

Ferroelectric Phase Transition Mechanism in $C_5H_6NBF_4$ by X-ray Crystal Analysis

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Pyridinium Tetrafluoroborate $C_5H_6NBF_4$ (abbreviated to $PyBF_4$) undergoes a ferroelectric-paraelectric phase transition at $T_1=238.7K$, and another phase transition at $T_2=204K$ [1, 3]. From the NMR studies [2], the pyridinium and tetrafluoroborate ions were the dynamical disorder state at room temperature. It was suggested that the ordering of these ions was linked to the successive phase transitions. From the X-ray diffraction study [3], the disorder state of the pyridinium and tetrafluoroborate ions was also reported. However, a report of the crystal structure analysis at low temperature was not found. The crystal structure analyses at low temperature phases in $PyBF_4$ were very important in order to clarify the mechanism of the successive phase transition in this material.

Re-investigation of the single-crystal X-ray structure analysis in $PyBF_4$ at room temperature was carried out, and we confirmed that the pyridinium and tetrafluoroborate ions were in the disorder state. Now, we are doing the X-ray structure analyses of low temperature phases in $PyBF_4$ single-crystal. In congress, we will show the crystal structures of low temperature phases and discuss the successive phase transition mechanism in $PyBF_4$.

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Keywords: single-crystal x-ray analysis, ferroelectric phase transitions, pyridinium tetrafluoroborate $C_5H_6NBF_4$