

Controlled assemblies of hepta- and trideca-Co^{II} clusters by a rational derivation of salicylaldehyde Schiff bases: Microwave-assisted synthesis, crystal structures, ESI-MS solution analysis and magnetic properties†

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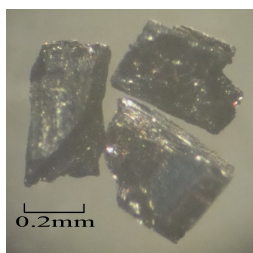


Fig. S1. Photo of some single crystals of 2 showing the morphology and size.

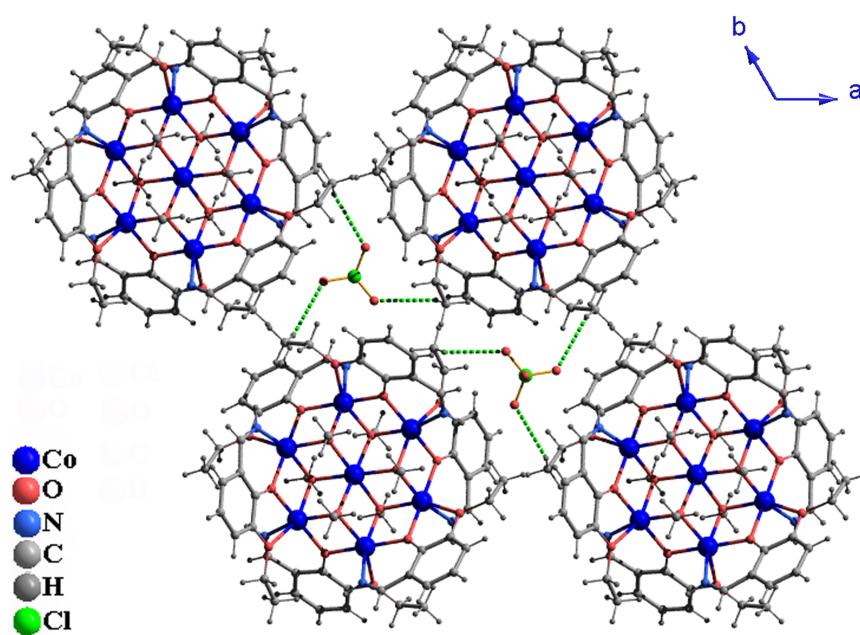


Fig. S2 The crystal packing of the Co₇ clusters.

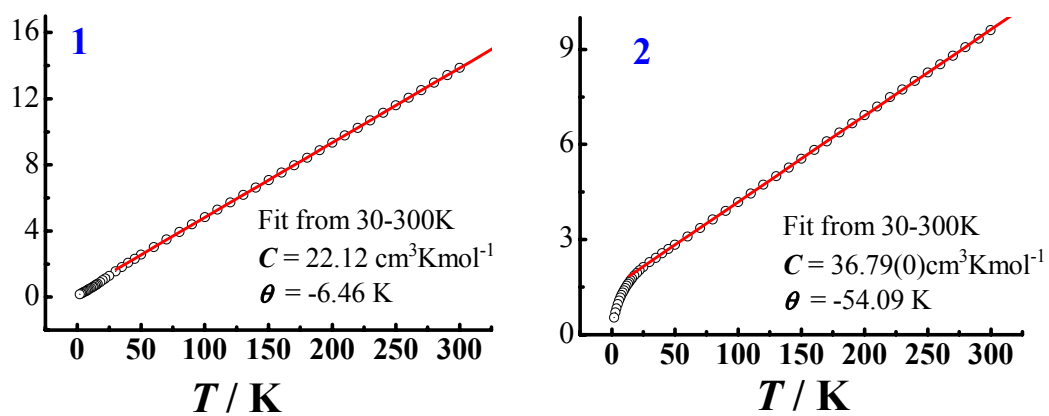


Fig. S3 Plots of χ^{-1} vs. T and the fit of Curie-Weiss law (solid curve) of **1** and **2**.

