TABLE IV

ANGLES IN $B_9C_2H_{11}Re(CO)_3$

Angle, deg		Angle, deg	
O(1)CO–C(1)CO–Re(1)	175	C(3)–B(8)–B(7)	60
O(2)CO–C(2)CO–Re(1)	178	C(2)–B(11)–B(6)	58
O(3)CO–C(3)CO–Re(1)	176	C(2)–B(11)–B(7)	59
C(1)CO–Re(1)–C(2)CO	89	B(5)–B(4)–B(9)	61
C(2)CO–Re(1)–C(3)CO	92	B(8)–B(4)–B(9)	59
C(3)CO–Re(1)–C(1)CO	88	B(4)–B(5)–B(9)	60
C(2)–Re(1)–C(3)	41	B(6)–B(5)–B(10)	58
C(3)–Re(1)–B(4)	43	B(9)–B(5)–B(10)	59
B(4)–Re(1)–B(5)	44	B(5)–B(6)–B(10)	61
B(5)–Re(1)–B(6)	45	B(10)–B(6)–B(11)	60
B(6)–Re(1)–C(2)	43	B(8)–B(7)–B(12)	60
Re(1)–C(2)–C(3)	70	B(11)–B(7)–B(12)	60
Re(1)–C(2)–B(6)	70	B(4)–B(8)–B(9)	60
Re(1)–C(3)–C(2)	70	B(7)–B(8)–B(12)	60
Re(1)–C(3)–B(4)	69	B(9)–B(8)–B(12)	61
Re(1)–B(4)–C(3)	68	B(4)–B(9)–B(5)	59
Re(1)–B(4)–B(5)	69	B(4)–B(9)–B(8)	60
Re(1)–B(5)–B(4)	67	B(5)–B(9)–B(10)	60
Re(1)–B(5)–B(6)	68	B(8)–B(9)–B(12)	60
Re(1)–B(6)–C(2)	67	B(10)–B(9)–B(12)	61
Re(1)–B(6)–B(5)	67	B(5)–B(10)–B(6)	62
C(2)–B(7)–C(3)	56	B(5)–B(10)–B(9)	61
C(3)–C(2)–B(7)	63	B(6)–B(10)–B(11)	61
C(2)–C(3)–B(7)	62	B(9)–B(10)–B(12)	60
B(6)–C(2)–B(11)	63	B(11)–B(10)–B(12)	60
B(7)–C(2)–B(11)	62	B(6)–B(11)–B(10)	59
B(4)–C(3)–B(8)	63	B(7)–B(11)–B(12)	60
B(7)–C(3)–B(8)	62	B(10)–B(11)–B(12)	61
C(3)–B(4)–B(8)	59	B(7)–B(12)–B(8)	60
C(2)–B(6)–B(11)	59	B(7)–B(12)–B(11)	60
C(2)–B(7)–B(11)	59	B(8)–B(12)–B(9)	59
C(3)–B(7)–B(8)	58	B(9)–B(12)–B(10)	59
C(3)–B(8)–B(4)	59	B(10)–B(12)–B(11)	59

Such increases are expected since large motions cause the observed distance to be shorter than the true average value.

In the carbonyl portion of the ion, the Re to C to O linkages are almost linear with a slight bend of a few degrees in an outward direction away from the axis of the molecule. At the Re atom the three carbonyl carbons make very nearly right angles with respect to each other. This tricarbonyl structure is quite similar to that reported in hexamethylbenzenechromium tricarbonyl,[8] thiophenechromium tricarbonyl,[8] benzenechromium tricarbonyl,[8] and cyclopentadienylmanganese tricarbonyl.[9] The carbonyl oxygens are apparently free to flop around somewhat as their thermal parameters are larger than the carbons to which they are attached. In Table III we have included some thermally adjusted values for the C–O bond distances based on a calculation that assumes the oxygens are "riding" on the carbons. These three bonds were the only bonds in the structure where this type of a correction was larger than the estimated standard deviation of the bond length. We do not fully understand the thermal motion and report these thermally corrected bond lengths primarily as an indication of the magnitude of the thermal effect rather than as accurate values.

The cesium ion has as its closest neighbors at 3.2 A three oxygen atoms of three symmetry unrelated carbonyls from three different anions.

The hydrogen atoms were poorly resolved in this structure determination. One hydrogen atom, H(10), was not resolved at all in the difference function.

