Infrared and Raman Studies of Temperature Induced Neutral-Ionic Phase Transition in \((\text{EDT-TTF-I}_2)_2\text{TCNQF}\)

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The low-dimensional charge-transfer \((\text{EDT-TTF-I}_2)_2\text{TCNQF}\) complex is a unique organic material of 2:1 stoichiometry that undergoes a neutral-ionic phase transition (NIT). The crystal lattice is composed of the iodinated ethylenedithiotetrathiafulvalene (EDT-TTF-I₂) donors (D) and the fluorinated tetracyanoquinodimethane (TCNQF) acceptors (A). Donor dyads alternate with acceptor along a stack.

To study the charge distribution and the origin of the phase transition in \((\text{EDT-TTF-I}_2)_2\text{TCNQF}\) we have measured polarized infrared and Raman spectra of the single crystals in the 8-293 K temperature range. In our spectral analysis we focus on charge sensitive C-S, C-I and C≡N stretching modes of EDT-TTF-I₂ and TCNQF, respectively. We present the schematic representation of the NIT in the 2:1 material and discuss the charge distribution in the ionic phase.

References: