Supporting information (SI)

Self-Assembly, Structures, Magnetic Properties and Solution Behaviors of Six Mixed-Valence Cobalt Clusters

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Single Crystal X-Ray Crystallography.

Single crystal of **SD/Co1-SD/Co6** with appropriate dimensions were chosen under an optical microscope and quickly coated with high vacuum grease (Dow Corning Corporation) before being mounted on a glass fiber for data collection. Data for them were collected on a Bruker Apex II CCD diffractometer with graphite-monochromated Mo Kα radiation source (λ = 0.71073 Å). A preliminary orientation matrix and unit cell parameters were determined from 3 runs of 12 frames each, each frame corresponds to a 0.5° scan in 6 s, followed by spot integration and least-squares refinement. For **SD/Co1-SD/Co6**, data were measured using ω scans of 0.5° per frame for 20 s until a complete hemisphere had been collected. Cell parameters were retrieved using SMART software and refined with SAINT on all observed reflections.[S1] Data reduction of **SD/Co1-SD/Co6** were performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS.[S2] In all cases, the highest possible space group was chosen. All structures were solved by direct methods using SHELXS-97 and refined on F^2 by full-matrix least-squares procedures with SHELXL-97.[S3] Atoms were located from iterative examination of difference F-maps following least squares refinements of the earlier models. Hydrogen atoms were placed in calculated positions and included as riding atoms with isotropic displacement parameters 1.2-1.5 times U_{eq} of the attached C atoms. Pertinent crystallographic data collection and refinement parameters are collated in Table 1. Selected bond lengths and angles are collated in Table S1.

References:

S1 R. H. Blessing, *ActaCrystallogr., Sect. A*, 1995, **51**, 33.

S2 G. M. Sheldrick, *SADABS 2.05*; University Göttingen: Gottingen, Germany, 1997.

S3 G. M. Sheldrick, *SHELXS97, Program for Crystal Structure Solution*; University of Göttingen: Göttingen, Germany, 1997.

Scheme S1 Metal-mediated nitrile−pyrazole coupling reaction in **SD/Co6**.

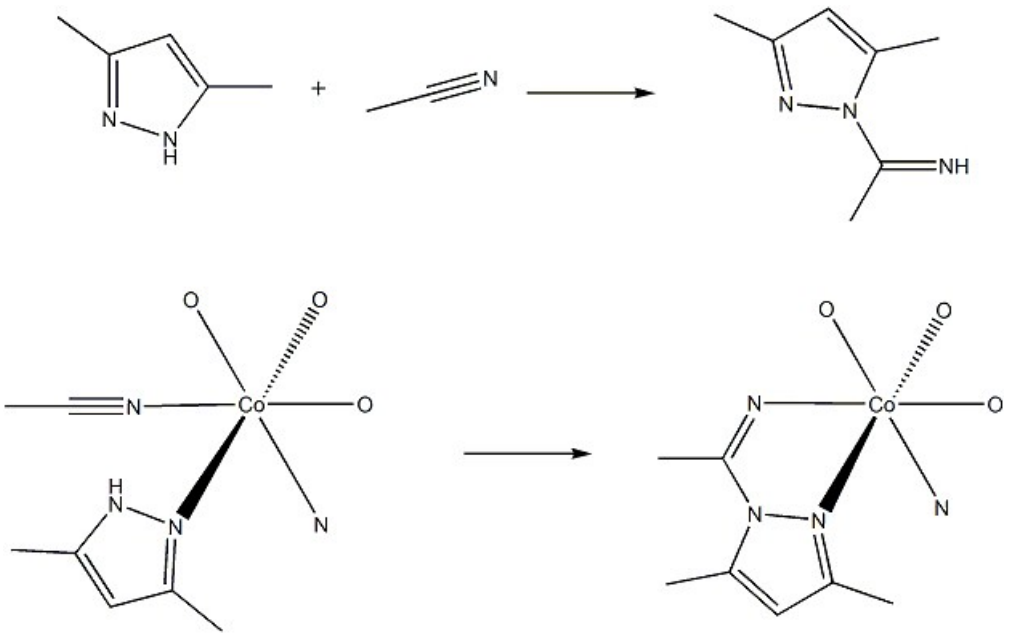

Fig. S1 IR spectrum of compound **SD/Co1**.

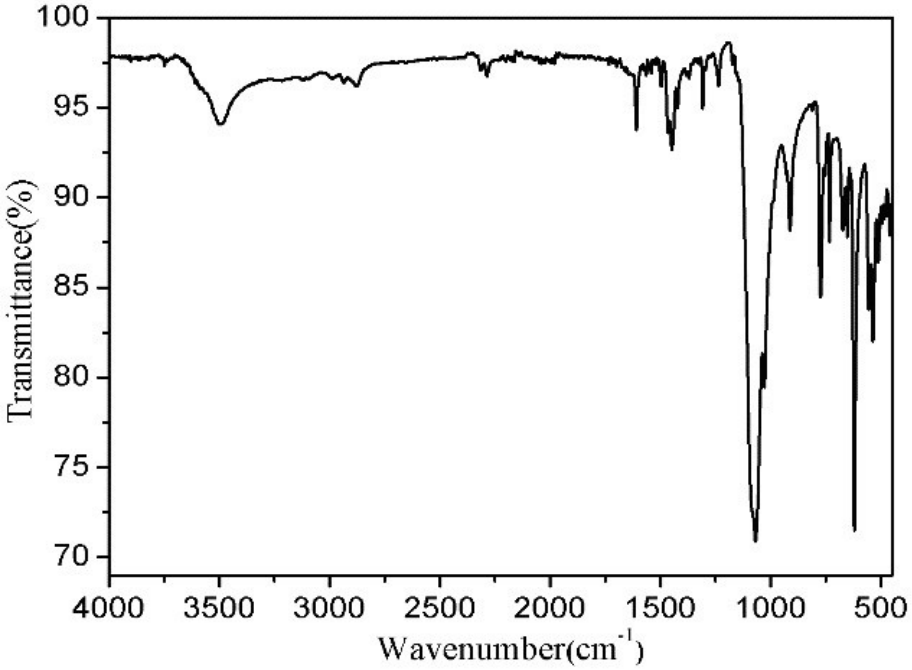

Fig. S2 IR spectrum of compound **SD/Co2**.

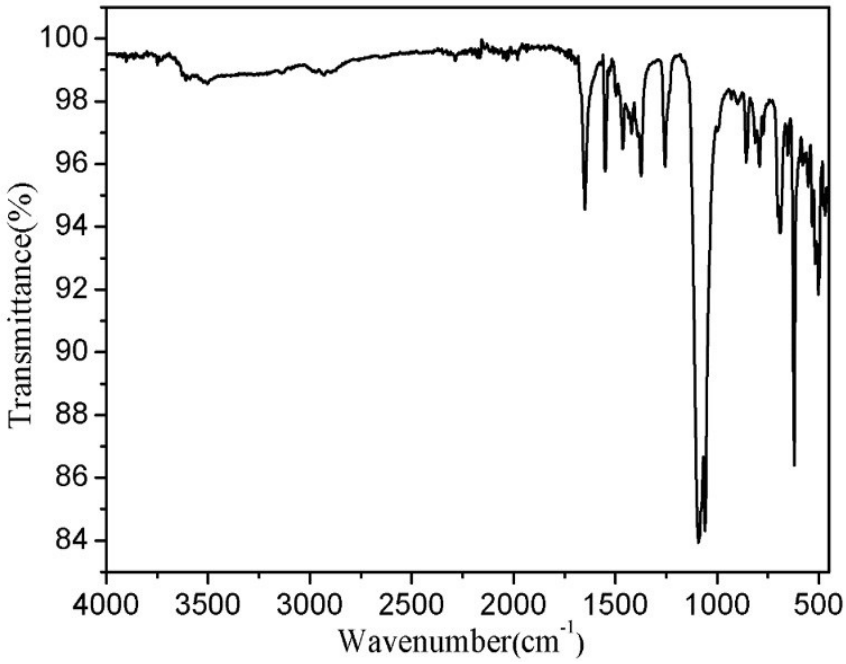

Fig. S3 IR spectrum of compound **SD/Co3**.

