)-C(23)-N(9)	122.46(19)	N(8)-N(9)-C(26)-C(25)	178.1(2)
O(11)-Co(2)-N(11)	94.14(7)	N(8)-C(22)-C(21)-N(12)	163.0(2)
N(12)-C(21)-N(7)	109.24(18)	N(8)-C(22)-C(21)-N(7)	17.1(4)
N(12)-C(21)-C(22)	125.41(19)	Co(2)-N(11)-C(23)-N(9)	177.91(15)
N(7)-C(21)-C(22)	125.36(19)	Co(2)-N(11)-C(23)-N(10)	2.2(4)
N(12)-C(17)-C(16)	106.46(18)	O(10)-N(12)-C(21)-N(7)	175.9(2)
N(12)-O(10)-Co(2)	122.13(13)	O(10)-N(12)-C(21)-C(22)	4.2(4)
N(1)-O(1)-Co(1)	122.17(13)	O(10)-N(12)-C(17)-C(20)	161.25(19)
O(1)-N(1)-C(7)	127.35(18)	O(10)-N(12)-C(17)-C(16)	80.1(2)
C(8)-N(5)-Co(1)	122.88(14)	O(10)-N(12)-C(17)-C(15)	39.6(3)
C(9)-N(5)-Co(1)	133.53(15)	O(1)-N(1)-C(7)-N(2)	177.0(2)
C(9)-N(5)-C(8)	103.03(16)	O(1)-N(1)-C(7)-C(8)	0.5(4)
C(22)-N(11)-Co(2)	123.51(14)	C(23)-N(9)-N(8)-C(22)	0.6(2)
C(23)-N(11)-Co(2)	133.78(14)	C(23)-N(9)-C(26)-C(25)	2.4(4)
C(23)-N(11)-C(22)	102.70(17)	C(23)-N(10)-C(24)-C(25)	2.0(4)
O(10)-N(12)-C(21)	126.73(18)	N(1)-C(7)-C(8)-N(5)	10.6(3)
O(10)-N(12)-C(17)	121.32(17)	N(1)-C(7)-C(8)-N(3)	165.7(2)
C(21)-N(12)-C(17)	111.78(17)	N(11)-C(22)-C(21)-N(12)	18.0(4)
N(3)-N(4)-C(9)	111.43(16)	N(11)-C(22)-C(21)-N(7)	161.9(2)
N(3)-N(4)-C(12)	126.52(18)	C(21)-N(12)-C(17)-C(16)	95.4(2)
C(12)-N(4)-C(9)	121.99(19)	Co(1)-N(5)-C(9)-N(4)	169.78(15)
Co(1)-O(1)-N(1)-C(7)	32.4(3)	Co(1)-N(5)-C(9)-N(6)	11.9(4)
N(10)-C(24)-C(25)-C(26)	1.0(4)	Co(2)-O(10)-N(12)-C(21)	39.1(3)
Co(1)-N(5)-C(8)-N(3)	170.99(15)	Co(2)-O(10)-N(12)-C(17)	135.74(17)
Co(1)-N(5)-C(8)-C(7)	12.5(3)	Co(2)-N(11)-C(22)-N(8)	178.47(15)
Co(2)-N(11)-C(22)-C(21)	2.5(3)		

Symmetry transformations used to generate equivalent atoms: <sup>#1</sup> -X,1-Y,1-Z; <sup>#2</sup> 1-X,1-Y,1-Z

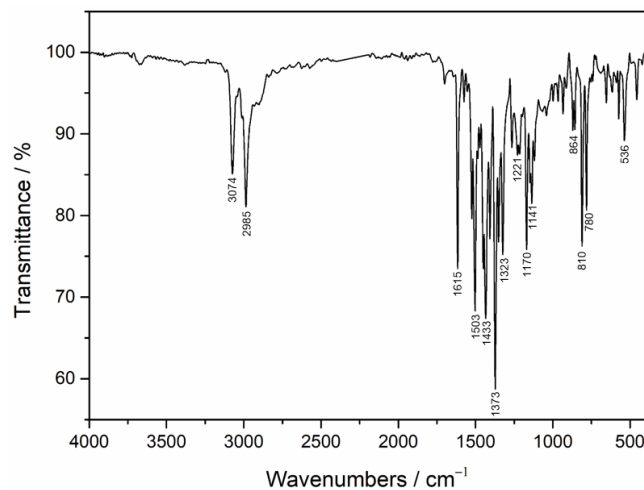
**Table S9** SHAPE analyses for **1<sub>Mn</sub>-6<sub>Co</sub>**.

