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Supplementary Information

The diversities of magnetic behaviors appearing simultaneously in three isomorphism based on 1H-tetrazolyl-acetic acid ligands

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Table S1. Selected bond lengths (Å) and angle (°) for **1**.

Mn1−O1	2.1528(11)	Mn1−O2$^{\#3}$	2.1659(10)
Mn1−O1$^{\#1}$	2.1528(11)	Mn1−N1$^{\#4}$	2.3015(12)
Mn1−O2$^{\#2}$	2.1659(10)	Mn1−N1$^{\#5}$	2.3015(12)
O1−Mn1−O1	188.12(6)	O2$^{\#2}$−Mn1−N1$^{\#4}$	88.62(4)
O1−Mn1−O2$^{\#2}$	178.44(4)	O2$^{\#3}$−Mn1−N1$^{\#4}$	90.99(4)
O1$^{\#1}$−Mn1−O2$^{\#2}$	91.44(4)	O1−Mn1−N1$^{\#5}$	87.54(5)
O1 −Mn1−O2$^{\#3}$	91.44(4)	O1$^{\#1}$−Mn1−N1$^{\#5}$	92.86(5)
O1$^{\#1}$−Mn1−O2$^{\#3}$	178.44(4)	O2$^{\#2}$−Mn1−N1$^{\#5}$	90.99(4)
O2$^{\#2}$−Mn1−O2$^{\#3}$	89.03(6)	O2$^{\#3}$−Mn1−N1$^{\#5}$	88.62(4)
O1−Mn1−N1^{4}	92.86(4)	N1$^{\#4}$−Mn1−N1$^{\#5}$	179.45(6)
O1$^{\#1}$−Mn1−N1$^{\#4}$	87.54(5)	C3−O1−Mn$^{\#1}$	130.56(9)
C3−O2−Mn1$^{\#3}$	131.39(8)	C1−N1−Mn1$^{\#5}$	129.47(10)

Symmetry codes:#1,2-x,+y,3/2-z; #2,+x,-y,-1/2+z; #3,2-x,-y,2-z; #4,-1/2+x,1/2-y,-1/2+z;#5,5/2-x,1/2-y,2-z.

Table S2. Selected bond lengths (Å) and angle (°) for **2**.

Co1−O2	2.0736(10)	Co1−N4$^{\#4}$	2.1731(13)
Co1−O2$^{\#1}$	2.0736(10)	Co1−N4$^{\#5}$	2.1731(13)
Co1−O1$^{\#2}$	2.0881(11)	O1−Co1$^{\#3}$	2.0881(11)
Co1−O1$^{\#3}$	2.0881(11)	N4−Co1$^{\#6}$	2.1731(13)
O2−Co1−O2$^{\#1}$	91.69(6)	O1$^{\#3}$−Co1−N4$^{\#4}$	86.01(5)
O2−Co1−O1$^{\#2}$	177.12(4)	O2$^{\#1}$−Co1−N4$^{\#5}$	88.40(4)
O2$^{\#1}$−Co1−O1	290.54(4)	O1$^{\#2}$−Co1−N4$^{\#5}$	86.01(5)
O2−Co1−O1$^{\#3}$	90.54(4)	O1$^{\#3}$−Co1−N4$^{\#5}$	93.34(5)
O2$^{\#1}$−Co1−O1$^{\#3}$	177.12(4)	O1$^{\#3}$−Co1−N4#4	86.01(5)
O1$^{\#2}$−Co1−O1$^{\#3}$	87.29(6)	O2$^{\#1}$−Co1−N4$^{\#5}$	88.40(4)
O2−Co1−N4$^{\#4}$	88.40(4)	O1$^{\#2}$−Co1−N4$^{\#5}$	86.01(5)
O2$^{\#1}$−Co1−N4$^{\#4}$	92.23(4)	O1$^{\#3}$−Co1−N4$^{\#5}$	93.34(5)
O1$^{\#2}$−Co1−N4$^{\#4}$	93.34(4)	C1−N4−Co1$^{\#6}$	129.45(10)

Symmetry codes:

#1,1-x,+y,3/2-z;#2,+x,-y,1/2+z;#3,1-x,-y,1-z;#4,-1/2+x,1/2+y,+z;#5,3/2-x,1/2+y,3/2-z;#6,1/2+x,-1/2+y,+z.

