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Thermal and Quantum Peierls Transitions in Organic Charge-Transfer Salts SHARON BEWICK, ZOLTAN SOOS, Princeton University — The choice of donors (D) and acceptors (A) governs the charge-transfer ρ in organic CT salts with mixed one-dimensional DADA stacks. Strong D and A yield $\rho \sim 0.9$ stacks of radical ions with thermally accessible spin and charge degrees of freedom whose Peierls transition can be described by a Hubbard model with site energies. The same microscopic model describes CT salts with smaller and variable $\rho \sim 0.5$ in which neutral-ionic and/or Peierls transitions occur in the ground electronic state. Quantum transitions are driven by volume changes, with negligible thermal population of excite states. CT salts with thermal or quantum Peierls transitions are identified. Conflicting magnetic, vibrational and structural data in several CT salts are resolved in terms of mobile spin solitons, a dimerized ground state and a Peierls transition beyond the crystal's thermal stability.

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