The structure of a-Lactose Monohydrate

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α-lactose monohydrate, $C_{12}H_{22}O_{11}\cdot H_2O$, hereafter designated as (I), is a reducing disaccharide consisting of a moiety of β-D-galactose and a moiety of α-D-glucose, linked by a 1,4 glycosidic bond. Lactose is known as milk sugar and (I) is the most common form of lactose. The structure of (I) was studied by Beevers & Hansen [1], Fries *et al*. [2] and Noordik *et al*. [3] at *ca* 296 K and by Smith *et al*. [4] at 150 K. Since they were used X-ray-diffraction data, obtained thermal parameters for carbon and oxygen atoms were anisotropic, while those for hydrogen atoms were determined as isotropic. In this study, we have performed single-crystal neutron diffraction experiment at R.T. using a four-circle neutron diffractometer, T22, FONDER and obtain accurate information of nuclear positions and anisotropic thermal displacements for hydrogen atoms of (I).

The lattice parameters obtained in the present experiment are $a = 7.8022(82)$ Å, $b = 21.5677(271)$ Å, $c = 4.8308(84)$ Å and $\beta = 105.711(84)$ with space group of $P2_1$ ($Z = 2$), which are consistent with previous X-ray measurements. The final reliable factor is $R = 4.35\%$ for 996 independent reflections with $|F| > 4\sigma$. Figure(a) shows the resultant molecular conformation of (I) with thermal ellipsoid in which the atoms are represented by a 50% probability. To visualize the distribution of nuclear density (ND), distribution of scattering amplitudes was calculated by the maximum entropy method (MEM). The final reliability factors of MEM analysis was $R = 5.6\%$. The calculated ND was plotted over the thermal ellipsoids in Fig.(b) with negative(blue parts) and positive (yellow parts) scattering amplitudes. The distributions of ND and the thermal ellipsoids of the hydrogen atoms show similar shapes, indicating that ND directly reflects the vibrations of the hydrogen atoms.

[1] C. A. Beevers & H. N. Hansen : Acta Cryst. B**27** (1971) 1323. [2] D.C.Fries *et al*.: Acta Cryst. B**27** (1971) 994. [3] J. H. Noordik *et al*.: Z. Kristallogr. **168** (1984) 59. [4] J.H. Smith *et al*. : Acta. Cryst. E**61** (2005) o2499.

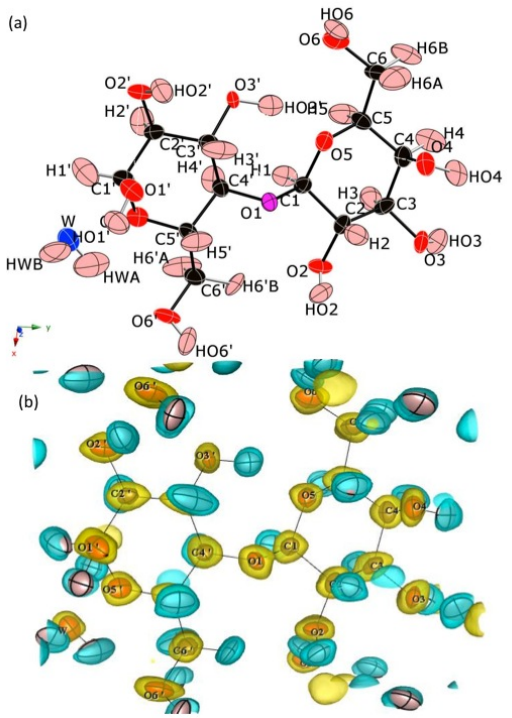

Fig. 1. (a)Molecular conformation of (I) with thermal ellipsoids and (b)ND calculated by MEM.