Table S3. Selected bond lengths (Å) and angle (°) for **3**.

Ni1−O1	2.0665(15)	Ni1−N4$^{\#4}$	2.1082(17)
Ni1−O1$^{\#1}$	2.0665(15)	Ni1−N4$^{\#5}$	2.1082(17)
Ni1−O2$^{\#2}$	2.0686(14)	O2−Ni1$^{\#3}$	2.0686(14)
Ni1−O2$^{\#3}$	2.0686(14)	N4−Ni1$^{\#4}$	2.1082(17)

O1−Ni1−O1$^{\#1}$	86.93(8)	O2$^{\#2}$−Ni1−N4$^{\#4}$	92.75(6)
O1−Ni1−O2$^{\#2}$	176.85(5)	O2$^{\#3}$−Ni1−N4$^{\#4}$	87.80(6)
O1$^{\#1}$−Ni1−O2$^{\#2}$	90.18(6)	O1−Ni1−N4$^{\#5}$	93.25(6)
O1−Ni1−O2$^{\#3}$	90.18(6)	O1$^{\#1}$−Ni1−N4$^{\#5}$	86.17(6)
O11−Ni1−O2$^{\#3}$	176.85(5)	C3−O2−Ni1$^{\#3}$	132.24(12)
O22−Ni1−O2$^{\#3}$	92.75(8)	C3−O1−Ni1	128.90(13)
O1−Ni1−N4$^{\#4}$	86.17(6)	C1−N4−Ni1$^{\#4}$	129.54(15)
O1$^{\#1}$−Ni1−N4$^{\#4}$	93.25(6)	N3−N4−Ni1$^{\#4}$	124.51(14)

Symmetry codes:#1,1-x,+y,3/2-z; #2,+x,-y,-1/2+z; #3,1-x,-y,2-z; #4,3/2-x,1/2-y,2-z;# 5,-1/2+x,1/2-y,-1/2+z.

Table S4. The θ Angles in complexes **1**,**2** and iso-**1**,**2**.

Compound	θ_1-1 / °	θ_1-2 / °	θ_1-3 / °	θ_1-4 / °	θ_2 / °	θ_3 / °	θ_4 / °	θ_5 / °	mode
1	87.54(5)	88.62(4)	90.99(4)	92.86(4)	179.45(6)	112.80(11)	84.486(32)	79.307(53)	I
Iso-1	81.90(5)	83.21(5)	96.79(5)	98.10(6)	180.00(1)	113.1(2)	73.202(29)	0.000(85)	II
2	86.01(5)	88.40(4)	92.23(4)	93.34(5)	179.11(6)	112.93(11)	86.176(34)	80.667(45)	I
Iso-2	82.48(10)	83.81(9)	96.19(9)	97.52(10)	180.000(1)	113.1(2)	76.814(46)	0.000(152)	II