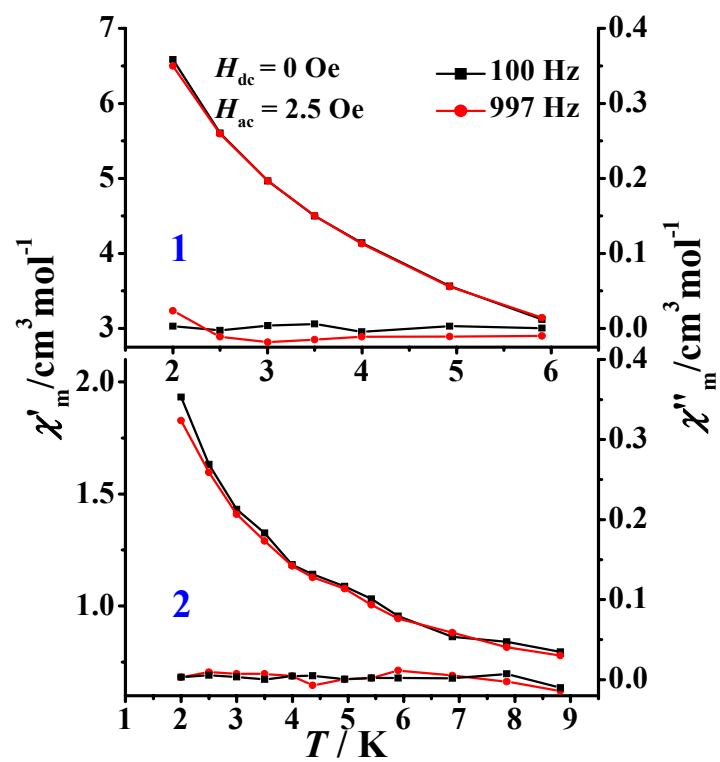


Fig. S4 Plots of in-of-phase (χ') and out-of-phase (χ'') ac susceptibility signals for **1** and **2**.

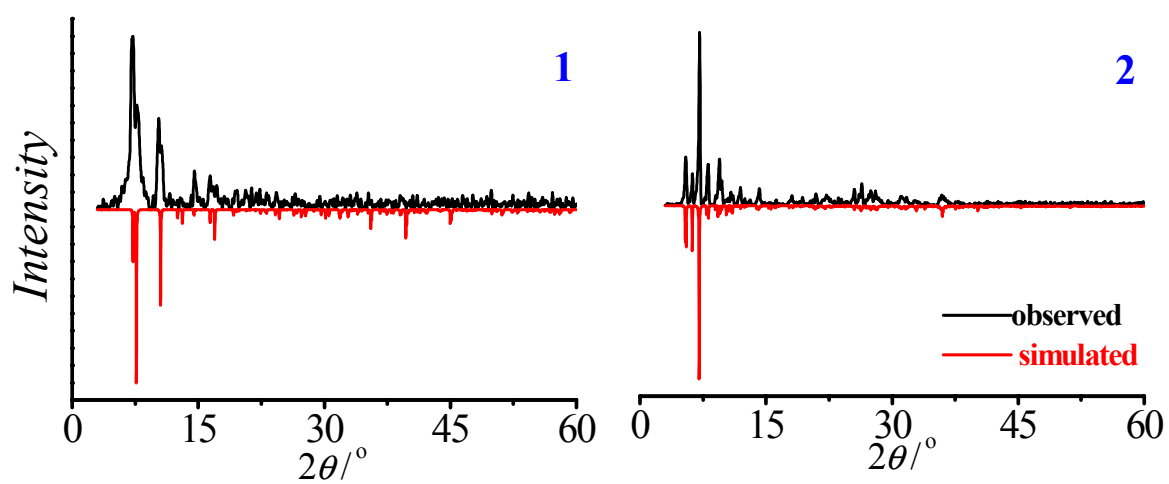


Fig. S5 The experimental (black) powder X-ray diffraction and simulated patterns (red) of **1** and **2**.