Complexes Label	<b>1<sub>Mn</sub></b>	<b>2<sub>Co</sub></b>	<b>3<sub>Mn</sub></b>		<b>4<sub>Co</sub></b>		<b>5<sub>Mn</sub></b>	<b>6<sub>Co</sub></b>	
			<b>Mn1</b>	<b>Mn2</b>	<b>Co1</b>	<b>Co2</b>		<b>Co1</b>	<b>Co2</b>
OC-6	<b>0.890</b>	<b>0.243</b>	<b>1.014</b>	<b>2.162</b>	<b>0.369</b>	<b>1.094</b>	<b>0.803</b>	<b>0.185</b>	<b>0.211</b>
TPR-6	12.295	14.374	12.486	8.970	13.271	10.615	13.037	16.170	15.891
JPPY-6	28.081	30.625	27.426	25.240	30.448	26.722	27.992	31.687	32.029

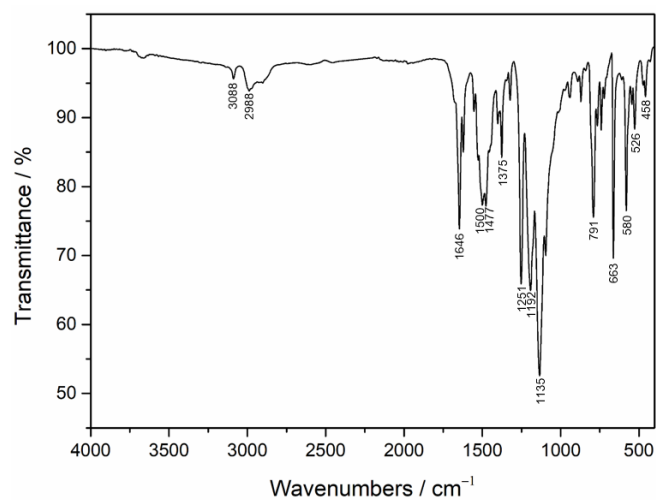
Code	Label	Symmetry	Shape
1	OC-6	<i>O<sub>h</sub></i>	Octahedron
2	TPR-6	<i>D<sub>3h</sub></i>	Trigonal prism
3	JPPY-6	<i>C<sub>5v</sub></i>	Johnson pentagonal pyramid J2



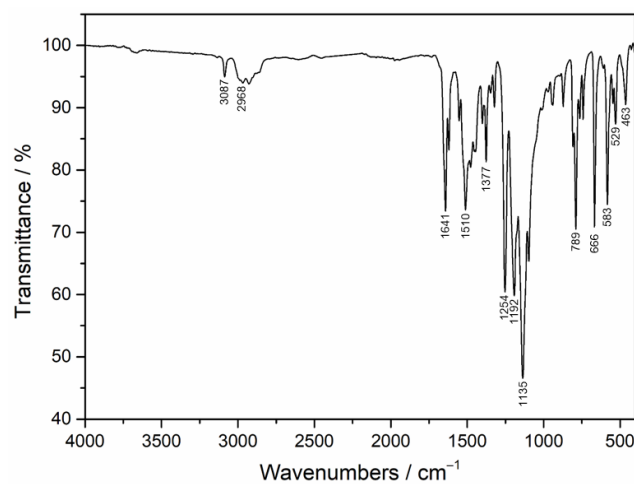
**Figure S1** X-ray powder diffraction patterns of NIT-2-TrzPm radical and complexes **1<sub>Mn</sub>**-**6<sub>Co</sub>**.



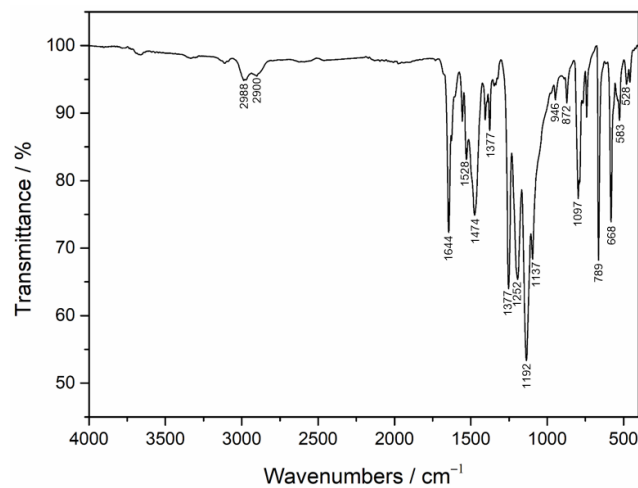
**Figure S2** Infrared spectrum of NIT-2-TrzPm radical at room temperature.