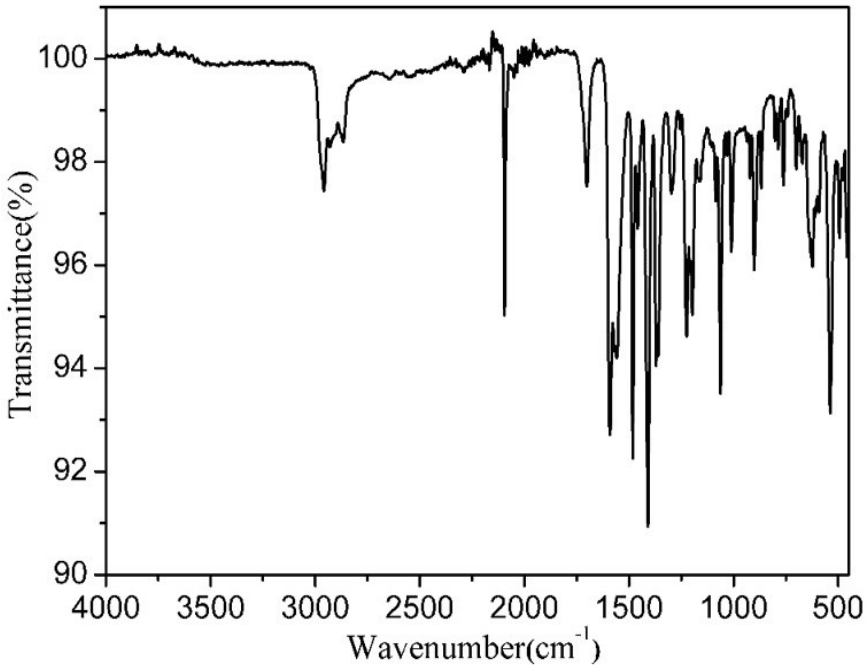

Fig. S4 IR spectrum of compound **SD/Co4**.

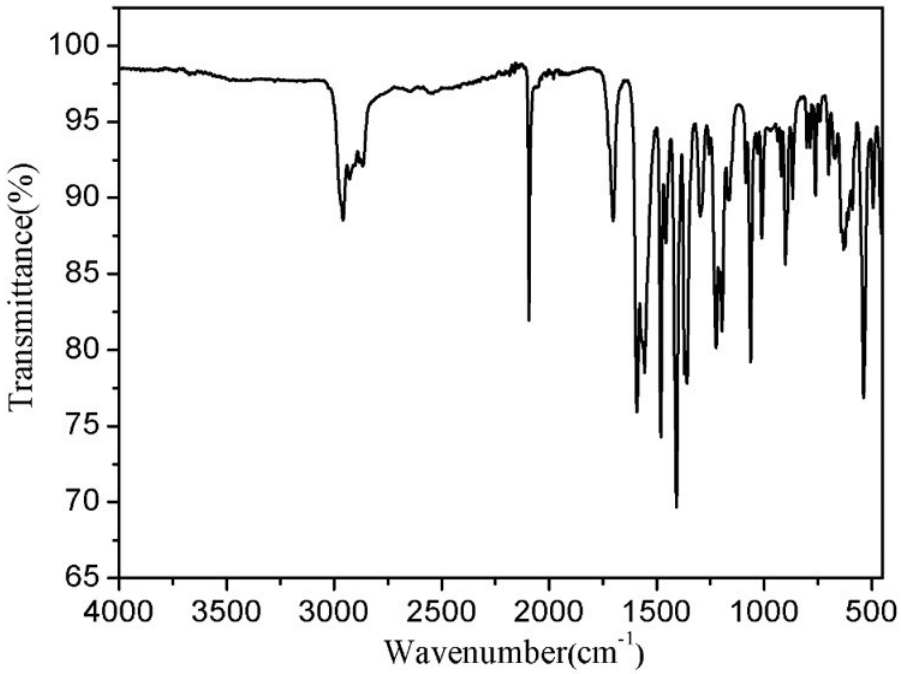

Fig. S5 IR spectrum of compound **SD/Co5**.

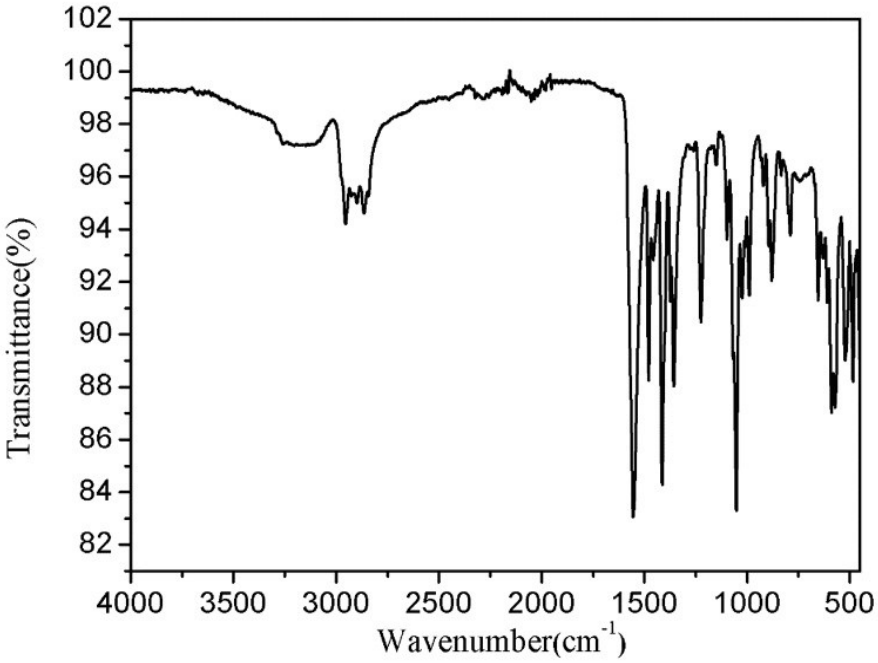

Fig. S6 IR spectrum of compound **SD/Co6**.

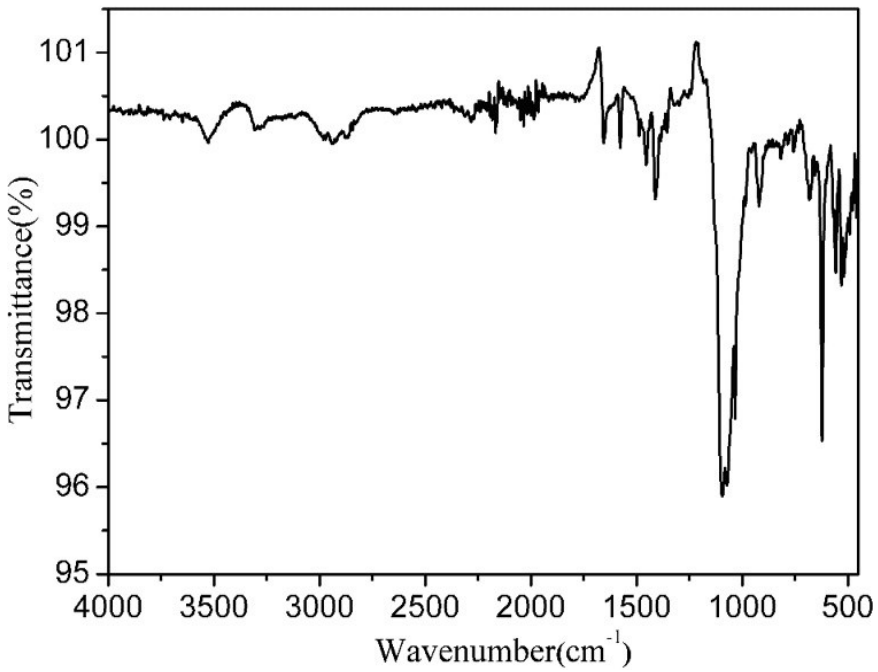

Fig. S7 TG curve of compound **SD/Co1**.

