

Table 2. Water molecule environment in  $\text{KBO}_2 \cdot \frac{4}{3}\text{H}_2\text{O}$  (Zviedre, Ozols & Ievins, 1974)

Bond distances (Å)				
Atom role		$\text{H}_2\text{O}(9)$	$\text{H}_2\text{O}(10)$	
Proton acceptors	O(8)'	2.71	O(8)'	2.58
	OH(5)'	2.85	OH(3)'	2.77
C1	K(3)'	2.97	K(2)'	2.91
C4	K(3)''	2.88	K(2)''	3.09
C2	OH(5)''	2.83	OH(3)''	2.72
C3	K(1)'	2.77	K(1)'	2.90
Bond angles (°)				
$\text{H}_2\text{O}(9)$				
O(8)', OH(5)'	107	K(3)', K(3)''	87	
O(8)', K(3)'	96	OH(5)'', K(1)'	164	
OH(5)', K(3)'	157	K(3)', OH(5)''	69	
O(8)', K(3)''	159	K(3)', K(1)'	95	
OH(5)', K(3)''	70	K(3)'', OH(5)''	87	
O(8)', OH(5)''	113	K(3)'', K(1)'	87	
OH(5)', OH(5)''	105	Planes		
O(8)', K(1)'	72	$\pi$ -C1, C4	21	
OH(5)', K(1)'	87	$\pi$ -C2, C3	76	
		C1, C4-C2, C3	94	
$\text{H}_2\text{O}(10)$				
O(8)', OH(3)'	115	K(2)', K(2)''	85	
O(8)', K(2)'	94	OH(3)'', K(1)'	158	
OH(3)', K(2)'	150	K(2)', OH(3)''	68	
O(8)', K(2)''	161	K(2)', K(1)'	91	
OH(3)', K(2)''	64	K(2)'', OH(3)''	84	
O(8)', OH(3)''	113	K(2)'', K(1)'	89	
OH(3)', OH(3)''	107	Planes		
O(8)', K(1)'	72	$\pi$ -C1, C4	21	
OH(3)', K(1)'	89	$\pi$ -C2, C3	76	
		C1, C4-C2, C3	89	

Bond distances and angles were recalculated (BONDLA, Stewart, Kruger, Ammon, Dickinson & Hall, 1972) from the coordinates given by Zviedre *et al.*; the values are not always the same as those reported by them [e.g. they give O(8)'-O(10) as 2.64 Å]. Our assignment of proton acceptors and C atoms is considered the most probable; notation follows that of Ferraris & Franchini-Angela (1972). The  $\pi$  plane was defined as that of the water oxygen atom and its two proton acceptors. For usage of primes, see Fig. 1.

hydroxyl ion. Further experimental data are needed to determine the precise character of this group of oxygen atoms.

Two other borate structures have been reported with another kind of unusual hydrogen bond. In both cases the proton appears to be located between two ring oxygen atoms of tetrahedra in adjacent borate rings, and the O...O distance is about 2.4 Å. Such oxygen atoms are charge-deficient by approximately 0.5 v.u., so their bonding to a proton is reasonable. For the structure of kaliborite,  $\text{HKMg}_2[\text{B}_5\text{O}_7(\text{OH})_3 \cdot \text{OB}(\text{OH})_2]_2 \cdot 4\text{H}_2\text{O}$  (Corazza & Sabelli, 1966; formula from Christ & Clark, 1977), most hydrogen atoms were located from a three-dimensional difference synthesis. However, the hydrogen H(10) associated with the 2.412 Å bond (and lying on a twofold axis) could not be found in this way. Possibly H(10) is a resonating proton and hence the residual electron density is smeared out. The structure of preobrazhenskite,  $\text{HMg}_3\{\text{B}_9\text{O}_{12}(\text{OH})_4 \cdot [\text{O}_2\text{B}(\text{OH})_2]_2\}$  (Rumanova, Razmanova & Belov, 1972; formula from Christ & Clark, 1977), has a similar bond. No hydrogen atoms were located in that study. Again, experimental determinations of hydrogen positions in both these structures would provide further useful information about this kind of hydrogen bond.