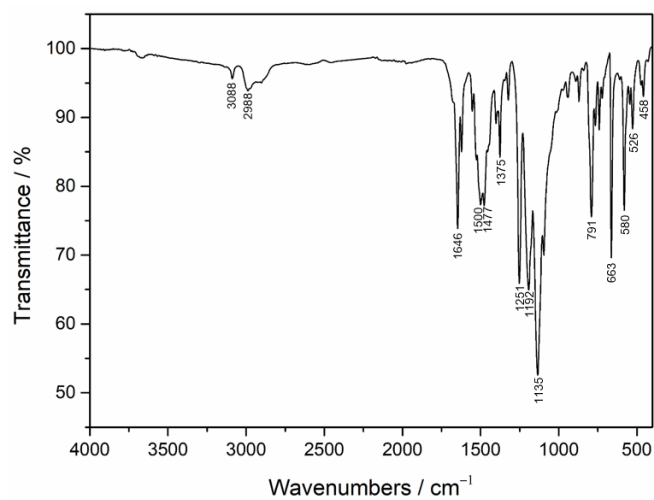
**Figure S3** Infrared spectrum of complex **1<sub>Mn</sub>** at room temperature.



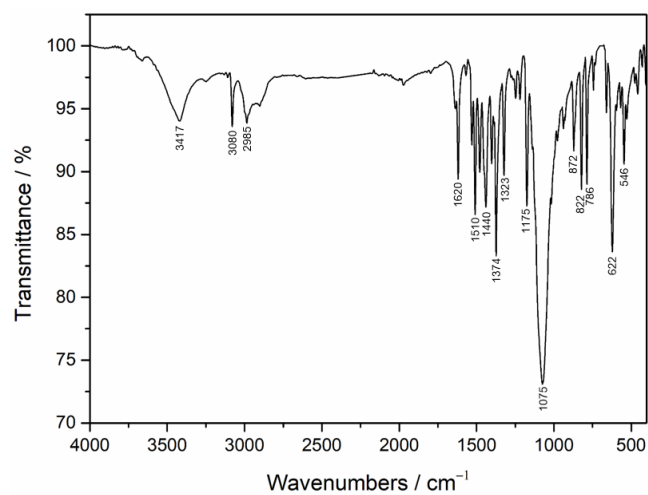
**Figure S4** Infrared spectrum of complex **2<sub>Co</sub>** at room temperature.



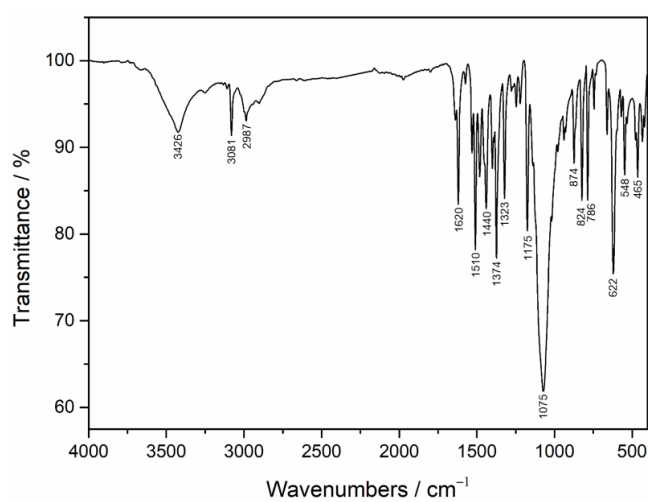
**Figure S5** Infrared spectrum of complex **3<sub>Mn</sub>** at room temperature.



