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Hexaamminecobalt(III) hexacyanidomanganate(III)

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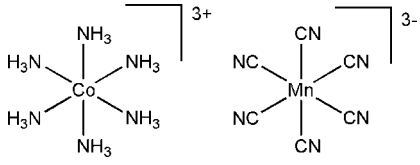
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(N–C) = 0.003 Å; R factor = 0.025; wR factor = 0.071; data-to-parameter ratio = 19.6.

The asymmetric unit of the title compound, $[Co(NH_3)_6][Mn(CN)_6]$, contains one Co and one Mn atom, both lying on threefold inversion axes, and one NH_3 and one CN group. The octahedral environments around Co^{II} and Mn^{II} are generated by symmetry and show very slight deviations from ideal geometry. A three-dimensional network is created by N—H···N hydrogen bonds.

Related literature

For related structures, see: Buschmann *et al.* (1999). For the construction of clusters and networks with adjustable magnetic properties, see: Przychodzen *et al.* (2006); Withers *et al.* (2005).



Experimental

Crystal data

$[Co(NH_3)_6][Mn(CN)_6]$
M_r = 372.19
Trigonal, $R\overline{3}$
a = 10.963 (5) Å
c = 10.779 (5) Å
V = 1121.9 (9) Å^3
Z = 3
Mo $K\alpha$ radiation
μ = 1.96 mm^{-1}
T = 100 (2) K
0.35 × 0.26 × 0.25 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.546, T_{max} = 0.614
3602 measured reflections
628 independent reflections
497 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.071
S = 0.93
628 reflections
32 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.89	2.09	2.979 (2)	173

Symmetry code: (i) $-y+1, x-y+1, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97* and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2122).

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supporting information

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Hexaamminecobalt(III) hexacyanidomanganate(III)

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S1. Comment

Our interest is in the use of cyanometalates as molecular building blocks for potentially constructing clusters and networks with adjustable magnetic properties [Przychodzen *et al.*, (2006), Withers *et al.*, (2005)].

The title compound crystallizes in the trigonal *R*-3 space group with *Z* = 3. The main part of the asymmetric unit contains one Co and one Mn atom, both lying on threefold rotational axes.

The octahedral environments around Co^{II} and Mn^{II} are generated by symmetry and shows very slight deviation from ideal geometry as illustrated by the C—Mn—C angles of 180.00 (7), 89.80 (7) and 90.20 (7) and N—Co—N angles of 180.00 (7), 89.47 (6) and 90.53 (6) ° respectively.

A three dimensional network is created by hydrogen bonds of the type N—H—N.

S2. Experimental

Equimolar amounts of $K_3[Mn(CN)_6]$ and $[Co(NH_3)_6]Cl_3$ were dissolved in water, added together and allowed to stand. Orange crystals separated out after a few days.

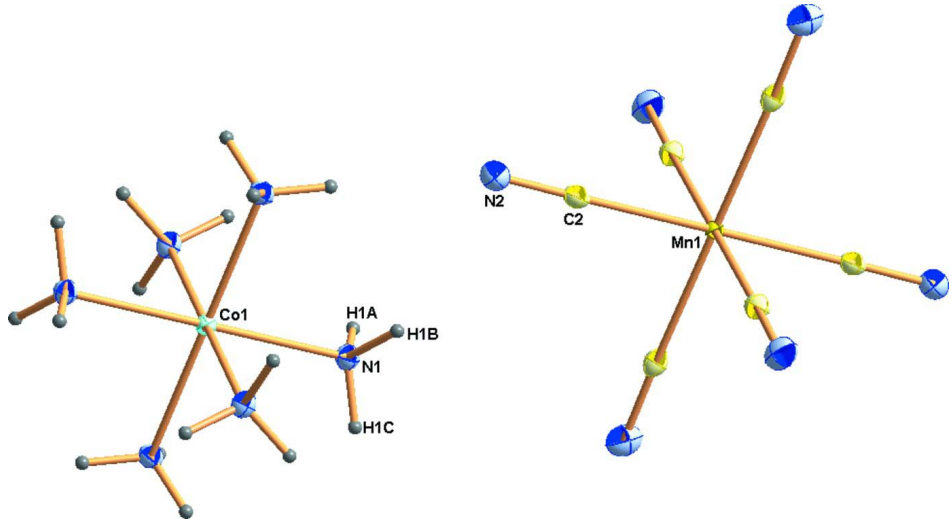

Figure 1

An ellipsoid plot of the title compound (50% probability displacement ellipsoids).