Acknowledgment.—We wish to thank Professor M. F. Hawthorne of the Riverside campus of the University of California for providing us with the crystals which made this work possible.

[8] M. F. Bailey and L. F. Dahl, *Inorg. Chem.*, **4**, 1302, 1306, 1314 (1965).

[9] A. F. Berndt and R. E. Marsh, *Acta Cryst.*, **16**, 118 (1963).

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The Crystal Structure of $AgC(CN)_3$

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Silver tricyanomethide, $AgC(CN)_3$, forms orthorhombic crystals in the space group I2cm with a = 6.21 A, b = 10.19 A, c = 7.98 A with four molecules per unit cell. Each Ag atom is coordinated in a flat pyramid to three N atoms, one at 2.11 ± 0.06 A and two at 2.25 ± 0.04 A, with one N–Ag–N angle of 99.7° and two of 123.9°. Owing to the large uncertainties in the light-atom positions, the $C(CN)_3^-$ group cannot be said to deviate from D_{3h} symmetry. The bonding leads to puckered, hexagonal, infinite nets of $AgC(CN)_3$. These nets interpenetrate in pairs to form a layer structure.

In the course of crystal structure studies of several silver compounds[1] and of the potassium salt of cyanoform,[2] $KC(CN)_3$, it occurred to us that $AgC(CN)_3$ might provide an example of silver atoms with coordination number three, and in particular that the planar arrangement shown in Figure 1 might exist. Accordingly, we have determined the crystal structure of $AgC(CN)_3$.

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[1] D. Britton and J. D. Dunitz, *Acta Cryst.*, **18**, 424; **19**, 662; **19**, 815 (1965).

[2] J. Witt and D. Britton, unpublished work. A preliminary report of this structure has been made by P. Andersen and B. Klewe, *Nature*, **200**, 464 (1963), who have also determined the structure of $NaC(CN_3)$ (private communication).

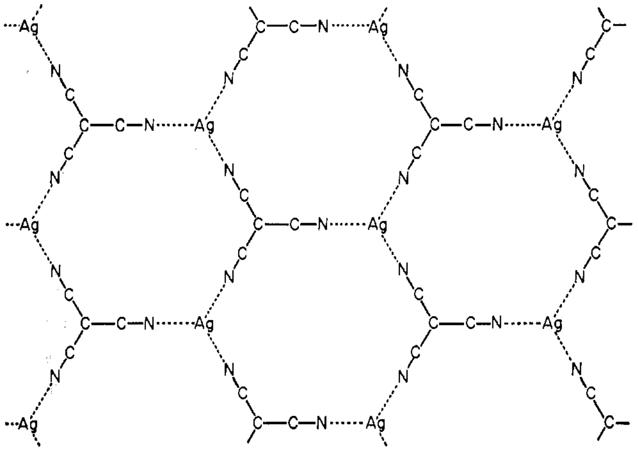

Figure 1.—Possible planar arrangement for $AgC(CN)_3$, involving three-coordinate silver.

Experimental Section

Preparation and Properties.—Silver tricyanomethide, $AgC(CN)_3$, was prepared by precipitation from a mixture of solutions of $AgNO_3$ and $KC(CN)_3$. Flat needles large enough for single crystal X-ray studies were grown by recrystallization from dilute ammonia solution. An infrared spectrum of the recrystallized compound showed only a single peak between 1400 and 4000 cm^{-1}. This peak, at 2200 cm^{-1}, compares reasonably with the peak[3] in the $KC(CN)_3$ spectrum at 2175 cm^{-1}. In particular, there was no peak attributable to NH_3, showing that an ammoniate had not been formed. The spoon test described by Bunn[4] showed the crystals to be pyroelectric and therefore acentric.

Space Group and Unit Cell.—Weissenberg and precession photographs taken with Mo Kα radiation (λ 0.7107 A) showed the needle axis to be the a axis of an orthorhombic crystal with $a = 6.21 \pm 0.01$ A, $b = 10.19 \pm 0.02$ A, $c = 7.98 \pm 0.01$ A. The assumption of four molecules per unit cell leads to a molecular volume of 126.2 A^3 and a calculated density of 2.603 g/cc, both of which are reasonable. Systematic extinctions for hkl $(h + k + l = 2n + 1)$ and $h0l$ $(h = 2n + 1, l = 2n + 1)$ indicate the space group to be either Imam, Ima2, or I2cm, of which the last was shown to be correct by the complete structure determination.

