Poster Presentation

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Neutron powder diffraction analysis of guanosine dihydrate using MEM

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In majority of the crystals of pharmaceutical compounds, hydrogen bonds play a crucial role. Determination of a hydrogen position is highly important, in order to investigate hydrogen bonds especially in the case of hydrates. We have been investigating humidity-induced phase transitions of hydrates systematically [1,2]. Unique characteristics of hydration water molecules have prompted us to explore the phenomena more precisely. Neutron diffraction analysis is a powerful tool to determine hydrogen positions. However, large single crystals are required because of weak neutron diffraction intensities. Under such background, we carried out neutron powder diffraction analysis of guanosine dihydrate using the Maximum Entropy Method (MEM). Neutron powder diffraction data of guanosine dihydrate ($C_{10}H_{13}N_5O_5.2H_2O$; crystal data: monoclinic, space group P21, a = 17.518, b = 11.278, c = 6.658 Å, β= 98.17°, Z = 4) were measured by iMATERIA at MLF in J-PARC (Figure 1(a)). Rietveld analysis was carried out using atomic coordinates of non-hydrogen atoms determined by X-ray analysis and those of hydrogen atoms which were placed on the geometrically calculated positions using the averaged X-H bond lengths determined by neutron analysis referencing the hydrogen positions estimated by X-ray analysis. Using Fo and σ by Rietveld analysis, the nuclear density distribution was calculated by MEM (Figure 1(b)). Nuclear densities of the hydrogen atoms of one water molecule (W1 in Figure 1) were elongated, which is consistent with the results of molecular dynamic simulation [2]. The effective usage of MEM to elucidate hydrogen atom positions from neutron powder diffraction data will be discussed together with that of difference Fourier calculations.

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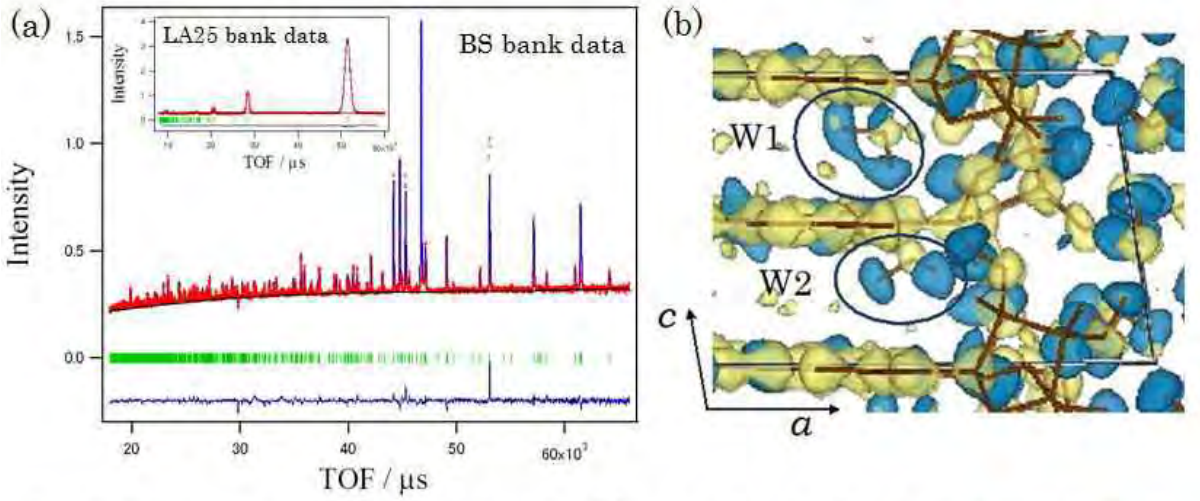

Fig.1 Neutron powder diffraction data (a) and nuclear density of guanosine dihydrate calculated by MEM (b). Dark blue and light green isosurfaces in (b) indicate negative densities for H atoms and positive ones for non-H atoms, respectively, with a level of -/+ 1.2 fm/Å^3.

Keywords: neutron powder diffraction, hydrogen bond, MEM