Charge-sensitive vibrational modes in the (EDT-TTF-OX)2AsF6 chiral molecular conductors

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Résumé en anglais	Infrared and Raman spectra of three chiral molecular conductors (EDT-TTF-OX)2AsF6, comprising of two salts based on enantiopure EDT-TTF-OX donor molecules and one based on their racemic mixture, have been measured as a function of temperature. In the frequency range of the C=C stretching vibrations of EDT-TTF-OX, charge-sensitive modes are identified based on theoretical calculations for neutral and oxidized EDT-TTF-OX using density functional theory (DFT) methods. The positions of C=C stretching modes in both Raman and infrared spectra of the (EDT-TTF-OX)2AsF6 materials are analyzed assuming a linear relationship between the frequency and charge of the molecule. The charge density on the EDTTTF-OX donor molecule is estimated to be +0.5 in all investigated materials and does not change with temperature. Therefore we suggest, that M-I transition observed in (EDT-TTF-OX)2AsF6 chiral molecular conductors at low temperature is not related to the charge ordering mechanism.
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