**Figure S6** Infrared spectrum of complex **4<sub>Co</sub>** at room temperature.

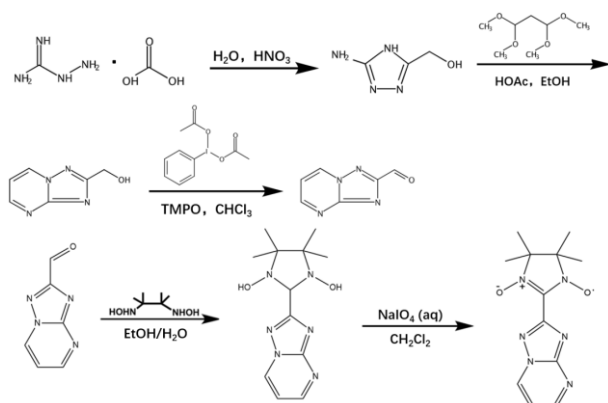


**Figure S7** Infrared spectrum of complex **5<sub>Mn</sub>** at room temperature.

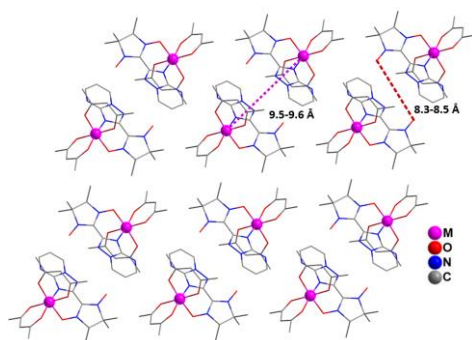


**Figure S8** Infrared spectrum of complex **6<sub>Co</sub>** at room temperature.

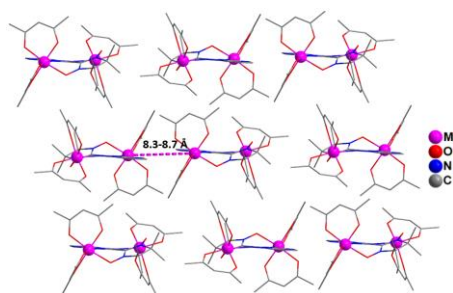
## 2. The synthesis of NIT-2-TrzPm radical



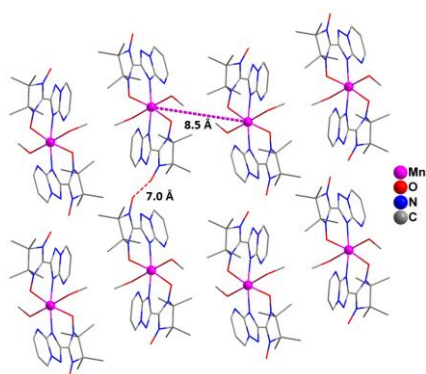
**Scheme S1** The synthesis of **NIT-2-TrzPm** radical.



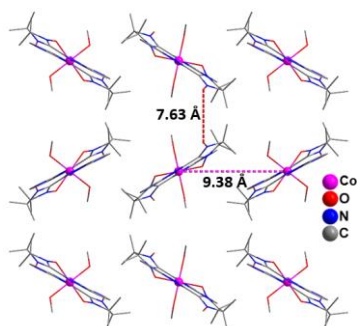
**Figure S9** Packing diagram of **1<sub>Mn</sub>** and **2<sub>Co</sub>** (H, F, and CH<sub>2</sub>Cl<sub>2</sub> molecules are omitted).



**Figure S10** Packing diagram of **3<sub>Mn</sub>** and **4<sub>Co</sub>** (H and F are omitted).



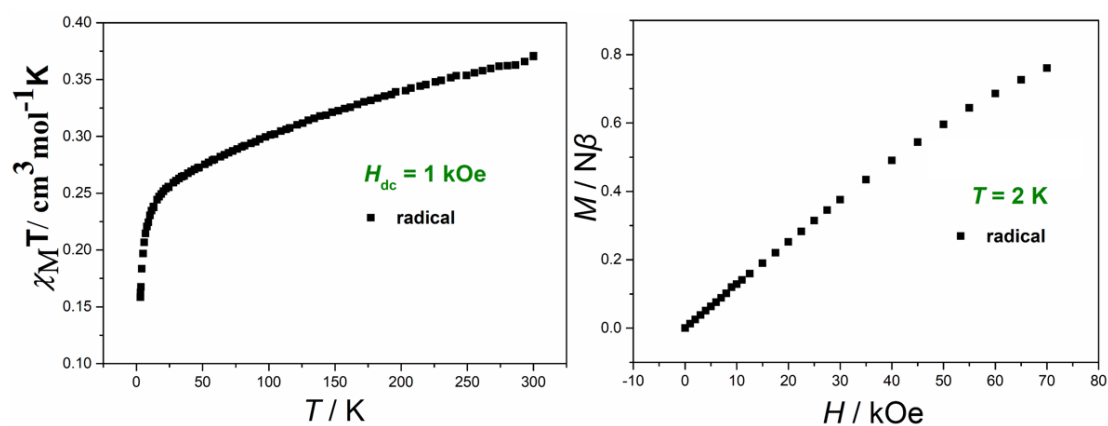
**Figure S11** Packing diagram of **5<sub>Mn</sub>** (H, ClO<sub>4</sub><sup>-</sup> and methanol solvent molecules are omitted).