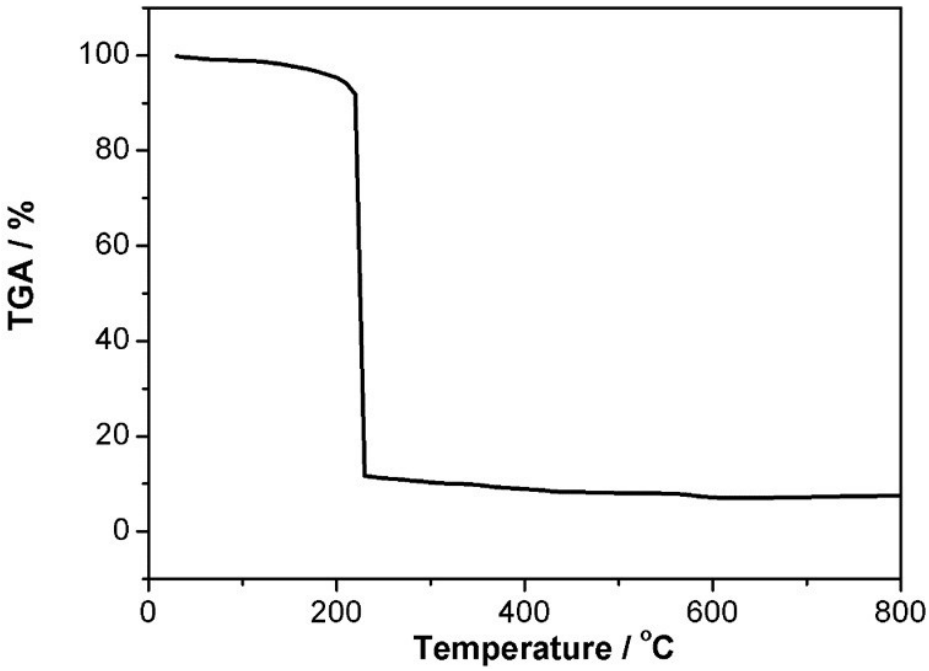

Fig. S8 TG curve of compound **SD/Co2**.

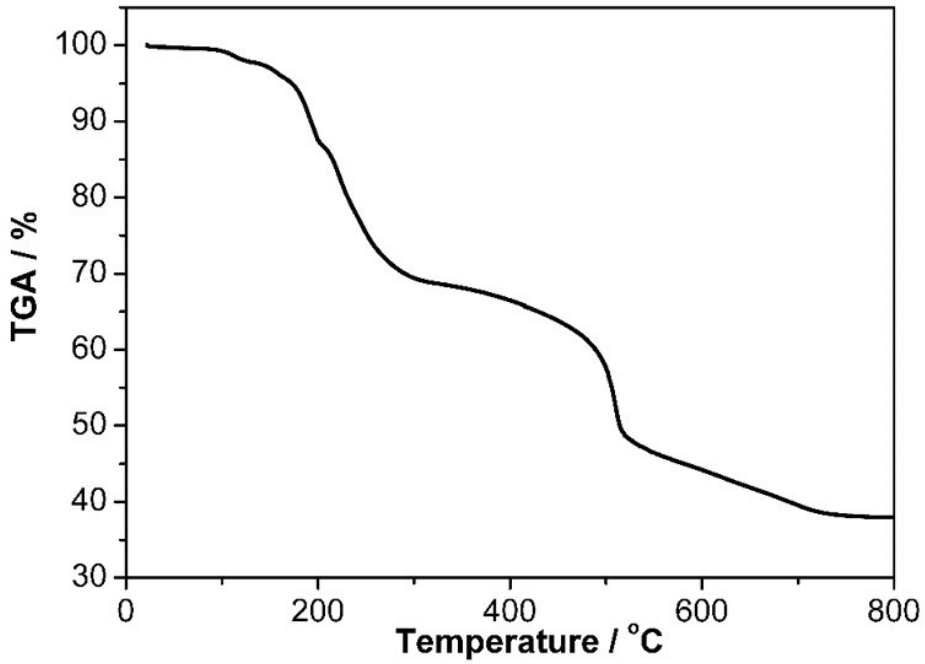

Fig. S9 TG curve of compound **SD/Co3**.

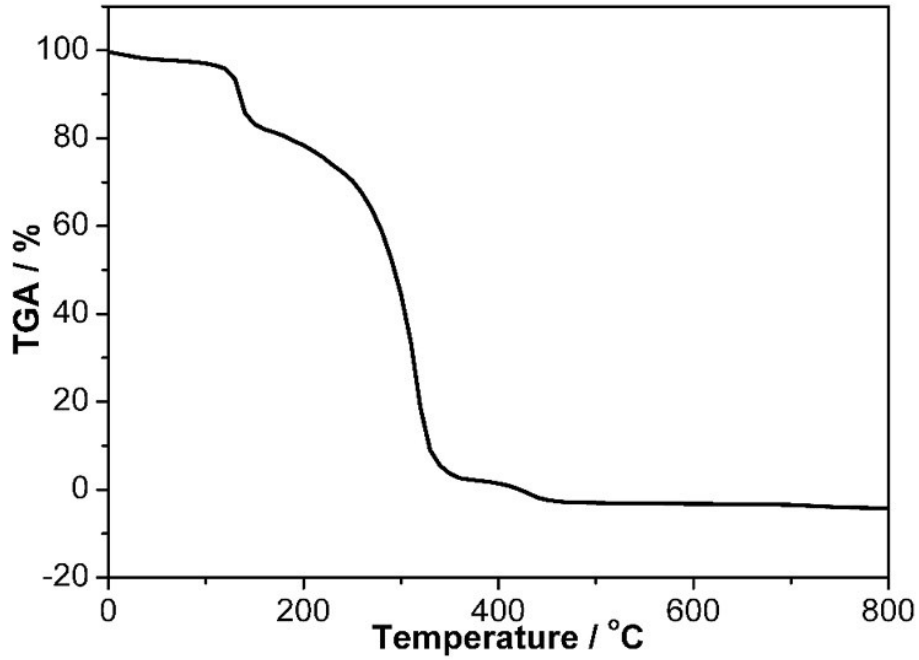

Fig. S10 TG curve of compound **SD/Co4**.

