

SHORT STRUCTURAL PAPERS

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Acta Cryst. (1974). B30, 1117

Silver Dicyanonitrosomethanide, $\text{AgC}(\text{CN})_2\text{NO}$

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(Received 17 August 1973; accepted 10 December 1973)

Abstract. $\text{AgC}(\text{CN})_2\text{NO}$ was prepared by the method of Longo [*Gazz. chim. Ital.* (1931). 61, 575] and recrystallized from aqueous solution; orthorhombic, $Pbca$, $Z=8$, $a=11.729$ (14), $b=10.299$ (4), $c=7.868$ (5) Å, $V=950$ Å³, $D_{\text{calc}}=2.82$, $D_{\text{obs}}=2.81$ (2) g cm⁻³. Each of the nitrogen and oxygen atoms bonds to a silver atom to give roughly tetrahedral four-coordinate silver. The packing is closely related to that of $\text{AgC}(\text{CN})_3$.

Introduction. 744 independent reflections were collected for $0 < \theta < 24^\circ$ on a Hilger and Watts 4-circle automated diffractometer using Zr-filtered Mo $K\alpha$ ($\lambda=0.7170$ Å) radiation. Only the 463 reflections with $I > 2\sigma(I)$ were used in the subsequent calculations. A crystal $0.10 \times 0.28 \times 0.42$ mm was used; absorption corrections were made (transmission coefficients ranged from 0.349 to 0.674). The space group was uniquely identified through systematic extinctions ($0kl$, $l=2n+1$; $h0l$, $l=2n+1$; $hk0$, $h=2n+1$). A trial structure was found from Patterson and Fourier maps and refined by full-matrix least squares with all atoms with anisotropic thermal parameters. The details of the experimental arrangements, the weighting scheme, and the programs used have all been described previously (Chow & Britton, 1974). No corrections were made for anomalous scattering. The refinement converged with $R=0.070$. The final parameters are given in Table 1.*

* A table of observed and calculated structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 30317 (10 pp.). Copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England, or from the authors.

Discussion. $\text{AgC}(\text{CN})_3$ (Konnert & Britton, 1966) has a structure with interwoven, infinite two-dimensional layers. The present study was undertaken to see whether the replacement of a cyanide group in the $\text{C}(\text{CN})_3$ anion by a nitroso group would lead to the same basic arrangement, which would require bonding through the oxygen atom to the silver atom, or whether the nitrogen atom in the nitroso group would act as the ligating atom, which would lead to a basically different structure.

The packing in the $\text{AgC}(\text{CN})_2\text{NO}$ structure is shown in Fig. 1. Somewhat to our surprise both the oxygen and the nitrogen atoms in the nitroso group are bonded to silver atoms. The oxygen atoms are bonded in such a way that the infinite two-dimensional layers analogous to those in $\text{AgC}(\text{CN})_3$ are present. On the other hand the bonding between the nitroso nitrogen atoms in one double layer and the silver atoms in the next require that the layers be arranged differently, with the consequence that the space group here is not simply derived from that of $\text{AgC}(\text{CN})_3$. Fig. 1 is drawn to facilitate comparison with the previous drawing showing the structure of $\text{AgC}(\text{CN})_3$ (Konnert & Britton, 1966, Fig. 2).

The anion is planar as suggested by Köhler & Seifert (1970). The interatomic distances and angles are also shown in Fig. 1 except for the angles about silver, which are: O–Ag–N(1), 111.7° ; O–Ag–N(2), 114.0° ; O–Ag–N(3), 97.5° ; N(1)–Ag–N(2), 95.1° ; N(1)–Ag–N(3), 128.2° ; N(2)–Ag–N(3), 111.2° . The estimated standard deviations are 0.02–0.03 Å for the bond lengths, $1-2^\circ$ for the angles with light atoms at the center, and 0.5° for the angles with silver at the center.

Table 1. Positional and thermal parameters for $\text{AgC}(\text{CN})_2\text{NO}$

Anisotropic temperature factors are of the form $\exp[-(\beta_{11}h^2 + \dots + 2\beta_{12}hk + \dots)]$. All parameters have been multiplied by 10^4 . E.s.d.'s are given in parentheses.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ag	99 (1)	5796 (1)	2861 (2)	71 (1)	142 (2)	180 (3)	-2 (1)	-8 (2)	2 (2)
O	1596 (10)	6014 (15)	4970 (19)	74 (12)	117 (17)	327 (37)	7 (13)	8 (16)	30 (21)
N(1)	1249 (15)	5792 (18)	6352 (24)	164 (19)	100 (17)	220 (33)	54 (19)	168 (25)	101 (25)
C(1)	1993 (15)	6304 (16)	7639 (30)	60 (13)	94 (18)	278 (57)	-2 (14)	-69 (27)	-57 (31)
C(2)	3008 (16)	6990 (16)	7349 (21)	92 (16)	102 (19)	86 (37)	1 (16)	16 (21)	4 (24)
N(2)	3819 (14)	7514 (17)	7158 (19)	90 (12)	130 (17)	238 (33)	-33 (16)	38 (20)	12 (26)
C(3)	1552 (13)	6025 (19)	9373 (27)	53 (14)	71 (20)	194 (42)	2 (15)	-8 (19)	-5 (23)
N(3)	1175 (14)	5836 (18)	10632 (21)	99 (15)	120 (17)	205 (34)	-12 (16)	59 (18)	31 (24)

