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Potassium silver thiocyanate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(N–C) = 0.006 Å
R factor = 0.036
wR factor = 0.095
Data-to-parameter ratio = 25.6

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

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The structure of $K[Ag(SCN)_2]$ forms a three-dimensional network consisting of seven-coordinated K atoms and four-coordinated Ag atoms connected together by bridging thiocyanate groups.

Comment

There has been considerable investigation into thiocyanates. A valuable synthetic study was published about 100 years ago (Wells, 1902) and treated mostly double and triple thiocyanates. At that time, most studies were synthetic and analytical. Many crystal structure determinations relating to metal thiocyanates have been solved since. Silver forms simple thiocyanate AgSCN, which has two polymorphic forms, *Pmnn* and *C*2/*c*. There are also double silver thiocyanates, and triple thiocyanates such as $Cs_3Sr[Ag_2(SCN)_7]$ and $Cs_3Ba[Ag_2(SCN)_7]$. These two triple thiocyanates have also interesting optical, electro-optic and electrostrictive properties (Bohaty & Fröhlich, 1992).

Although potassium silver thiocyanate, $K[Ag(SCN)_2]$, has been known for 150 years, there is little data available in the literature. The unit cell has been published (Chateau *et al.*, 1962). Potassium silver thiocyanate, $K[Ag(SCN)_2]$, is not isostructural with $AgNH_4(SCN)_2$, unlike many potassium and ammonium compounds.

Potassium is seven-coordinated, with five N and two S atoms around the K atom. The coordination polyhedron is a distorted monocapped trigonal prism, as shown in Fig. 1. N1 is the capping atom which is at a distance of 2.986 (4) Å from K1.

Four S atoms surround the Ag atom in the form of a tetrahedron. The tetrahedron is slightly distorted: Ag—S distances vary between 2.579 (1) and 2.739 (1) Å. The six S—Ag—S angles vary between 95.29 (3) and 126.49 (4)°.

There are two different thiocyanate groups in the structure. The bond lengths and angles are normal and similar in both groups, but differ in coordination. In thiocyanate group one (S1/C1/N1), the S atom is connected to two Ag atoms and the N atom to three K atoms, whereas in thiocyanate group two (S2/C2/N2), the S atom is connected to two Ag atoms and two K atoms and the N atom to two K atoms.

The structure forms a three-dimensional network. It can be thought of as consisting of infinite AgS_2 layers, so that the tetrahedra around the Ag atoms are approximately at planes xz with y = 0.0 and 0.5 (Fig. 2) and the potassium polyhedra approximately at planes xz with y = 0.25 and 0.75. Tetrahedra around the Ag atoms share one common edge and two common corners so that one tetrahedron is connected to three other tetrahedra. The monocapped trigonal prisms around the

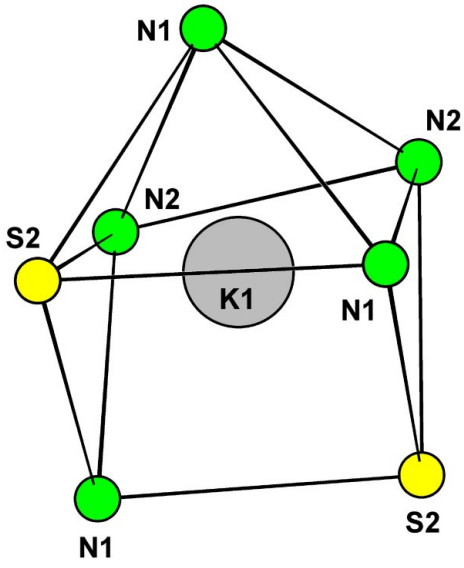

Figure 1
The coordination polyhedron around the K atom.

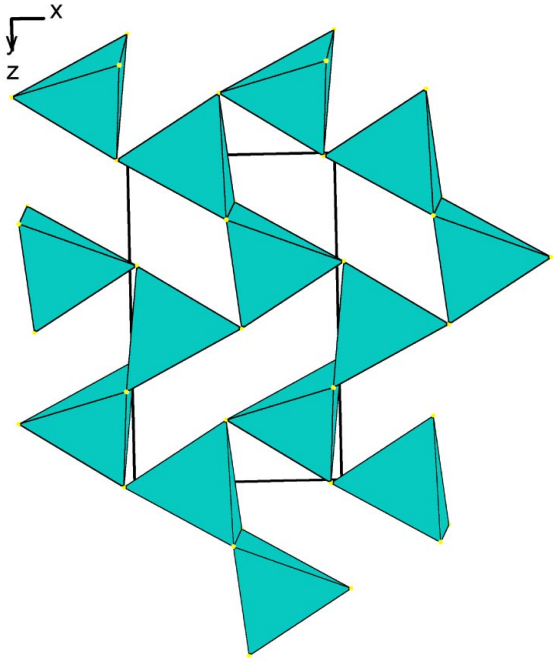

Figure 2
The AgS_2 layer viewed along the *y* axis. The *x* axis is horizontal.