Multiple film Weissenberg photographs (Mo Kα radiation) were collected for the $0kl$–$5kl$ layers using a flat needle 0.05 × 0.26 × 2.0 mm, and for the $h0l$–$h8l$ layers using a section (cut from a flat needle) approximately 0.3 × 0.3 × 0.05 mm. Multiple film oscillation photographs were also taken to help with the correlation. The intensities were measured by comparison to a series of timed exposures of a selected spot. The usual Lorentz and polarization corrections were made. No corrections for absorption were made ($\mu = 37.4$ cm^{-1}). This is undoubtedly a large source of error in the data, but at the time of the work no program was available for making absorption corrections on irregularly shaped crystals and the shapes precluded spherical or cylindrical approximations. Intensities were measured for 221 independent reflections; 31 more reflections in the same region of reciprocal space with intensities too weak to measure were included in the subsequent refinement with intensities corresponding to four-ninths the minimum observable intensity.

Determination and Refinement of the Structure

The programs used in these calculations were prepared by L. W. Finger of the Geology Department and were carried out on the Control Data 1604 computer of the Numerical Analysis Center of the University of Minnesota.

The silver atom positions were readily determined from a three-dimensional Patterson map. A three-dimensional Fourier map based on the Ag only had Imcm symmetry and showed the light atoms plus their mirror images. The only reasonable arrangement was in I2cm, and one set of light-atom positions with this symmetry was chosen. A full-matrix least-squares refinement of the function $\Sigma w(|F_o|^2 - |F_c|^2)^2$ was carried out with weights: $w = {}^1/_2$ for unobserved F_o; $w = 1$ for $F_o < 40$; $w = (40/F_o)^4$ for $F_o > 40$. The refinement was monitored with the usual R function and with $r = [\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w|F_o|^4]^{1/2}$. A comparison of the values, $R = 0.142$ and 0.094, $r = 0.342$ and 0.214, with all atoms isotropic and with Ag only anisotropic, respectively, shows that the improvement with the Ag anisotropic is significant at better than the 99.5% confidence level according to the test suggested by Hamilton.[5] The original correlation of the various data had been made by using oscillation photographs about a to correlate the $0kl$–$5kl$ layers, and then using these data to correlate the lower quality $h0l$–$h8l$ layers. After the first refinements it was clear from a comparison of the observed and calculated structure factors that the scaling of the latter set of data could be improved, and the individual layers in h were rescaled by 2–5%. The corrections showed no regular trend with h and should not have affected the anisotropic thermal parameters in any misleading way. At this point the unobserved reflections were also included and refinement was then continued. With Ag only anisotropic and with all atoms anisotropic, respectively, convergence was reached at $R = 0.0996$ and 0.0994, $r = 0.207$ and 0.197. The improvement is only significant at the 75% confidence level so we report the results of the refinement with Ag only anisotropic. The final parameters and standard deviations calculated from the full matrix are given in Table I. The observed and calculated structure factors are given in Table II.

TABLE I

FINAL PARAMETERS FOR $AgC(CN)_3$
(INCLUDING STANDARD DEVIATION)

		x	y	z	B
Ag	(4b)	(0.0000)	0.1519(4)	$^1/_4$	(3.5)
N_1	(4b)	0.759(9)	−0.007(6)	$^3/_4$	5.9(10)
N_2	(8c)	0.229(7)	0.186(3)	0.464(5)	5.4(7)
C_1	(4b)	0.613(10)	0.057(8)	$^3/_4$	5.1(13)
C_2	(8c)	0.296(4)	0.155(4)	0.594(3)	3.0(5)
C_3	(4b)	0.396(8)	0.130(6)	$^3/_4$	3.4(9)
		β_{11}	β_{22}	β_{33}	β_{12}
Ag		0.0238(9)	0.0137(5)	0.0114(4)	−0.0046(15)

[a] The anisotropic temperature factor is exp $-(h^2\beta_{11} \ldots + 2hk\beta_{12} \ldots)$.

Discussion

The bond lengths and bond angles in this compound along with comparative values from other compounds are given in Table III.

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(3) F. A. Miller and W. K. Baer, *Spectrochim. Acta*, **19**, 73 (1963); D. A. Long, R. A. G. Carrington, and R. B. Gravenor, *Nature*, **196**, 371 (1962).

(4) C. W. Bunn, "Chemical Crystallography," 2nd ed, Oxford University Press, 1961, p 321.

(5) W. C. Hamilton, *Acta Cryst.*, **19**, 502 (1965).

