The structure and phase transition in the one-dimensional semiconductor C$_5$H$_{10}$NH$_2$PbI$_3$ has been investigated by using neutron and x-ray single crystal diffraction methods. C$_5$H$_{10}$NH$_2$PbI$_3$ has a lead-based inorganic-organic perovskites structure consisting of semiconducting parts which are composed of one-dimensional chains of face-sharing lead-iodide octahedra and barrier parts composed of C$_5$H$_{10}$NH$_2^+$ molecules. It has been shown by Raman scattering that the structure undergoes successive phase transitions below the room temperature which involves rotational/orientational ordering of the organic C$_5$H$_{10}$NH$_2^+$ parts [1]. However, its precise structure has not been determined even for the room temperature. The aim of the present study is to clarify the structural change and its effects on the electronic state in the phase transitions of C$_5$H$_{10}$NH$_2$PbI$_3$ by combining the data obtained by neutron and x-ray single crystal diffraction.

The neutron data were obtained at T2-2, FONDER at room temperature (R.T.), and analyzed by using program SHELXL with 199 unique reflections. In the refinement, positional parameters for Pb and I are fixed to the values previously obtained by x-ray structural analysis [2]. Positional information for nitrogen and hydrogen atoms which were not taken into account in the x-ray data analysis is obtained with R = 0.09. The nitrogen atom in the C$_5$H$_{10}$NH$_2^+$ molecule tends to occupy C1 and C2 carbon sites, which are closer to the lead-iodide chain than the C3 site. The occupancies of nitrogen atoms at C1 and C2 sites are found to be 0.42 and 0.58, respectively. The hydrogen atoms are found as CH$_2$ groups with the distances of the hydrogen bonds being 0.8769 Å from C1, 1.0687 Å from C2 and 1.1403 Å from C3. Figure 1 shows the structure of the organic C$_5$H$_{10}$NH$_2^+$ part at R.T. obtained from the neutron data. In the figure, C3 site obtained from the x-ray data is shown together as C3’ for a comparison. The structure of the molecule obtained by the neutron data clearly shows a chair form which has greater strain than that obtained by the x-ray data. It is expected that the twisting motion between the two identical chair conformers is present in the molecule and plays an important role in the phase transitions.

References

Fig. 1. Structure of the organic C$_5$H$_{10}$NH$_2^+$ part obtained from neutron data. C3’ site is positional data obtained from x-ray data.