Acta Cryst. (1966). 20, 321

Errata in den International Tables for X-Ray Crystallography, Vol. I (1. Ausgabe). Von ERNST SCHULTZE-RHONHOF, Anorganisch-Chemisches Institut der Universität, 53 Bonn, Meckenheimer Allee 168, Deutschland

(Eingegangen am 20. Juli 1965)

- 1. Zu S. 377, Raumgruppe Pm (Nr. 6): Die Phasenbedingungen müssen heissen: Für c als $\overline{2}$: $\alpha(hkl) = -\alpha(hkl)$ und für b als $\overline{2}$: $\alpha(hkl) = -\alpha(hkl)$.
- 2. Zu S. 426, Raumgruppe $P4_122$ (Nr. 91) und S. 429, Raumgruppe $P4_322$ (Nr. 95): Die Phasenbedingungen für l=4n+1 und l=4n+3 müssen heissen: $\alpha(hkl) = \ldots = \pi - \alpha(hkl)$.
- 3. Zu S.436, Raumgruppe *I*4*cm* (Nr.108):
 - Die Phasenbedingungen für h+k+l=2n, l=2n müssen heissen:

 $\alpha(hkl) = \ldots \qquad \ldots = -\alpha(hkl).$

4. Zu S.488, Raumgruppe P6₃/mcm (Nr.193): Die Beziehung zwischen den Strukturamplituden F(ħkl) und F(ħkl) für l=2n+1 muss heissen: F(ħkl)=-F(ħkl).

Acta Cryst. (1966). 20, 321

Degeneracy between interlayer scale factors and b_{ii} in structure refinement. By E. C. LINGAFELTER, Department of Chemistry, University of Washington, Seattle, Wash. 98105, and JERRY DONOHUE, Department of Chemistry, University

of Southern California, Los Angeles, California 90007.*

(Received 19 May 1965 and in revised form 28 July 1965)

It is apparently not uniformly realized that the usual expression for the anisotropic temperature factor may be factored by removal of terms which vary with h, k, or l alone. It follows that when intensity data are collected by the Weissenberg method with rotation about only one axis, i, so that, in general, data affording interlayer scaling are wanting, then there is complete degeneracy between b_{tt} and the scale factors, and it is accordingly *impossible* to evaluate them individually. If a least-squares refinement is attempted which includes both the b_{tt} and the K_t as variable parameters, meaningless (and sometimes catastrophic) results, or a singular matrix, will be obtained. Data from a zero level Weissenberg photograph may be placed, by statistical methods, on an approximate absolute scale only if the corresponding projection is resolved. This situation does not hold for the upper levels: these cannot be scaled by such methods because of the above mentioned degeneracy.

* This work was supported in part by the U.S. Atomic Energy Commission.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Rekencentrum der Rijksuniversiteit, Grote Appelstraat 11, Groningen, The Netherlands). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.

Summer School in Boboty, Mala Tatra, CSR, 24–29 July 1966

This Summer School is organized by the Commission on Crystallographic Teaching of the International Union of Crystallography, with the sponsorship of the Slovak Academy of Sciences and the Komensky and Slovak Technical Universities (Bratislava). It will be devoted to the *Dynamical Theory of Diffraction by Crystals and its Applications (Study* of Crystal Defects).

The school is intended for teachers of crystallography and advanced students in crystallography and physics. There will be lectures and informal discussions.

The attendance fee will be *ca*. U.S.\$10 per day, which includes full-board accommodation. The nearest airport is

Bratislava. Bus services will be available from Bratislava to Boboty on 23 July.

For information and application please contact Dr F. Hanic, Institute of Inorganic Chemistry of the Slovak Academy of Sciences, Dubravska cesta, Patronka, Bratislava, Czechoslovakia, before 31 March 1966.

Shubnikov groups

The Publishing House of Moscow State University will shortly publish a book on the above subject, written by Professor V. Kopcik and edited by Academician N. V. Belov. It will contain about 700 pages and cost 2.30 roubles. It is expected that copies will be available through the X-ray Analysis Group of The Institute of Physics and The Physical