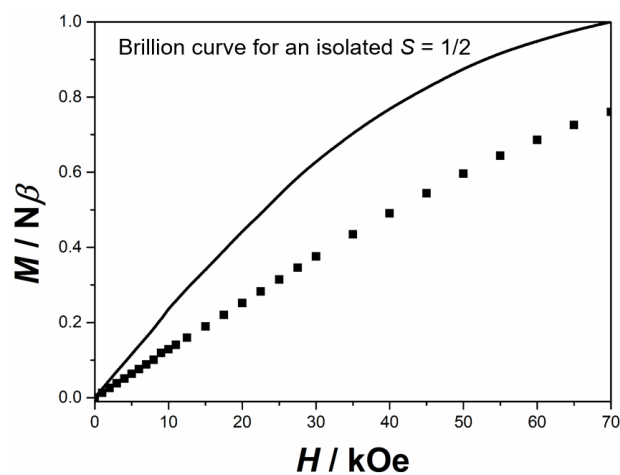
**Figure S12** Packing diagram of **6<sub>Co</sub>** (H, ClO<sub>4</sub><sup>-</sup> and methanol solvent molecules are omitted).



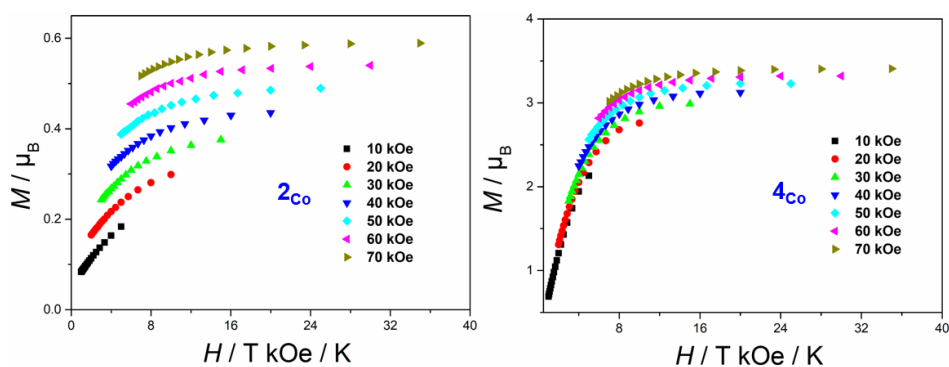
### 3. Magnetic Properties



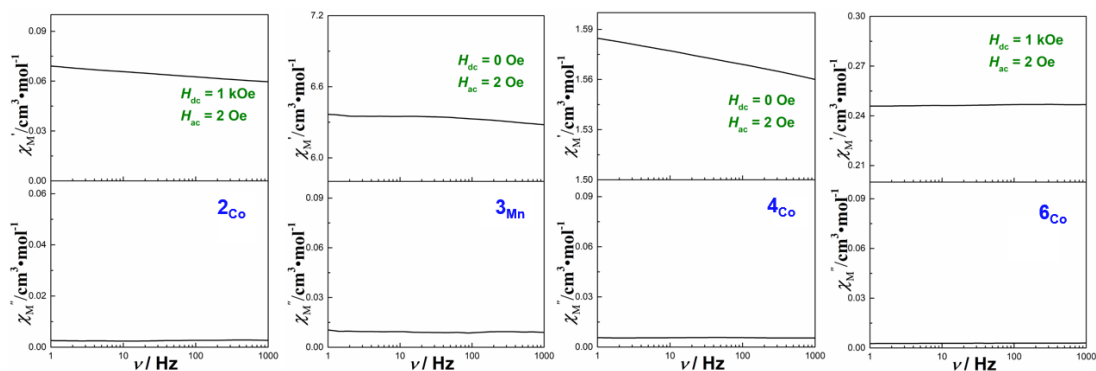
**Figure S13** Temperature-dependent dc magnetic susceptibility data measured at 1 kOe (left) and field-dependent magnetizations at 2 K (right) of NIT-2-TrzPm radical.



