Table 1. *Atom coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* ($Å^2 \times 10^3$)

	x	y	z	U_{eq}*
Al	3752 (3)	4402 (2)	3739 (2)	25 (1)
O(1)	6083 (5)	4914 (4)	4756 (3)	25 (2)
O(2)	1293 (5)	3873 (4)	2860 (4)	29 (2)
O(3)	4338 (6)	6327 (4)	3473 (4)	28 (3)
O(4)	3825 (5)	3747 (4)	2295 (3)	29 (2)
O(5)	2865 (5)	2365 (4)	3779 (3)	30 (2)
C(1)	7486 (8)	4808 (7)	4524 (6)	31 (4)
C(2)	7034 (9)	3165 (7)	4024 (6)	46 (5)
C(3)	7952 (9)	5791 (7)	3760 (6)	45 (4)
C(4)	599 (9)	4446 (7)	2089 (5)	29 (4)
C(5)	1561 (9)	5826 (7)	1965 (6)	34 (4)
C(6)	3376 (10)	6705 (7)	2684 (6)	34 (4)
C(7)	−1372 (9)	3590 (7)	1337 (6)	43 (4)
C(8)	−2055 (10)	1914 (7)	974 (7)	67 (5)
C(9)	4328 (10)	8259 (7)	2557 (7)	44 (5)
C(10)	5723 (10)	8333 (8)	2164 (7)	64 (6)
C(11)	2961 (9)	2401 (7)	1546 (6)	35 (4)
C(12)	2075 (9)	1125 (7)	1797 (6)	38 (4)
C(13)	2089 (8)	1155 (7)	2915 (6)	34 (4)
C(14)	3073 (10)	2315 (7)	377 (5)	45 (4)
C(15)	2640 (11)	3446 (8)	−182 (6)	59 (5)
C(16)	1150 (11)	−271 (7)	3172 (7)	55 (5)
C(17)	1763 (15)	−269 (9)	4347 (8)	170 (9)

* Equivalent isotropic U defined as one-third of the trace of the orthogonalized U_{ij} tensor.

difference map and constrained to have C—H = 0·96 Å and isotropic thermal parameters, $U = 0{\cdot}06$ Å^2. 208 parameters refined. All non-H atoms treated as anisotropic. $R_{int} = 0{\cdot}0302$; $R = 0{\cdot}0837$; $wR = 0{\cdot}0672$; $w^{-1} = \sigma^2(F) + 0{\cdot}0003F^2$. $(\Delta/\sigma)_{max} = 0{\cdot}094$, $(\Delta\rho)_{max} = 0{\cdot}37$, $(\Delta\rho)_{min} = -0{\cdot}40$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Programs: *SHELXTL* (Sheldrick, 1981). Atomic coordinates are contained in Table 1.* Bond lengths and angles, structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited. Fig. 1 illustrates the molecule with the numbering scheme employed. Note that the large thermal motion for C(17) leads to an incorrect bond distance for C(16)—C(17). Efforts to refine this disorder were unsuccessful.

Related literature. For additional information on structures and chemistry of aluminium alkoxide and siloxide complexes, see Garbauskas, Wengrovius, Going & Kasper (1984) and Wengrovius *et al.* (1986).

* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44206 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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The Silver Salt of Cyanourea

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Abstract. $Ag^+.C_2H_2N_3O^-$, $M_r = 191{\cdot}93$, orthorhombic, *Pbca*, $a = 6{\cdot}530$ (6), $b = 9{\cdot}882$ (4), $c = 12{\cdot}973$ (3) Å, $Z = 8$, $V/Z = 104{\cdot}6$ (2) Å^3; $D_x = 3{\cdot}045$ (5), $D_m > 2{\cdot}96$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71073$ Å, $\mu = 46{\cdot}2$ cm^{-1}, $F(000) = 720$, $T = 297$ (2) K, $R = 0{\cdot}040$ for 909 reflections. The anion is formed from the neutral cyanourea molecule by loss of the H ion attached to the central N atom. The bond distances indicate considerable electron delocalization in the anion. The NH_2 group is bent out of the plane of the N_2CO fragment by 23 (6)° and the nitrile group is bent out of the same plane by 4·5 (3)°. The NH_2 H atoms are both involved in hydrogen bonds to O atoms in adjacent anions. The Ag ion has two close contacts [2·143 (4) Å to a nitrile N atom and 2·180 (4) Å to a central N atom] 144·7 (2)° apart as well as two longer contacts [2·576 (3) Å to an O atom and 2·733 (5) Å to another nitrile N atom].

