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Dipotassium sodium hexacyanocobalt(III)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(N–C) = 0.002 Å
R factor = 0.019
wR factor = 0.056
Data-to-parameter ratio = 20.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The polymeric structure of the title compound, $K_2Na[Co(CN)_6]$, contains a three-dimensional network of centrosymmetric CoC_6 and NaN_6 octahedra and K^+ cations.

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Comment

Hexacyanometallates(III) of alkali metals $M_2M'[M''(CN)_6]$ (M = Cs, Rb; M' = Rb, K, Na; M'' = Cr, Mn, Fe, Co) (Peschel *et al.*, 2000) crystallize in the monoclinic system (space group $P2_1/n$). Recently, we reported the synthesis of the isostructural hexacyanometallates $K_2Na[M''(CN)_6]$ (M'' = Fe, Co; Zhilov *et al.*, 2003).

The coordination polyhedra of the Co and Na ions, both of which lie on inversion centres, are octahedra. The $[Co(CN)_6]^{3-}$ complexes and the Na^+ cations form a three-dimensional network. The crystallographically unique K^+ ion has an irregular coordination geometry formed by six N and five C atoms, with K—N and K—C distances in the ranges 2.855 (1)–3.405 (1) and 3.181 (1)–3.387 (1) Å, respectively.

Experimental

The title compound was prepared by applying an aqueous $K_3[Co(CN)_6]$ (Aldrich) solution to an ion-exchange column (H^+ form). The acidic solution obtained was boiled and then neutralized with $NaHCO_3$. Isothermal evaporation of the hydrolysed solution thus obtained (298 K) produced single crystals of $K_2Na[Co(CN)_6]$.

Crystal data

$K_2Na[Co(CN)_6]$
M_r = 316.24
Monoclinic, $P2_1/n$
a = 7.0276 (7) Å
b = 7.5566 (6) Å
c = 10.2883 (8) Å
β = 90.665 (12)°
V = 546.32 (8) Å^3
Z = 2
D_x = 1.922 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
θ = 13.7–14.9°
μ = 2.35 mm^{-1}
T = 296 (2) K
Prism, colourless
0.25 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Non-profiled $\omega/2\theta$ scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.534, T_{max} = 0.625
3025 measured reflections
1598 independent reflections
1461 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 30.0°
$h = -2 \rightarrow 9$
$k = -3 \rightarrow 10$
$l = -14 \rightarrow 14$
2 standard reflections
frequency: 120 min
intensity decay: 3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.056
S = 1.00
1598 reflections
77 parameters
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0093 (18)

Table 1
Selected bond lengths (Å).

Co1—C3	1.8901 (12)	Na1—N2^{iii}	2.5190 (12)
Co1—C1	1.8928 (12)	N1—C1	1.1461 (17)
Co1—C2	1.8958 (12)	N2—C2	1.1479 (17)
Na1—N1^{i}	2.4953 (12)	N3—C3	1.1482 (17)
Na1—N3^{ii}	2.5019 (12)		

Symmetry codes: (i) $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; (ii) $x,y,z-1$; (iii) $\frac{1}{2}-x,y-\frac{1}{2},\frac{1}{2}-z$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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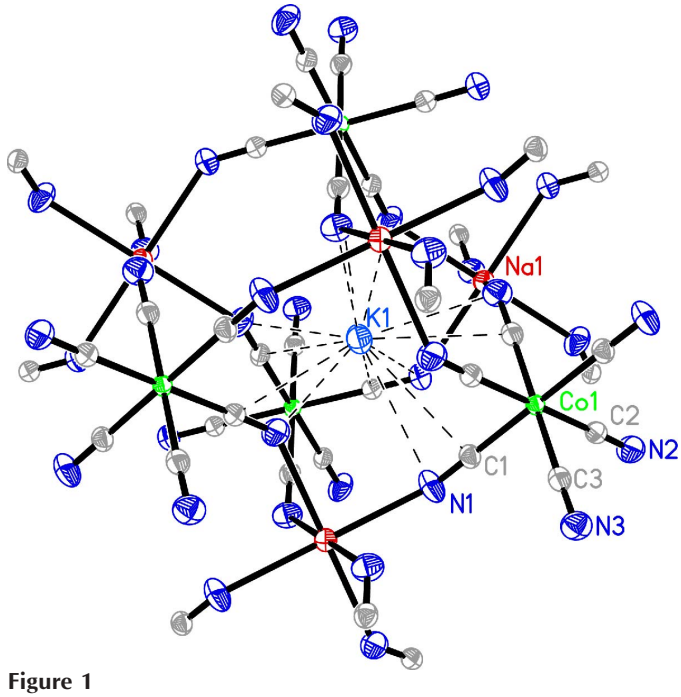

Figure 1
A fragment of the structure of $K_2Na[Co(CN)_6]$ (50% probability displacement ellipsoids).

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