

the final cycles of refinement the positional and anisotropic thermal parameters were included for all atoms except H. The contributions of these atoms were included in the structure-factor calculations, keeping the atoms fixed in their calculated positions and with their isotropic temperature factors equal to those of the atoms to which they are covalently bonded. These factors were obtained from the earlier cycles of refinement. The final values of the coordinates of the non-hydrogen atoms are given in Table 1.*

* Lists of anisotropic thermal parameters, hydrogen atom parameters and structure factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33230 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Bond lengths and angles are given in Tables 2 and 3. An important feature of the structure is the closest approach of the O atom of one molecule to the N atom of the neighbouring molecule. This distance was found to be 2.858 Å, which reveals hydrogen bonding between these atoms. All other contacts are consistent with the sum of the van der Waals radii. The numbering scheme is shown in Fig. 1 and a stereoview of the structure is given in Fig. 2.

References

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A neutron diffraction study of the crystal structure of β -D-fructopyranose: errata. By SHOZO TAKAGI and G. A. JEFFREY, *Chemistry Department, Brookhaven National Laboratory, Upton, New York 11973, USA and The Crystallography Department, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA*

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The atomic coordinates in the paper by Takagi & Jeffrey [*Acta Cryst.* (1977), **B33**, 3510–3515] refer to the L enantiomer. To obtain the data for the D enantiomer, a – sign should be added to the z coordinates. Fig. 1 in the paper is the stereoview of the L enantiomer. That of the D enantiomer is now given. The signs of the torsion angles in Fig. 2 should be changed. The ring conformation is ${}^2C_5-D$ and the Cremer & Pople [*J. Am. Chem. Soc.* (1975), **97**, 1354–1358] parameters are $q_3 = -0.555$ Å, $\varphi_2 = 47.9^\circ$, $\theta = 177.3^\circ$. In Table 3, the signs of T_{13} and T_{23} should be interchanged; the signs of ω_{13} and ω_{23} should be –. Corrected values for the directions relative to the axes are given.

A stereoview of the molecule of β -D-fructopyranose is given in Fig. 1.

In Table 3 of Takagi & Jeffrey (1977) the directions relative to the axes should be as follows:

	<i>a</i>	<i>b</i>	<i>c</i>
T	135.7°	77.8°	131.8°
	45.9	82.6	134.9
	93.6	165.7	103.9
ω	83.2	113.7	24.8
	26.8	110.9	106.0
	64.2	32.5	71.6

References

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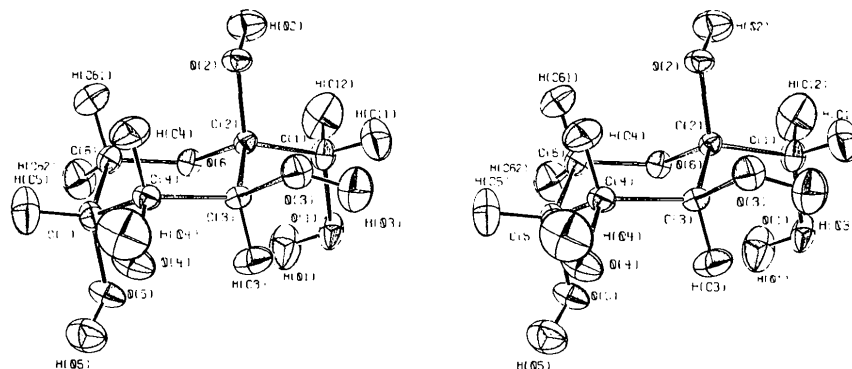


Fig. 1. Stereoview of the molecule of β -D-fructopyranose. Thermal ellipsoids are at 50% probability (Johnson, 1976).