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Table 1. *Atomic coordinates and equivalent isotropic thermal parameters*

$B_{eq} = (B_{11} + B_{22} + B_{33})/3.$

	x	y	z	B_{eq}(Å²)
Ag	0·05322 (7)	0·20941 (4)	0·17250 (4)	3·741 (8)
N3	0·1750 (6)	0·5880 (4)	0·1771 (4)	3·07 (9)
C2	0·0580 (7)	0·5062 (5)	0·1551 (4)	2·31 (9)
N2	−0·0692 (6)	0·4089 (3)	0·1357 (3)	2·19 (7)
C1	−0·2529 (8)	0·4486 (4)	0·0930 (3)	1·98 (8)
O1	−0·2886 (5)	0·5693 (3)	0·0710 (3)	2·41 (7)
N1	−0·3896 (6)	0·3513 (3)	0·0780 (4)	2·77 (8)
H1	−0·366 (8)	0·274 (4)	0·077 (3)	3 (1)*
H2	−0·498 (9)	0·373 (6)	0·039 (4)	5 (1)*

* Atoms refined isotropically.

Table 2. *Interatomic distances* (Å) *and angles* (°)

Ag environment			
Ag–N3	2·143 (4)	N3–Ag–N2	144·7 (2)
Ag–N2	2·180 (4)	N3–Ag–O1	105·6 (1)
Ag–O1	2·576 (3)	N3–Ag–N3′	100·7 (1)
Ag–N3′	2·733 (5)	N2–Ag–O1	97·4 (1)
		N2–Ag–N3′	110·7 (1)
		O1–Ag–N3′	76·3 (1)
Anion			
N1–C1	1·327 (6)	N1–C1–O1	122·2 (5)
C1–O1	1·248 (5)	N1–C1–N2	116·0 (4)
C1–N2	1·378 (6)	N2–C1–O1	121·8 (4)
N2–C2	1·295 (6)	C1–N2–C2	115·1 (4)
C2–N3	1·149 (6)	N2–C2–N3	175·9 (6)
N1–H1	0·78 (5)	C1–N1–H1	125 (5)
N1–H2	0·90 (7)	C1–N1–H2	116 (4)
Anion environment			
N1···O1 (H1)	3·021 (5)	C1–N1···O1 (H1)	112·4 (4)
N1···O1 (H2)	2·961 (5)	C1–N1···O1 (H2)	114·5 (4)
H1···O1	2·26 (6)	N1–H1···O1	165 (6)
H2···O1	2·08 (7)	N1–H2···O1	170 (6)
		C1–N2–Ag	131·6 (3)
		C2–N2–Ag	113·2 (3)
		C2–N3–Ag	159·8 (5)

Experimental. Lath-shaped crystals suitable for X-ray diffraction were obtained from the hydrolysis of $N(CN)_2^-$ in acid solution during an attempt to grow crystals of $AgN(CN)_2$; the crystals were identified by the X-ray analysis. The crystal used measured 0·05 × 0·13 × 0·35 mm. The crystals were denser than the densest liquid available, tetrabromoethane. Data were collected on an Enraf–Nonius CAD-4 diffractometer equipped with a graphite monochromator. 25 reflections with $12 < \theta < 20°$ were used to determine the cell parameters. Systematic extinctions (0*kl*, *k* odd; *h*0*l*, *l* odd; *hk*0, *h* odd) uniquely determined the space group. Data were collected, using ω scans, in the range $0 < \theta < 30°$ for one hemisphere (ranges: h −9 to 9, k 0 to 13, l −18 to 18). Empirical absorption corrections were made; the maximum variation in intensity in the ψ scans was 24·5%. After the absorption corrections the equivalent reflections were combined ($R_{int} = 0·027$) to give 1217 unique allowed reflections, of which the 909 with $I > \sigma(I)$ were used in the calculations. Three check reflections measured every 3000 s of exposure time showed no systematic change with time. The Ag position was found from a Patterson synthesis and the remaining atoms from successive electron density maps. All the atoms except H were given anisotropic thermal parameters. All parameters were refined by full-matrix least-squares refinement on F's. Refinement converged with $R = 0·040$, $wR = 0·034$ and $S = 0·939$; $w = 1/\sigma^2(F)$ was calculated from $\sigma^2(I) = \sigma^2(I)_c + (0·03I)^2$, where $\sigma(I)_c$ is the standard deviation in I based on counting statistics alone. $(\Delta/\sigma)_{max}$ in the final cycle was 0·09. The eight highest peaks (0·52 to 0·99 e Å^{-3}) in the final difference electron density map were all within 1·1 Å of the Ag position. Atomic scattering factors and anomalous-dispersion corrections for all atoms were taken from *International Tables for X-ray Crystallography* (1974). The computer programs used were all from the Enraf–Nonius *Structure Determination Package* and have been described by Frenz (1978).

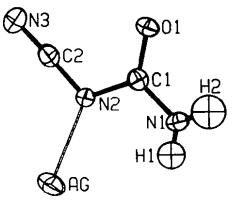

Fig. 1. View of the title compound. Thermal ellipsoids are shown at the 50% probability level.

Atomic coordinates are given in Table 1, and interatomic distances and angles in Table 2.* The atom labelling and thermal ellipsoids for one asymmetric unit are shown in Fig. 1.

Related literature. Magomedova & Zvonkova (1974) made a preliminary report of the structure of the potassium salt of cyanourea. The bond distances in their anion are similar to those reported here.

* Lists of anisotropic thermal parameters, deviations from planarity, and observed and calculated structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44315 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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