Structural Phase Transitions in $(TMTTF)_2AsF_6$ and $(TMTTF)_2PF_6$ Organic Conductors

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The $(TMTTF)_2XF_6$ salts are a series of quasi one-dimensional organic conductors that exhibit a variety of ordered phases in close proximity.[1] They are part of one of the major families of strongly correlated materials. The salts have a zigzag stack of inversion-related donor molecules with high conductivity separated by anion chains. Two phase transitions are especially interesting for the x-ray studies: spin-Peierls transition (around 10K) and recently found ferroelectric transition (around 70K). The spin-Peierls transition occurs when pairs of neighboring spins dimerize and form spin singlets, giving rise to superlattice peaks, which are possible to detect by x-ray scattering. The ferroelectric transition occurs as a result of a dimerization when donors move toward each other. The ferroelectric nature of this transition has been recently revealed by the dielectric permeability measurements.[2] The shift in the anion positions should give rise to a change in the structure factor, i.e., relative intensities of structural Bragg peaks. The present project is devoted to the studies of both spin-Peierls and ferroelectric phase transitions.

Preliminary studies of $(TMTTF)_2AsF_6$ and $(TMTTF)_2PF_6$ have been conducted at the APS. The results indicate that the samples tested were good single crystals with a mosaic spread of <0.05 degree. A number of peaks were measured, and the twin structure was found to be that detailed in the literature. Special care was taken to minimize the exposure of the samples to x-rays since they are susceptible to x-ray damage.

The samples are roughly needle shaped, and there is a flat surface along the needle. The long axis of the needle was found to be the *a*-direction, that is the direction of the stack of donor molecules. The flat surface is the a*b*-plane hence the *c**-axis is perpendicular to the surface. The good correspondence between the appearance of the sample and their local structure greatly facilitates alignment during scattering experiments. A number of Bragg peaks was measured across the ferroelectric transition temperature, but the results need further analysis and are not yet fully conclusive at the present stage of this project.

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