

Structures of New Molecular Conductors Based on Functionalized Organic Donors

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Functionalized organic donors are remarkable for the ability to form hydrogen bonds of cation···cation and cation···anion types, which can effectively control the crystal architecture of molecular conductors [1]. Hydrogen bond network is well developed in the crystals of four new radical cation salts based on amide functionalized EDT-TTF donors EDT-TTF-CONH₂ (D1) and EDT-TTF-(CONH₂)₂ (D2) [2].

Semiconducting α' -(D1)₄[FeNO(CN)₅] (**1**), α' -(D1)₄[Co(CN)₆] (**2**), β -(D1)₆[Fe(CN)₆] (**3**) and (D2)₄[FeNO(CN)₅]NB (**4**) salts have been prepared and characterized by X-ray single crystal diffraction experiments and band structure calculations. (D1)₂-dimers or (D2)_n-extended zigzag chains of donors connected through functional groups are found to be stable structural motifs in **1-4**. The **1** and **2** salts are isostructural but contain anions of different charge, -2 and -3, respectively. The degree of charge transfer affects on electronic structures of the crystals that results in changing their transport properties: $\sigma_{RT}(\mathbf{2})/\sigma_{RT}(\mathbf{1})=50$. In the crystals **4** a superstructure with incommensurate vector $\pm(0.5, 0.3, 0.2)$ has been observed and studied.

[1] Fourmigue M., Batail P., *Chem. Rev.*, 2004, **104**, 5379. [2] Shibaeva R., Khasanov S., Zorina L., et al., *J. Phys. IV France*, 2004, **114**, 481.

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