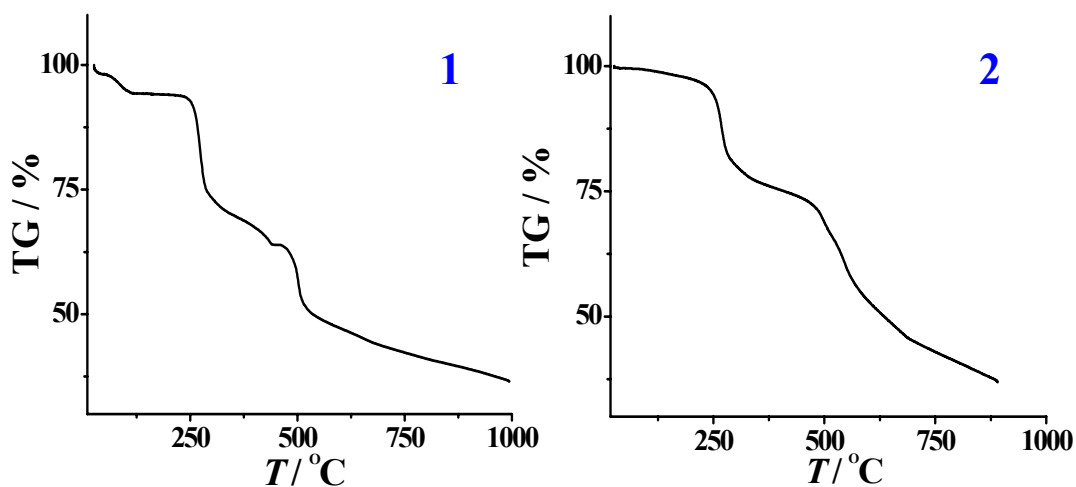


Fig. S5 TG curve of **1** and **2**.

Table S1. Bond lengths (Å) and angles (°) for **1** and **2**.

1					
Co1-O3a	2.129(3)	Co1-O3e	2.129(3)	Co2-O3c	2.066(3)
Co1-O3b	2.129(3)	Co2-O1a	2.019(3)	Co2-O3	2.110(3)
Co1-O3c	2.129(3)	O3-Co2a	2.066(3)	Co2-O2	2.374(4)
Co1-O3d	2.129(3)	Co2-O1	2.026(3)	N1-Co2c	2.059(4)
Co1-O3	2.129(3)	Co2-N1a	2.059(4)	O1-Co2c	2.019(3)
O3a-Co1-O3b	81.88(12)	O3c-Co1-O3e	98.12(12)	Co2a-O3-Co2	98.59(14)
O3a-Co1-O3c	98.12(12)	O3d-Co1-O3e	81.88(12)	C10-O3-Co1	125.6(3)
O3b-Co1-O3c	180.000	O3-Co1-O3e	180.000	Co2a-O3-Co1	97.63(14)
O3a-Co1-O3d	180.000	O1a-Co2-O1	171.69(7)	Co2-O3-Co1	96.28(14)
O3b-Co1-O3d	98.12(12)	O1a-Co2-N1a	85.91(15)	O1-Co2-N1a	99.86(15)
O3c-Co1-O3d	81.88(12)	O3c-Co2-O3	83.85(18)	O1a-Co2-O3c	105.28(14)
O3a-Co1-O3	81.88(12)	O1a-Co2-O2	103.07(13)	O1-Co2-O3c	79.53(13)
O3b-Co1-O3	98.12(12)	O1-Co2-O2	71.61(12)	N1a-Co2-O3c	101.86(16)
O3c-Co1-O3	81.88(12)	N1a-Co2-O2	86.03(16)	O1a-Co2-O3	78.64(13)
O3d-Co1-O3	98.12(12)	O3c-Co2-O2	151.01(13)	O1-Co2-O3	95.36(14)
O3a-Co1-O3e	98.12(12)	O3-Co2-O2	95.94(14)	N1a-Co2-O3	164.47(15)
O3b-Co1-O3e	81.88(12)	Co2c-O1-Co2	103.00(14)		