TABLE II

OBSERVED AND CALCULATED STRUCTURE FACTORS

H	K	L	OBS	CALC	ALPHA
0	0	2	139.1	162.8	-180.0
0	0	4	141.8	141.0	.0
0	0	6	99.1	93.3	-180.0
0	0	8	50.4	49.5	.0
0	0	10	21.3	26.0	-180.0
0	1	3	108.4	98.7	.0
0	1	5	91.3	75.2	-180.0
0	1	7	27.1	30.7	.0
0	1	9	24.4	30.3	-180.0
0	2	2	17.4	8.4	-180.0
0	2	4	25.6	23.3	-180.0
0	2	6	15.3	17.7	.0
0	2	8*	6.4	10.3	-180.0
0	3	1	20.1	10.7	-180.0
0	3	3	29.8	26.8	.0
0	3	5	10.1	9.4	-180.0
0	3	7*	6.4	9.8	.0
0	3	9*	8.2	6.0	-180.0
0	4	0	110.8	109.2	-180.0
0	4	2	92.8	73.8	.0
0	4	4	61.6	54.6	-180.0
0	4	6	45.8	48.3	.0
0	4	8	23.8	27.1	-180.0
0	5	1	89.4	83.9	.0
0	5	3	108.0	86.4	-180.0
0	5	5	64.0	56.1	.0
0	5	7	30.8	29.3	-180.0
0	5	9	25.8	25.7	.0
0	6	0	100.7	96.6	.0
0	6	2	51.1	49.6	-180.0
0	6	4	51.9	46.8	.0
0	6	6	39.2	38.8	-180.0
0	6	8	20.2	21.1	.0
0	7	1	26.3	23.4	-180.0
0	7	3	20.6	20.6	.0
0	7	5	21.1	19.1	-180.0
0	7	7*	6.4	6.0	.0
0	8	0*	8.4	6.7	.0
0	8	2	21.1	19.6	-180.0
0	8	4*	6.4	6.8	.0
0	8	6	19.3	8.3	-180.0
0	9	1	16.9	17.9	-180.0
0	9	3	23.8	25.7	.0
0	10	0	30.1	27.9	-180.0
0	10	2	22.2	22.8	.0
0	11	1*	6.4	10.9	.0
0	12	0*	8.2	6.6	.0
1	1	2	81.7	76.8	-210.8
1	1	4	55.3	54.7	-12.5
1	1	6	28.6	32.8	-179.2
1	1	8	14.0	21.5	-4.2
1	1	10*	9.4	13.3	-187.2
1	2	1	140.4	167.5	-185.0
1	2	3	135.5	117.2	2.6
1	2	5	100.5	84.8	-177.3
1	2	7	54.1	54.2	-11.1
1	2	9	26.4	30.4	-172.1
1	3	0	133.2	149.3	-143.8
1	3	2	118.6	111.2	-5.3
1	3	4	62.1	87.4	-172.5
1	3	6	62.0	54.0	13.2
1	3	8	35.2	34.2	-176.4
1	4	1	68.5	66.4	-9.4
1	4	3	51.0	47.6	-187.8
1	4	5	44.9	39.2	4.4
1	4	7	25.3	27.3	-202.1
1	4	9*	8.7	15.1	9.8
1	5	0	14.5	14.2	20.8
1	5	2	37.5	30.2	-253.4
1	5	4	13.2	9.6	-27.5
1	5	6	13.0	7.1	-231.5
1	5	8*	8.7	4.5	-50.0
1	6	1	42.5	40.7	-10.9
1	6	3	33.4	33.3	-166.9
1	6	5	22.3	25.0	-12.3
1	6	7	12.6	17.5	-181.2
1	7	0	48.3	48.6	9.4
1	7	2	50.9	48.7	-178.8
1	7	4	41.2	39.2	-6.6
1	7	6	24.0	26.2	-166.2
1	8	1	42.9	44.6	-188.7
1	8	3	38.6	35.0	9.3
1	8	5	28.7	28.5	-184.0
1	8	7	21.9	20.7	-11.6
1	9	0	21.5	20.2	-162.4
1	9	2	21.3	20.7	-17.9
1	9	4	15.2	17.6	-193.3
2	0	0	75.0	70.6	-7.6
2	0	2	155.0	151.0	-181.3
2	0	4	102.3	88.4	4.5
2	0	6	54.0	55.3	-186.6
2	0	8	37.6	38.8	-1.8
2	0	10	18.7	24.3	-177.3
2	1	1	102.0	111.3	-173.5
2	1	3	93.8	85.4	-6.2
2	1	5	60.0	53.4	-174.7
2	1	7	50.7	47.4	3.0
2	1	9	16.0	19.3	-181.5
2	2	0	29.7	30.6	-205.1
2	2	2	75.8	69.2	-11.3
2	2	4	32.9	32.2	-186.3
2	2	6	24.7	21.7	-16.5
2	2	8	12.5	13.9	-190.4
2	2	10*	9.6	7.9	-3.9
2	3	1	32.1	30.6	-170.7
2	3	3	17.9	15.4	10.5
2	3	5	21.8	19.4	-172.1
2	3	7	10.2	10.8	18.7
2	3	9*	8.8	6.6	-170.5
2	4	0	69.8	77.4	-189.2
2	4	2	94.1	84.1	-1.1
2	4	4	65.4	64.4	-179.2
2	4	6	37.1	36.0	-6.7
2	4	8	20.2	25.0	-181.8
2	5	1	94.3	87.3	11.5
2	5	3	64.7	60.2	-177.8
2	5	5	49.8	48.7	9.1
2	5	7	40.3	38.3	-171.2
2	5	9*	9.6	17.2	2.0
2	6	0	30.8	33.0	-21.1
2	6	2	58.2	56.5	-186.9
2	6	4	38.2	38.7	-2.1
2	6	6	27.7	24.2	-195.6
2	6	8	13.2	18.3	-6.9
