

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 $\bar{\sigma}$ 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.

This research is supported by the National Science Foundation, Grant No. CHE-8316882.

References

- BERGLUND, B. & VAUGHAN, R. W. (1980). *J. Chem. Phys.* **73**, 2037–2043.
- CRAVEN, B. M. & SWAMINATHAN, S. (1984). *Trans. Am. Crystallogr. Assoc.* **20**, 133–135.
- DITCHFIELD, R. (1976). *J. Chem. Phys.* **65**, 3123–3129.
- FALK, M. & GIGUERE, P. A. (1958). *Can. J. Chem.* **36**, 1680–1685.
- FYFE, C. A. (1983). *Solid State NMR for Chemists*. Guelph, Canada: GEC Press.
- JEFFREY, G. A. & RUBLE, J. R. (1984). *Trans. Am. Crystallogr. Assoc.* **20**, 129–132.
- JEFFREY, G. A., WOOD, R. A., PFEFFER, P. E. & HICKS, K. B. (1983). *J. Am. Chem. Soc.* **106**, 2128–2133.
- KENNEDY, N. S. J., NELMES, R. J., THORNLEY, F. R. & ROUSE, K. D. (1976). *Ferroelectrics*, **14**, 591–593.
- MEHRING, M. (1983). *Principles of High Resolution NMR in Solids*. Berlin: Springer-Verlag.
- ROHLFING, C. M., ALLEN, L. C. & DITCHFIELD, R. (1983). *J. Chem. Phys.* **79**, 4958–4966.
- TAYLOR, M. G., MARCHESSAULT, R. H., PEREZ, S., STEPHENSON, P. J. & FYFE, C. A. (1985). *Can. J. Chem.* **63**, 270–273.
- TAYLOR, R. & KENNARD, O. (1983). *Acta Cryst.* **B39**, 133–138.

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.

Acta Cryst. (1986). **B42**, 413–414

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