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Phase Transitions in Hexafluorophosphate Salts, *K. Vedam, R. Pepinsky, Joseph

Lajzerowicz, Y. Okaya and N. Stemple, The Pennsylvania State University. —

$\text{NH}_4\text{PF}_6 \cdot \text{NH}_4\text{F}$ is tetragonal at room temperature, and has two low-temperature transitions: at -45°C ($= T_{\text{UC}}$) and at -101°C ($= T_{\text{LC}}$).¹ Both low-temperature phases are orthorhombic. The dielectric constant $\epsilon_{[110]}$ exhibits a small anomaly at T_{UC} , and a pronounced anomaly at T_{LC} . X-ray examination reveals superstructuring along the a and b axes below T_{UC} , and a doubling of the c axis below T_{LC} . The lowest phase is antiferroelectric. A detailed structural investigation is required to reveal the dielectric character of the intermediate phase.

An order-disorder transition has been observed in KPF_6 at 4°C .¹ A detailed x-ray structure analysis reveals hindered rotation of the $(\text{PF}_6)^{-1}$ octahedra. A large thermal anomaly at the transition temperature suggests a "freezing in" of the hindered rotations in the lower phase.

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¹R. Pepinsky *et al.*, Acta Cryst. 10, 835 (1957).

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