might be regarded as an incipient second Lewis acidbase interaction, but the geometry at the chlorine atom, where C-Cl···N is approximately 90°, makes it unlikely. Returning to the bromo compound, if we make the same calculation, but with a $CN \cdots Br$ distance of 3.06 Å between the cyanide group and the bromine atom in the para position on the next molecule, and further require that all $Br \cdots Br$ distances be 4.00 Å or greater, with interlayer spacing of 3.45 Å, thus shifting the CN...Br interaction from the ortho to the para bromine atom, we find a molecular volume of 230 Å³, about 3% larger than in the actual structure. Presumably, the actual structure occurs because its greater packing efficiency, and therefore greater van der Waals energy, more than offsets the failure to make the best (linear) $CN \cdots Br$ contact.

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The Crystal Structures of BrC(CN)₃, ClC(CN)₃, and CH₃C(CN)₃

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Bromotricyanomethane, BrC(CN)₃, is orthorhombic, space group *Pbca* (D_{2h}^{15}) , with a=6.09 (1), b=11.49 (2), and c=17.62 (3) Å; there are eight molecules in the unit cell. The structure has been determined from three-dimensional Weissenberg film data and refined by least-squares methods to a conventional *R* of 0.15. The structure contains tetrahedral BrC(CN)₃ molecules with normal bond distances and angles. The packing is dominated by a short intermolecular N···Br distance of 3.03 Å and two short N···C distances of 3.18 and 3.20 Å. Chlorotricyanomethane, ClC(CN)₃, and 1,1,1-tricyano-ethane, CH₃C(CN)₃, are isomorphous, both hexagonal, space group $P6_3/m$ (C_{6h}^2), with identical cell constants a=10.23 (2) and c=9.95 (2) Å; there are six molecules in the unit cell. Both structures were solved from three-dimensional Weissenberg data and were refined by least-squares methods: ClC(CN)₃ to an *R* of 0.155. The structures contain tetrahedral molecules with required mirror symmetry; these molecules also have normal bond distances and angles. Short intermolecular distances were found between a nitrogen atom on one molecule and three cyanide carbon atoms on the next; N···C is approximately 3.10 Å in all cases. These interactions lead to the formation of weakly bound trimers. Orthorhombic and monoclinic modifications of ClC(CN)₃ were also found.

Introduction

As part of a continuing study of weak Lewis acid-base interactions (see the preceding paper for a more extensive introduction) we have determined the crystal structures of bromo-, chloro-, and methyltricyanomethane, $XC(CN)_3$, where X=Br, Cl, or CH₃, to deter-

mine whether any unusual intermolecular interactions are present. These compounds are all unstable and volatile so that low-temperature measurements would be required for accurate structure determinations. However, since our main interest is in the packing, we have used the available equipment to determine the structures at room temperature.

Experimental

Preparation

BrC(CN)₃ was prepared by the procedure of Dr H. D. Hartzler (1963) of E. I. du Pont de Nemours and Co., Central Research Department. A solution of 0.03 mole of bromine in 10 ml of benzene was added dropwise to a suspension of 0.03 mole AgC(CN)₃ in 30 ml benzene, under dry nitrogen at room temperature. After 30 minutes of stirring, the solution was decanted from the silver bromide precipitate and evaporated to dryness under vacuum. The pale yellow powder was sublimed at 50° to give small white needles of the desired product. The melting point, 74°, agrees with that of Hartzler $(72-74\cdot2^\circ)$ and with that reported earlier by Birkenback & Huttner (1929) (74°). Crystals suitable for X-ray diffraction were grown by sublimation under reduced pressure at a few degrees above room temperature; it was necessary to coat the condensation surface with stopcock grease in order to be able to remove the crystals without serious damage. The crystals decomposed slowly on standing; crystals exposed to X-rays turned red in a few days, and decomposed to a powder in less than two weeks. This instability had a severe effect on the quantity and quality of the X-ray data.

A sample of ClC(CN)₃, prepared by Dr S. Trofimenko, was supplied by Dr Hartzler (Trofimenko, Little & Mower, 1962). Crystals suitable for X-ray diffraction studies were grown by sublimation under reduced pressure at slightly above room temperature. The crystals (m.p. 47°) sublimed very readily and the problem was to avoid crystals that were too large. The heat of the hand provided better control than any other heating method found.

