

methods. The usual Lorentz and polarization corrections were made,* but no absorption corrections were made (linear absorption coefficient, μ , for $\text{K}(\text{C}(\text{CN})_3)$ is 66 cm^{-1} for $\text{Cu K}\alpha$ radiation).

Approximate locations of all atoms were found from Patterson and Fourier maps. After several cycles of least-squares refinement, using isotropic thermal parameters and including refinement of the layer scaling factors, agreement factors converged to $R=0.100$ and $r=0.040$.†

The F_o and F_c values on an absolute scale are listed in Table 1, final atomic parameters in Table 2, and final interatomic distances and angles in Table 3. The structure is shown in Fig. 1.

Table 2. Final atomic coordinates and temperature factors‡

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> (Å ²)
K	0.1724 (2)	0.2020 (2)	0.2116 (5)	1.77 (2)
N(1)	0.2272 (8)	0.4513 (8)	0.6918 (19)	4.41 (15)
N(2)	0.6038 (7)	0.8521 (7)	0.2730 (18)	3.63 (14)
N(3)	0.0887 (7)	0.8656 (7)	0.2669 (17)	3.26 (13)
C(1)	0.2623 (8)	0.5779 (8)	0.5680 (21)	2.79 (15)
C(2)	0.4683 (8)	0.7968 (8)	0.3375 (21)	2.76 (14)
C(3)	0.1902 (8)	0.8049 (8)	0.3329 (20)	2.38 (14)
C(4)	0.3062 (7)	0.7256 (7)	0.4151 (19)	1.96 (13)

‡ Standard deviations (in parentheses) occur in the last digit.

Table 3. Final interatomic distances and angles

K–N(1)	2.92 (1) Å	N(1)–C(1)–C(4)	178.3 (15)°
	2.85 (1)	N(2)–C(2)–C(4)	178.2 (15)
		N(3)–C(3)–C(4)	177.3 (15)
K–N(2)	2.88 (1)	N(1)–C(4)–N(3)	119.2 (7)
	2.87 (1)	N(1)–C(4)–N(2)	118.6 (7)
		N(2)–C(4)–N(3)	122.1 (10)
K–N(3)	2.88 (1)	C(1)–C(4)–C(3)	120.0 (6)
	2.88 (1)	C(2)–C(4)–C(3)	120.2 (10)
	2.98 (1)	C(1)–C(4)–C(2)	119.8 (10)
N(1)–C(1)	1.16 (1)		
N(2)–C(2)	1.17 (1)		
N(3)–C(3)	1.17 (1)		
C(1)–C(4)	1.37 (1)		
C(2)–C(4)	1.41 (1)		
C(3)–C(4)	1.40 (1)		

The average C–C distance in the tricyanomethide anion is $1.39 (2) \text{ \AA}$, in agreement with the distance of 1.38 \AA we would expect for a $C_{sp}-C_{sp2}$ bond with a bond order of $\frac{4}{3}$ (Bent, 1961). The average C–N distance, $1.17 (1) \text{ \AA}$, is not significantly greater than the usual 1.156 \AA for the C–N distance in nitriles (Britton, 1967). All angles about the central carbon atom are 120° and all the N–C–C angles are 180° within two e.s.d.'s. All this information is in substantial agreement with the results for $\text{NaC}(\text{CN})_3$ and $\text{NH}_4\text{C}(\text{CN})_3$.

Atoms C(1), C(2), C(3), and the central C(4) atom are calculated to be 0.026 , 0.020 , 0.018 , and 0.026 \AA , respect-

* These and most subsequent calculations were made on a Univac 1103 computer with programs developed by Professor W. N. Lipscomb and co-workers at the University of Minnesota. Final refinements were made with programs, supplied by Professor R. Jacobson of Princeton University, for a CDC 1604 computer. Plane calculations were made with a local program (PLANE) on a CDC 6600 computer. All calculations were made at the University of Minnesota Computer Center.