2	7	1	19.8	20.9	-204.9
2	7	3	22.3	20.5	-37.4
2	7	5*	6.8	10.8	-209.8
2	7	7*	8.8	12.8	-17.9
2	8	0	12.5	12.5	-16.0
2	8	2*	6.8	.9	-151.0
2	8	4	10.2	7.9	-7.9
2	8	6*	8.8	3.2	-183.7
2	9	1	20.0	23.5	-162.7
2	9	3*	6.9	12.6	16.9
2	9	5	13.7	16.3	-166.6
2	10	0	18.1	20.5	-186.4
2	10	2	19.4	21.4	7.5
2	10	4	18.8	21.2	-173.6
2	11	1	13.7	16.1	-6.4
2	11	3*	8.8	9.7	-209.5
3	1	0	75.1	73.5	-2.3
3	1	2	74.8	63.9	-162.6
3	1	4	45.4	42.5	10.1
3	1	6	37.6	35.0	-176.9
3	1	8	21.3	20.2	7.0
3	2	1	81.0	78.9	-178.6
3	2	3	98.5	84.8	-2.3
3	2	5	57.9	50.4	-184.9
3	2	7	33.1	33.4	8.2
3	2	9	15.9	24.0	-188.2
3	3	0	85.7	99.1	-196.3
3	3	2	95.0	83.1	9.5
3	3	4	56.2	55.7	-181.0
3	3	6	50.7	49.4	-3.7
3	3	8	26.8	28.3	-178.6
3	4	1	42.9	47.7	-15.5
3	4	3	52.6	52.1	-190.6
3	4	5	31.8	30.9	-22.0
3	4	7	21.1	19.9	-179.3
3	4	9	14.3	14.8	-19.5
3	5	0	21.7	17.1	-94.0
3	5	2*	8.7	4.6	-152.5
3	5	4	10.2	8.3	-95.7
3	5	6*	6.6	4.6	-244.5
3	5	8*	8.5	3.0	-72.3
3	6	1	21.4	26.7	4.3
3	6	3	26.2	26.2	-191.5
3	6	5	16.9	18.9	8.9
3	6	7*	8.5	10.5	-179.3
3	7	0	43.3	46.7	10.7
3	7	2	33.1	35.3	-162.7
3	7	4	28.9	29.4	22.7
3	7	6	26.7	24.8	-173.9
3	8	1	31.5	28.0	-176.6
3	8	3	32.7	32.4	-8.4
3	8	5	21.2	20.3	-180.9
3	9	0	22.6	24.7	-213.9
3	9	2	14.6	16.6	-20.5
4	0	0	94.7	94.1	3.1
4	0	2	59.7	59.4	-179.7
4	0	4	59.6	57.7	-8.9
4	0	6	41.0	41.0	-172.6
4	0	8	26.5	24.8	-.6
4	1	1	72.3	69.7	-185.5
4	1	3	66.7	58.6	10.5
4	1	5	51.8	47.0	-184.2
4	1	7	26.7	25.5	-4.3
4	2	0	32.4	32.7	-193.2
4	2	2	19.8	15.3	-18.7
4	2	4	22.7	20.7	-205.0
4	2	6*	6.7	12.8	-5.7
4	2	8*	8.6	8.2	-194.2
4	3	1	24.6	25.4	-164.2
4	3	3	26.5	25.2	17.9
4	3	5	17.6	15.4	-158.7
4	3	7*	8.6	11.1	11.7
4	4	0	43.1	43.4	-167.9
4	4	2	34.9	35.0	-.5
4	4	4	27.3	28.4	-183.7
4	4	6	23.5	23.8	11.7
4	5	1	46.9	48.2	-2.2
4	5	3	42.9	46.1	-167.0
4	5	5	33.3	34.1	.2
4	5	7	18.6	21.2	-184.0
4	6	0	41.8	46.8	-.9
4	6	2	34.9	33.0	-189.4
4	6	4	34.2	30.9	-15.9
4	6	6	22.3	22.6	-178.1
4	7	1	17.8	17.6	-219.7
4	7	3*	6.7	11.7	-20.0
4	8	0*	6.7	9.0	66.7
5	1	0	33.8	36.1	4.0
5	1	2	35.9	36.9	-183.9
5	1	4	36.4	32.6	1.0
5	1	6	15.2	18.1	-178.7
5	1	8	13.7	13.5	1.1
5	2	1	47.4	49.2	-178.4
5	2	3	33.5	29.9	-.1
5	2	5	33.1	32.2	-175.5
5	2	7	21.8	23.0	-2.0
5	3	0	39.9	44.7	-172.2
5	3	2	47.5	45.5	-5.4
5	3	4	46.4	43.1	-178.6
5	3	6	21.8	22.8	-.9
5	3	8	20.0	18.1	-182.1
5	4	1	34.5	32.8	-7.1
5	4	3	24.9	19.9	-196.8
5	4	5	24.9	21.5	-3.7
5	4	7	14.5	15.0	-195.3
5	5	0*	6.5	7.3	-73.6
5	5	2	11.8	12.8	83.7
5	5	4*	6.5	6.8	-73.3
5	6	1	19.3	18.2	26.2
5	6	3	16.9	14.8	-143.0
5	6	5	13.5	11.0	25.7
5	7	0	20.5	20.0	2.4
5	7	2	23.6	26.1	-176.7
5	7	4	22.5	22.3	1.0
5	8	1	18.1	22.1	-186.0
6	0	0	33.8	32.8	-6.3
6	0	2	29.2	34.7	-180.4
6	0	4	31.3	25.7	11.2
6	0	6	27.4	21.6	-189.6
6	1	1	30.7	32.1	-177.5
6	1	3	32.9	32.2	-14.3
6	4	0	26.0	24.8	-173.9
6	4	2	23.8	23.5	19.0
6	4	4	20.5	19.6	-157.6
6	5	1	26.7	27.1	2.0
6	5	3	17.3	26.5	-194.4
6	6	0	24.1	19.1	-19.0
7	1	0	27.4	16.5	9.1