 $CH_3C(CN)_3$ was prepared from $AgC(CN)_3$ and CH_3I by the method of Hantzsch & Osswald (1899). The m.p. (95°) and the analysis (C-56.92%, H-3.02%) agreed with the expected values of m.p. 93.5° and C-57·13%, H-2·88%. Suitable crystals were grown by sublimation at reduced pressure.

In all cases, crystals were sealed in glass capillaries before being used for X-ray studies.

Unit cells and space groups

The crystals were examined by precession photography (Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å) and by Weissenberg and oscillation photography (Mo $K\alpha$ radiation and Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å). Crystal data are listed in Table 1. Although individual photographs gave smaller errors, we regard the probable errors to be one part in 600 for the precession photographs and one part in 300 for the Weissenberg and oscillation photographs.

Systematic extinctions (0kl, k=2n+1; h0l, l=2n+1; hk0, h=2n+1) for BrC(CN)₃ indicate the space group to be *Pbca*. Fensch & Wagner (1938) concluded that the space group was *Pbcm*, but their list of observed reflections agrees with ours and with space group *Pbca*.

The first crystal of ClC(CN)₃ examined appeared to be monoclinic; it decomposed during the third photograph taken, and no other monoclinic crystals were ever found. Nevertheless, it would appear from the molecular volume, that this was ClC(CN)₃ and no accidental impurity. Numerous orthorhombic crystals were found, all of which gave poor diffraction photographs and which were probably twinned. Systematic extinctions (0kl, none; h0l, h=2n+1; hk0, not determined; hkl, none) indicate the diffraction symbol to be P-a?. The dimensions and the part of the diffraction symmetry that could be determined, make it clear that this form of ClC(CN)₃ is not isomorphous with the bromo compound. No crystals of this form suitable for intensity photographs were found. A hexagonal third form, which was exactly isomorphous with the methyl compound, was also found. Systematic extinctions (00/, l=2n+1) indicate the space group to be

	Table I. Crystal		CN_3 , $CIC(CN)$	$r_3, unu Ch_3C(0)$	$(1N)_3$	
	BrC(CN) ₃	BrC(CN)	3 ClC(CN)3	ClC(CN) ₃	ClC(CN) ₃	CH ₃ C(CN) ₃
	This work	Fensch & Wagner (19)	t This work 38)	This work	This work	This work
a	6·09 (1) *Å	6·06† Å	6·55 (1) Å	5·57 (2)‡ Å	10·23 (2) Å	10·23 (2) Å
b	11.49 (2)	11.35†	9.45 (2)	9.26 (3)	-	- ``
с	17.62 (3)	17.20	18.3 (1)	11.48 (4)	9.95 (2)	9.95 (2)
		(17.74)†		.,	.,	
System	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic	Hexagonal	Hexagonal
Space group	Pbca	Pbcm†	P-a?	?	$P 6_3/m$	$P6_3/m$
Z	8	8	8	4	6	6
Dobs	_	1.8 g. cm ⁻³	1·46 g.cm ⁻³		-	1.18 g. cm ⁻³
Dcal	1.831 (6)	1.91	1.47	1.46	1.387 (4)	1.161 (4)
		(1.84)				
Volume per molecule	154 Å ³	148 Å ³ (153)	142 Å ³	143 Å ³	150 Å ³	150 Å ³

Table 1. Crystal data for BrC(CN)₃, ClC(CN)₃, and CH₃C(CN)₃

* Errors given are probable errors based on the method used for measurement.

† These are converted from kX units. It seems likely that c = 17.17 kX was a misprint for c = 17.71 kX, since they gave $D_{cal} = 1.82$ g.cm⁻³. See the text for a discussion of the space group.

 \ddagger This is $a/\sin\beta$. β was not determined.

Table 2. Positional and thermal parameters

Form of the anisotropic temperature factor is: $\exp\left[-\frac{1}{4}\left(B_{11}h^2a^{*2}+\ldots+2B_{12}hka^*b^*+\ldots\right)\right]$.