Hexaamminecobalt(III) hexacyanidomanganate(III)

Crystal data

$[Co(NH_3)_6][Mn(CN)_6]$
$M_r = 372.19$
Trigonal, $R\overline{3}$
Hall symbol: -R 3
$a = 10.963$ (5) Å
$c = 10.779$ (5) Å
$V = 1121.9$ (9) Å^3
$Z = 3$
$F(000) = 570$
$D_x = 1.653$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 1532 reflections
$\theta = 2.9$–$28.3°$
$\mu = 1.96$ mm^{-1}
$T = 100$ K
Cuboid, orange
0.35 × 0.26 × 0.25 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.546$, $T_{max} = 0.614$
3602 measured reflections
628 independent reflections
497 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.9°$
$h = -12 \rightarrow 14$
$k = -14 \rightarrow 9$
$l = -10 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.071$
$S = 0.93$
628 reflections
32 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 3.8029P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0	0	0	0.00732 (17)
Mn1	0.3333	0.6667	0.1667	0.00607 (17)
N1	−0.02748 (15)	0.13048 (15)	−0.10659 (13)	0.0107 (3)
H1A	0.0238	0.2179	−0.0777	0.016*
H1B	−0.1181	0.1061	−0.1065	0.016*
H1C	−0.0006	0.1264	−0.1837	0.016*
C2	0.31385 (18)	0.80238 (18)	0.06080 (16)	0.0119 (3)
N2	0.30018 (17)	0.87891 (17)	−0.00283 (15)	0.0184 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0076 (2)	0.0076 (2)	0.0067 (3)	0.00381 (10)	0	0

Mn1	0.0064 (2)	0.0064 (2)	0.0055 (3)	0.00318 (10)	0	0
N1	0.0117 (7)	0.0099 (7)	0.0111 (7)	0.0058 (6)	0.0007 (5)	0.0010 (5)
C2	0.0108 (8)	0.0144 (8)	0.0115 (8)	0.0070 (7)	0.0001 (6)	−0.0026 (6)
N2	0.0200 (8)	0.0248 (9)	0.0159 (7)	0.0152 (7)	0.0014 (6)	0.0013 (6)

Geometric parameters (Å, º)

Co1—N1^{i}	1.9718 (16)	Mn1—C2^{vii}	1.9696 (19)
Co1—N1^{ii}	1.9718 (16)	Mn1—C2^{viii}	1.9696 (19)
Co1—N1^{iii}	1.9718 (15)	Mn1—C2^{ix}	1.9696 (19)
Co1—N1^{iv}	1.9718 (15)	Mn1—C2^{x}	1.9696 (19)
Co1—N1	1.9718 (15)	N1—H1A	0.89
Co1—N1^{v}	1.9718 (15)	N1—H1B	0.89
Mn1—C2^{vi}	1.9696 (19)	N1—H1C	0.89
Mn1—C2	1.9696 (19)	C2—N2	1.150 (2)
N1^{i}—Co1—N1^{ii}	180.00 (7)	C2—Mn1—C2^{viii}	89.80 (7)
N1^{i}—Co1—N1^{iii}	89.47 (6)	C2^{vii}—Mn1—C2^{viii}	89.80 (7)
N1^{ii}—Co1—N1^{iii}	90.53 (6)	C2^{vi}—Mn1—C2^{ix}	89.80 (7)
N1^{i}—Co1—N1^{iv}	89.47 (6)	C2—Mn1—C2^{ix}	90.20 (7)
N1^{ii}—Co1—N1^{iv}	90.53 (6)	C2^{vii}—Mn1—C2^{ix}	180
N1^{iii}—Co1—N1^{iv}	89.47 (6)	C2^{viii}—Mn1—C2^{ix}	90.20 (7)
N1^{i}—Co1—N1	90.53 (6)	C2^{vi}—Mn1—C2^{x}	89.80 (7)
N1^{ii}—Co1—N1	89.47 (6)	C2—Mn1—C2^{x}	90.20 (7)
N1^{iii}—Co1—N1	180.00 (10)	C2^{vii}—Mn1—C2^{x}	90.20 (7)
N1^{iv}—Co1—N1	90.53 (6)	C2^{viii}—Mn1—C2^{x}	180.00 (7)
N1^{i}—Co1—N1^{v}	90.53 (6)	C2^{ix}—Mn1—C2^{x}	89.80 (7)
N1^{ii}—Co1—N1^{v}	89.47 (6)	Co1—N1—H1A	109.5
N1^{iii}—Co1—N1^{v}	90.53 (6)	Co1—N1—H1B	109.5
N1^{iv}—Co1—N1^{v}	180.00 (10)	H1A—N1—H1B	109.5
N1—Co1—N1^{v}	89.47 (6)	Co1—N1—H1C	109.5
C2^{vi}—Mn1—C2	180	H1A—N1—H1C	109.5
C2^{vi}—Mn1—C2^{vii}	90.20 (7)	H1B—N1—H1C	109.5
C2—Mn1—C2^{vii}	89.80 (7)	N2—C2—Mn1	178.31 (17)
C2^{vi}—Mn1—C2^{viii}	90.20 (7)		

Symmetry codes: (i) $y, -x+y, -z$; (ii) $-y, x-y, z$; (iii) $-x, -y, -z$; (iv) $x-y, x, -z$; (v) $-x+y, -x, z$; (vi) $-x+2/3, -y+4/3, -z+1/3$; (vii) $-y+1, x-y+1, z$; (viii) $-x+y, -x+1, z$; (ix) $y-1/3, -x+y+1/3, -z+1/3$; (x) $x-y+2/3, x+1/3, -z+1/3$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N2^{vii}	0.89	2.09	2.979 (2)	173

Symmetry code: (vii) $-y+1, x-y+1, z$.