*indicates unobserved reflection. Value given corresponds to one-half minimum observable intensity.

TABLE III

BOND LENGTHS (A) AND ANGLES (DEG)

Compound	Bond or angle	Value	Ref
AgC(CN)$_3$	Ag–N$_1$	2.11 ± 0.06	*a*
AgC(CN)$_3$	Ag–N$_2$	2.26 ± 0.04	*a*
AgC(CN)$_3$	Ag–N$_2$′	2.91 ± 0.04	*a*
AgCN·2AgNO$_3$	Ag–N(av)	2.058 ± 0.008	*b*
AgNCO	Ag–N(av)	2.115 ± 0.008	*b*
AgN$_3$	Ag–N(av)	2.561 ± 0.008	*c*
AgC(CN)$_3$	N$_1$–Ag–N$_2$	123.9 ± 1.3°	*a*
AgC(CN)$_3$	N$_2$–Ag–N$_2$	99.7 ± 2.6°	*a*
AgC(CN)$_3$	C$_3$–C$_1$	1.54 ± 0.09	*a*
AgC(CN)$_3$	C$_3$–C$_2$	1.41 ± 0.07	*a*
	C$_1$–N$_1$	1.10 ± 0.09	*a*
	C$_2$–N$_2$	1.16 ± 0.05	*a*
NH$_4$C(CN)$_3$	C–C	1.40 ± 0.01	*d*
	C–N	1.15 ± 0.01	*d*
KC(CN)$_3$	C–C	1.39 ± 0.02	*e*
	C–N	1.17 ± 0.01	*e*
AgC(CN)$_3$	C$_1$–C$_3$–C$_2$	118.0 ± 3.6°	*a*
AgC(CN)$_3$	C$_2$–C$_3$–C$_2$	123.5 ± 7.2°	*a*
AgC(CN)$_3$	C$_3$–C$_1$–N$_1$	172.7 ± 12.8°	*a*
AgC(CN)$_3$	C$_3$–C$_2$–N$_2$	172.9 ± 7.0°	*a*