#### References

- CHRIST, C. L. & CLARK, J. R. (1977). *Phys. Chem. Miner.* **1**. In the press.
- CORAZZA, E. & SABELLI, C. (1966). *Accad. Nazl. Lincei, Rend. Cl. Sci. Fis. Mat. Nat.* **41**, 527-552.
- FERRARIS, G. & FRANCHINI-ANGELA, M. (1972). *Acta Cryst.* **B28**, 3572-3583.
- RUMANOVA, I. M., RAZMANOVA, Z. P. & BELOV, N. V. (1972). *Sov. Phys. Dokl.* **16**, 518-521.
- STEWART, J. M., KRUGER, G. J., AMMON, H. L., DICKINSON, C. & HALL, S. R. (1972). Tech. Rep. TR-192. Univ. of Maryland, USA.
- ZVIEDRE, I., OZOLS, J. & IEVINS, A. (1974). *Latv. PSR Zinat. Akad. Vestis, Kim. Ser.* pp. 387-394 (in Russian).

## Book Review

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.

**Atlas of steroid structure.** Vol. 1. Edited by W. L. DUAX and DORITA A. NORTON. Pp. xiii + 572. New York, Washington and London: IFI/Plenum, 1975. Price \$59.40, £31.19.

This book, modestly termed an 'Atlas', is a superbly organized reference work on the detailed structures of those

steroids that have been studied by X-ray crystallography. Written by crystallographers, it is intended primarily for a non-crystallographic readership: workers in organic chemistry, biochemistry, biology and medicine.

Dr Duax points out in his preface that the average crystallographic paper presents results in terms of atomic coordinates, from which many other molecular parameters

can be calculated. However, the average biologist – or even organic chemist – does not know how to do this, and therefore tends to disregard work which carries concealed information of vital importance to his own studies, or else misinterprets it. The *Atlas* overcomes all these difficulties by presenting the available data on the shapes of about 100 steroids in half-a-dozen different fashions.

A general introduction of about 50 pages explains the ways in which the data are presented, and an outline of the conformational patterns found. The data for 103 steroids (30 oestrans, 39 androstanes and 34 pregnanes) are then presented in great detail, four pages being allotted to each compound. The items given for each compound include the following: two large perspective drawings; full tables of atomic coordinates (except for hydrogen), interatomic distances, interatomic angles and torsional angles; a projection formula in the general plane of the nucleus; detailed discussion of the conformation in words and figures, and often with additional diagrams of special features; molecular packing with several projections.

Appendices give summaries of formulae, projections, systematic names and references.

All non-crystallographers are, we hope, aware that the conformation of a given molecule in solution is not necessarily the same as that in the crystal. However, the 'conformation-in-the-crystal' is often a guide to what happens in solution, and may generally be used as a starting-point for discussion, unless evidence from other physical methods indicates a different conformation.

This book is a model for those who seek to put the results of one specialized technique at the disposal of other scientists. The reviewer hopes that it will be copied in other fields of organic chemistry, and that Dr Duax and his colleagues will produce further volumes on other sub-classes of steroids (*e.g.* sterols, bile acids, cardiac glycosides). This first volume must serve as a living memorial to Dr Dorita Norton who worked on it for some years before her untimely death in 1972.

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### Book Received

*The following book has been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.*

**New applications of organometallic reagents in organic synthesis.** Edited by D. SEYFERTH. Pp. v + 488. Amsterdam: Elsevier, 1976. Price \$44.75, Dfl. 116.00. **Organosilicon reviews.** Edited by D. SEYFERTH, A. G. DAVIES, E. O. FISCHER, J. F. NORMANT and O. A. REUTOV. Pp. viii + 404. Amsterdam: Elsevier, 1976. Price \$39.75, Dfl. 103.00. **Organometallic chemistry reviews.** Edited by D. SEYFERTH, A. G. DAVIES, E. O.

FISCHER, J. F. NORMANT and O. A. REUTOV. Pp. viii + 342. Amsterdam: Elsevier, 1977. Price \$39.75, Dfl. 103.00.

These three are respectively Vols 1, 2 and 3 of the *Journal of Organometallic Chemistry Library*. Vol. 1 consists of the proceedings of a symposium held in New York, USA, in April 1975.