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Organic molecular crystals: materials with competing orders GIANLUCA GIOVANNETTI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, 34136 Trieste, Italy, SANJEEV KUMAR, Indian Institute of Science Education and Research Mohali, MGSIPAP Complex, Sector 26, Chandigarh 160 019, India, JEAN-PAUL POUGET, Laboratoire de Physique des Solides, Université Paris Sud, CNRS, UMR 8502, 91405 Orsay, France, MASSIMO CAPONE, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, 34136 Trieste, Italy — The search for multiferroics has become an important research topic in the last few years. Almost all newly discovered multiferroics are transition metal compounds where spin, lattice and charge degrees of freedom are strongly entangled. The possibility of finding organic multiferroics can open up a new area of research where new mechanisms, different from those active in standard transition metal oxide multiferroics, may have a role for the simultaneous occurrence of magnetic and ferroelectric order. By means of ab-initio and model calculations, we show an instability towards multiferroicity in the organic molecular crystal TMTTF₂-PF₆. Coexistence of charge ordering with a structural dimerization results in a ferroelectric phase with the tendency to the dimerization magnetically driven. The Multiferroicity is induced by competing orders: charge distribution and lattice distortions coupled with the magnetic state.

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