

unpaired valence electrons. It is, however, not known if the substituents have their highest oxidation numbers and if they prefer specific lattice sites.

A discussion of the electron configuration of these phases is not feasible at the present stage. More knowledge of the physical and structural properties seems necessary; in particular are electrical measurements on single-crystals and single-crystal X-ray data required.

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The Crystal Structure of $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NH}_3]\cdot 2\text{H}_2\text{O}$

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The crystal structure of $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NH}_3]\cdot 2\text{H}_2\text{O}$ has been determined by single crystal methods. Crystals of $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NH}_3]\cdot 2\text{H}_2\text{O}$ were prepared from $\text{Na}_3[\text{Fe}(\text{CN})_5\text{NH}_3]$, the original method of preparation described by Brauer¹ being slightly modified. X-Ray data were recorded with a single crystal diffractometer (Philips Pailred) using $\text{MoK}\alpha$ -radiation.

The crystals are orthorhombic with space group $Pnmm$, and cell constants of $a = 6.1 \text{ \AA}$, $b = 11.9 \text{ \AA}$ and $c = 15.5 \text{ \AA}$. There are four formula units per unit cell.

It was obvious by inspection of the raw diffraction data that the structure of $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NH}_3]\cdot 2\text{H}_2\text{O}$ was closely related to that of sodium nitroprusside, $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}]\cdot 2\text{H}_2\text{O}$.² This similarity was exploited in the location of the heavy atoms, while subsequent electron density calculations yielded the light atom parameters. After anisotropic least squares refinement, the R -factor converged to 0.086. The atomic parameters thus obtained are listed in Table I.

Table I. Atomic parameters for $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NH}_3]\cdot 2\text{H}_2\text{O}$. Space group $Pnmm$. The Fe and Na atoms, as well as the NH_3 group and C_1-N_1 , occupy fourfold positions. All other atoms lie in eightfold positions.

Atom	x	y	z
Fe	0.495	0.278	0.500
Na(1)	0.500	0.000	0.247
Na(2)	0.000	0.000	0.378
C(1)	0.251	0.180	0.500
C(2)	0.614	0.183	0.590
C(3)	0.345	0.364	0.412
N(1)	0.100	0.120	0.500
N(2)	0.673	0.125	0.644
N(3)	0.245	0.412	0.361
N(4)	0.768	0.372	0.500
O	0.174	0.125	0.269

The complex ion $[\text{Fe}(\text{CN})_5\text{NH}_3]^{2-}$ lies in the mirror plane and has approximately C_{4v} symmetry if the three hydrogen atoms are not taken into consideration. The Fe—C—N bonds are approximately linear, and the cyanide group *trans* to the ammonia molecule appears to be more firmly bonded than the rest of the ligands. There is no significant hydrogen bonding to the water molecules.

A projection of the unit cell of $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NH}_3] \cdot 2\text{H}_2\text{O}$ along the *a*-axis is shown in Fig. 1 and the most important distances are listed in Table 2.

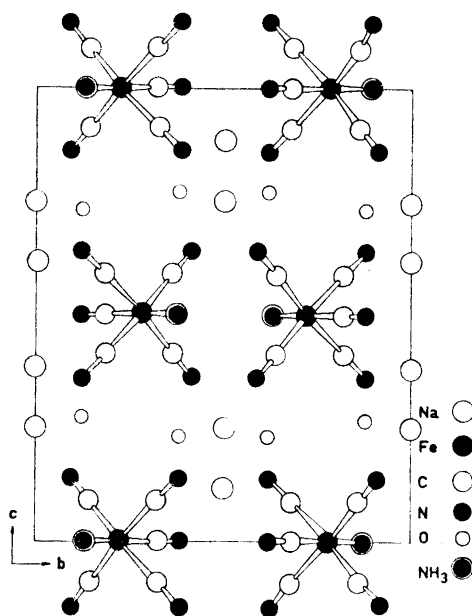


Fig. 1. Projection of the structure of $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NH}_3] \cdot 2\text{H}_2\text{O}$ along the *a*-axis.

Table 2. Interatomic distances and angles within the complex ion $[\text{Fe}(\text{CN})_5\text{NH}_3]^{2-}$.

Bond	<i>d</i> (Å)	Angle	Value(°)
Fe—C ₁	1.89	Fe—C ₁ —N ₁	179.8
C ₁ —N ₁	1.17	Fe—C ₂ —N ₂	176.2
Fe—C ₂	1.94	Fe—C ₃ —N ₃	176.0
C ₂ —N ₂	1.14		
Fe—C ₃	1.94		
C ₃ —N ₃	1.15		
Fe—N ₄	2.00		

A complete report of the investigation will be published in due course.

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2-Arylfurans from 2-Furylcopper and Halogenoarenes

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2-Arylfurans can be prepared by the decarboxylative coupling between 2-furoic acid and iodoarenes in quinoline in the presence of copper(I) oxide, but the yields (so far) are low.¹ 2-Iodofuran itself is rather unstable² and has apparently not been used in Ullmann reactions.³ The use of organocopper compounds often provides a useful method for the formation of carbon-carbon bonds. Recently the preparation of 2-arylthiophenes from 2-thienylcopper and halogenoarenes was described together with a preliminary result for 2-furylcopper.⁴

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