In (1) the proposed hydrogen-bonding scheme consists of closed loops, with the donor–acceptor sequence:

$$\begin{array}{ccccc} O(6)H & \rightarrow & O(1)H & \rightarrow & O(3) \\ & \nwarrow & & & H \\ & & & & \downarrow \\ & & HO(2) & \leftarrow & HO(4) \end{array} .$$

The hydrogen bond H···O distances range from 1·70 to 2·13 Å, the longest being that from the anomeric hydroxyl O(1)H to O(3), and the shortest from O(6)H to the anomeric O(1). The O–H···O angles are exceptionally linear, ranging from 179·6 to 179·9° (a rather unlikely circumstance because of the well-known geometrical factor).

In (2) the position of one hydrogen, H(O4), was poorly defined and placed in an unlikely position which was only 1·797 Å from H(O3). A more reasonable position is that deduced from the structure (1) which places it close to the line between O(4) and O(2) at a hydrogen-bonding distance of 1·89 Å from O(2). The hydrogen-bond scheme for structure (2) consists of infinite chains with two-link side chains, *i.e.*

$$\begin{array}{ccccccccccc} \rightarrow & O(4)H & \rightarrow & O(2)H & \rightarrow & O(3)H & \rightarrow & O(4)H & \rightarrow & O(2)H & \rightarrow \\ & & & \uparrow & & & & & & & \\ & & & HO(6) & \leftarrow & HO(1) & & & & & \end{array} .$$

The H···O bond distances then span a narrower range, from 1·89 to 2·02 Å, and the O–H···O angles have values from 114 to 180°. The anomeric O(1)H···O(6) remains the longest hydrogen bond, making an unusually small O–H···O angle. The anomeric O is not a hydrogen-bond acceptor.

Our interest in this problem arises from the prediction by Tse & Newton (1977) and the observations by Jeffrey, Gress & Takagi (1977) and Jeffrey & Lewis (1977) that anomeric hydroxyls in simple pyranoses are generally strong hydrogen-bond donors, but very weak acceptors. The hydrogen-bonding proposed in (1) provided one of the few strong exceptions to this hypothesis, whereas that in (2) is in better agreement, especially if the true position for H(O1) is closer to the line between O(1) and O(6), thereby shortening the H···O bond distance. For this reason, we favor the hydrogen-bonding scheme (2). Final resolution of this question must come from a neutron diffraction study, which must await the growth of suitable crystals, an experiment which hitherto has been unsuccessful.

This research was supported in part by NIH Research Grant GM-21794.

References

ABRAHAMS, S. C. & KEVE, E. T. (1971). *Acta Cryst.* A**27**, 157–165.

JEFFREY, G. A., GRESS, M. E. & TAKAGI, S. (1977). *J. Amer. Chem. Soc.* **99**, 609–611.

JEFFREY, G. A. & LEWIS, L. (1977). *Carbohydr. Res.* In the press.

NYBURG, S. C. (1974). *Acta Cryst.* B**30**, 251–252.

OHANESSIAN, J. & GILLIER-PANDRAUD, H. (1976). *Acta Cryst.* B**32**, 2810–2812.

SHELDRICK, B. (1976). *Acta Cryst.* B**32**, 1016–1020.

TSE, Y.-C. & NEWTON, M. D. (1977). *J. Amer. Chem. Soc.* **99**, 611–613.

International Union of Crystallography

Structure Reports

Volumes 40B and 41A of *Structure Reports* have recently been published. Volume 40B, covering the literature for organic compounds for 1974, is bound in two parts (viii + 582 pages and ii + 645 pages) and costs 320 Netherlands guilders. Volume 41A, covering the literature for metals and inorganic compounds for 1975, (viii + 477 pages) costs 150 Netherlands guilders. A 47-page supplement for 1974–1975 to Section A (Metals and Inorganic Compounds) of the 60-*Year Structure Index* is being sold with Volume 41A, and is included in the price for that volume. Additional copies of the supplement are available at a price of 10 Netherlands guilders.

Orders for these publications may be placed direct with the publisher, Bohn, Scheltema & Holkema, Emmalaan 27, Utrecht, The Netherlands, with Polycrystal Book Service, PO Box 11567, Pittsburgh, Pennsylvania 15238, USA, or with any bookseller.

World Directory of Crystallographers

Fifth Edition

The Fifth Edition of this most useful Directory has just been published on behalf of the International Union of Crystallography by Polycrystal Book Service, PO Box 11567, Pittsburgh, Pennsylvania 15238, USA, from whom copies may be ordered direct at a price of US $10.00 post free. It contains short biographical data on 7641 scientists from 71 countries, arranged in alphabetical order by countries, and by individuals within the countries. The biographical data include full name and title, address, year of birth, highest degree, field of study, university and year of highest degree, present position, telephone number and major scientific interests. There is also a comprehensive name index.

The General Editor of the Directory is Dr S. C. Abrahams and the Associate Editor is Dr A. L. Bednowitz. Crystallog-