

Neutral to Ionic phase Transition in TTF-Fluoranil, DimethylTTF-Fluoranil and DimethylTTF-Chloranil: a comparative high pressure study

Elena Ferrari¹ and Matteo Masino¹

¹*Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Parco Area delle Scienze 11°, I-43124 Parma, Italy, e-mail: elena.ferrari2@unipr.it*

The Neutral to Ionic phase Transition (NIT) occurs in few mixed stack charge transfer cocrystals at high pressure or low temperature[1]. The lattice contraction, increasing the 3-D Coulomb interactions, favors a higher degree of charge transfer. Due to Peierls instability, this leads to the dimerization of the stack, breaking its inversion symmetry. Thus, the NIT is a charge and a structural instability. It can be first or second order: while the 3-D interactions induce discontinuous NIT, the electron-lattice phonon coupling drives the stack to a continuous dimerization. The 3-D interactions also affect the arrangement of the adjacent stacks, making the ionic phase ferroelectric or antiferroelectric.

The role of these parameters has been widely studied in Tetrathiafulvalene-haloquinone cocrystals. We compare three of them: the newly synthesized TTF-FA[2] and DimethylTTF-FA with the known DMTTF-CA, isostructural with DMTTF-FA. We characterized them by Raman and infrared spectroscopy at high pressure. While the FA based crystals undergo strongly first order NIT, DMTTF-CA shows continuous behavior.

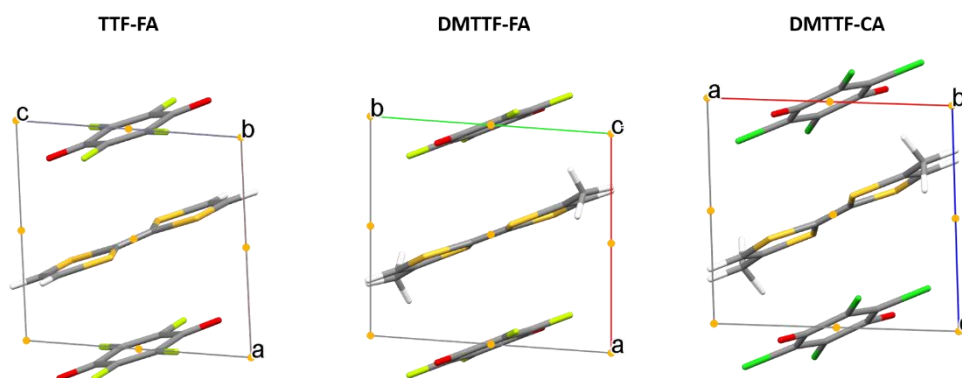


Fig. 1. Unit cell of the three charge transfer crystals

References

- [1] J. B. Torrance et al., *Phys. Rev. Lett.*, **vol. 46**, no. 4, pp. 253–257 (1981)
- [2] E. Ferrari et al., *Phys. Rev. B*, **vol. 105**, no. 5, pp. 1–6 (2022)