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 <b>MLF Experimental Report</b>	提出日 Date of Report 2011/06/29
課題番号 Project No. 2010A0084 実験課題名 Title of experiment Crystal structure of a lead-based inorganic-organic perovskite (C <sub>5</sub> H <sub>10</sub> NH <sub>2</sub> )PbBr <sub>3</sub> 実験責任者名 Name of principal investigator Miwako Takahash 所属 Affiliation Univ. of Tsukuba	装置責任者 Name of responsible person Ichirho Tanaka 装置名 Name of Instrument/(BL No.) iBIX 実施日 Date of Experiment 2010/10/17 – 2010/10/21

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.
C <sub>4</sub> H <sub>10</sub> NOPbBr <sub>3</sub> 3×3×0.8mm <sup>3</sup> , 0.03g

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. Single crystal diffraction measurement was performed at 120K. The experiment was successful and obtained data were analyzed using program GSAS. The final reliable factors are R=15% and the nuclear positions of hydrogen atoms are determined accurately. Figure 1 shows crystal structure of C <sub>4</sub> H <sub>10</sub> NOPbBr <sub>3</sub> obtained by the present neutron data. In the figure, orientation of the molecules and distortion tendency of PbBr <sub>6</sub> octahedra shows existence of chemical bonding between lead and oxygen atoms. By comparing the electron density distribution obtained by X-ray diffraction, it is suggested that the bonding between organic and inorganic parts is of an ionic character.
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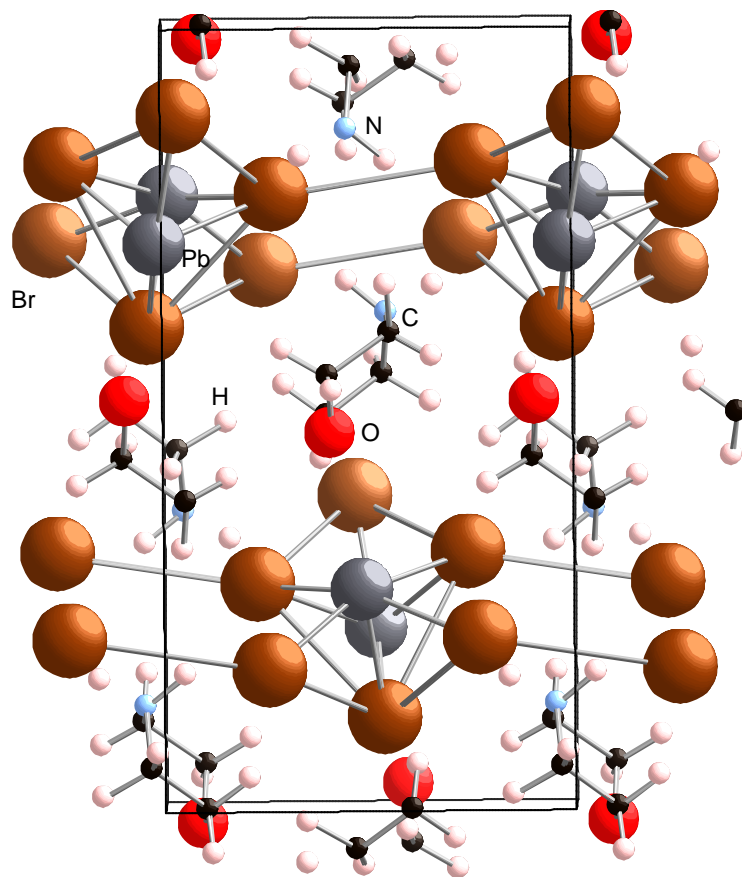


Fig. 1 Crystal structure of  $C_4H_{10}NO PbBr_3$  obtained by present experimental data.