Acta Cryst. (1980). B36, 2858

The structure of $K_2(K_{0.41}, H_2O_{0.59})_6Na_{3.98}H_3O_{0.78}^+X_{0.68}^+(Fe_{0.05}^{2+}, \square_{0.95})Fe_6^{3+}O_2(SO_4)_{12}$. 11.91 H_2O : erratum. By Fernando Scordari, Istituto di Mineralogia e Petrografia, Piazza Umberto I°, 70121 Bari, Italy

(Received 22 September 1980)

Abstract

A printer's error is corrected. In the paper by Scordari [Acta Cryst. (1980), B36, 1733-1738] the sentence beginning on the nineteenth line of the left-hand column of p. 1735 should read: After several attempts we preferred to fix the

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coordinates of the atoms refined in $P\bar{3}$ and then to proceed to refine in $P\bar{3}$ the occupancy coefficients of all the other atoms deduced from the Fourier map and steric considerations.

All the information is given in the Abstract.

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Acta Cryst. (1980). B36, 2859-2860

Computing in Crystallography

(Editors: R. Diamond, S. Ramaseshan and K. Venkatesan)

This book has recently been published by the Indian Academy of Sciences for the International Union of Crystallography. It contains 29 chapters incorporating the lectures presented at the International Winter School on Crystallographic Computing, which was held at the Indian Institute of Science, Bangalore, India, 4-14 January 1980, and was organized by the Union's Commission on Crystallographic Computing. The titles of the chapters are: Diffractometer control with minicomputers; Absorption corrections for single-crystal X-ray and neutron data; The strategy of extinction corrections; Microdensitometry; Vector-space Patterson search and other stored-function sampling procedures; Automatic interpretation of the Patterson function; Symbolic addition; Multisolution methods; Other multisolution methods; Structure invariants and seminvariants; The method of least squares in crystallography; Error analysis; Incorporation of stereochemical information into crystallographic refinement; Thermal motion analysis; A systems approach to computing for charge density studies; Derivation of molecular properties by charge density integration; Heavy atom positions in macromolecules; The refinement of crystal structures by Fast-Fourier least squares; Phase evaluation and some aspects of the Fourier refinement of macromolecules; A matrix approach to the phase problem; Some problems in macromolecular map interpretation; XTAL: New concepts in program system design; Mini-computers in structure analysis; Microprocessors and microcomputers; Molecular conformation; Computer-generated illustrations; Interactive graphics;