K atoms share four common edges and two common corners. These layers are held together by the thiocyanate groups (Fig. 3).

Experimental

Potassium thiocyanate was obtained from Fluka Chemie AG and silver thiocyanate from the Aldrich Chemical Company Inc. Potassium silver thiocyanate was made by dissolving 1670 mg KSCN in 3.3 ml deionized water and then dissolving 1230 mg AgSCN in that solution at room temperature. After slow evaporation at room temperature, white crystals of $K[Ag(SCN)_2]$ formed after two days. The crystal used for analysis was mounted on a glass fibre.

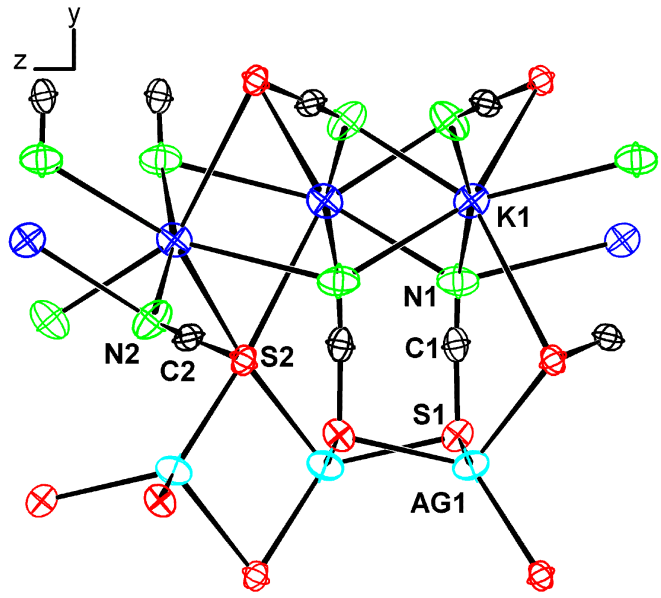

Figure 3
The partial structure along the *a* axis. The *z* axis is horizontal. Ellipsoids are presented at the 50% probability level.

Crystal data

$K[Ag(SCN)_2]$
M_r = 263.13
Orthorhombic, *Pbca*
a = 6.719 (1) Å
b = 18.024 (1) Å
c = 10.826 (2) Å
V = 1311.0 (3) Å^3
Z = 8
D_x = 2.666 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 14.6–25.4°
μ = 4.23 mm^{-1}
T = 293 (2) K
Prism, colourless
0.2 × 0.2 × 0.1 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.56, T_{max} = 0.65
1897 measured reflections
1897 independent reflections
1137 reflections with $I > 2\sigma(I)$
θ_{max} = 30.0°
h = 0 → 9
k = 0 → 25
l = 0 → 15
2 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.095
S = 1.00
1897 reflections
74 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0460P)^2 + 0.2326P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0148 (6)

Table 1
Selected geometric parameters (Å, °).

Ag1—S1	2.5788 (13)	K1—N1^{vii}	3.228 (4)
Ag1—S2	2.5836 (11)	K1—S2	3.3771 (15)
Ag1—S1^{i}	2.6068 (12)	K1—S2^{viii}	3.4431 (15)
Ag1—S2^{ii}	2.7393 (11)	S1—C1	1.658 (5)
K1—N2^{iii}	2.779 (4)	S2—C2	1.666 (4)
K1—N1^{iv}	2.823 (5)	C1—N1	1.162 (6)
K1—N2^{v}	2.885 (4)	C2—N2	1.145 (6)
K1—N1^{vi}	2.986 (4)		
S1—Ag1—S2	126.49 (4)	S2—Ag1—S2^{ii}	95.29 (3)
S1—Ag1—S1^{i}	100.64 (3)	S1^{i}—Ag1—S2^{ii}	101.75 (4)
S2—Ag1—S1^{i}	119.21 (4)	N1—C1—S1	177.4 (4)
S1—Ag1—S2^{ii}	110.78 (4)	N2—C2—S2	177.6 (4)

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

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2000).

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