Co1-N3	2.01(2)	Co5-O7	2.151(17)	Co9-O25	2.23(2)
Co1-O2	2.025(16)	Co5-O33	2.15(2)	Co9-O39	2.27(2)
Co1-N2	2.03(2)	Co5-O4	2.169(19)	Co10-O29	2.032(18)
Co1-O11	2.047(18)	Co5-O30	2.194(19)	Co10-O20	2.05(2)
Co1-O7	2.11(2)	Co6-O31	2.022(19)	Co10-N14	2.07(3)
Co1-O4	2.151(17)	Co6-N11	2.06(3)	Co10-O40	2.067(18)
Co2-O2	2.000(18)	Co6-O8	2.064(17)	Co10-O16	2.224(18)
Co2-N7	2.03(2)	Co6-O26	2.08(2)	Co10-O18	2.31(2)
Co2-N6	2.06(2)	Co6-O4	2.221(19)	Co11-O40	1.98(2)
Co2-O5	2.084(15)	Co6-O6	2.28(2)	Co11-O13	2.01(2)
Co2-O16	2.155(18)	Co7-O28	2.010(18)	Co11-O16	2.100(16)
Co2-O19	2.193(16)	Co7-N10	2.05(2)	Co11-O42	2.16(2)
Co3-N4	1.92(2)	Co7-O5	2.055(18)	Co11-O19	2.232(19)
Co3-N1	1.94(2)	Co7-O20	2.08(2)	Co11-O15	2.25(2)
Co3-O23	1.95(2)	Co7-O7	2.220(19)	Co12-O37	2.03(2)
Co3-O17	1.958(19)	Co7-O9	2.25(2)	Co12-O23	2.06(2)
Co3-O10	2.00(2)	Co8-O32	1.99(2)	Co12-N13	2.08(3)
Co3-O1	2.021(18)	Co8-O26	2.05(2)	Co12-O25	2.109(19)
Co4-O11	2.015(18)	Co8-O34	2.05(2)	Co12-O10	2.17(2)
Co4-N8	2.03(2)	Co8-N12	2.11(4)	Co12-O27	2.17(3)
Co4-N9	2.05(2)	Co8-O22	2.19(2)	Co13-N5	2.02(3)
Co4-O8	2.06(2)	Co8-O24	2.25(3)	Co13-O13	2.04(2)
Co4-O22	2.17(2)	Co9-O37	1.98(2)	Co13-O17	2.053(18)
Co4-O25	2.22(2)	Co9-O34	2.03(2)	Co13-O19	2.10(2)
Co5-O31	2.03(2)	Co9-O22	2.11(2)	Co13-O1	2.171(19)
Co5-O28	2.031(19)	Co9-O36	2.18(3)	Co13-O21	2.17(2)
N3-Co1-O2	100.1(8)	O23-Co3-O1	89.4(8)	O26-Co6-O4	110.7(8)
N3-Co1-N2	166.2(8)	O17-Co3-O1	83.2(7)	O31-Co6-O6	94.9(8)
O2-Co1-N2	89.2(8)	O10-Co3-O1	95.7(8)	N11-Co6-O6	115.3(9)
N3-Co1-O11	90.7(9)	O11-Co4-N8	95.6(8)	O8-Co6-O6	148.3(8)
O2-Co1-O11	89.2(7)	O11-Co4-N9	95.9(9)	O26-Co6-O6	78.8(8)
N2-Co1-O11	99.7(8)	N8-Co4-N9	163.4(9)	O4-Co6-O6	69.9(7)
N3-Co1-O7	83.5(8)	O11-Co4-O8	90.2(8)	O28-Co7-N10	89.6(8)
O2-Co1-O7	90.6(7)	N8-Co4-O8	99.9(9)	O28-Co7-O5	103.5(7)
N2-Co1-O7	86.2(8)	N9-Co4-O8	92.1(9)	N10-Co7-O5	90.4(9)
O11-Co1-O7	174.1(8)	O11-Co4-O22	172.4(8)	O28-Co7-O20	168.8(8)
N3-Co1-O4	87.0(8)	N8-Co4-O22	82.2(8)	N10-Co7-O20	84.8(9)
O2-Co1-O4	172.9(7)	N9-Co4-O22	87.9(9)	O5-Co7-O20	86.3(7)
N2-Co1-O4	83.8(8)	O8-Co4-O22	83.1(8)	O28-Co7-O7	75.1(7)
O11-Co1-O4	90.8(7)	O11-Co4-O25	97.4(8)	N10-Co7-O7	164.3(8)