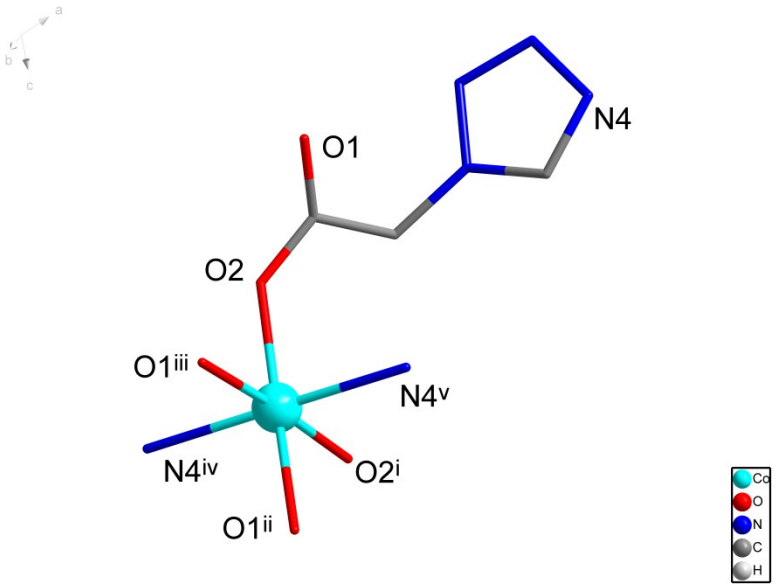

Figure S1. Coordination environment of the Co(II) ion in complex 2 with hydrogen atoms omitted for clarity. Symmetry codes: (i) −x+1, y, −z+3/2; (ii) x, −y, z+1/2; (iii) −x+1, −y, −z+1; (iv) −x+3/2, y+1/2, −z+3/2; (v) x−1/2, y+1/2, z; (vi) x+1/2, y−1/2, z.

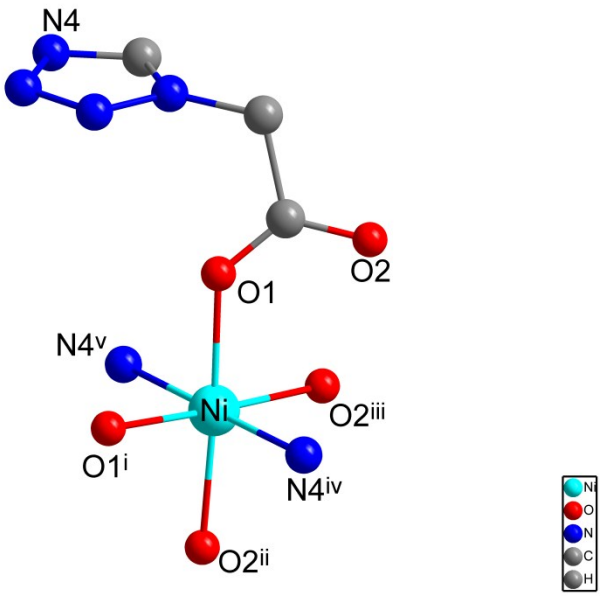

Figure S2. Coordination environment of the Ni (II) ion in complex 3 with hydrogen atoms omitted for clarity. Symmetry codes: (i) −x+1, y, −z+3/2;

(ii) x, −y, z−1/2; (iii) −x+1, −y, −z+2; (iv) x−1/2, −y+1/2, z−1/2; (v) −x+3/2, −y+1/2, −z+2.

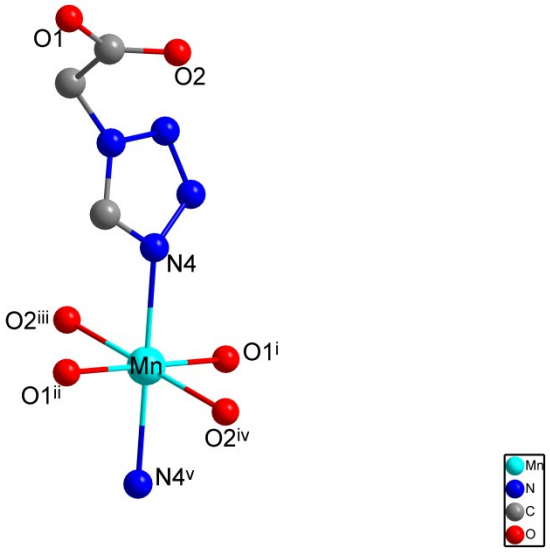

Figure S3. Coordination environment of the Mn (II) ion in iso-1 with hydrogen atoms omitted for clarity. Symmetry codes: (i) x+1/2, −y+5/2, z−1/2; (ii) −x−1/2, y−1/2, −z+5/2; (iii) x−1/2, −y+5/2, z−1/2; (iv) −x+1/2, y−1/2, −z+5/2; (v) −x, −y+2, −z+2.