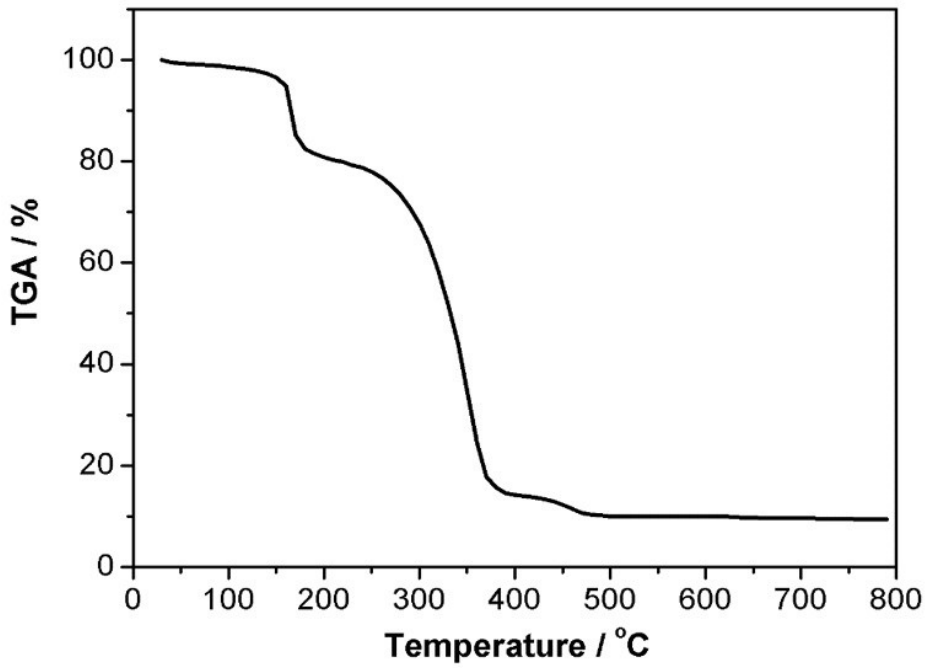

Fig. S11 TG curve of compound **SD/Co5**.

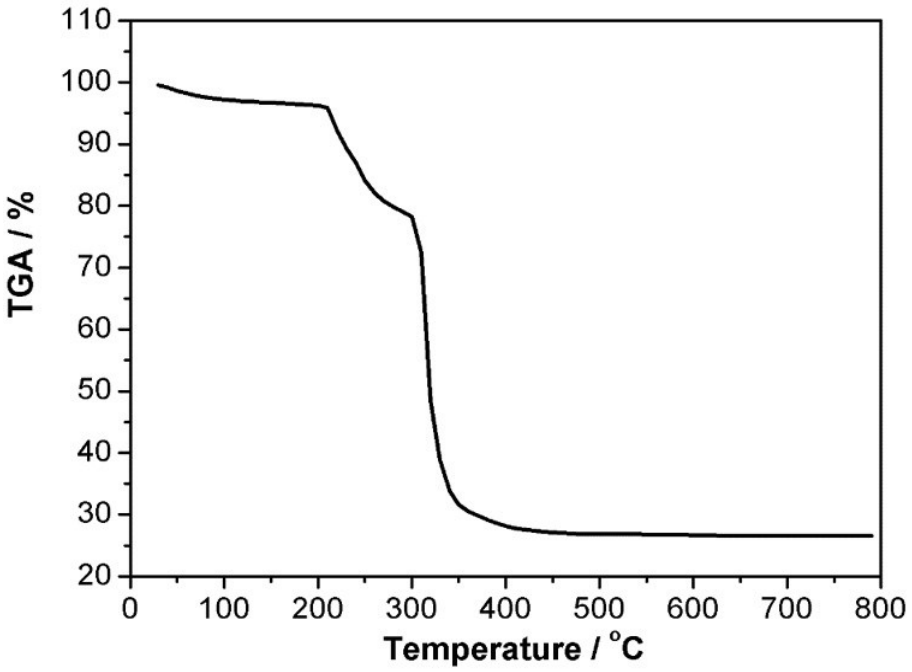

Fig. S12 Calculated (black) and experimental (red) ESI-MS isotopic distribution patterns of the species **1a-1e**, **2a-2d**, **3a-3c**, **4a-4b**, **5a**, and **6a-6b.**

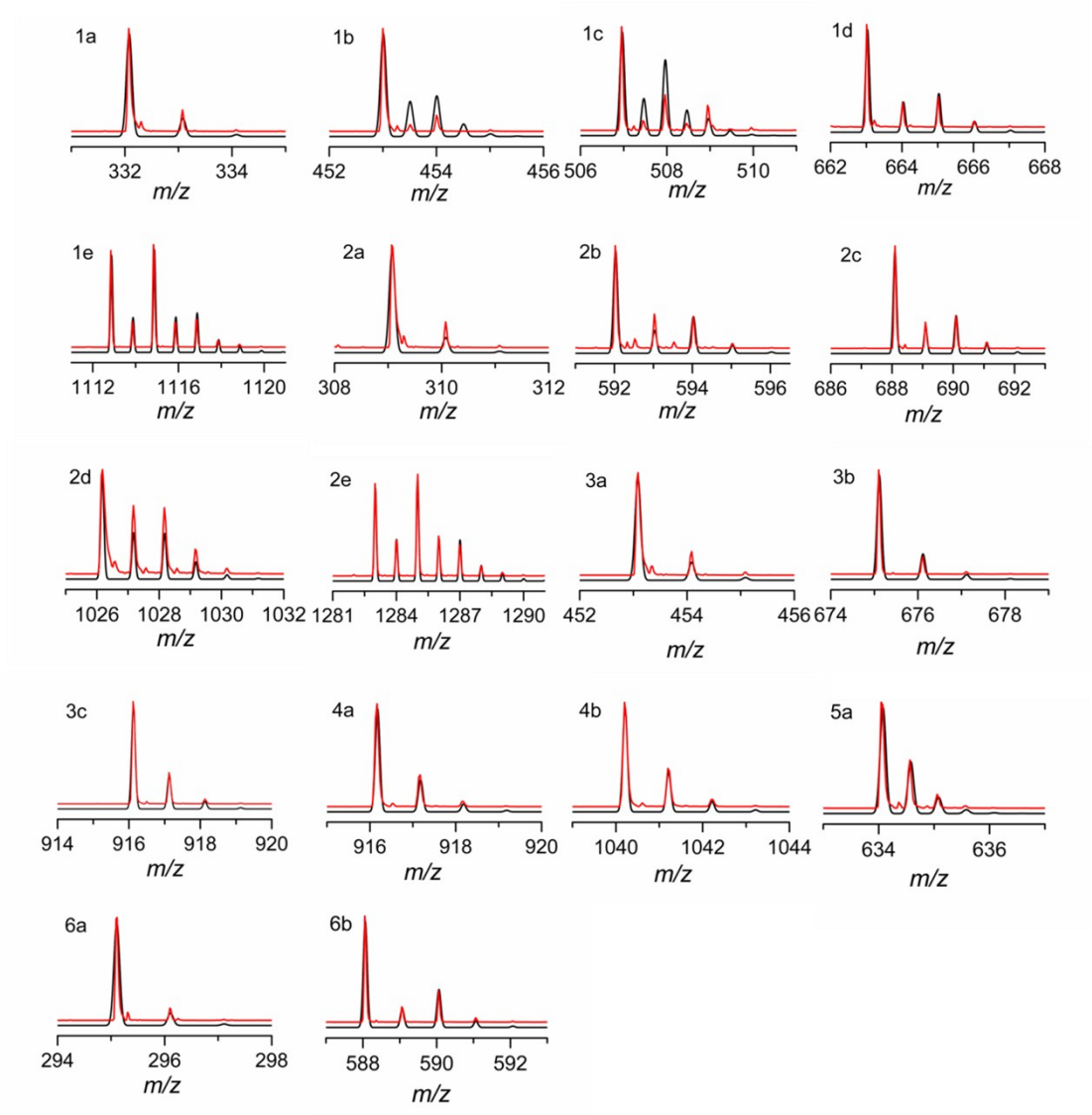

Fig. S13 The HRESI-MS of **SD/Co5** disolved in different solvents.