O7-Co1-O4	90.1(7)	N8-Co4-O25	85.2(8)	O5-Co7-O7	89.4(7)
O2-Co2-N7	95.5(9)	N9-Co4-O25	81.4(8)	O20-Co7-O7	110.9(7)
O2-Co2-N6	95.3(8)	O8-Co4-O25	170.4(8)	O28-Co7-O9	93.4(8)
N7-Co2-N6	163.5(9)	O22-Co4-O25	89.6(8)	N10-Co7-O9	113.9(9)
O2-Co2-O5	88.9(6)	O31-Co5-O28	173.1(7)	O5-Co7-O9	150.5(6)
N7-Co2-O5	93.0(8)	O31-Co5-O7	108.2(7)	O20-Co7-O9	80.1(8)
N6-Co2-O5	99.6(8)	O28-Co5-O7	76.3(7)	O7-Co7-O9	71.6(7)
O2-Co2-O16	171.2(7)	O31-Co5-O33	76.1(8)	O32-Co8-O26	86.0(9)
N7-Co2-O16	89.0(8)	O28-Co5-O33	98.6(8)	O32-Co8-O34	166.(1)
N6-Co2-O16	82.0(8)	O7-Co5-O33	94.2(8)	O26-Co8-O34	102.8(9)
O5-Co2-O16	83.3(7)	O31-Co5-O4	76.1(7)	O32-Co8-N12	84.2(13)
O2-Co2-O19	98.8(7)	O28-Co5-O4	109.6(8)	O26-Co8-N12	93.1(13)
N7-Co2-O19	81.5(8)	O7-Co5-O4	88.6(7)	O34-Co8-N12	84.5(12)
N6-Co2-O19	84.6(8)	O33-Co5-O4	151.5(8)	O32-Co8-O22	117.3(9)
O5-Co2-O19	170.9(7)	O31-Co5-O30	100.7(7)	O26-Co8-O22	94.9(8)
O16-Co2-O19	89.3(7)	O28-Co5-O30	75.6(7)	O34-Co8-O22	73.3(8)
N4-Co3-N1	95.7(9)	O7-Co5-O30	150.4(8)	N12-Co8-O22	157.5(11)
N4-Co3-O23	94.4(9)	O33-Co5-O30	98.7(8)	O32-Co8-O24	79.5(9)
N1-Co3-O23	91.7(9)	O4-Co5-O30	92.4(7)	O26-Co8-O24	151.9(9)
N4-Co3-O17	93.0(9)	O31-Co6-N11	89.3(10)	O34-Co8-O24	96.6(9)
N1-Co3-O17	96.1(9)	O31-Co6-O8	103.7(8)	N12-Co8-O24	109.0(14)
O23-Co3-O17	168.6(7)	N11-Co6-O8	90.8(9)	O22-Co8-O24	71.3(8)
N4-Co3-O10	84.9(9)	O31-Co6-O26	168.9(8)	O37-Co9-O34	173.9(10)
N1-Co3-O10	174.2(9)	N11-Co6-O26	85.3(1)	O37-Co9-O22	110.5(9)
O23-Co3-O10	82.5(9)	O8-Co6-O26	86.1(8)	O34-Co9-O22	75.5(9)
O17-Co3-O10	89.7(8)	O31-Co6-O4	75.0(8)	O37-Co9-O36	96.8(10)
N4-Co3-O1	176.2(9)	N11-Co6-O4	164.(1)	O34-Co9-O36	77.3(1)
N1-Co3-O1	84.1(8)	O8-Co6-O4	90.1(7)	O22-Co9-O36	152.2(9)
O37-Co9-O25	73.8(8)	O16-Co10-O18	69.8(7)	O23-Co12-O10	75.9(8)
O34-Co9-O25	107.5(8)	O40-Co11-O13	172.1(8)	N13-Co12-O10	86.5(1)
O22-Co9-O25	91.0(8)	O40-Co11-O16	75.5(8)	O25-Co12-O10	108.5(7)
O36-Co9-O25	91.9(9)	O13-Co11-O16	112.4(8)	O37-Co12-O27	97.1(9)
O37-Co9-O39	75.8(9)	O40-Co11-O42	76.8(9)	O23-Co12-O27	158.0(8)
O34-Co9-O39	103.7(9)	O13-Co11-O42	95.3(9)	N13-Co12-O27	108.3(1)
O22-Co9-O39	91.9(8)	O16-Co11-O42	152.0(9)	O25-Co12-O27	74.5(8)
O36-Co9-O39	99.9(9)	O40-Co11-O19	105.4(8)	O10-Co12-O27	90.1(9)
O25-Co9-O39	148.4(8)	O13-Co11-O19	75.2(8)	N5-Co13-O13	88.8(9)
O29-Co10-O20	84.6(8)	O16-Co11-O19	89.7(7)	N5-Co13-O17	88.9(9)
O29-Co10-N14	85.4(9)	O42-Co11-O19	94.0(8)	O13-Co13-O17	97.1(8)
O20-Co10-N14	91.7(1)	O40-Co11-O15	106.7(9)	N5-Co13-O19	166.4(9)
O29-Co10-O40	167.2(9)	O13-Co11-O15	74.0(8)	O13-Co13-O19	77.6(8)
O20-Co10-O40	104.3(8)	O16-Co11-O15	91.7(7)	O17-Co13-O19	92.4(7)