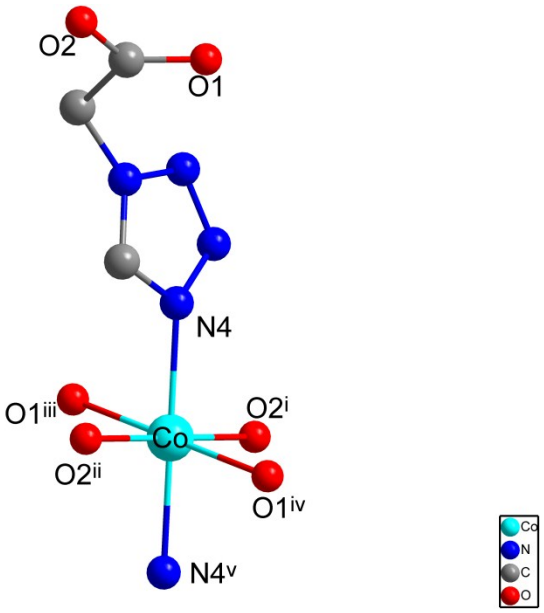

Figure S4. Coordination environment of the Co (II) ion in iso-1 with hydrogen atoms omitted for clarity. Symmetry codes: (i) x+1/2, −y+5/2, z−1/2; (ii) −x−1/2, y−1/2, −z+5/2; (iii) x−1/2, −y+5/2, z−1/2; (iv) −x+1/2, y−1/2, −z+5/2; (v) −x, −y+2, −z+2.

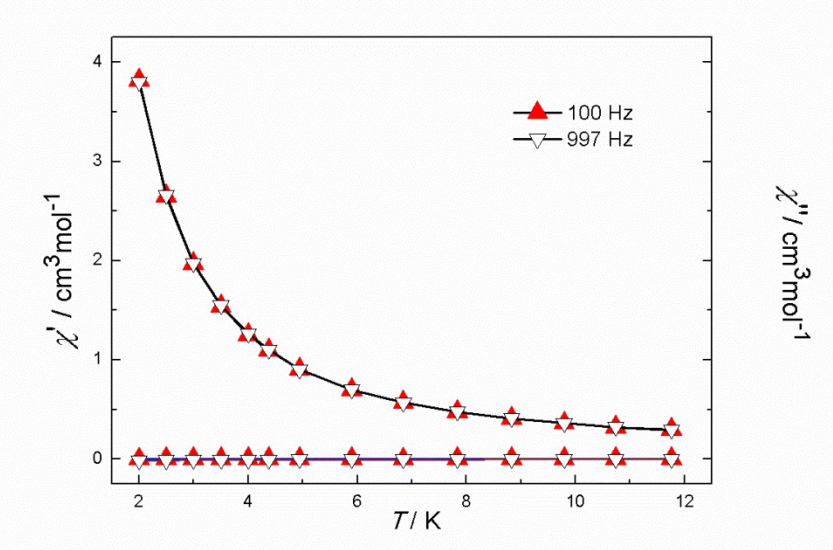

Figure S5. Temperature dependence of the in-phase (χ′) and out-of-phase (χ″) ac susceptibilities at H_{ac} = 2.5 Oe for complex **2** measured without an applied dc field.

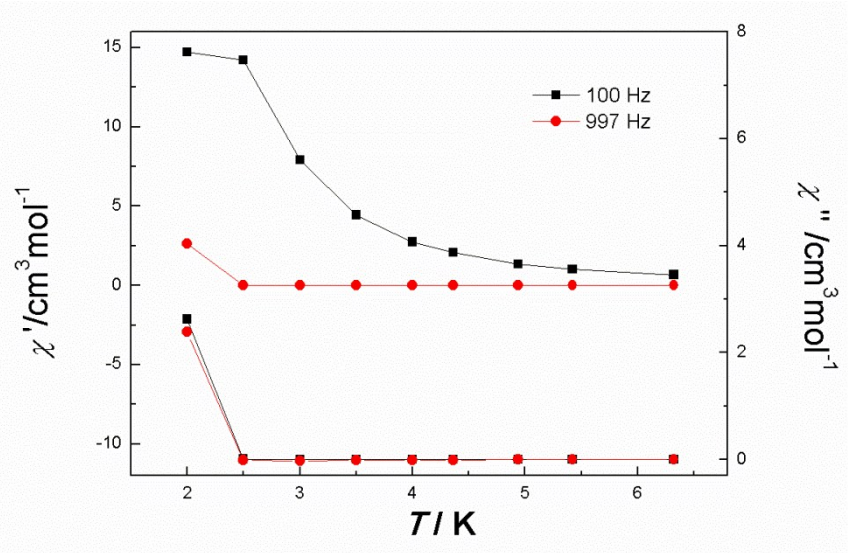

Figure S6. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibilities at H_{ac} = 2.5 Oe for complex **3** measured without an applied dc field.

