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SUPPLEMENTARY MATERIAL TO

Spectroscopic and structural characterization of hexaamminecobalt(III) dibromide permanganate

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Table S-I. Crystal data and structure refinement

	$[Co(NH_3)_6]Br_2(MnO_4)$	$[Co(NH_3)_6]Cl_2(MnO_4)$[12]
Empirical formula	$Br_2H_{18}CoMnN_6O_4$	$Cl_2H_{18}CoMnN_6O_4$
Formula weight	439.89	350.97
Temperature	103(2)	163(2)
Radiation and wavelength	Mo-Kα, λ=0.71073Å	Mo-Kα, λ=0.71075Å
Crystal system	monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
Unit cell dimensions	a =13.9533(6)Å	a =13.6133(7)Å
	b =7.4499(4)Å	b =7.3658(5)Å
	c =12.3766(7)Å	c =12.3682(6)Å
	α = 90°	α = 90°
	β = 108.453(8)°	β = 108.547(8)°
	γ = 90°	γ = 90°
Volume	1220.41(12)Å^3	1175.78(13)Å^3
Z	4	4
Density (calculated)	2.394 Mg/m^3	1.983 Mg/m^3

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Absorption coefficient, μ	8.944 mm^{-1}	2.941 mm^{-1}
F(000)	856	712
Crystal color	red	Red
Crystal description	prism	Platelet
Crystal size	0.45 x 0.43 x 0.11 mm	0.56 x 0.41 x 0.11 mm
Absorption correction	numerical	Numerical
Max. and min. transmission	0.4820.889	0.8680.987
θ - range for data collection	$3.078 \le \theta \le 30.504°$	$3.157 \le \theta \le 27.473°$
Index ranges	$-19 \le h \le 19;-10 \le k \le 10;-17 \le l \le 17$	$-17 \le h \le 17;-9 \le k \le 9;-16 \le l \le 15$
Reflections collected	39290	18320
Completeness to 2θ	1.000	1.000
Independent reflections	3727 [*R*(int) =0.1132]	2684 [*R*(int) =0.0588]
Reflections $I>2\sigma(I)$	3309	2351
Refinement method	full-matrix least-squares on F^2	full-matrix least-squares on *F*2
Data/restraints/parameters	3727 /0 /136	2684 /0 /136
Goodness-of-fit on F^2	1.188	1.152
Final *R* indices [$I>2\sigma(I)$]	R_1 =0.0438, wR_2 =0.0759	R_1 =0.0422, wR_2 =0.0854
R indices (all data)	R_1 =0.0531, wR_2 =0.0783	R_1 =0.0528, wR_2 =0.0892

Table S-II. Bond lengths [Å] of compound **1**.

Mn1-O1	1.608(3)		Mn1-O4	1.614(3)
Mn1-O3	1.620(3)		Mn1-O2	1.627(3)
Co1-N1#1	1.958(3)		Co1-N1	1.958(3)
Co1-N2#1	1.960(3)		Co1-N2	1.960(3)
Co1-N3#1	1.965(3)		Co1-N3	1.965(3)
Co2-N4#2	1.957(3)		Co2-N4	1.957(3)
Co2-N5#2	1.962(3)		Co2-N5	1.962(3)
Co2-N6	1.982(3)		Co2-N6#2	1.982(3)

Table S-III. Bond angles [°] of compound **1.**

O1-Mn1-O4	109.3(1)		O1-Mn1-O3	110.3(1)
O4-Mn1-O3	109.9(1)		O1-Mn1-O2	110.1(1)
O4-Mn1-O2	108.5(1)		O3-Mn1-O2	108.8(2)
N1#1-Co1-N1	180.0		N1#1-Co1-N2#1	89.6(1)
N1-Co1-N2#1	90.4(1)		N1#1-Co1-N2	90.4(1)
N1-Co1-N2	89.6(1)		N2#1-Co1-N2	180.0
N1#1-Co1-N3#1	90.3(1)		N1-Co1-N3#1	89.7(1)
N2#1-Co1-N3#1	89.0(1)		N2-Co1-N3#1	91.0(1)
N1#1-Co1-N3	89.7(1)		N1-Co1-N3	90.3(1)
N2#1-Co1-N3	91.0(1)		N2-Co1-N3	89.0(1)
N3#1-Co1-N3	180.0(2)		N4#2-Co2-N4	180.0(2)
N4#2-Co2-N5#2	89.9(1)		N4-Co2-N5#2	90.1(1)
N4#2-Co2-N5	90.1(1)		N4-Co2-N5	89.9(1)
N5#2-Co2-N5	180.0(2)		N4#2-Co2-N6	89.2(1)
N4-Co2-N6	90.8(1)		N5#2-Co2-N6	88.9(1)
N5-Co2-N6	91.1(1)		N4#2-Co2-N6#2	90.8(1)
N4-Co2-N6#2	89.2(1)		N5#2-Co2-N6#2	91.1(1)
N5-Co2-N6#2	88.9(1)		N6-Co2-N6#2	180.00(9)