† $[R = \sum(|F_o| - |F_c|) / \sum |F_o|; r = \sum w(|F_o|^2 - |F_c|^2) / \sum w|F_o|^4; w = 1 \text{ for } F_o \leq 4.0, w = (4.0/F_o)^4 \text{ for } F_o > 4.0$. Numerator of r is the function refined.

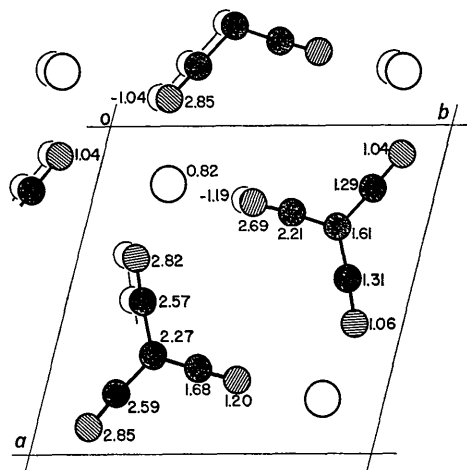


Fig. 1. The structure of $\text{K}(\text{C}(\text{CN})_3)$. View is along the c^* direction. Numbers give the distance in Å from the plane in which $z=0$. Displacement of successive layers can be seen for a few of the atoms near the origin.

ively, above the plane through the N atoms. Thus, the four carbon atoms are coplanar within experimental error; yet there does seem to be a slight, but real difference, between the plane of the carbon atoms and the plane of the nitrogen atoms. The same nearly planar geometry is found in $\text{NaC}(\text{CN})_3$ and $\text{Cu}[\text{C}(\text{CN})_3]$. There is a larger deviation from a planar anion in $\text{NH}_4\text{C}(\text{CN})_3$, and probably also in $\text{AgC}(\text{CN})_3$. Steric arguments have been used to explain the distortions in the latter two cases.

The potassium ion has seven near nitrogen neighbors at 2.86 to 2.98 \AA away. It is at the center of an imaginary tetragonal prism of dimensions $3.39 \times 3.39 \times 3.89 \text{ \AA}$; six N atoms are at the corners of the imaginary prism and the 7th is on the edge between the unoccupied corners. A comparison of the cation environment in $\text{K}(\text{C}(\text{CN})_3)$, $\text{NH}_4\text{C}(\text{CN})_3$, and $\text{NaC}(\text{CN})_3$ is given in Fig. 2 of the article on the $\text{NaC}(\text{CN})_3$ structure (Andersen, Klewe & Thom, 1967). The same illustration (plus an extensive discussion of these compounds) is also given in the review article by Andersen (1967).

We thank the National Science Foundation for their support of this work, and Dr Carol Mahon for her assistance.

References

- ANDERSEN, P. (1967). In *Selected Topics in Structure Chemistry*, p. 125. Ed. P. ANDERSEN *et al.* Oslo: Universitetsforlaget.
- ANDERSEN, P. & KLEWE, B. (1963). *Nature, Lond.* **200**, 464.
- ANDERSEN, P., KLEWE, B. & THOM, E. (1967). *Acta Chem. Scand.* **21**, 1530.
- BENT, H. A. (1961). *Chem. Rev.* **61**, 275.
- BIONDI, C., BONAMICO, M., TORELLI, L. & VACIAGO, A. (1965). *Chem. Commun.* **10**, 191.
- BRITTON, D. (1967). *Perspectives Struct. Chem.* **1**, 109.
- COX, E. & FONTAINE, A. (1954). *Bull. Soc. Chim. Fr.* 948.
- DESIDERATO, R. & SASS, R. L. (1965). *Acta Cryst.* **18**, 1.
- KONNERT, J. & BRITTON, D. (1966). *Inorg. Chem.* **5**, 1193.
- LONG, D. A., CARRINGTON, R. A. & GRAVENOR, R. B. (1962). *Nature, Lond.* **196**, 371.
- MILLER, F. A. & BAER, W. K. (1963). *Spectrochim. Acta*, **19**, 73.