

with  $n$  so we have taken our predicted values slightly modified to fit exactly the known values for  $n=6, 8$  and  $18$ . The two sets of parameters are given in Table 1.

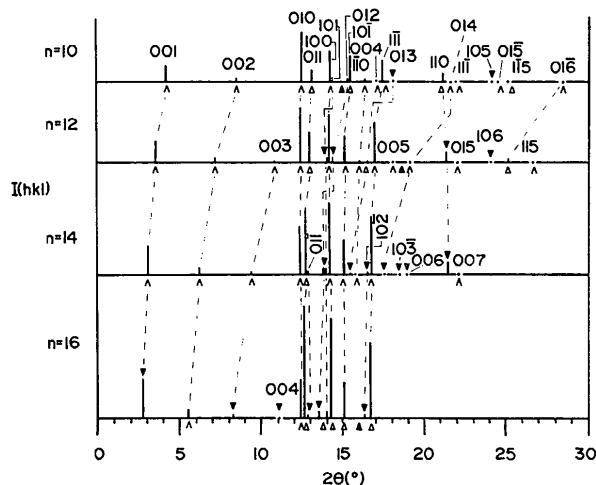


Fig. 1. Indices,  $2\theta$  values and relative intensities predicted and observed by N & M for powder diagrams of the  $n$ -alkanes ( $n=10, 12, 14, 16$ ). See Table 2.

- ▲ Indices and measured  $2\theta$  agreeing with those of N & M.
- ▲ Lines recorded by N & M but not predicted.
- ▼ Lines predicted but not observed by N & M.
- ◻ Observed and predicted positions agreeing but with indices different from those assigned by N & M.

It will be seen from Fig. 1 that the agreement between observed and predicted positions of the powder lines is on the whole very good for all four alkanes; where both the position and N & M's indexing agree with our predictions we have indicated this by  $\Delta$ . The discrepancies are of three kinds and are set out in Table 2. The most serious discrepancies concern the moderately strong reflexions (one each for  $n=12, 14$  and  $16$ ) which were not observed by N & M. We do not know the reason for this. It should be noted from Table 2 that for  $n=16$  there is virtually no agreement in the indexing. This is due to the differences in  $c$  and  $\beta$  parameters (Table 1). We agree with the  $\gamma$  parameter assigned by N & M but are uncertain how this value was obtained by them since no  $hk0$  or  $hkl$  indices were assigned.

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### References

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### 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 Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).*

#### New volume of *International Tables for X-ray Crystallography*

Volume IV, entitled *Revised and Supplementary Tables* and edited by James A. Ibers and the late Walter C. Hamilton, has just been published for the Union by The Kynoch Press, Witton, Birmingham B6 7BA, England, at a price of £10.00. Orders may be placed direct with The Kynoch Press, with Polycrystal Book Service, P.O. Box 11567, Pittsburgh, Pa. 15238, U.S.A., or with any bookseller.

Since the publication of Volume III in 1962, experimental and theoretical activity in all areas of crystallography has greatly increased. The principle motivation for a new volume was to provide revised values for atomic scattering factors, X-ray wavelengths and atomic absorption coefficients.

Volume IV has a cumulative index for all four volumes. When specific information included in Volume IV supersedes material in an earlier volume, the reference to the earlier volume is included in parenthesis. In such cases, the numerical values given in Volume IV should be used, but the earlier volume should also be consulted for the

sometimes extensive textual material accompanying the tables.

A number of special topics, mainly mathematical in content, which were not included in Volume II, have developed considerably and have been incorporated in Volume IV. Such new material, selected by the Editors, includes diffractometer calculations, analysis of thermal motion in crystals, and some aspects of direct methods for phase determination. Although some of this material is more textual than tabular, it has been included because of its great importance to most structural crystallographers. Omission of other topics should not be taken as indicative of their relative unimportance. Selection had to be made by the Editors. The Union is greatly indebted to the Editors and to all the contributing authors for making the publication of this volume possible.

Volumes I, II and III in this series are still available but it has been necessary to increase the price slightly to £8.00 per volume. Prospectuses for all volumes and details of preferential prices for personal subscribers may be obtained from The Kynoch Press or from Polycrystal Book Service.

