

Abstract Submitted
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Metastable domains at the pressure induced neutral-ionic transition of TTF-CA ZOLTAN SOOS, Princeton University, ANNA PAINELLI, Parma University — Tetrathiafulvalene-Chloranil (TTF-CA) is the prototypical organic charge transfer (CT) salt whose neutral-ionic and dimerization (Peierls) transitions have been studied on cooling or under pressure. Volume changes switch the ground state from a band insulator with a fractional CT from TTF to CA of $\rho \sim 0.3$ in a regular stack to a Mott insulator with $\rho > 0.5$ in a dimerized stack. TTF-CA spectra indicate electron-vibration coupling to both lattice (e-ph) and molecular (e-mv) modes that lead to competing instabilities. Near the metallic point of the rigid system, a one-dimensional adiabatic Hubbard model with linear e-ph and e-mv coupling leads to metastable domains with different ρ, ρ' that are thermally accessible at 300 K over a limited bistability range. The transition of TTF-CA single crystals at 1 GPa indicates a pressure range with two resolved ρ, ρ' . The model also describes the first order transition at 81 K at ambient pressure and generates anharmonic potential energy surfaces. These quantum transitions are driven by volume changes without contributions from electronic excited states.

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