

# Vibrational Spectra of Coordination Polymers Based on TCE-TTF

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Coexistence of magnetism and electrical conductivity is one of the most important directions in the synthesis of multifunctional organic-based materials. Here we present infrared and Raman spectra of the series of TCE-TTF-based isostructural polymeric salts with paramagnetic (Co<sup>II</sup>, Mn<sup>II</sup>), and diamagnetic (Zn<sup>II</sup>, Cd<sup>II</sup>) metal ions [1]. Infrared and Raman active modes are identified and assigned based on theoretical calculations for neutral and ionized TCE-TTF using density functional theory (DFT) methods. The vibrational modes related to the C=C stretching vibrations of TCE-TTF are analyzed assuming the existence of the electron-molecular vibration coupling (EMV). The presence of the antisymmetric C=C dimeric mode provides an evidence that charge transfer takes place between TCE-TTF molecules belonging to neighboring polymeric networks.

1. J. Olivier et al., Inorg. Chem. 2009, 22, 3282-3290.

13.4 cm

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9.7 cm