

**BTDMTTF–TCNQ ($C_{10}H_8S_6^+ \cdot C_{12}H_4N_4^-$):
Topological bonding analysis of a charge transfer crystal**

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The organic charge-transfer complex BTDMTTF–TCNQ ($C_{10}H_8S_6^+ \cdot C_{12}H_4N_4^-$) behaves as an almost pure 1D metal, showing metallic character down to 26 K [1]. The magnitude of the intermolecular charge transfer at $T = 130$ K was initially estimated at approximately 0.7 e from the values of the multipolar parameters obtained in an experimental charge density study [2]. Recently, a QTAIM (Quantum Theory of Atoms in Molecules) analysis [3] applied to the same multipolar charge density model revealed more accurate atomic charges. Indeed, while charges inferred from multipoles replicate integrated charges for coarse grained atomic groups, they fail when fine granularity (e.g C, N) is demanded. In addition, contributions to charge-transfer are spread amongst several atoms instead of being localized in sulphur atoms, as previously pointed out [2]. Also, we have systematically identified the interactions present in the crystal phase using the topology of the electrostatic potential [4, 5] and the Laplacian of the electron density with MoPro [6] and Critic [7] programs. Theoretical calculations on the molecules and solids involved are examined to help advancing in the knowledge of the experimental measured densities.

References:

- [1] N. Santalo, J. Tarres, E. Espinosa, J. Llorca, E. Molins, J. Veciana, C. Rovira, M. Mays, S. Yang, D. Cowan, et al., *Synthetic Metals* **56** (1993) 2050.
- [2] E. Espinosa, E. Molins, and C. Lecomte, *Phys. Rev. B* **56** (1997) 1820.
- [3] R. Bader, *Atoms in Molecules: A Quantum Theory*. Oxford University Press, (1994).
- [4] I. Mata, E. Molins, I. Alkorta, and E. Espinosa, *J. Phys. Chem. A* **111**, 6425 (2007).
- [5] I. Mata, E. Molins, and E. Espinosa, *J. Phys. Chem. A* **111**, 9859 (2007).
- [6] C. Jelsch, B. Guillot, A. Lagoutte, and C. Lecomte, *J. Appl. Cryst.* **38**, 38 (2005).
- [7] A. Otero de-la-Roza, et. al., *Comput. Phys. Commun.* **180** (2009) 157; **185** (2014) 1007.