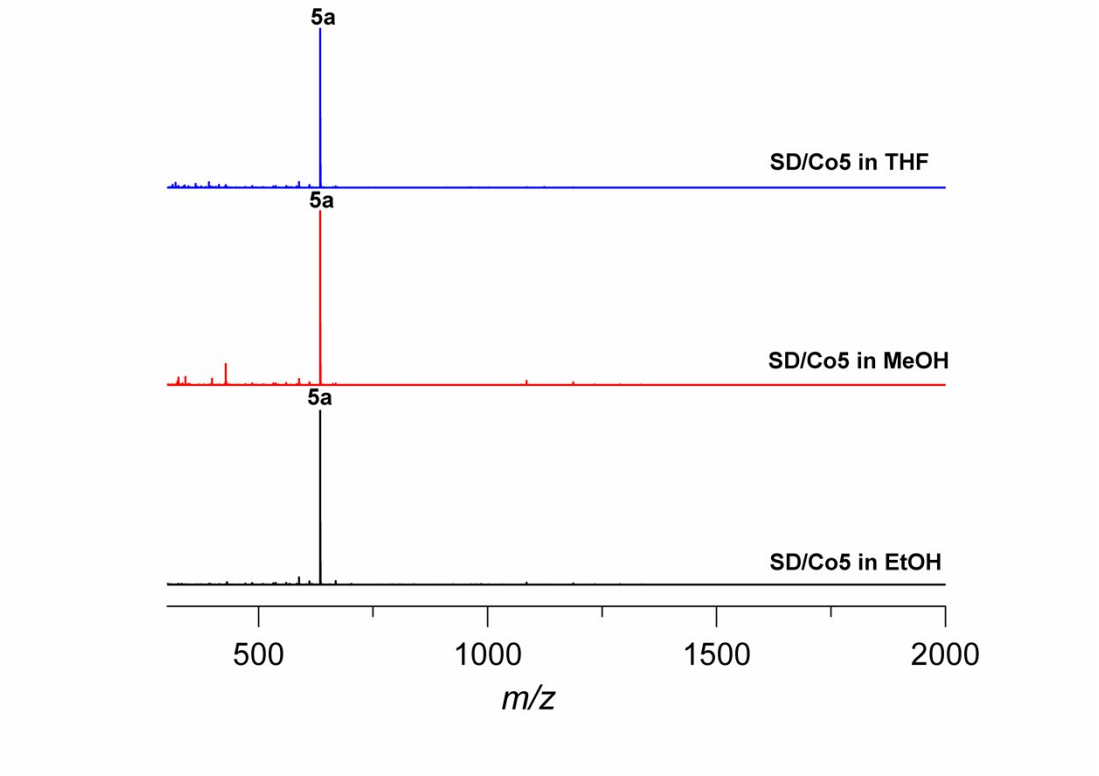

Fig. S14 The solid state UV-Vis spectra of **SD/Co1-SD/Co6**.

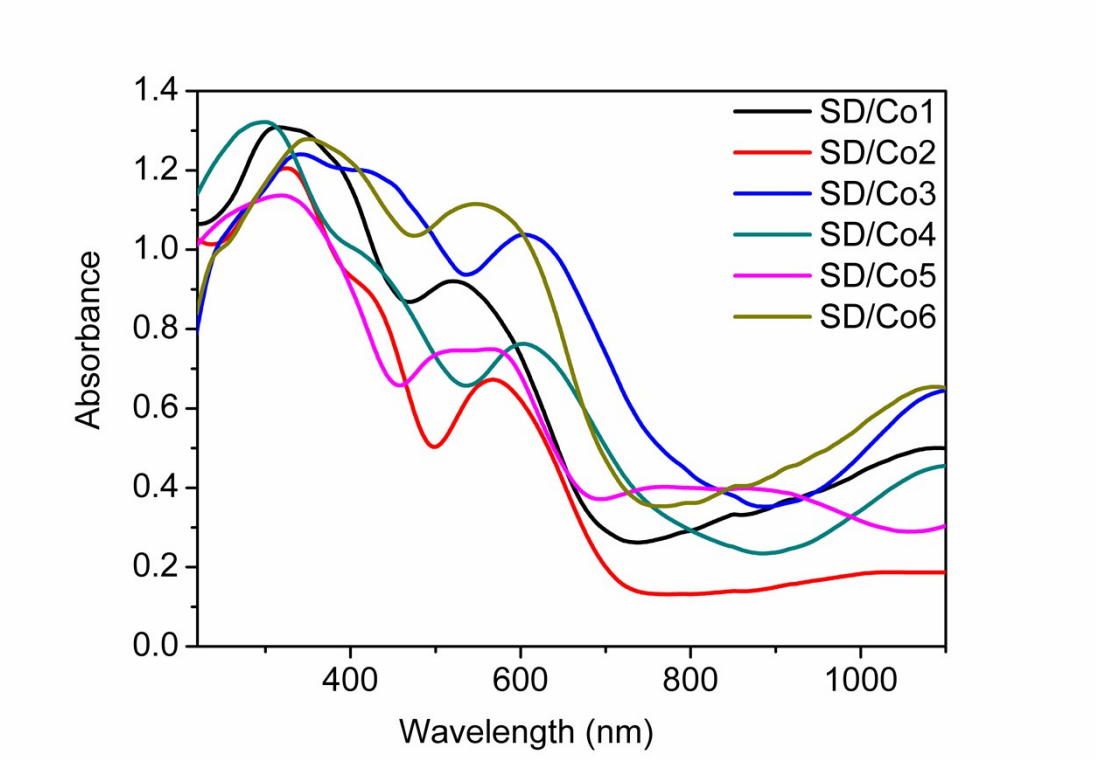

Table S1 Selected bond lengths [Å] and angles [º] for SD/Co1-SD/Co6.

Compound SD/Co1			
Bond lengths			
Co(1)-O(1)	1.872(4)	Co(3)-O(5)	1.873(5)
Co(1)-O(2)	1.877(5)	Co(3)-O(6)	1.875(5)
Co(1)-O(3)	1.930(5)	Co(3)-O(4)	1.924(5)
Co(1)-N(3)	1.942(6)	Co(3)-N(9)	1.943(6)
Co(1)-N(2)	1.950(5)	Co(3)-N(8)	1.949(6)
Co(1)-N(1)	1.966(6)	Co(3)-N(10)	1.985(6)
Co(2)-O(2)	2.008(4)	Co(4)-O(1)	2.003(4)
Co(2)-O(6)	2.008(5)	Co(4)-O(5)	2.024(5)
Co(2)-N(5)	2.107(7)	Co(4)-N(6)	2.095(7)
Co(2)-N(4)	2.125(7)	Co(4)-N(7)	2.109(7)
Co(2)-O(3)	2.128(5)	Co(4)-O(4)	2.129(5)
Co(2)-O(4)	2.154(5)	Co(4)-O(3)	2.140(5)
Bond angles			
O(1)-Co(1)-O(2)	94.2(2)	O(5)-Co(3)-O(6)	94.6(2)
O(1)-Co(1)-O(3)	81.79(19)	O(5)-Co(3)-O(4)	82.1(2)
O(2)-Co(1)-O(3)	81.9(2)	O(6)-Co(3)-O(4)	81.6(2)
O(1)-Co(1)-N(3)	91.2(2)	O(5)-Co(3)-N(9)	172.1(2)
O(2)-Co(1)-N(3)	173.4(2)	O(6)-Co(3)-N(9)	92.5(2)
O(3)-Co(1)-N(3)	95.3(2)	O(4)-Co(3)-N(9)	95.6(2)
O(1)-Co(1)-N(2)	172.8(2)	O(5)-Co(3)-N(8)	90.7(2)
O(2)-Co(1)-N(2)	92.2(2)	O(6)-Co(3)-N(8)	174.1(2)
O(3)-Co(1)-N(2)	95.9(2)	O(4)-Co(3)-N(8)	96.7(2)
N(3)-Co(1)-N(2)	82.2(2)	N(9)-Co(3)-N(8)	82.0(3)
O(1)-Co(1)-N(1)	87.2(2)	O(5)-Co(3)-N(10)	87.5(2)
O(2)-Co(1)-N(1)	87.4(2)	O(6)-Co(3)-N(10)	86.1(2)
O(3)-Co(1)-N(1)	164.0(2)	O(4)-Co(3)-N(10)	163.1(2)
N(3)-Co(1)-N(1)	96.5(2)	N(9)-Co(3)-N(10)	96.4(2)
N(2)-Co(1)-N(1)	96.3(2)	N(8)-Co(3)-N(10)	96.7(2)
O(2)-Co(2)-O(6)	171.60(19)	O(1)-Co(4)-O(5)	165.94(19)
O(2)-Co(2)-N(5)	89.1(2)	O(1)-Co(4)-N(6)	89.7(2)
O(6)-Co(2)-N(5)	96.1(2)	O(5)-Co(4)-N(6)	101.5(2)
O(2)-Co(2)-N(4)	97.5(2)	O(1)-Co(4)-N(7)	101.0(2)
O(6)-Co(2)-N(4)	88.8(2)	O(5)-Co(4)-N(7)	87.4(2)
N(5)-Co(2)-N(4)	92.5(3)	N(6)-Co(4)-N(7)	91.4(3)
O(2)-Co(2)-O(3)	74.12(18)	O(1)-Co(4)-O(4)	97.01(18)
O(6)-Co(2)-O(3)	100.47(18)	O(5)-Co(4)-O(4)	73.75(18)
N(5)-Co(2)-O(3)	163.2(2)	N(6)-Co(4)-O(4)	94.7(2)