### A format for a File of Inorganic Crystal Structure Data

The increased rate of publication of crystal structure determinations has led to a number of statistical surveys of structure and bonding, each of which has resulted in its author building up a large file of crystal structure data (usually atomic coordinates and cell constants). FICS-FORM is a format which allows such files and the programs which read them to be exchanged between workers as well as providing a method of file management.

A tentative version of FICS-FORM (FICS-FORM-73) is now available. The definitive version should be ready about the time of The Tenth International Congress of Crystallography but files written in FICS-FORM-73 should be compatible with later versions. Ultimately, it may be possible to edit the various users' programs and files into a single file. In the meantime, the use of FICS-FORM will ensure that these programs and files can be exchanged privately.

Copies of FICS-FORM and further information may be obtained from Dr I. D. Brown, Institute for Materials

Research, McMaster University, Hamilton, Ontario, Canada L8S 4M1. Periodic news letters describing files and programs that are available as well as changes in the definition will be sent to those who ask to be placed on the mailing list.

### Index of French laboratories producing mineral crystals

The Montpellier Documentation Centre has just issued a new index of French industrial and university laboratories which produce mineral crystals. This index supersedes the index prepared in 1967.

This index may be obtained by sending the sum of three francs (postage stamps) or four international reply coupons to Professor Vergnoux, Centre de Documentation sur les Synthèses Cristallines, Université des Sciences et Techniques du Languedoc, Place Eugène Bataillon, F-34060 Montpellier Cedex, France.

### Book Reviews

*Works intended for notice in this column should be sent direct to the Book-Review Editor (M.M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.*

**Molecular structures and dimensions. Vol. A1. Interatomic distances 1960-1965.** Edited by OLGA KENNARD, D. G. WATSON, F. H. ALLEN, N. W. ISAACS, W. D. S. MOTHERWELL, R. C. PETERSON AND W. G. TOWN. Pp. xix + 637. Utrecht: Oosthoek's. Price £24.50 (personal price £17.50)

This volume is of such obvious value to crystallographers and others interested in structural chemistry, and it has been prepared with such thoroughness, that it is difficult at first sight to venture any criticism. Nearly 1300 organic and metal-organic compounds, in 86 different classifications, have been listed, cross-referenced in terms of authors, chemical names and formulae. Where possible, each entry contains the name, formula, structural formula, stereo illustrations, publication references, bond lengths, bond angles and torsional angles. The structural details have been recalculated and compared with published values, and in many cases errors in published values have been cited.

Looking ahead to the publication of future editions of this series, one wonders whether it will be possible to devote as much space to each compound, in view of the increasing publication rate. Structural organic chemists will still require a complete list of bond distances, bond angles and torsion angles, but a reduction of type size would be tolerable, and would effect a substantial saving in space. One hesitates to recommend the elimination of the stereo illustrations with their obvious usefulness, but perhaps they could be dispensed with for simple structures and for those where steric features are obvious or of little importance. With the present style of presentation, one feels a little cheated by the omission of such things as water molecules, heavy ions and intermolecular hydrogen bonds. In many instances, these features represent the main purpose of the

investigation. With the current tendency to present stereo illustrations in original publications, such features would be quickly ascertainable, and could perhaps be included in cases where they were judged to be of sufficient importance. Finally, a cross-index according to space group would be of value to many users, and would add little to the preparation time or volume size.

In conclusion, those responsible for the planning and compilation of the volume are to be commended for its general excellence and clarity. The criticisms and suggestions above are relatively minor, in the category of suggestions requested in the preface. Features deserving of praise are so numerous as to be impossible to list, but one in particular should be mentioned. In the few cases where a check was made, the elimination of redundant publications was found to have been thoroughly carried out. Such a policy will be of even greater importance in future volumes.

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**Crystal structures - a working approach.** By HELEN D. MEGAW. Pp. xviii + 563. Figs. 208, Tables 42. London: Saunders, 1973. Price £8.30

The results of a crystal structure analysis can be summarized in a set of data (space group, lattice parameters, atomic coordinates, etc.) which usually constitute an essential part