N14-Co10-O40	85.1(9)	O42-Co11-O15	99.9(9)	N5-Co13-O1	86.5(9)
O29-Co10-O16	117.9(8)	O19-Co11-O15	147.2(9)	O13-Co13-O1	172.8(9)
O20-Co10-O16	94.7(7)	O37-Co12-O23	97.8(9)	O17-Co13-O1	77.4(7)
N14-Co10-O16	156.3(8)	O37-Co12-N13	89.4(1)	O19-Co13-O1	107.0(7)
O40-Co10-O16	71.1(8)	O23-Co12-N13	88.1(1)	N5-Co13-O21	105.9(9)
O29-Co10-O18	79.5(8)	O37-Co12-O25	75.5(8)	O13-Co13-O21	97.3(8)
O20-Co10-O18	148.5(8)	O23-Co12-O25	93.6(8)	O17-Co13-O21	159.4(8)
N14-Co10-O18	113.7(1)	N13-Co12-O25	164.9(1)	O19-Co13-O21	76.5(7)
O40-Co10-O18	96.4(8)	O37-Co12-O10	172.6(9)	O1-Co13-O21	89.2(8)

Symmetry Codes: a:1+x-y, x, -z; b:2-y, 1+x-y, z; c: y, 1-x+y, -z; d:1-x+y, 2-x, z; e:2-x, 2-y, -z for **1**.

Electrospray mass spectroscopic experiments:

The ESI mass spectra were acquired using a HCT mass spectrometer (Bruker Daltonics, Germany).

For compound **1**, Sprayed solution was prepared by dissolving ~1 mg of sample in 1 mL of MeCN solvent. Data were collected in positive ion mode in the conditions that the needle and capillary exit voltage were set at 4 kV and 152V, respectively; and the desolvation chamber temperature was set in 573 K. Scan scale from 100-1800 m/z.

For compound **2**, Sprayed solution was prepared similar with 1 in MeCN solvent. Data were collected in positive ion mode in the conditions that the needle and capillary exit voltage were set at 4 kV and 200V, respectively; and the desolvation chamber temperature was set in 573 K. Scan scale from 50-3000 m/z.