Symmetry codes to generate equivalent atoms:
1. -x+1,-y+1,-z+1
2. -x,-y+1,-z

Table S-IV. Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg in compound **1.**

Nr	Donor --- H....Acceptor	Symm. op.	D - H	H...A	D...A	D - H...A
1	N1 --H1A ..Br2	x,y,z	0.91	2.87	3.402(3)	119
2	N1 --H1A ..O1	x,1+y,z	0.91	2.45	2.937(4)	113
3	N1 --H1B ..Br1	1-x,1/2+y,1/2-z	0.91	2.57	3.460(3)	165
4	N1 --H1C ..Br1	x,3/2-y,1/2+z	0.91	2.70	3.518(3)	149
5	N2 --H2A ..Br1	x,y,z	0.91	2.66	3.539(3)	164
6	N2 --H2B ..O3	x,y,z	0.91	2.59	3.273(4)	132
7	N2 --H2C ..Br1	1-x,-1/2+y,1/2-z	0.91	2.70	3.513(3)	149
8	N3 --H3A ..Br2	x,y,z	0.91	2.86	3.555(3)	134
9	N3 --H3A ..O1	x,1/2-y,1/2+z	0.91	2.49	2.930(4)	110
10	N3 --H3B ..Br1	1-x,1-y,1-z	0.91	2.62	3.484(3)	159
11	N3 --H3C ..Br1	x,1/2-y,1/2+z	0.91	2.88	3.703(3)	152
12	N4 --H4A ..O2	-x,1-y,-z	0.91	2.37	3.179(4)	149
13	N4 --H4A ..O4	-x,1-y,-z	0.91	2.30	3.070(4)	142
14	N4 --H4B ..O2	x,1+y,z	0.91	2.03	2.922(4)	166
15	N4 --H4C ..O3	-x,1/2+y,1/2-z	0.91	2.14	3.028(4)	165

16	N5	--H5A	..O2	x,y,z	0.91	2.34	3.181(4)	154
17	N5	--H5A	..Br2	-x,-1/2+y,1/2-z	0.91	2.89	3.417(3)	118
18	N5	--H5B	..O2	-x,1/2+y,1/2-z	0.91	2.45	3.120(4)	131
19	N5	--H5B	..O3	-x,1/2+y,1/2-z	0.91	2.38	3.243(4)	159
20	N5	--H5C	..Br2	x,y,z	0.91	2.53	3.423(3)	167
21	N6	--H6A	..Br2	x,3/2-y,-1/2+z	0.91	2.72	3.619(3)	169
22	N6	--H6B	..O4	x,y,z	0.91	2.47	3.163(4)	133
23	N6	--H6C	..Br2	x,y,z	0.91	2.86	3.704(2)	155
24	N6	--H6C	..O1	x,1+y,z	0.91	2.58	3.063(4)	114

