each niobium atom (Dahl & Wampler, 1959). M.O. symmetry arguments based on a model of idealized D_{2h} symmetry for the localized structural unit, $(NbI_4)_2$, (not given here to conserve space) are consistent with our proposal of weak metal–metal interaction involving the direct overlap of pairs of d_{xy} niobium orbitals.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

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A preliminary investigation of the crystal and molecular structure of α-D-glucose monohydrate.

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α-D-Glucose (1α-D-glucopyranose) is easily crystallized as a monohydrate. The needle crystals are monoclinic and the cell dimensions obtained from Weissenberg photographs are

$$a = 8{\cdot}84 \pm 0{\cdot}03,\ b = 5{\cdot}10 \pm 0{\cdot}02,\ c = 9{\cdot}69 \pm 0{\cdot}03\ \text{Å};$$
$$\beta = 98{\cdot}25 \pm 0{\cdot}25°.$$

The density is $1{\cdot}512 \pm 0{\cdot}005$ g.cm.$^{-3}$, indicating that there are two molecules per unit cell. The only systematic absences observed were $0k0$ for k odd, and the space group is thus $P2_1$.

Equi-inclination Weissenberg photographs were taken with Cu radiation, a multi-film technique being used, and the intensities were estimated visually for some thousand reflections. Several small crystal specimens were employed and no absorption corrections have been applied.

Since the unique axis is comparatively short, good resolution of the atoms in the (010) projection was expected and a modification of the method of Karle & Hauptman (1953) to take account of the effect on the invariant and semi-invariant phases of possible asymmetric unit symmetry was used to determine the phases of the structure factors in this centrosymmetric projection. Several stages of successive Fourier refinement were applied to give an eventual $R(h0l)$ of 19%. On the basis of stereochemical considerations reasonable values for the y coordinates of the atoms were chosen and a three-dimensional least-squares refinement, first with an overall isotropic temperature factor and then with individual isotropic temperature factors, resulted in an $R(hkl)$ of 17%, the contributions of the hydrogen atoms having been neglected at this stage. The coordinates and temperature factors are listed in Table 1, and confirm that the glucose molecule is a Sachse–Mohr 'chair-shaped' pyranose ring.

Table 1. *Atomic coordinates and isotropic temperature factors*

	x/a	y/b	z/c	B (Å^2)
C_1	0·190	0·138	0·070	4·7
C_2	0·107	−0·001	0·180	1·9
C_3	0·193	0·032	0·324	2·0
C_4	0·363	−0·046	0·325	2·2
C_5	0·429	0·103	0·215	2·2
C_6	0·598	0·029	0·200	3·0
O_1	0·179	0·406	0·085	3·5
O_2	−0·047	0·085	0·168	2·8
O_3	0·124	−0·158	0·412	3·5
O_4	0·446	0·012	0·458	2·8
O_5	0·345	0·066	0·081	2·1
O_6	0·613	−0·254	0·188	3·0
O_7	−0·119	−0·470	0·322	2·7

In this crystal only 14 of the 28 hydrogen atoms in the unit cell are bonded to the carbon atoms and hence occur in predictable positions. It has been reported by Mann & Marrinan (1958) that the results of infra-red analysis show that the structure is fully hydrogen-bonded; from the coordinates of Table 1 there are seven inter-molecular distances between oxygen atoms less than 2·85 Å. Fig. 1 is a plan of the structure projected down the b axis with the hydrogen bonds shown by broken lines. Some evidence for the positions of the hydrogen atoms was obtained from this hydrogen-bonding scheme, and those hydrogens which can be placed with certainty are marked as right crosses on Fig. 1. The remaining hydrogen bonds form two separate infinite chains about two of the screw axes. Due to high anisotropy of the oxygen atoms it is not yet possible to fix the hydrogen positions in these chains. Indeed it is not impossible that they exist as a statistical distribution throughout the crystal.

One short inter-molecular distance (C_6–O_7''') exists (2·61 Å). All other inter-molecular and intra-molecular distances are normal and the bond lengths and bond

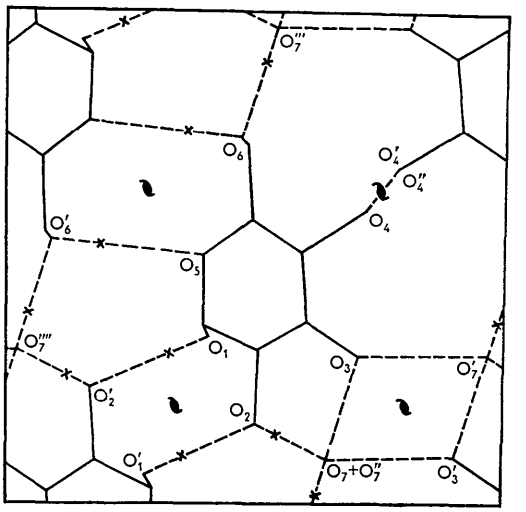

Fig. 1. Plan of the structure projected down the b axis. The hydrogen bonds are shown by broken lines, and the bonding hydrogen atoms that can be placed with certainty are shown as right crosses. The c-axis is parallel to the bottom edge of the diagram.

angles are similar to those found in α-D-glycose (McDonald & Beevers, 1952) with the exceptions that there seems to be no undue shortening in the C_1–O_1 bond (1·38 Å) or the C_6–O_6 bond (1·46 Å).

It is intended to carry out a full three-dimensional refinement with anisotropic temperature factors and full details of the analyses will be published when the work is completed.

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