**Figure S14** The field-dependent magnetization curve of NIT-2-TrzPm radical at 2 K. The solid line represents the calculated Brillouin curve for an isolated  $S = 1/2$ .



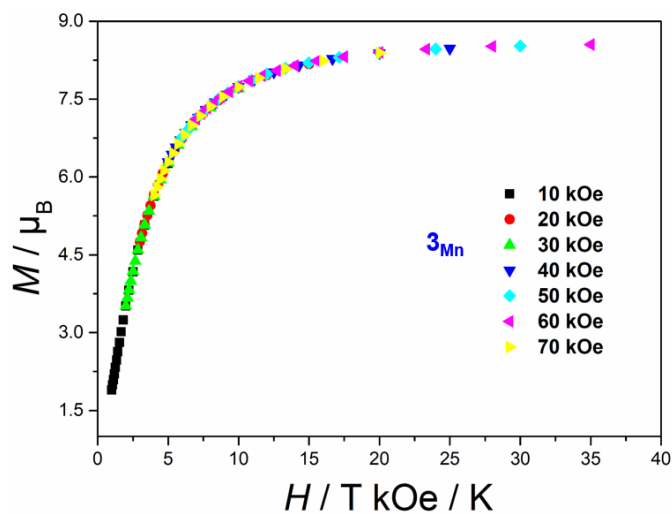
**Figure S15** The reduced magnetization data of  $2\text{Co}$  and  $4\text{Co}$  collected under various applied DC fields.



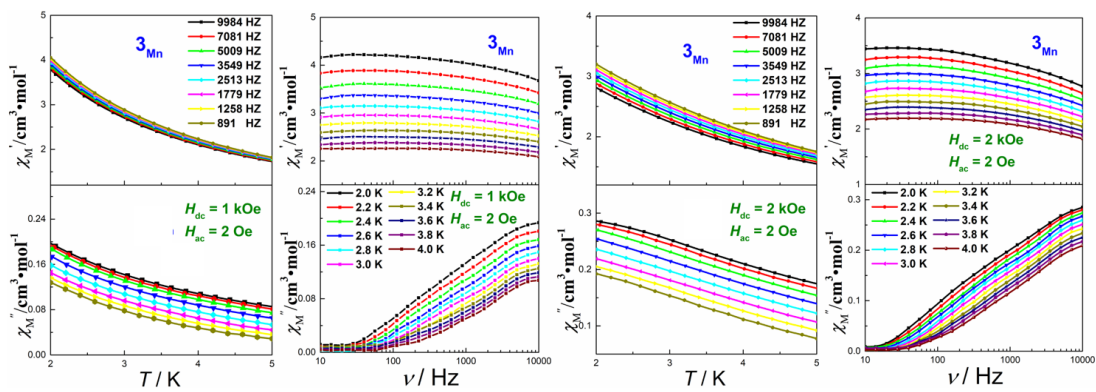
**Figure S16** Frequency-dependent ac signals for **2Co**, **3Mn**, **4Co** and **6Co** at 2 K under a 0 or 1 kOe dc field.

**Table S10** Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **4Co** under a 1 kOe dc field according to the generalized Debye model.

Temperature / K	$\chi_s / \text{cm}^3\text{mol}^{-1}$	$\chi_T / \text{cm}^3\text{mol}^{-1}$	$\tau / \text{s}$	$\alpha$
2.0	0.186	2.09	0.000891	0.21120
2.2	0.163	1.91	0.000697	0.21386
2.4	0.204	1.75	0.000562	0.17164
2.6	0.206	1.62	0.000448	0.14763
2.8	0.222	1.51	0.000359	0.11213
3.0	0.226	1.43	0.000283	0.095347
3.2	0.226	1.31	0.000217	0.047837
3.4	0.215	1.24	0.000169	0.029989
3.6	0.199	1.20	0.000128	0.031412
3.8	0.231	1.15	0.000104	0.013481
4.0	0.295	1.11	0.0000883	0.00073194



**Figure S17** The reduced magnetization data of **3Mn** collected under various applied DC fields.



**Figure S18** Temperature- and frequency-dependent ac magnetic susceptibility data obtained for complex  $3_{Mn}$  in a 1000 and 2000 Oe dc field.