	Position	x	у	Z	B or B_{11}	\mathbf{B}_{22}	B ₃₃	B_{12}	B_{13}	B_{23}
BrC(CN) ₃										
Br	8(c)	0.4485 (6)	0.7291 (4)	0.1768 (2)	8.0 (2)	13.6 (6)	6.4 (2)	-1.0 (2)	-2·2 (1)	1.8 (2)
N(1)	8(c) -	-0.0087 (38)	0.9063 (31)	0.1097 (15)	8.8 (7)					
N(2)	8(c)	0.5715 (35)	1.0412 (27)	0.2027 (13)	6.8 (5)					
N(3)	8(c)	0.5931 (38)	0.8578 (23)	-0·0135 (12)	7·9 (6)					
C(1)	8(c)	0.1780 (33)	0.8910 (22)	0.1142 (11)	4.8 (5)					
C(2)	8(c)	0.5053 (35)	0.9642 (33)	0.1637 (14)	5.2 (5)					
C(3)	8(c)	0.5033 (29)	0.8676 (27)	0.0465 (12)	4.8 (5)					
C(4)	8(c)	0.4003 (26)	0.8719 (21)	0.1195 (9)	3.4 (4)					
ClC(CN) ₃										
Cl	6(h)	0.5146 (4)	0.4492 (5)	1	3.0(1)	4.7 (2)	9.6 (7)	0.4 (1)	-	-
N(1)	6(h)	0.2149(15)	0.0551 (14)	4	5.0 (6)	3.6 (6)	15.3 (22)	2.5 (5)	-	-
N(2)	12(i)	0.2172(14)	0.4201 (15)	0.0228 (24)	7.4 (6)	8.1 (7)	13.6 (23)	3.8 (6)	1.7 (9)	2.4 (9)
$\mathbf{C}(1)$	6(h)	0.2571 (14)	0.1822 (15)	4	2.5 (5)	3.1 (6)	13.2 (24)	1.3 (4)	-	_
C(2)	12(i)	0.2578 (14)	0.3876 (12)	0.1347 (25)	5.4 (5)	3.7 (4)	5.0 (21)	2.0 (4)	<i>−</i> 0·4 (8)	0.6 (7)
C(3)	6(h)	0.3137 (13)	0.3500 (14)	4	3.2 (5)	3.1 (5)	1.5 (21)	1.2 (4)	-	-
CH ₃ C(CN) ₃										
C(H)	6(h)	0.4989 (13)	0.4282 (14)	1	1.2 (5)	2.3 (5)	6.8 (18)	-0.2(4)	-	-
N(1)	6(h)	0.2172 (13)	0.0512 (12)	1	3.6 (5)	2.6 (5)	8.9 (17)	2.2 (4)	-	-
N(2)	12(i)	0.2274 (12)	0.4276 (12)	0.0358 (18)	4.4 (4)	4.9 (5)	8.2 (18)	2.2 (4)	0.1 (6)	-0.1 (6)
C(1)	6(h)	0.2567 (12)	0.1779 (12)	4	1.5 (4)	0.5 (4)	9.9 (19)	0.3 (3)	-	-
C(2)	12(i)	0.2662 (11)	0.3846 (11)	0.1316 (25)	2.6 (4)	2·8 (4)	6.8 (17)	1.3 (3)	0.4 (7)	-0.6 (7)
C(3)	6(<i>h</i>)	0.3222 (13)	0.3453 (11)	4	2.0 (5)	0.9 (4)	3.2 (18)	0 ∙8 (4)	-	-

 $P6_3$ or $P6_3/m$; the latter was shown to be correct by the complete structure determination.

Determination of the structures

BrC(CN)₃

The original data, from which the structure was solved approximately using Patterson and Fourier maps, were visually estimated three-dimensional Weissenberg film data (Mo K α radiation, 0kl-3kl) obtained with a rather large crystal. Layers were correlated with a small number of precession film intensities. Quality of these data was poor and a second set of Weissenberg film data was collected (Cu K α radiation, h0l-h5l) using an acicular crystal, elongated along b and approximately cylindrical with a diameter of 0.1 mm. Oscillation data were also collected for layer correlation. Lorentz and polarization corrections were made, but not absorption corrections ($\mu = 94.3 \text{ cm}^{-1}$ for Cu Ka radiation).* There were 303 independent reflections of measurable intensity and 172 reflections in the same region of reciprocal space with intensities too weak to measure; the latter were included in the refinement, with intensities equal to half the minimum

