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Optical investigations of organic semiconductors truecm (tTTF)₂X (X=Br, I)*

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The organic semiconductors (tTTF)₂X (where: tTTF= trimethylene-tetrathiafulvalene and X = Br, I) are low-dimensional antiferromagnets with the highest Nel temperatures for charge-transfer salts based on TTF derivatives: about 35 K for Br salt and about 43 K for I salt [1]. The studied salts are isomorphous and within conducting layers, the donors are arranged in dimeric units (tTTF)₂. We studied the corresponding IR and Raman spectra of (tTTF)₂X crystals over a temperature range of 5 - 300 K. Our spectroscopic data provide evidence of charge localization over this range. Within the region of C=C stretching (1400-1600 cm⁻¹) and ring breathing modes (400 - 550 cm⁻¹), Raman bands related to tTTF molecules with charge +1 were observed; i.e. the charge in dimers is not uniformly distributed. The bands assigned to the ring breathing mode show a specific splitting due to interactions between (tTTF)₂ dimers. We suggest that these modes could be used for evaluation of the strength of interactions between dimers. The IR spectra also give clear evidence of non-uniform charge distribution as two charge transfer transitions (centred at about 4000 and 8000 cm⁻¹) were observed. The spectroscopic data will be discussed in relation to formation of the antiferromagnetic states in (tTTF)₂X salts.

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[1] M. Fourmigué *et al.*, *Inorg. Chem.* **50**, 4171 (2012).