

Coordinates of the C, N, and B atoms are given in Table 1.\* Difference maps in the planes of the methyl hydrogen atoms suggested that these groups are disordered, and they were represented by six half-populated sites with C—H = 0.95 Å; after unsatisfactory attempts to refine the coordinates of the remaining four H atoms, these were placed in idealized positions with C—H = 1.0, B—H = 1.1 Å. Bond lengths for the *P1* structure are given in Table 2. The Cu atom now lies at a center of symmetry and the two HB(3,5-Me<sub>2</sub>pz)<sub>3</sub> ligands are equivalent by symmetry; within each ligand there is no discernible difference between corresponding bond lengths in the three pyrazole rings. However, there are large differences among the three Cu—N bond lengths; the coordination about Cu is best described as 2 + 2 + 2 rather than the more usual 4 + 2 (or 4 + 1). There appears to be little correlation between the Cu—N distance and other bond lengths within the ligand; however, all three pyrazole rings are distorted as a result of the strength of the N—B bond compared to N—Cu (see Fig. 1).

\* Coordinates of the H atoms,  $U_{ij}$ 's of the heavier atoms, and a listing of observed and calculated structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51731 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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**Structure of ErFe(CN)<sub>6</sub>·4H<sub>2</sub>O. Corrigendum.** By RICHARD E. MARSH, *A. A. Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena,\* California 91125, USA*

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#### Abstract

The crystal structure of the title compound has been described as monoclinic, space group  $P2_1/m$ , with  $a = 7.431$  (1),  $b = 13.729$  (2),  $c = 7.435$  (2) Å,  $\beta = 120.02$  (2)°,  $Z = 2$  [Mullica, Perkins, Sappenfield & Leschnitzer (1989). *Acta Cryst.* **C45**, 330–331.] It should be described as orthorhombic, space group *Cmcm*, with  $a = 7.435$ ,  $b = 12.868$ ,  $c = 13.729$  Å,  $Z = 4$ . Revised coordinates are given.

The vectors defining the new cell edges are  $[00\bar{1}]$ ,  $[\bar{2}0\bar{1}]$ , and  $[010]$ ; the corresponding coordinate transformations are  $x' = (x/2) - z$ ,  $y' = -(x/2)$ ,  $z' = y$ . After averaging the transformed coordinates over appropriate pairs of atoms, the *Cmcm* coordinates in Table 1 result. No atom needed to be shifted as much as its reported e.s.d. [Mullica, Perkins, Sappenfield & Leschnitzer (1989) (hereafter MPSL), Table 1] in order to comply with the symmetry of *Cmcm*. Thus, there are no significant changes in the bond lengths or angles (MPSL, Table 2).

\* Contribution No. 7922.

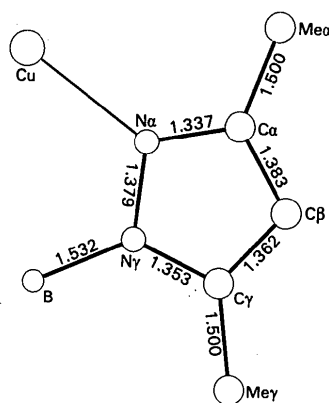


Fig. 1. Average bond lengths within the dimethylpyrazole groups. Except for the Cu—N distances, values for the three rings within each ligand agree approximately within the e.s.d.'s (see Table 2). The e.s.d.'s in the average values are about 0.003–0.004 Å.

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Table 1. Coordinates, space group *Cmcm*

	Site	x	y	z
Er	4(c)	0.50	−0.17647	0.25
Fe	4(a)	0.00	0.00	0.50
C(1,3)	16(h)	0.1844	−0.0466	0.4110
C(2)	8(f)	0.00	−0.1362	0.5596
N(1,3)	16(h)	0.2965	−0.0756	0.3608
N(2)	8(f)	0.00	−0.2160	0.5964
O(1)	8(f)	0.50	0.1553	0.4001
O(2,3)	8(g)	0.265	0.215	0.25

As MPSL note, the compound is isotypic with BiFe(CN)<sub>6</sub>. Interestingly, however, this latter compound was also first reported as monoclinic, space group  $P2_1/m$ , but with a different choice of axes (Mullica, Perkins & Sappenfield, 1988), and also had its space group revised to *Cmcm* (Marsh, 1989).

#### References

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