Table 3. Observed and calculated structure factors for $BrC(CN)_3(\times 1)$

<u>v. t. ro</u>	<u>r 1</u>	<u> 50 55</u>	<u>E 1</u>	F0 70	<u>r_1</u>	<u>50 _ FC</u>	£1.	.7072	K L FC FC
h = 0	2.9	25 24	8 J	78 70	1 1	8 -9	1 3	24 19	2 1 11 -9
0 2 106 -118	2 10	33 -28	1 9	26 20	1 2	64 -64	1 4	31 20	2 2 41 35 2 3 9 10
0 4 138 -124	2 12	2R 23	1 11	81 1	1 4	51 /8	1 6	46 .46	2 4 4 30
0 3 105 -90	2 14	ax -5	1 13	01	1 6	10 -7	1 8	45 40	2 6 14 15
0 10 46 41	2 15	Qe 3	1 14	32 31	1 7	7. 4	1 0	9* 11	2 7 0
0 14 86 -76	2 17	9. 3	1 16	21 -10	1 0	8. 7	1 11	0. 7	2 0 0 4
0 16 25 25	2 18	8+ 8	1 17	11+ 0	1 10	33 37	112	· -14	2 10 23 -22
0 20 17 -17	3 2	135 135	2 0	79 -85	1 12	95	1 14	26 27	2 12 17 15
2 2 78 77	3 3	129 130	2 1	10 -14	1 13	Q = 3 Q = 16	1 15	R = 2	3 1 3 9
2 4 39 20	3 5	45 -42	23	10 14	1 15	0. 1	2 0	A	3 3 10- 10
2 6 151 -115	37	51	2 5	20 21	2 1	14 -17	21	×, -3	3 5 10 5
2 7 101 -92	3 8	33 18	2 6	87 -78	2 2	70 60	2 1	5 5	3 6 27 -23
2 9 24 24	5 10	76 -65	2.8	60 55	3 4		5	17 19	5 8 84 -1
2 10 11* 4	3 12	50 50	2 10	0+ 11 12+ 3	2.6	27 -25	3 4	87 -11	3 9 14
2 12 64 -54	3 13	12 - 2	2 11	· • •	2 7	74 0	2.8	9. 4	41 9 6
2 14 55 51	3 15	8+ 14	2 13	12 -14	2 9	10 17	2 10	0 1	4 2 20 -31
2 15 25 -10	3 16	14 - 18	2 14	31 52	7 10	46 -44	2 11	9. 1	4 4 22 13
217 9 -6	3 19	19 17	3 1	5 2	2 12	40 15	5 6	33 37	4 6 9 4
2 18 84 -7 7 10 84 -0	3 19	13 ⁺ -1 20 -23	3 2	5 - 20	3 1	6* -10 36	3 1	27 . 27	4 7 9 0
20 14 15	4 2	4+ Q	3 4	6 -5	3.3	46 1	3 3	• - •	4 9
4 3 33 32	4 4	43 40	3 6	1/ =1/ 54 55	3 5	21 -1	3 4	8 -10	4 10 12 13
4 4 67 1	4 5	22 20	37	15 14	1.5	7.0		41 44	3.5.6.6
4 6 115 108	4 7	61 -0	3 9	16 -12	3.0	1 1/		17 .10	5 4 4 5
4 8 113 -115	4 9	73	3 10	17 -17	3 10	25 -26	7 10	8 1	5 6 6 13
