



Chirality Driven Metallic versus Semiconducting Behavior in a Complete Series of Radical Cation Salts Based on Dimethyl-Ethylenedithio-Tetrathiafulvalene (DM-EDT-TTF)

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Résumé en anglais	<p>Enantiopure (S,S) and (R,R) dimethyl-ethylenedithio-tetrathiafulvalene (DM-EDT-TTF) 1donors are synthesized by cross coupling followed by decarboxylation reactions. In the solid state the methyl groups are arranged in axial positions within sofa-type conformation for the six-membered rings. Crystalline radical cation salts formulated as [(S,S)-1]2PF6, [(R,R)-1]2PF6, and [(rac)-1]2PF6 are obtained by electrocrystallization. When the experiment is conducted with enantioenriched mixtures both enantiopure and racemic phases are obtained. The monoclinic enantiopure salts, containing four independent donors in the unit cell, show semiconducting behavior supported by band structure calculations of extended Hückel type. The racemic salt contains only one independent donor in the mixed valence oxidation state +0.5. Under ambient pressure the racemic material is metallic down to 120 K, while an applied pressure of 11.5 kbar completely suppresses the metal-insulator transition. Band structure calculations yield an open Fermi surface, typical for a pseudo-one-dimensional metal, with unperfected nesting, thus ruling out the possibility of charge or spin density modulations to be at the origin of the transition. Raman spectroscopy measurements, in agreement with structural analysis at 100 K, show no indication of low-temperature charge ordering in the racemic material at ambient pressure, thus suggesting Mott-type charge localization for the observed metal-insulator transition.</p>
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