N(4)-Co(2)-O(3)	90.5(2)	N(7)-Co(4)-O(4)	161.0(2)
O(2)-Co(2)-O(4)	99.79(18)	O(1)-Co(4)-O(3)	73.77(17)
O(6)-Co(2)-O(4)	73.09(18)	O(5)-Co(4)-O(3)	94.66(18)
N(5)-Co(2)-O(4)	96.9(3)	N(6)-Co(4)-O(3)	163.4(2)
N(4)-Co(2)-O(4)	160.3(2)	N(7)-Co(4)-O(3)	93.5(2)
O(3)-Co(2)-O(4)	85.41(18)	O(4)-Co(4)-O(3)	85.75(19)
Compound SD/Co2			
Bond lengths			
Co(1)-O(8)	1.878(2)	Co(2)-N(8)	2.077(3)
Co(1)-O(10)	1.906(2)	Co(2)-O(10)	2.083(2)
Co(1)-O(9)	1.916(2)	Co(2)-N(7)	2.096(3)
Co(1)-N(2)	1.918(3)	Co(2)-O(9)	2.116(2)
Co(1)-N(3)	1.928(3)	Co(2)-O(9)#1	2.215(2)
Co(1)-N(5)	1.945(3)	O(8)-Co(2)#1	1.984(2)
Co(2)-O(8)#1	1.984(2)	O(9)-Co(2)#1	2.215(2)
Bond angles			
O(8)-Co(1)-O(10)	91.22(10)	O(8)#1-Co(2)-N(8)	93.49(11)
O(8)-Co(1)-O(9)	83.40(9)	O(8)#1-Co(2)-O(10)	160.56(9)
O(10)-Co(1)-O(9)	84.96(9)	N(8)-Co(2)-O(10)	93.16(10)
O(8)-Co(1)-N(2)	83.65(11)	O(8)#1-Co(2)-N(7)	93.98(10)
O(10)-Co(1)-N(2)	93.14(11)	N(8)-Co(2)-N(7)	89.42(12)
O(9)-Co(1)-N(2)	166.87(11)	O(10)-Co(2)-N(7)	104.33(10)
O(8)-Co(1)-N(3)	90.71(11)	O(8)#1-Co(2)-O(9)	97.21(9)
O(10)-Co(1)-N(3)	167.23(11)	N(8)-Co(2)-O(9)	168.97(10)
O(9)-Co(1)-N(3)	82.73(11)	O(10)-Co(2)-O(9)	75.84(9)
N(2)-Co(1)-N(3)	99.62(12)	N(7)-Co(2)-O(9)	92.47(10)
O(8)-Co(1)-N(5)	173.93(11)	O(8)#1-Co(2)-O(9)#1	73.66(9)
O(10)-Co(1)-N(5)	83.00(10)	N(8)-Co(2)-O(9)#1	99.57(10)
O(9)-Co(1)-N(5)	97.90(11)	O(10)-Co(2)-O(9)#1	87.23(8)
N(2)-Co(1)-N(5)	94.76(12)	N(7)-Co(2)-O(9)#1	165.02(10)
N(3)-Co(1)-N(5)	95.34(11)	O(9)-Co(2)-O(9)#1	81.00(9)
Symmetry transformations used to generate equivalent atoms: #1: -x+1, -y, -z+2.			
Compound SD/Co3			
Bond lengths			
Co(1)-O(6)	1.866(6)	Co(6)-O(15)	1.885(6)
Co(1)-O(11)	1.888(6)	Co(6)-O(13)	1.907(6)
Co(1)-O(9)	1.910(6)	Co(6)-O(18)	1.909(5)
Co(1)-O(10)	1.922(6)	Co(6)-O(17)	1.921(6)
Co(1)-N(3)	1.932(8)	Co(6)-N(19)	1.932(8)
Co(1)-N(12)	1.937(8)	Co(6)-N(20)	1.957(8)
Co(2)-O(8)	1.879(6)	Co(7)-O(17)	1.884(6)
Co(2)-O(12)	1.891(6)	Co(7)-O(16)	1.893(6)
Co(2)-O(9)	1.907(6)	Co(7)-O(18)	1.901(6)