4 0 7 1	4 10	40 35	3 12	24 20	3 21	11 -14		10 -14	5 7 4 - 2
4 11 23 - 25	4 12	100 -5	14	29 - 24	3 13	12 -10	5 13	10 0	5 8, 4 7 - 6
4 1 3 10 37	4 12	°	4 1	54 58	3 14	8* 10 21 18	4 0	10	h = 0
4 14 26 -22	51	25 24	4 2	69 -77	4 3	29 -27	4 1	20 10	0 0 4 -4
H = 1	5 3	41 -30	4 4	32 -27	4 4	43 49	4 3	6 2	0 4 13 -4
0 2 100 -105	5 5	37 42	2 6	69 65	4 6	2/ -25	4 5	16 -15 20 -17	0 6 0 -4
0 6 16 9	56	21 -16	47	34 31	47	81 -2	4 6	18 17	0 10 15 -15
0 8 15 -15	5 R	41 - 1	4 0	F +1	4 0	12 -13	4 8	o	1 1 0 7
0 17 43 -36	5 10	44 -41 50 49	4 10	22 + 23	4 10	20 15	4 9	0. 1	1 2 9: 11
0 14 4* R	5 11	17 15	4 12	37 31	4 12	21 -17	5 0	36 -33	1 4 0 3
0 18 19 -15	5 13	5 0	4 14	18 -19	4 14	0 1		20 -23	1 5 0+ 4
0 20 34 0	5 14	12 -16	5 0	46 - 61	5 1	14 14	5 3	4 -5	2 0 16 10
1 2 118 -175	5 16	8 10	5 2	24 24	5 5	16 -16	5 5	15 18	2 2 0 -5
1 4 177 178	5 18	12 -12	5 6	13 -19	5 5	*C 34	5 7	10 -25	2 4 8 - 2
1 5 80 -61	1/ = 2		5 5	15 16	5 6		5 8	21 25	2 5 8+ 4
1 7 64 7			5 7	24 - 23	5 8	15 +15	5 10	4: -5	2 7 Pe 5
1 9 7 4	0 2	70 -75	5 8	34 34	5 0	13 -16	1. = 4		2 8 P+ -6
1 10 97 105	04	57 -48	5 10	17 -18	5 11	1. 4			3 1 R+ 7
1 12 38 -38	0.8	90 -84	5 12	9 .0	5 12	44	õ i	· · · ·	
115 8 2	0 12	10 -7	5 13	8 -9 10 0	2 = 4		0 6	20 -13	5 4 5 - A
1 15 69	0 14	47 -47			0.0	40 21	0.10	37 24	3 / 3 11
1 17 9. 4	0 18	12 16	1 = 3		0 2		0.12	10 -1.2	5 0 9 -10
1 19 16 -20	0,20	10 -10	0 2	77 - 22	0.6	23	1 2	··· 6	5 2 4
2 2 51 54	1 1	34 -51	0 6	19 -22	0 10	M	1 4	ê. <u>5</u>	5 4 6 4
2 3 40 -39	1 2	23 23	0 8	38 -36 43 - 40	017	1 21	1 5	00	5 5 3 4
2 5 56 -10	14	44 35	6 12	50 - 60	0.1	15 -12	1 2	o. 4	5 7 3 7
2 7 6	1 6	62 -59	0.16	1 19	1 1	A- 0	1 0	21 15	
 7 N 17 0 Indicates wooh 	2 7 cerved =	16 -15 effection	C 18	25 -21	1 2	53 50	1 10	15 5	