[a] This work. [b] Ref 1. [c] H. H. Dewing, Jr., and E. W. Hughes (1962), private communication quoted in ref 1. [d] R. Desiderato and R. L. Sass, *Acta Cryst*, **18**, 1 (1965). [e] Ref 2.

The C(CN)$_3^-$ group appears to be distorted from D$_{3h}$ symmetry with apparently nonequivalent bond lengths and with the central C atom 0.16 A from the plane of the three N atoms, but the standard deviations in the light-atom positions are so large that we cannot say with confidence that the structure of the anion is different from that in NH$_4$-, Na-, or KC(CN)$_3$. Several Fourier and difference Fourier maps were prepared in an attempt to find the light-atom positions, particularly C$_1$ and C$_3$, with more certainty, but without success.

Also, the C(CN)$_3^-$ group was put in with its normal dimensions in the mean position of the observed group. The *r* factor increased to such an extent that if this had been the result of a refinement we would have concluded that the distorted model gave a better fit at between the 99.0 and 99.5% confidence levels. However, this was not the result of a refinement, and we do not have a program that allows the refinement of the C(CN)$_3$ as a group. It is possible that if the group refinement were carried out the confidence level of the significance of the difference would fall considerably.

The Ag–N distances of 2.11 and 2.25 A may just be significantly different from each other. (These would be 2.17 and 2.29 A if the rigid C(CN)$_3$ group were used.) They differ by approximately three standard deviations, and in addition the bond angles of 99° opposite the short bond and 124° opposite the long bond are consistent with a larger amount of s character in the short bond. The deviation of the arrangement from planar is beyond question in this case, the Ag being over 0.5 A from the plane of the three N atoms. The CN groups do not point straight at the Ag: the angles C$_1$–N$_1$–Ag and C$_2$–N$_2$–Ag are 172.2 and 151.3°. The deviations of these bonds from linear as well as the distortion from planar about the Ag atom can be understood in terms of the packing.

The crystal structure is shown in Figure 2. The most interesting feature is that the infinite layers, which were suggested in Figure 1, are presented in distorted form. These layers are puckered and occur in pairs, completely interwoven. The structure as a whole is made up of these double layers stacked in the *b* direction, which is the direction of least growth of the

