Raman studies of the charge ordering in organic electronic ferroelectrics \((TMTTF)_2X\) \((X = \text{SbF}_6, \text{AsF}_6, \text{PF}_6, \text{ReO}_4, \ldots)\)

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The organic donor TMTTF (teramethyl-tetrathiafulvalene) and various anions (octahedral: \(X = \text{SbF}_6, \text{AsF}_6, \text{PF}_6\); and tetrahedral: \(X = \text{ReO}_4, \text{ClO}_4, \text{BF}_4\)) form one-dimensional 2:1 charge-transfer salts with metallic properties. At low temperatures \((T = 64 - 230 \text{ K})\) in these salts a charge ordering (CO) is observed which is mainly due to strong electron-electron correlations. The CO effect is directly related with the so-called electronic ferroelectricity. We studied temperature dependence of Raman spectra of the \((TMTTF)_2X\) salts focusing mainly on the charge sensitive \(\text{C=\text{C}}\) and \(\text{C-S}\) stretching modes which can be used for evaluation of the charge distribution in conducting TMTTF stacks. The \(\text{C-S}\) bands of molecules with charge +0.5 are assigned to ferroelectric domains, while the bands of neutral \(\text{TMTTF}^0\) and fully ionized \(\text{TMTTF}^+\) molecules to domain walls \([1]\).

References: