

実験報告書様式(一般利用課題・成果公開利用)

(※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。)

	提出日 Date of Report 9 October 2012
課題番号 Project No. 2012A0069 実験課題名 Title of experiment Crystal structure and hydrogen bonds of trisaccharide raffinose-pentahydrate 実験責任者名 Name of principal investigator Takuro Kawasaki 所属 Affiliation Japan Atomic Energy Agency	装置責任者 Name of responsible person Takashi Ohhara 装置名 Name of Instrument/(BL No.) SENJU (BL18) 実施日時 Date and time of Experiment 20 Jun. 2012 – 24 Jun. 2012

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.
Name : Raffinose pentahydrate Chemical formula : $C_{18}O_{16}H_{32} \cdot 5H_2O$ Physical form : Single crystal

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.
<p><u>Method</u></p> <p>The raffinose single crystal was attached to the Cd stick using the Al tape and mounted to the goniometer. Neutron diffraction intensities were collected on the following conditions.</p> <p>-----</p> <p>Crystal orientation: 6                  Exposure time: 8 hrs. / orientation                  Temperature: 120 K</p> <p>-----</p>

## 2. 実験方法及び結果(つづき) Experimental method and results (continued)

### Result

The crystal structure refinement of raffinose – pentahydrate was performed. The structural parameters including atomic positions and anisotropic displacement parameters of H atoms were converged reasonable values (Fig. 1). The resultant reliability factor was  $R = 7.6\%$ . The geometrical parameters of the atoms suggest the hydrogen bonds connecting the water molecules in the raffinose – pentahydrate crystal are categorized as “moderate hydrogen bond”. The five water molecules in the crystal are connected each other by the bonds and form the finite chain. The three water molecules have the four hydrogen bonds and the other two molecules have the three bonds. It is expected that the former three molecules are more stable than the latter two molecules in the crystal.

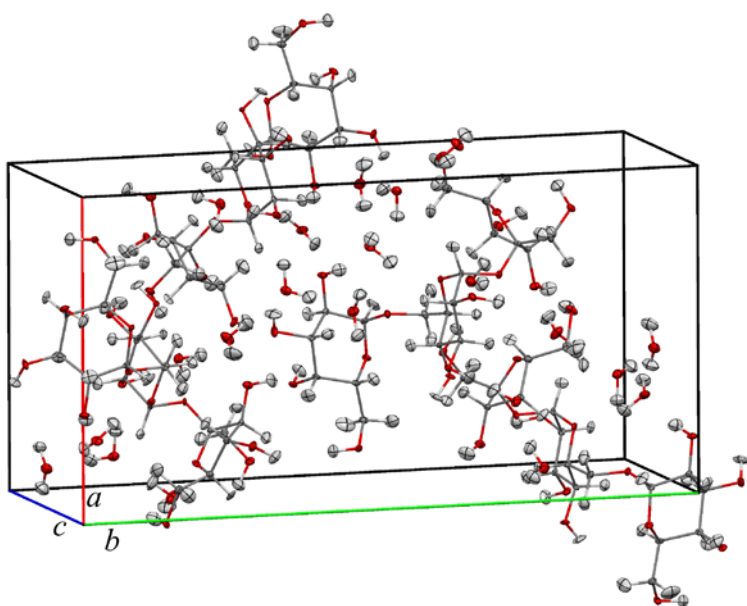


Fig. 1

Crystal structure of raffinose –  
pentahydrate

Data: 5194 reflections

$R = 7.6\%$

Space group: P212121

Lattice parameters:  $a = 12.33 \text{ \AA}$ ,  
 $b = 23.84 \text{ \AA}$ ,  $c = 8.96 \text{ \AA}$