Vidal-Valat, Vidal, Zeyen & Kurki-Suonio (1979) have reported values of the thermal-vibration parameters of the atoms in the magnesium difluoride crystal as determined by a neutron-diffraction study at 300 K and 52 K. They conclude from the observed strong anisotropy of the vibration of the F atom at 300 K that there is strong excitation of a libration-like mode of a nearly rigid, linear MgF_2 molecule in the xy plane of the tetragonal crystal. Another way of discussing the observations may, however, have greater significance.

Magnesium difluoride has the rutile structure, with $a = 4{\cdot}628$, $c = 3{\cdot}045$ Å, and the oxygen parameter $x = 0{\cdot}3032$. With these values the linear F–Mg–F group has bond lengths of 1·984 Å, as stated by Vidal-Valat *et al.* (1979). The value of x, however, is close to $[(c/a)^2 + 2]/8 = 0{\cdot}3041$, which places six atoms at the same distance from the Mg atom (Pauling, 1928); in fact, with $x = 0{\cdot}3032$ there are four F atoms with Mg–F bond lengths of 1·994 Å, only 0·5% greater than for the other two.

It is accordingly not justified to describe the crystal as containing linear F–Mg–F molecules. Instead, it has a framework structure, with each Mg atom forming six bonds with F atoms at the corners of a somewhat distorted octahedron (two opposite edges, shared between octahedra, shortened to 2·576 Å) and each F atom forming three bonds in a vertical plane, with bond angles 99·5, 130·2, 130·2°. All vibrations of atoms relative to their neighbors would thus involve a change in length of strong bonds except the vibration of the F atom perpendicular to the plane of its three bonds. The values of the mean-square principal amplitudes of vibration given by Vidal-Valat *et al.* (1979) (averages of seven values corresponding to different assumptions about extinction) are the following, in order U_{33} (along the c axis), U_{11}, and $U_{\perp}$, all in units 10^{-4} Å; at 52 K, 13, 19, 14 for Mg and 23, 31, 40 for F; and at 300 K, 31, 42, 52 for Mg and 56, 49, 115 for F. As pointed out by Vidal-Valat *et al.* (1979), the strikingly large amplitude is that of the F atom at 300 K; also it is in the direction that does not involve first-order stretching and compression of Mg–F bonds.

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Change of publisher of *Structure Reports, Molecular Structures and Dimensions* and other publications

As from 1 January 1980, D. Reidel Publishing Company, PO Box 17, 3300 AA Dordrecht, The Netherlands, has taken over the publication and sales of all the publications of the International Union of Crystallography previously handled by Bohn, Scheltema and Holkema. These publications include *Structure Reports, Molecular Structures and Dimensions, Symmetry Aspects of M.C. Escher's Periodic Drawings, Fifty Years of X-ray Diffraction, Early Papers on Diffraction of X-rays by Crystals*, and miscellaneous other publications of the Union such as the bibliographies and the *Index of Crystallographic Supplies*. Orders for all these publications may be placed direct with the publishers or with Polycrystal Book Service, PO Box 11567, Pittsburgh, PA 15238, USA, or with any bookseller.

Notes and News

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Proceedings of the International Symposium on Biomolecular Structure, Conformation, Function & Evolution held at Madras in January 1978

These proceedings, covering over a hundred articles presented at the above Symposium, are being published by Pergamon Press in two volumes edited by Professor R. Srinivasan and others. The volumes are expected to be available in early 1980. Vol. I might be of interest to crystallographers as it deals with 'Diffraction and Related Studies' on biomolecules.