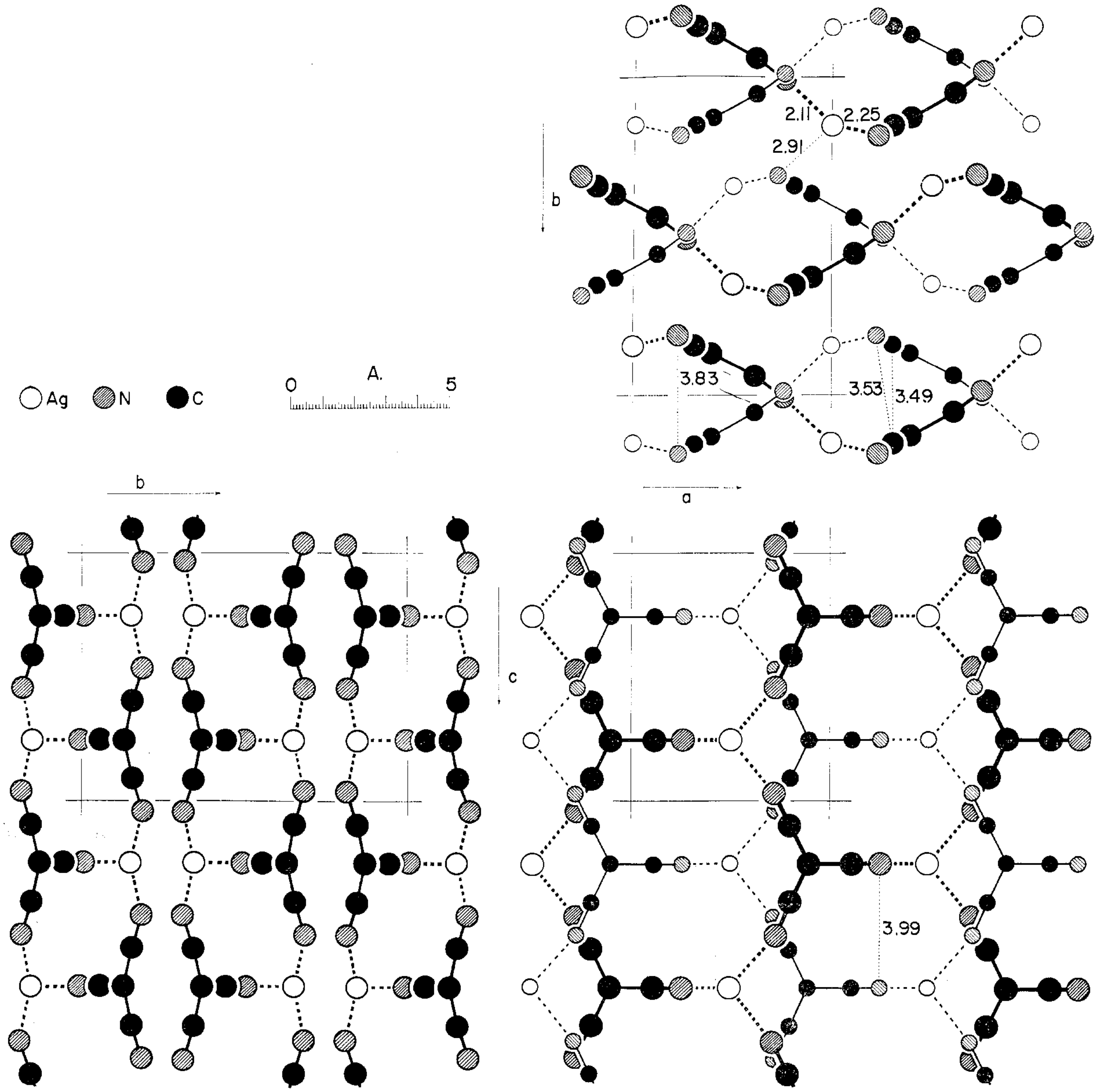

Figure 2.—The structure of $AgC(CN)_3$. The double layers are clearly seen in the upper view. In the lower left view one half of the double layer eclipses the other half. In the lower right view only one double layer (the central one from the view above) is shown. The large and small atoms indicate the two separate halves of interpenetrating layers. The lower right view should be compared with Figure 1.

crystal, not surprisingly. The shortest Ag–light atom distance between layers is a pair of 2.91 A distances to each Ag from opposite N_2 atoms. Other interatomic distances are shown in Figure 2.

The question arises: why does the complex packing occur? The answer must be that the simple planar sheets leave too large a fraction of empty space in the crystal. A conservative estimate of the molar volume for the planar arrangement gives 175 A^3 compared to 125 A^3 in the actual structure. We are left with the pleasant speculation that it might be possible for the planar form to be stable as a clathrate compound with some inert species filling the holes in each of the layers and thereby allowing the undistorted bonding arrangement to occur.

Although threefold coordination is uncommon for Ag, it is more common for Cu(I). The Cu atom in[6] $KCu(CN)_2$ is coordinated to two C atoms at 1.92 A and one N atom at 2.05 A in a nearly planar arrangement. In[7] $KCu_2(CN)_3 \cdot H_2O$ the arrangement is very similar to the one reported here with infinite distorted hexagonal sheets of composition $Cu_2(CN)_3^-$. There are two kinds of Cu, one bonded to two C atoms at 1.89 and 1.90 A and one N atom at 1.98 A, and the other bonded to one C atom at 1.87 A and two N atoms at 1.96 and 2.02 A. The K and H_2O fill in the large holes in the hexagons, so interpenetration of the sheets is not necessary to fill space.

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(6) D. T. Cromer, *J. Phys. Chem.*, **61**, 1388 (1957).

(7) D. T. Cromer and A. C. Larson, *Acta Cryst.*, **15**, 397 (1962).