Co(2)-O(11)	1.912(6)	Co(7)-O(14)	1.904(6)
Co(2)-N(15)	1.942(9)	Co(7)-N(22)	1.914(9)
Co(2)-N(16)	1.949(7)	Co(7)-N(21)	1.961(9)
Co(3)-O(7)	1.974(6)	Co(8)-O(16)	1.983(6)
Co(3)-O(6)	1.994(6)	Co(8)-O(19)	1.991(6)
Co(3)-O(8)	2.006(6)	Co(8)-O(20)	1.996(6)
Co(3)-O(5)	2.006(6)	Co(8)-O(15)	2.005(5)
Co(4)-O(7)	1.874(6)	Co(9)-O(20)	1.866(6)
Co(4)-O(4)	1.897(6)	Co(9)-O(22)	1.890(6)
Co(4)-O(1)	1.903(6)	Co(9)-N(31)	1.915(9)
Co(4)-O(3)	1.913(6)	Co(9)-O(21)	1.917(6)
Co(4)-N(6)	1.923(9)	Co(9)-O(24)	1.924(7)
Co(4)-N(7)	1.970(8)	Co(9)-N(32)	1.981(7)
Co(5)-O(5)	1.889(6)	Co(10)-O(22)	1.865(6)
Co(5)-O(4)	1.891(6)	Co(10)-O(19)	1.878(6)
Co(5)-O(3)	1.911(6)	Co(10)-O(21)	1.914(6)
Co(5)-O(2)	1.929(6)	Co(10)-O(23)	1.936(7)
Co(5)-N(11)	1.953(8)	Co(10)-N(28)	1.951(8)
Co(5)-N(8)	1.958(9)	Co(10)-N(27)	1.953(9)
Bond angles			
O(6)-Co(1)-O(11)	87.1(3)	O(15)-Co(6)-O(13)	178.2(3)
O(6)-Co(1)-O(9)	88.9(2)	O(15)-Co(6)-O(18)	89.2(2)
O(11)-Co(1)-O(9)	81.8(3)	O(13)-Co(6)-O(18)	92.5(2)
O(6)-Co(1)-O(10)	178.4(3)	O(15)-Co(6)-O(17)	87.0(3)
O(11)-Co(1)-O(10)	94.3(2)	O(13)-Co(6)-O(17)	94.0(3)
O(9)-Co(1)-O(10)	92.1(3)	O(18)-Co(6)-O(17)	79.7(2)
O(6)-Co(1)-N(3)	92.1(3)	O(15)-Co(6)-N(19)	92.5(3)
O(11)-Co(1)-N(3)	97.8(3)	O(13)-Co(6)-N(19)	85.9(3)
O(9)-Co(1)-N(3)	178.9(3)	O(18)-Co(6)-N(19)	178.1(4)
O(10)-Co(1)-N(3)	86.9(3)	O(17)-Co(6)-N(19)	99.4(4)
O(6)-Co(1)-N(12)	89.0(3)	O(15)-Co(6)-N(20)	87.2(3)
O(11)-Co(1)-N(12)	165.7(3)	O(13)-Co(6)-N(20)	92.1(3)
O(9)-Co(1)-N(12)	84.3(3)	O(18)-Co(6)-N(20)	86.9(3)
O(10)-Co(1)-N(12)	89.8(3)	O(17)-Co(6)-N(20)	165.4(3)
N(3)-Co(1)-N(12)	96.1(4)	N(19)-Co(6)-N(20)	94.2(4)
O(8)-Co(2)-O(12)	177.6(3)	O(17)-Co(7)-O(16)	88.6(3)
O(8)-Co(2)-O(9)	87.9(3)	O(17)-Co(7)-O(18)	80.8(2)
O(12)-Co(2)-O(9)	92.8(3)	O(16)-Co(7)-O(18)	85.9(2)
O(8)-Co(2)-O(11)	89.9(2)	O(17)-Co(7)-O(14)	93.0(3)
O(12)-Co(2)-O(11)	92.5(2)	O(16)-Co(7)-O(14)	178.3(3)
O(9)-Co(2)-O(11)	81.3(2)	O(18)-Co(7)-O(14)	94.7(3)
O(8)-Co(2)-N(15)	93.0(3)	O(17)-Co(7)-N(22)	178.7(3)
O(12)-Co(2)-N(15)	84.6(3)	O(16)-Co(7)-N(22)	92.5(3)

O(9)-Co(2)-N(15)	97.1(3)	O(18)-Co(7)-N(22)	98.6(3)
O(11)-Co(2)-N(15)	176.7(3)	O(14)-Co(7)-N(22)	85.8(3)
O(8)-Co(2)-N(16)	87.3(3)	O(17)-Co(7)-N(21)	85.6(3)
O(12)-Co(2)-N(16)	92.6(3)	O(16)-Co(7)-N(21)	87.7(3)
O(9)-Co(2)-N(16)	166.9(3)	O(18)-Co(7)-N(21)	165.1(3)
O(11)-Co(2)-N(16)	86.6(3)	O(14)-Co(7)-N(21)	92.1(3)
N(15)-Co(2)-N(16)	95.2(3)	N(22)-Co(7)-N(21)	95.1(4)
O(7)-Co(3)-O(6)	103.1(2)	O(16)-Co(8)-O(19)	104.1(3)
O(7)-Co(3)-O(8)	100.3(2)	O(16)-Co(8)-O(20)	103.4(2)
O(6)-Co(3)-O(8)	121.0(2)	O(19)-Co(8)-O(20)	119.5(2)
O(7)-Co(3)-O(5)	123.9(2)	O(16)-Co(8)-O(15)	123.5(2)
O(6)-Co(3)-O(5)	104.1(3)	O(19)-Co(8)-O(15)	103.8(2)
O(8)-Co(3)-O(5)	106.1(2)	O(20)-Co(8)-O(15)	103.8(2)
O(7)-Co(4)-O(4)	86.8(2)	O(20)-Co(9)-O(22)	86.5(3)
O(7)-Co(4)-O(1)	179.0(3)	O(20)-Co(9)-N(31)	91.6(3)
O(4)-Co(4)-O(1)	94.2(3)	O(22)-Co(9)-N(31)	98.9(3)
O(7)-Co(4)-O(3)	87.2(3)	O(20)-Co(9)-O(21)	90.0(3)
O(4)-Co(4)-O(3)	80.0(2)	O(22)-Co(9)-O(21)	80.9(3)
O(1)-Co(4)-O(3)	93.2(3)	N(31)-Co(9)-O(21)	178.3(3)
O(7)-Co(4)-N(6)	89.7(3)	O(20)-Co(9)-O(24)	177.9(3)
O(4)-Co(4)-N(6)	98.8(3)	O(22)-Co(9)-O(24)	94.1(3)
O(1)-Co(4)-N(6)	89.8(3)	N(31)-Co(9)-O(24)	86.3(3)
O(3)-Co(4)-N(6)	176.8(3)	O(21)-Co(9)-O(24)	92.0(3)
O(7)-Co(4)-N(7)	86.4(3)	O(20)-Co(9)-N(32)	88.3(3)
O(4)-Co(4)-N(7)	165.1(4)	O(22)-Co(9)-N(32)	162.8(3)
O(1)-Co(4)-N(7)	92.8(3)	N(31)-Co(9)-N(32)	97.6(4)
O(3)-Co(4)-N(7)	86.5(4)	O(21)-Co(9)-N(32)	82.7(3)
N(6)-Co(4)-N(7)	94.4(4)	O(24)-Co(9)-N(32)	91.7(3)
O(5)-Co(5)-O(4)	88.8(2)	O(22)-Co(10)-O(19)	88.7(3)
O(5)-Co(5)-O(3)	87.5(3)	O(22)-Co(10)-O(21)	81.6(3)
O(4)-Co(5)-O(3)	80.2(2)	O(19)-Co(10)-O(21)	87.3(3)
O(5)-Co(5)-O(2)	178.1(3)	O(22)-Co(10)-O(23)	92.5(3)
O(4)-Co(5)-O(2)	93.0(3)	O(19)-Co(10)-O(23)	178.6(3)
O(3)-Co(5)-O(2)	93.5(3)	O(21)-Co(10)-O(23)	92.2(3)
O(5)-Co(5)-N(11)	86.8(3)	O(22)-Co(10)-N(28)	86.1(3)
O(4)-Co(5)-N(11)	86.3(3)	O(19)-Co(10)-N(28)	88.0(3)
O(3)-Co(5)-N(11)	165.4(3)	O(21)-Co(10)-N(28)	166.9(3)
O(2)-Co(5)-N(11)	92.6(3)	O(23)-Co(10)-N(28)	92.7(4)
O(5)-Co(5)-N(8)	91.2(3)	O(22)-Co(10)-N(27)	179.2(4)
O(4)-Co(5)-N(8)	178.1(3)	O(19)-Co(10)-N(27)	92.0(3)
O(3)-Co(5)-N(8)	97.9(3)	O(21)-Co(10)-N(27)	98.0(3)
O(2)-Co(5)-N(8)	87.0(3)	O(23)-Co(10)-N(27)	86.8(3)
N(11)-Co(5)-N(8)	95.6(4)	N(28)-Co(10)-N(27)	94.4(4)

