

Structure analysis of trehalose dihydrate by neutron diffraction

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α, α -trehalose dihydrate is a non-reducing disaccharide, and very attractive from both academic and practical points of view, such as an additive for long term storage in food and pharmaceutical industries. It has high superiority as a protector of biological molecules compared with other carbohydrates such as sucrose. To understand the biological protective mechanism of α, α -trehalose, information on the hydrogen atom positions is indispensable.

Structure analysis of α, α -trehalose at room temperature was carried out by means of neutron diffraction method. Intensity data up to $\sin \theta / \lambda < 0.75 \text{ \AA}^{-1}$ was collected using crystals with approximate dimensions of $15 \times 4.5 \times 2.7 \text{ mm}^3$ by a four-circle diffractometer, FONDER at T2-2. The space group of α, α -trehalose is orthorhombic $P2_12_12_1$ ($Z = 4$) and the obtained lattice parameters at 300 K were $a = 12.2380 \text{ \AA}$, $b = 17.9087 \text{ \AA}$ and $c = 7.6032 \text{ \AA}$. Least square fitting analysis were performed to refine structural parameters; in the analysis, parameters obtained by previous X-ray study^[1,2] were used as initial parameters for atoms except for the hydrogen atom. Structure determined by 1711 neutron intensity data with R values of 0.068 is shown in Fig.1. Position of hydrogen atoms in both glucose (pink circle) and water molecules (red circle) are determined for the first time. It is found that the hydrogen atoms in water molecules are oriented to the glucose molecules, indicating that the molecules are connected to each other through the hydrogen bonding between the molecule and hydrogen atoms in water.

[1] G. M. Brown *et al.* Acta Crystallogr., B **283**(1972)3145.

[2] G. Taga *et al.* Acta Crystallogr., B **283**(1972)3258.

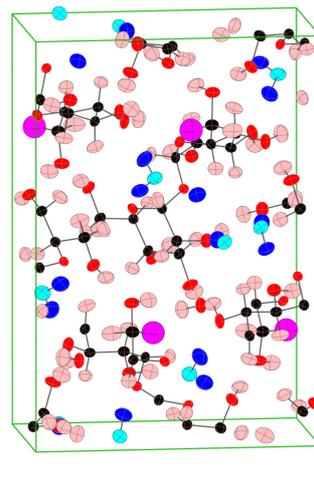


Fig. 1. Crystal structure of α, α -trehalose determined by neutron analysis. Hydrogen atom in glucose and water molecules are shown with pink and blue circles, respectively.