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	承認日 Date of Approval 2013/07/16 承認者 Approver Takashi Ohhara 提出日 Date of Report 2013/07/16
課題番号 Project No. 2013A0165 実験課題名 Title of experiment Neutron diffraction analysis of disodium inosine 5'-mono-phosphate heptahydrate 実験責任者名 Name of principal investigator Yoko Sugawara 所属 Affiliation Kitasato University, School of Science	装置責任者 Name of Instrument scientist Takashi Ohhara 装置名 Name of Instrument/(BL No.) Extreme Environment Single Crystal Neutron Diffractometer SENJU (BL-18) 実施日 Date of Experiment 2013/5/3 9:00 a.m. – 2013/5/8 9:00 a.m.

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)  
 Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form. Disodium inosine 5'-monophosphate heptahydrate ( $\text{Na}_2\text{IMP} \cdot 7\text{H}_2\text{O}$ ) $\text{C}_{10}\text{H}_{11}\text{N}_4\text{O}_8\text{PNa}_2 \cdot 7\text{H}_2\text{O}$ (The data collection of deuterated sample ( $\text{Na}_2\text{IMP} \cdot 7\text{D}_2\text{O}$ ) was scheduled. However, quality of the deuterated crystals was not sufficient. Therefore, data collection of non-deuterated sample ( $\text{Na}_2\text{IMP} \cdot 7\text{H}_2\text{O}$ ) was carried out.)
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2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。) Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.  As described in the section of "Name of sample(s)", the data collection of deuterated sample ( $\text{Na}_2\text{IMP} \cdot 7\text{D}_2\text{O}$ ) was scheduled. However, quality of the deuterated crystals was not sufficient. Therefore, data collection of non-deuterated sample ( $\text{Na}_2\text{IMP} \cdot 7\text{H}_2\text{O}$ ) was carried out. A single crystal ( $1.5 \times 1.0 \times 0.8 \text{ mm}^3$ ) sealed in a quartz capillary ( $1.5 \phi$ ) was mounted on the sample position of SENJU and was irradiated by the pulsed white neutron at room temperature. Measurements of Bragg reflections up to the resolution limit of $0.5 \text{ \AA}$ were carried out with 9 goniometer settings for the first frame and 3 goniometer settings for the second frame. Data reduction was carried out by STARGazer. Number of collected independent reflections ( $ F_o  > 0$ ) of the first frame and the second frame were 1593 and 97, respectively.
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## 2. 実験方法及び結果(つづき) Experimental method and results (continued)

Using 1593 independent reflections of the first frame up to 0.62 Å resolution, a tentative structure refinement was carried out starting from non-hydrogen atom positions of IMP determined by X-ray analysis. All hydrogen atoms of IMP molecules, two sodium ions, 8 oxygen and 11 hydrogen sites of 5.5 water molecules were located in the difference Fourier maps. Among 8 oxygen sites of water molecules, the occupancy factors of five were 0.5, because one was located at the special position and the others were disordered and treated as split atoms.

At the present stage, atomic displacement parameters of non-hydrogen atoms and hydrogen atoms were treated as anisotropic and isotropic, respectively, and  $R$  value was 0.13 for 1583 reflections ( $|F_o| > 4\sigma(|F_o|)$ ). We are going to continue refinement carefully paying special attention to the highly disordered regions using both the Fourier and the maximum entropy methods.

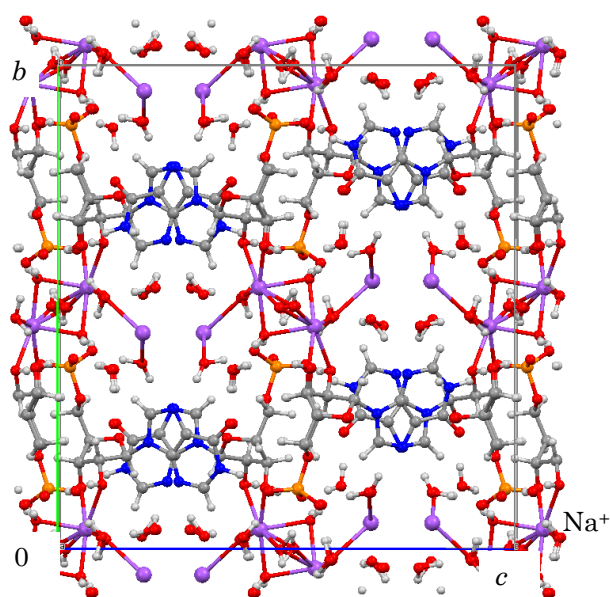


Figure 1 Crystal structure of  $\text{Na}_2\text{IMP}\cdot 7\text{H}_2\text{O}$  at the present stage.