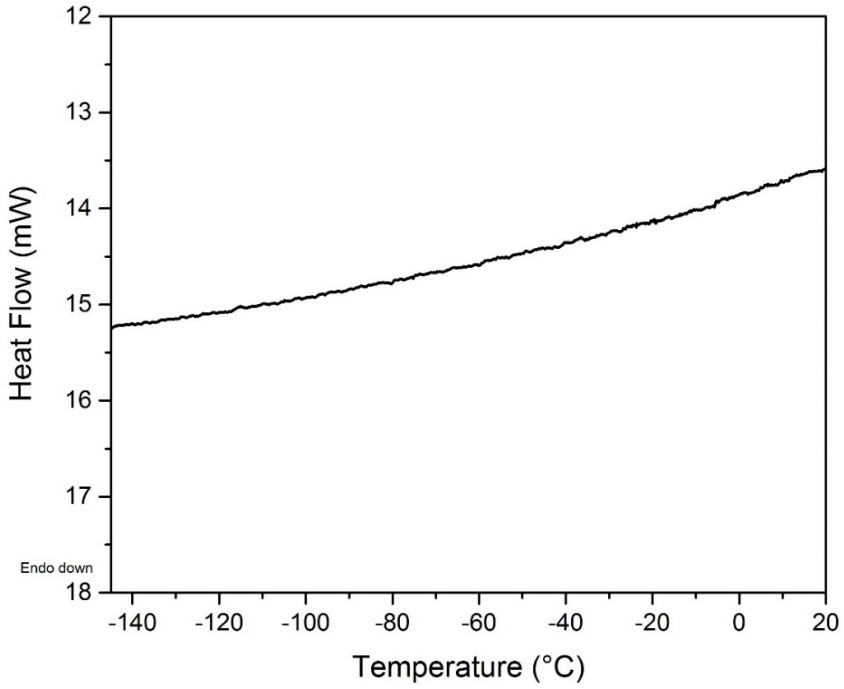

Fig. S-1. The low temperature (between -140 — 25 °C) DSC curve of compound **1**.

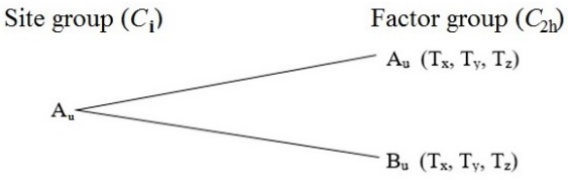

Fig. S-2. The correlation analysis for Co^{III} ions in compound **1**.

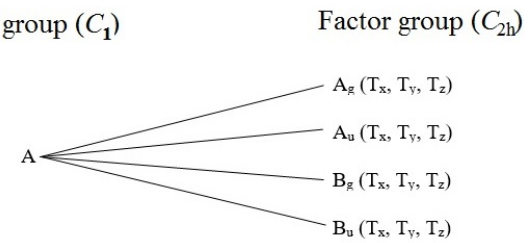

Fig. S-3. The correlation analysis for Br ions in compound **1**.

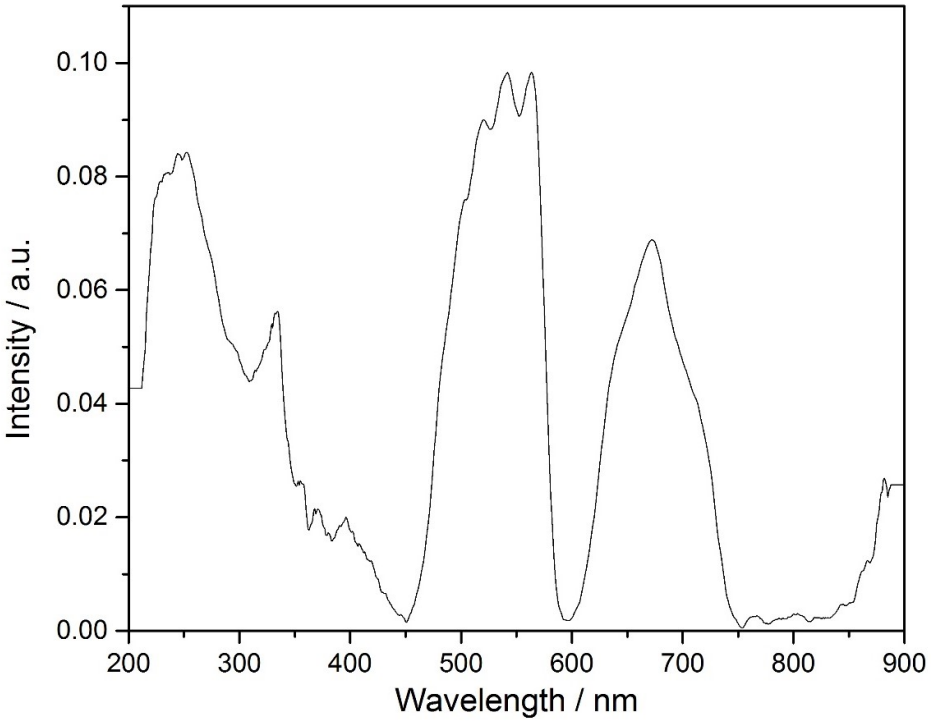

Fig. S-4. The UV-VIS spectra of compound **1**.