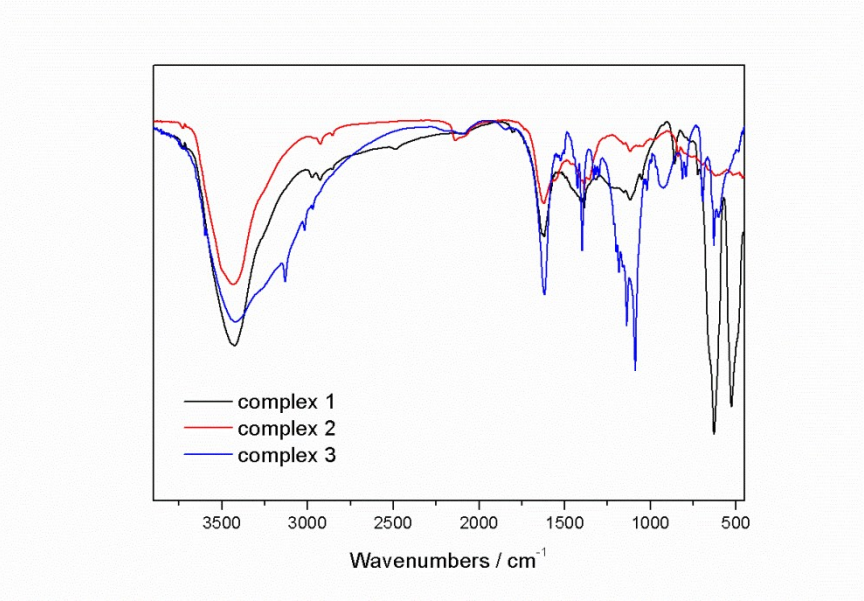

Figure S7. Infrared spectra of the complexes **1**-**3.**

In the spectra, characteristic bands at 3423, 2972, 2925, 2079, 1618, 1384, 1116, 857, 627 and 526 cm^{-1} for **1**, 3431, 2924, 2851, 2136, 1619, 1384, 1116, 836 and 617 cm^{-1} for **2,** 3421, 3130, 3016, 2962, 2079, 1617, 1400, 1137, 1087, 811 and 628 cm^{-1} for **3.**

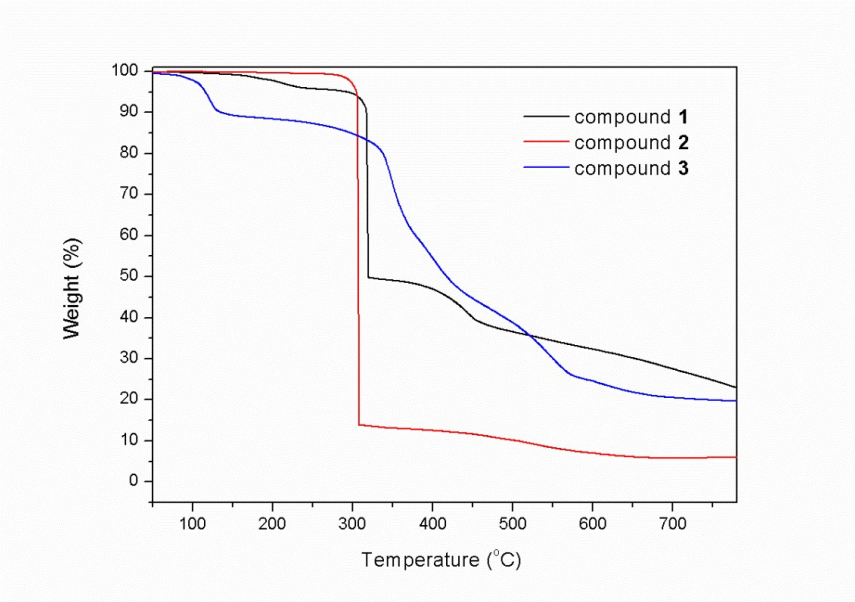

Figure S8. TGA plots of the complexes **1-3**