Infrared Studies of Pressure-Induced Neutral-Ionic Phase Transition in the (EDT-TTF-I_2)$_2$TCNQF Complex

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The (EDT-TTF-I_2)$_2$TCNQF charge-transfer salt belongs to a rare group of low-dimensional organic conductors of mixed-stacks that under external stimuli (i.e. temperature, pressure) undergo neutral-ionic phase transition (NIT) [1,2]. It is a complex phenomenon in which change of ionization phase is accompanied by a lattice distortion. Thus, it makes favorable conditions for electronic ferroelectricity that is highly attractive from the application perspective. Fundamental studies of the materials are focused on a better understanding of electronic correlations and on making a significant impact on the ground state stabilization parameters.

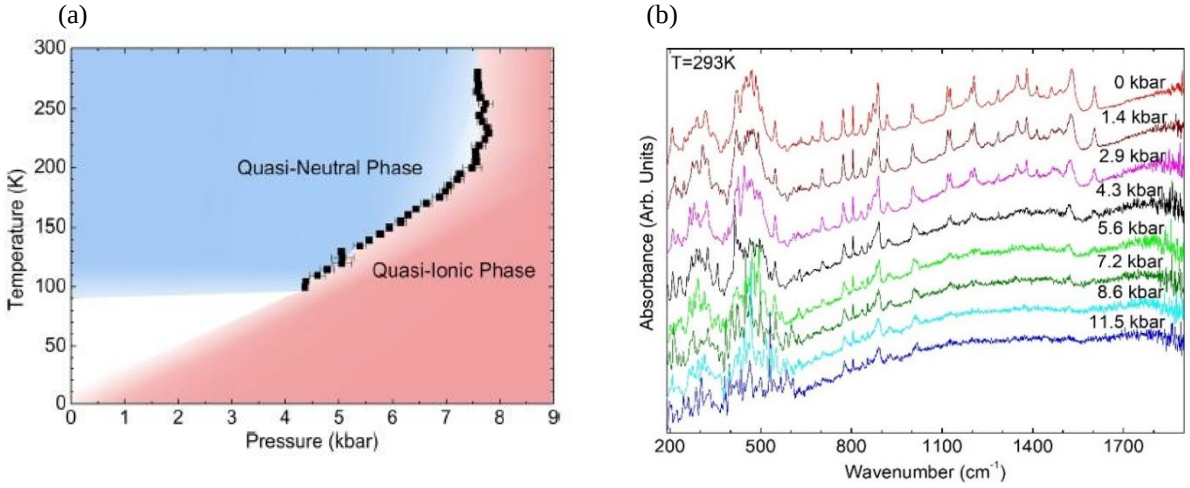

Fig. 1 (a) Pressure-temperature phase diagram of (EDT-TTF-I_2)$_2$TCNQF based on the results of the electrical resistance studies in a function of temperature (8-293 K) and pressure (0-11.8 kbar) [2]; (b) absorbance spectra of (EDT-TTF-I_2)$_2$TCNQF recorded at room-temperature in a function of pressure (0-11.5 kbar).

Based on the results of the electrical resistance studies of (EDT-TTF-I_2)$_2$TCNQF in a function of temperature (8-293 K) and hydrostatic pressure (0-11.8 kbar), the p-T phase diagram of the complex has been presented (Fig. 1a) [2]. In order to probe the local environment of the complex, infrared studies of (EDT-TTF-I_2)$_2$TCNQF in a function of temperature (10 – 293 K) and hydrostatic pressure (0 – 97 kbar) in the broad frequency range were performed. Figure 1b presents absorbance spectra recorded at 293 K in quasi-neutral phase, mixed-phase and quasi-ionic phase. To study charge distribution and lattice distortion, a detailed analysis of vibrational dynamics was performed. This work was supported by the Polish National Science Centre (Miniatura-3, DEC-2019/03/X/ST3/01653).

References

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