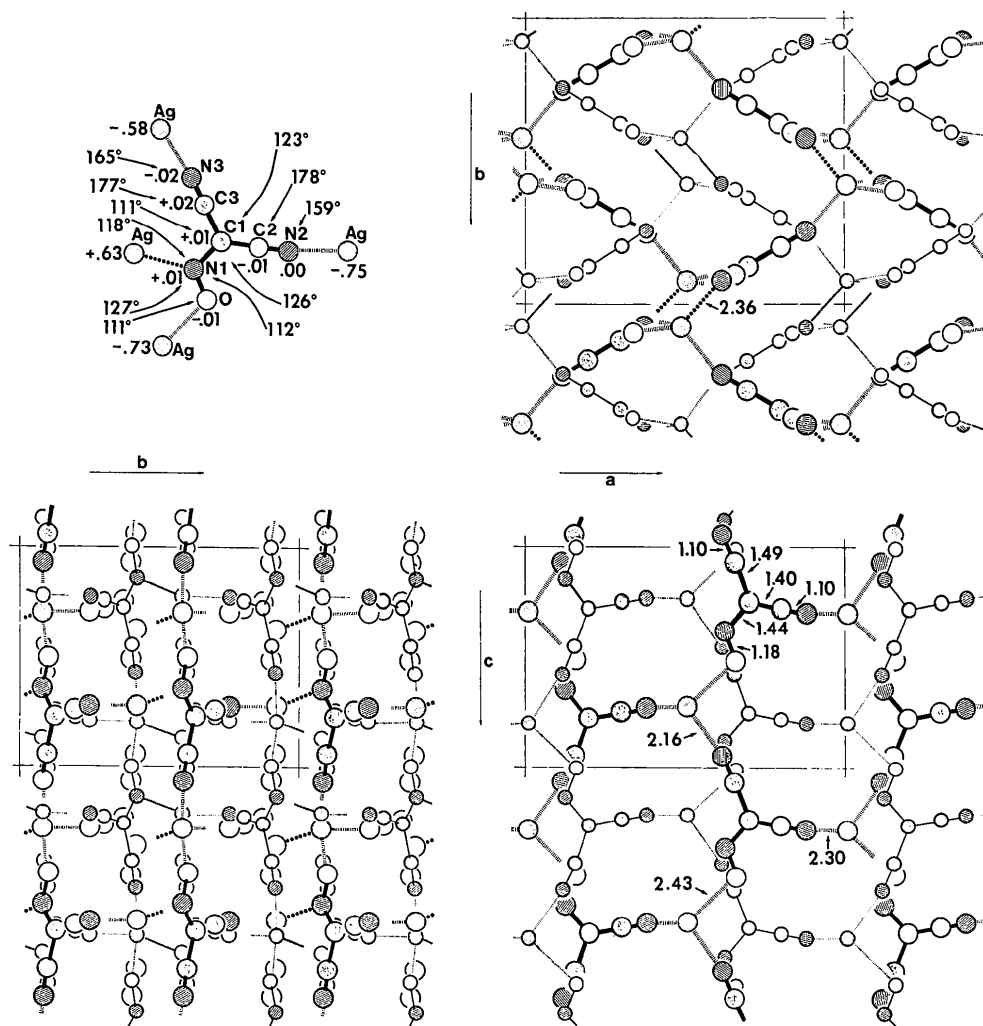


Fig. 1. The structure of $\text{AgC}(\text{CN})_2\text{NO}$. Upper left: an isolated anion and its nearest silver atoms, showing the labeling of the atoms, the distance in Å of each of the atoms out of the mean plane of the anion, and the bond angles (arrows point to the central atoms of each angle). Upper right and below: three views of the packing. Interatomic distances are given in Å. This figure should be compared with the drawing showing the structure of $\text{AgC}(\text{CN})_3$ [see Fig. 2, Konnert & Britton (1966)]. The different sized atoms are intended to distinguish between the two halves of an interpenetrating double layer. The $\text{N}\cdots\text{Ag}$ contacts between layers are shown as dotted lines to distinguish them from the $\text{N}\cdots\text{Ag}$ and $\text{O}\cdots\text{Ag}$ contacts within the layers. In the lower right only one double layer (the central one from the other two views) is shown.

The coordination about the silver atom is reasonably close to tetrahedral considering the constraints imposed by the geometry of the anion.

We thank the National Science Foundation for their support of this work.

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