Neutron Diffraction Analysis of Dehydrated State of Disodium Inosine 5′-monophosphate Hydrate

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Hydration around biomacromolecules draws attention from the viewpoint of correlation between hydrated structures and dynamic functions. Hydration schemes around proteins, nucleic acids, and oligonucleotides have been investigated by numerous methods, *e.g.*, crystallographic analysis, NMR, Raman spectroscopy, dielectric relaxation measurements. Determination of hydrogen positions in hydrogen bonds is inevitable to discuss the hydration networks. However, it is difficult to determine hydrogen positions by X-ray analysis, especially in the case of crystal water molecules, because they mostly fluctuate. From this point of view, neutron diffraction analysis is highly important.

In this paper, we report neutron diffraction analysis of disodium inosine 5′-monophosphate heptahydrate ($Na_2IMP.7H_2O$), which is stable in medium humidity range. IMP is one of the components of RNA. The hydration numbers of Na_2IMP crystals changes from zero to ten in the relative humidity of 0 to 90% at room temperature. In the case of the heptahydrate, there are some highly disordered region where we could not distinguish water sites and sodium ion sites on the basis of X-ray analysis. Neutron diffraction data were collected at FONDER in JAEA/JRR-3 (Proposal No. 2734) and SENJU in J-PARC/MLF (Proposal No. 2013A0165). On the basis of observed nuclear density distribution, the hydration of the heptahydrate will be discussed. Nucleotides are not macromolecules, but the neutron analysis of nucleotide hydrates has an advantage of high resolution. We believe that the hydration schemes in nucleotides give us an insight into the hydration schemes of biomacromolecules.