

proton anisotropic chemical shift is other than linear over the whole range, from very short almost symmetrical bonds to long hydration bonds.

The X-ray data, with one exception, lie on or systematically below the line correlating the neutron data. In correcting the hydrogen positions for the X-ray shortening effect, we used a standard O–H covalent bond length of 0.97 Å. For the shorter hydrogen bonds in the range 1.5 to 1.7 Å, the O–H covalent bond lengths are longer because of the correlation between O–H and H···O bond lengths. Corrections of 1.02 to 0.98 Å are more appropriate. This would move the six X-ray data in the range 1.58 to 1.72 Å closer to the line by 0.05 to 0.01 Å.

Of the neutron analyses, only three were carried out at liquid-nitrogen temperatures, and only for Ca(OH)₂ and ice were corrections made for the effects of thermal anharmonicity on the motion of the hydrogen atom relative to the oxygen atom to which it is covalently bonded. These corrections are significant, even at very low temperatures, ~15 K, and can affect hydrogen-bond lengths by as much as 0.04 Å (Craven & Swaminathan, 1984; Jeffrey & Ruble, 1984).

It is clear from these data that well coordinated proton NMR and single-crystal neutron diffraction measurements at low temperatures (~10 K) could establish a very precise experimental relationship between the trace σ and the H···O hydrogen-bond length, against which future theoretical calculations could be tested.

The correlations between the chemical-shift anisotropy, $\Delta\sigma$, and the hydrogen-bond lengths, shown in Fig. 2, have much more scatter, although there is a definite trend for the anisotropy to increase with the stronger bonds. We could find no correlation between the anisotropies and the O–H···O angles.

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International Union of Crystallography

Acta Cryst. (1986). **B42**, 413

Structure Reports

Volume 48B of *Structure Reports* has recently been published. It is in two parts (vi+772 and vi+1080 pages) and covers the literature for organic compounds (including organometallic compounds) for 1981. The price of the new volume is 510 Netherlands guilders for subscribers with standing orders. The full price for individual copies is 600 guilders but personal subscribers may buy a copy for their own use at 300 guilders. Orders for this publication may be placed direct with the publishers, D. Reidel Publishing Company, PO Box 17, 3300 AA Dordrecht, The Netherlands, with Polycrystal Book Service, PO Box 27, Western Springs, IL 60558, USA, or with any bookseller.

The last volume published in this series was Volume 46B, for 1980. Volume 47B will be the cumulative index for the years 1971–1980 inclusive.

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International Union of Crystallography announces the Ewald Prize

The International Union of Crystallography announces the establishment of the Ewald Prize for outstanding contributions to the science of crystallography. The name of the prize has been chosen with the kind consent of the late Paul Peter Ewald, to recognize Professor Ewald's significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography, especially his services as the President of the Provisional International Crystallographic Committee from 1946 to 1948, as the first Editor of the Union's publication *Acta Crystallographica* from 1948 to 1959, and as the President of the Union from 1960 to 1963.

The prize consists of a medal, a certificate and a financial award. It will be presented once every three years during

the triennial International Congresses of Crystallography. The first prize will be presented during the XIV Congress at Perth, Australia, in 1987. This year will be the seventy-fifth anniversary of the discovery of X-ray diffraction in 1912.

Any scientist who has made contributions of exceptional distinction to the science of crystallography is eligible for the Ewald Prize, irrespective of nationality, age or experience. No restrictions are placed on the time or the means of publication of his or her contributions. The prize may be shared by several contributors to the same scientific achievement.

Nominations for the Ewald Prize are invited. They should be submitted in writing, accompanied by supporting documentation, to the Executive Secretary of the International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, United Kingdom. The closing date for nominations is 30 September 1986.

TH. HAHN
President

K. V. J. KURKI-SUONIO
General Secretary

Acta Cryst. (1986). B42, 414

Commission on Journals Atomic Labelling

The Commission on Journals recently voted to simplify the form of atomic labelling. Atoms of the same chemical species within an asymmetric unit should be distinguished in future by an appended arabic numeral, with parentheses around the numeral required only in the event of ambiguity, such as C11 *versus* C1(1) or C(11).

Acta Cryst. (1986). B42, 414

Appointments in the IUCr Office

A notice concerning recent appointments in the IUCr office appeared in the July 1986 issue of *Acta Crystallographica*, section A, p. 288.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1986). B42, 414-415

International tables for crystallography: Brief teaching edition of Volume A: Space group symmetry. Edited by T. HAHN. Pp. viii + 119. Dordrecht: Reidel, 1985. Price Dfl27.50, \$8.50, £7.60.

This is a slim volume consisting of 24 selected space-group descriptions and several pages of the basic text sections from Volume A of *International tables for crystallography*. The declared purpose of the *Teaching edition* is:

(i) to provide a handy and inexpensive tool for researchers and students to become familiar with the use of the space-group tables in Volume A;

(ii) to be used in classroom teaching;

(iii) to serve as a laboratory handbook, because the 24 examples include most of the frequently occurring space groups, for both organic and inorganic crystals.

The basic text section consists of material found in chapters 1, 2, 3 and 5 of Volume A: namely *Symbols and terms used*, *Guide to the use of the space-group tables*, *Space-group determination and diffraction symbols*, and *Transformations in crystallography*.

I approve strongly of the idea of bringing out an introductory book on the excellent, but detailed, Volume A, as there is a serious need for material which can be read and understood by beginners and non-specialists. I was therefore delighted to hear that the International Union of Crystallography had, at last, brought out such a text. However, I am sorry to say that, when I opened my review copy, I felt

somewhat surprised and, even, disappointed. The title had suggested a digestible and specially written account, which could be recommended to someone meeting, for the first time, the beauty and mysteries of crystallographic symmetry. Instead of the elementary treatment I had anticipated, it seems that the basic text has been lifted entirely without change from Volume A.

As a result, I certainly could not expect a novice to take the text away and learn from it by him/herself. Indeed, because no attempt has been made to adapt the text to suit its declared aims, on almost every page peculiar inconsistencies can be found which ensure that it cannot stand alone as a teaching text. It is particularly irritating to encounter so many references to sections that are missing entirely. As typical examples, in the *Guide to the use of the space-group tables*, page 10, the reader is referred to sections 8.3.1 and 9.1 for further details on lattice centring and to section 9.3 for reduced bases. On page 30 the index of a maximal subgroup requires the footnote in section 8.1.5 to be consulted. Again, picking a page at random, I find on page 39 reference to a missing Table 4.3.1, and so on. This occurs so frequently throughout that one might as well use Volume A in the first place.

The main problem with the *Teaching edition* is that it falls between two stools. On the one hand, it is too difficult to act simply as a text for learning about the space-group tables and, on the other, it is not complete enough for the experienced researcher to use as a handbook. In any case, those who already know about space groups and the *International tables* are unlikely to want to consult the introduc-