Compound SD/Co4			
Bond lengths			
Co(1)-O(7)	1.874(3)	Co(2)-O(7)	2.003(3)
Co(1)-O(7)#1	1.874(3)	Co(2)-O(7)#2	2.003(3)
Co(1)-O(5)#1	1.922(3)	Co(2)-O(4)	2.043(5)
Co(1)-O(5)	1.922(3)	Co(2)-O(6)#2	2.054(4)
Co(1)-N(1)	1.966(6)	Co(2)-O(6)	2.054(4)
Co(1)-N(2)	2.050(3)	N(2)-Co(1)#3	2.050(3)
Bond angles			
O(7)-Co(1)-O(7)#1	88.9(2)	O(5)-Co(1)-N(2)	92.58(18)
O(7)-Co(1)-O(5)#1	176.46(14)	N(1)-Co(1)-N(2)	174.3(3)
O(7)#1-Co(1)-O(5)#1	94.22(14)	O(7)-Co(2)-O(7)#2	94.98(18)
O(7)-Co(1)-O(5)	94.22(14)	O(7)-Co(2)-O(4)	99.28(14)
O(7)#1-Co(1)-O(5)	176.46(14)	O(7)#2-Co(2)-O(4)	99.28(14)
O(5)#1-Co(1)-O(5)	82.6(2)	O(7)-Co(2)-O(6)#2	160.52(17)
O(7)-Co(1)-N(1)	86.85(16)	O(7)#2-Co(2)-O(6)#2	88.52(15)
O(7)#1-Co(1)-N(1)	86.85(16)	O(4)-Co(2)-O(6)#2	99.05(17)
O(5)#1-Co(1)-N(1)	91.68(17)	O(7)-Co(2)-O(6)	88.52(15)
O(5)-Co(1)-N(1)	91.68(17)	O(7)#2-Co(2)-O(6)	160.52(17)
O(7)-Co(1)-N(2)	89.11(17)	O(4)-Co(2)-O(6)	99.05(17)
O(7)#1-Co(1)-N(2)	89.11(17)	O(6)#2-Co(2)-O(6)	82.1(2)
O(5)#1-Co(1)-N(2)	92.58(18)		
Symmetry transformations used to generate equivalent atoms: #1: x, y, -z+3/2; #2: -x+1, y, z; #3: -x+1, y, -z+3/2.			
Compound SD/Co5			
Bond lengths			
Co(1)-O(7)	2.052(4)	Co(2)-O(12)	2.190(4)
Co(1)-O(6)	2.056(4)	Co(3)-O(5)	1.883(4)
Co(1)-O(1)#1	2.063(4)	Co(3)-O(6)	1.885(4)
Co(1)-O(4)#1	2.079(4)	Co(3)-O(12)	1.903(4)
Co(1)-O(4)	2.147(4)	Co(3)-O(8)	1.910(4)
Co(1)-O(12)	2.193(4)	Co(3)-N(2)	1.935(6)
Co(2)-O(2)	1.958(4)	Co(3)-N(3)	1.987(5)
Co(2)-O(5)	1.961(4)	O(4)-Co(1)#1	2.079(4)
Co(2)-O(4)	2.014(4)	O(1)-Co(1)#1	2.063(4)
Co(2)-N(1)	2.123(5)		
Bond angles			
O(7)-Co(1)-O(6)	91.01(17)	O(4)-Co(2)-N(1)	84.56(17)
O(7)-Co(1)-O(1)#1	94.04(18)	O(2)-Co(2)-O(12)	96.73(17)
O(6)-Co(1)-O(1)#1	92.11(17)	O(5)-Co(2)-O(12)	76.18(16)
O(7)-Co(1)-O(4)#1	98.17(16)	O(4)-Co(2)-O(12)	84.65(14)
O(6)-Co(1)-O(4)#1	166.49(16)	N(1)-Co(2)-O(12)	162.42(18)
O(1)#1-Co(1)-O(4)#1	97.08(15)	O(5)-Co(3)-O(6)	90.03(19)

O(7)-Co(1)-O(4)	170.54(15)	O(5)-Co(3)-O(12)	85.39(18)
O(6)-Co(1)-O(4)	86.20(16)	O(6)-Co(3)-O(12)	86.16(16)
O(1)#1-Co(1)-O(4)	95.09(16)	O(5)-Co(3)-O(8)	176.99(19)
O(4)#1-Co(1)-O(4)	83.15(15)	O(6)-Co(3)-O(8)	92.89(18)
O(7)-Co(1)-O(12)	89.02(16)	O(12)-Co(3)-O(8)	95.54(17)
O(6)-Co(1)-O(12)	74.94(15)	O(5)-Co(3)-N(2)	87.7(2)
O(1)#1-Co(1)-O(12)	166.76(16)	O(6)-Co(3)-N(2)	86.7(2)
O(4)#1-Co(1)-O(12)	95.23(15)	O(12)-Co(3)-N(2)	170.0(2)
O(4)-Co(1)-O(12)	81.52(14)	O(8)-Co(3)-N(2)	91.7(2)
O(2)-Co(2)-O(5)	119.00(19)	O(5)-Co(3)-N(3)	86.8(2)
O(2)-Co(2)-O(4)	111.72(17)	O(6)-Co(3)-N(3)	173.3(2)
O(5)-Co(2)-O(4)	127.21(18)	O(12)-Co(3)-N(3)	87.7(2)
O(2)-Co(2)-N(1)	100.1(2)	O(8)-Co(3)-N(3)	90.4(2)
O(5)-Co(2)-N(1)	99.63(19)	N(2)-Co(3)-N(3)	99.1(2)
Symmetry transformations used to generate equivalent atoms: #1: -x+2, -y, -z+1.			
Compound SD/Co6			
Bond lengths			
Co(1)-O(8)	1.984(4)	Co(2)-O(10)	1.872(4)
Co(1)-O(10)#1	2.040(4)	Co(2)-N(5)	1.911(5)
Co(1)-O(1W)	2.080(5)	Co(2)-O(9)	1.924(4)
Co(1)-O(9)#1	2.102(5)	Co(2)-N(3)	1.937(5)
Co(1)-N(1)	2.155(6)	Co(2)-N(2)	1.975(5)
Co(1)-O(9)	2.174(5)	O(9)-Co(1)#1	2.102(5)
Co(2)-O(8)	1.866(4)	O(10)-Co(1)#1	2.040(4)
Bond angles			
O(8)-Co(1)-O(10)#1	167.48(15)	O(8)-Co(2)-O(10)	94.29(18)
O(8)-Co(1)-O(1W)	96.85(19)	O(8)-Co(2)-N(5)	89.6(2)
O(10)#1-Co(1)-O(1W)	92.27(17)	O(10)-Co(2)-N(5)	174.7(2)
O(8)-Co(1)-O(9)#1	95.64(17)	O(8)-Co(2)-O(9)	82.10(18)
O(10)#1-Co(1)-O(9)#1	75.08(15)	O(10)-Co(2)-O(9)	83.33(18)
O(1W)-Co(1)-O(9)#1	167.34(18)	N(5)-Co(2)-O(9)	93.6(2)
O(8)-Co(1)-N(1)	89.36(18)	O(8)-Co(2)-N(3)	170.2(2)
O(10)#1-Co(1)-N(1)	99.36(18)	O(10)-Co(2)-N(3)	94.8(2)
O(1W)-Co(1)-N(1)	89.2(2)	N(5)-Co(2)-N(3)	81.1(2)
O(9)#1-Co(1)-N(1)	93.0(2)	O(9)-Co(2)-N(3)	95.2(2)
O(8)-Co(1)-O(9)	73.39(15)	O(8)-Co(2)-N(2)	86.34(18)
O(10)#1-Co(1)-O(9)	96.96(16)	O(10)-Co(2)-N(2)	87.31(18)
O(1W)-Co(1)-O(9)	97.6(2)	N(5)-Co(2)-N(2)	96.6(2)
O(9)#1-Co(1)-O(9)	84.03(19)	O(9)-Co(2)-N(2)	164.5(2)
N(1)-Co(1)-O(9)	162.06(19)	N(3)-Co(2)-N(2)	97.9(2)
Symmetry transformations used to generate equivalent atoms: #1: -x+1, -y+1, -z.			