^{*} Most of the calculations were done using programs prepared at Princeton University by Professor R. A. Jacobsen. The final refinements in each case were carried out using programs prepared by Dr L. W. Finger. Group refinements were made using a local modification of an earlier modification by Doedens of the program ORFLS (Busing, Martin & Levy, 1962). All computer calculations were run on CDC 1604 or 6600 computers of the University of Minnesota Computer Center.

observable intensity. Full-matrix least-squares refinement, with all atoms isotropic, converged with r= 0.216; R=0.228.* With the Br atom treated anisctropically, refinement converged at r=0.095; R=0.148. A difference Fourier map at this point showed no peak higher than 1.6 e.Å³. Final positional and thermal parameters are given in Table 2. Structure factors are given in Table 3.

CIC(CN)₃

Weissenberg film data (Cu K α radiation, hk0-hk4) were collected for the hexagonal modification of $ClC(CN)_3$, using an acicular crystal elongated along c, approximately cylindrical of diameter 0.1 mm. Oscillation data were collected for layer correlation. There were 218 independent reflections of measurable intensity and 187 more reflections in the same region of reciprocal space with intensities too weak to measure; the latter were not included in the calculations. Lorentz and polarization corrections were made, but not absorption corrections ($\mu = 39.7 \text{ cm}^{-1}$ for Cu Ka radiation). Atom positions were found from Patterson and Fourier maps.⁺ Full-matrix least-squares refinement, with all atoms isotropic, converged at r=0.140; R=0.198. Refinement converged at r = 0.079; R = 0.109, with the Cl atom anisotropic and the light atoms isotropic. The highest peak on a difference Fourier map calculated at this point was 0.6 e.Å⁻³, compared with $4.0 \text{ e.}\text{Å}^{-3}$, the height of the smallest atomic peak on the corresponding Fourier map. Although, as already mentioned, the quality of the data was not good (e.g. the C(2) and N(2) peaks were not resolved in the best Fourier map, and the amount of data was limited), it was decided to try refinement with all atoms anisotropic. Convergence was reached after three cycles with r = 0.0514, R = 0.088. Hamilton's (1965) test gives $\mathcal{R}_{19,176,0.005} = 1.15$ compared with $(0.0790/0.0514)^{1/2} =$ 1.24, so we report results of the final refinement.[‡] Parameters are given in Table 2. Structure factors are listed in Table 4.

* $R = \sum ||F_o| - |F_c|| / \sum |F_o|$, $r = \sum w(|F_o|^2 - |F_c|^2)^2 / \sum w|F_o|^4$, where the numerator of r is the function refined, $w = (F_w/F_o)^4$ for $F_o > F_w$ and w = 1 for $F_o \le F_w$; in the final refinement cycles, F_w was 18.5 for BrC(CN)₃, 8.6 for ClC(CN)₃, and 6.9 for CH₃C(CN)₃. Scattering factors for all atoms were taken from *International Tables for X-ray Crystallography* (1962). No anomalous dispersion corrections were made.

[†] The calculations for both the $ClC(CN)_3$ and $CH_3C(CN)_3$ were made by expanding the data and parameter lists to correspond to monoclinic symmetry, and all calculations were performed as if the crystal were monoclinic since the program used does not handle hexagonal symmetry.

[‡] To test the possibility that the proper space group is $P6_3$ rather than $P6_3/m$, data were refined with an idealized molecular geometry in $P6_3/m$ (starting as close to the final parameters given in Table 2 as possible) and in $P6_3$ (starting with the molecule rotated $3\cdot3^\circ$ away from coincidence with the mirror plane). After three cycles of refinement, the molecule in $P6_3$ had moved back toward the $P6_3/m$ positions to the extent that no corresponding pair of atom positions differed by as much as one standard deviation; therefore, $P6_3/m$ was accepted as the correct space group.

Table 4. Observed and calculated structure factors for $ClC(CN)_3$ and $CH_3C(CN)_3$ (×10)

н	ĸ	F 7	FC	н	×	FO	۴c	н	×	FO F	c ۲	ĸ	FO	۴c	н	ĸ	FO	۴c	н	ĸ	FO	PC
Ċ,	-1.02	0																				
L	• 0			5	6	67	-63	4	4	221 22	8 3	1	220	-255	1	2	64	-57	L	v 4		
٥	1	121 -	-98	ŝ	3	75	-61	4	6	78 7	6 3	4	126	-118 68	÷	4	139	-148	0	s	244	275
	2	107	89	6	5	67	-83	5	4	53 -4	7 3	- 5	56	-47	1	5	150	-88	0	3	172	-162
õ	د ه	246	216	7	1	241	-72	5	5	61 -7		ŝ	110	-113	1	ŝ	108	61	2	-	39	- 35
ç	2	77	77	Ż	5	188	172		ž	50 S	ż 4	i	127	125	i	10	56	-43	?	è	62	50
÷.	6	51 -	-64	9	1	74 62	-97	6	5	79 -7	94 76	ž	171	-103	2	1	200	214	ĉ	7	140	-127
1	1	659 -6	560					6	ē	80 9	5 4	4	78	75	2	3	492	462	1	ī	127	-147
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. INDICATES UNDESFRUED REFLECTIONS

