

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

A. Frąckowiak,¹ I. Olejniczak,¹ R. Świetlik,¹ O. Jeannin,² and M. Fourmigué²

¹*Institute of Molecular Physics Polish Academy of Sciences,
M. Smoluchowskiego 17, 60-179 Poznań (Poland)*

²*Institut des Sciences Chimiques de Rennes,
Université Rennes 1, CNRS UMR 6226, 35042 Rennes (France)*

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-I_2) 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 $\text{C}\equiv\text{N}$ stretching modes of EDT-TTF-I_2 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:

- [1] A. Frąckowiak et al., J. Phys. Chem. C 120, 23740 (2016).
- [2] J. Lieffrig et al., Chem. Eur. J. 19, 14804 (2013)