$CH_3C(CN)_3$

Weissenberg film data (Cu K α radiation, hk0-hk4) were collected using an acicular crystal elongated along c, approximately cylindrical with a diameter of 0.1mm. Oscillation data were collected for layer correlation. There were 191 reflections of measurable intensity and 54 reflections in the same region of reciprocal space with intensities too weak to measure: the latter were included in the eventual refinement with intensities equal to half the minimum observable intensity. Lorentz and polarization corrections were made, but not absorption corrections ($\mu = 6.7 \text{ cm}^{-1}$ for Cu Ka radiation). The compound was assumed to be isostructural with the chloro compound, and initial parameters were chosen on this basis. Full-matrix leastsquares refinement, with all atoms isotropic, converged at r=0.130, R=0.171. With all atoms anisotropic, refinement converged at r = 0.103, R = 0.154. As with the chloro compound, the same objections to anisotropic refinement apply, but again a comparison of $\mathcal{R}_{22,203,0.005} = 1.07$, with $(0.130/0.103)^{1/2} = 1.12$, leads us to report the results of the anisotropic refinement. The final parameters are given in Table 2; the structure factors are listed in Table 4. A final difference Fourier map showed the highest peak to be $0.4 \text{ e.} \text{Å}^{-3}$, compared with 5.4 e.Å⁻³ for the lowest atomic peak in the corresponding Fourier map. No attempt was made to include the hydrogen atoms.

Results and discussion

The interatomic distances in the molecules are given in Table 5. In view of the instability of the crystals and the consequent low quality of the data we believe that the error estimates are optimistic, and that there are no demonstrated deviations from normal geometry and bond lengths in these molecules. Similarly, the anisotropic thermal parameters do not warrant any extensive rationalization.

Table 5. Bond lengths and angles in XC(CN)₃

	$BrC(CN)_3$	ClC(CN) ₃	CH ₃ C(CN) ₃
XC(4)	1·95 (2) Å	1·78 (1) Å	1·57 (2) Å
C(4) - C(1)	1.37 (3)	1.51(2)	1.50 (2)
C(4) - C(2)	1.46 (4)	1.42(2)	1.45 (2)
C(4) - C(3)	1.43 (3)	-	-
C(1) - N(1)	1.15 (3)	1.15 (2)	1.15 (2)
C(2) - N(2)	1.19 (4)	1.29(3)	1.20(2)
C(3) - N(3)	1.20 (3)	-	-
X - C(4) - C(1)	108·6 (16)°	108·9 (10)°	110·8 (13)°
X - C(4) - C(2)	105.6 (16)	110.7 (6)	111.0 (7)
X - C(4) - C(3)	111.7 (17)	-``	-
C(1)-C(4)-C(2)	110.6 (20)	109.3 (10)	107.7 (7)
C(2)-C(4)-C(3)	108.1 (20)	108.0 (21)	108.5 (21)
C(3)-C(4)-C(1)	112.0 (15)		
C(4)-C(1)-N(1)	179.6 (30)	179.7 (16)	174.9 (14)
C(4)-C(2)-N(2)	173.7 (22)	174.0 (20)	175.3 (12)
C(4)-C(3)-N(3)	176.3 (30)	_ `	_ `

Table 6. Intermolecular distances in $ClC(CN)_3$ and $CH_3C(CN)_3$

Distance*		ClC(CN) ₃	CH ₃ C(CN) ₃
а	N(1) - C(1)	3.09 Å	3.09 Å
b	N(1) - C(2)	3.09	3.11
с	N(1) - C(3)	3.27	3.31
d	N(1) - N(1)	3.42	3.48
е	N(1) - N(2)	3.55	3.49
f	N(1)-X	3.39	3.58
g	N(2)-C(1)	3.14	3.29
h	N(2) - N(1)	3.30	3.43
i	N(2) - C(2)	3.45	3.49
j	N(2)-X	3.49	3.48
k	N(2)-X	3.65	3.78
l	XX	4.03	4 ∙07

^{*} See Fig. 2.

The point of interest for which these studies were undertaken, and which we believe is demonstrated in the results, is the packing of the molecules (Figs. 1 and 2). The short intermolecular distances in BrC(CN)₃ are shown in Fig. 1; all $N \cdots Br$ and $Br \cdots Br$ distances less than 4.0 Å, and all $N \cdots N$ and $N \cdots C$ distances less than 3.5 Å, are indicated, as well as a few additional distances. The short intermolecular distances in $ClC(CN)_3$ and $CH_3C(CN)_3$ are given in Table 6 (with reference to Fig. 2) for the same range of values.

We had expected in this study that $N \cdots X$ interactions might be stronger than the usual van der Waals interactions for X=Cl and Br, but not for X=CH₃. The results do, indeed, show such an $N \cdots Br$ interaction, as evidenced by the 3.03 Å distance and the approximately linear $CN \cdots Br$ geometry. This dis-



Fig. 1. The crystal structure of $BrC(CN)_3$. Top, view down c; lower left, view down a; lower right, view into b. The same chain of molecules held together by $N \cdots Br$ interactions is emphasized in all three views. Intermolecular distances (in Å) are given for all short contacts.



Fig. 2. The crystal structures of ClC(CN)₃ and CH₃C(CN)₃. The view is down the c axis. The molecules centered at $z=\frac{1}{4}$ are emphasized. The distances corresponding to the intermolecular contacts indicated by the letters are given in Table 6. tance may be compared with the sum of the usual van der Waals radii, 3.45 Å (Pauling, 1960; see also the discussion in the preceding paper). On the other hand, there is no unusual $N \cdots Cl$ contact in $ClC(CN)_3$, a conclusion that might have been drawn from the isomorphism with $CH_3C(CN)_3$.

Before continuing to the next type of interaction we need to discuss the van der Waals radius of nitrogen. Pauling (1960) suggests 1.5 Å and Kitaigorodskii (1961) suggests 1.57 Å for this radius. However, Donohue (1961), in refining the structure of α -nitrogen, pointed out that the $N \cdots N$ distance of 3.60 Å did not agree with Pauling's value for the radius. Pursuing his argument with more recent data, we find in α -nitrogen (Jordan, Smith, Streib & Lipscomb, 1964) a shortest $N \cdots N$ distance of 3.42 Å, and in the structure of y-nitrogen a shortest N····N distance of 3.275 Å at 20.5°K and 4015 atm (Schuch & Mills, 1970). If we use the expansion of β -nitrogen between 4015 and 0 atm to predict the corresponding expansion of y-nitrogen, then we should correct the 3.275 Å value to 3.44 Å, to agree with the α -nitrogen distance. From these results we conclude that 1.7 Å is a more reasonable value to use for the van der Waals radius for nitrogen, and that the smaller values given previously probably result from the frequent occurrence of weak but specific $N \cdots X$ interactions in crystals. This conclusion leads us to 3.4 Å as the van der Waals distance for a $N \cdots C$ contact with no acid-base character. Similarly, Klug (1965) has suggested that the usual $O \cdots C$ van der Waals distance of 3.10 Å should be replaced by 3.3-3.4 Å, and that a distance of 3.10 Å is abnormally short, *i.e.* it indicates an acid-base interaction.

Looking at our structures with the idea that $N \cdots C$ distances less than $3 \cdot 4$ Å are suggestive of acid-base contacts, we find several situations where there are such short distances. In each molecule there is one of these contacts that is also supported by the rest of the geometry. In the bromo compound, the CN group approximately parallel to the *a* axis points halfway between the two close CN groups in the next molecule, with $N \cdots C$ distances of $3 \cdot 18$ and $3 \cdot 20$ Å. In the chloro and methyl compounds, the mirror-plane CN group points toward the central carbon atom of the next molecule, so that all of the $N \cdots C$ distances to the cyanide carbon atoms are approximately equal at $3 \cdot 10$ Å in both compounds. This leads to weakly bonded cyclic trimers about the *c* axis.

For comparison the following are some of the short $N \cdots C$ distances previously reported : cyanogen,

3·18 and 3·26 Å (Parkes & Hughes, 1963); tetracyanoethylene, 3·09, 3·12, 3·20, and 3·23 Å (Bekoe & Trueblood, 1960); 1,2,3-tricyanopropane, 3·10 Å (Hartman & Hirshfeld, 1966); 1,2,3,4-tetracyanocyclobutane, 3·07, 3·16, 3·18, and 3·19 Å (Greenberg & Post, 1968); tetracyanothiophene, 2·98 and 3·07 Å (Rychnovsky & Britton, 1968); tetracyano-1,4-dithiin, 3·13, 3·15, 3·15, 3·18, and 3·19 Å (Dollase, 1965); tetracyanoquinodimethane, 3·18 and 3·22 Å (Long, Sparks & Trueblood, 1965).

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