Poster Presentation

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Adducts of Trimeric Perfluro-o-Phenylene Mercury with TTF or DTT

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Since the discovery of metallic conductivity in the TTF-TCNQ complex, the charge transfer (CT) complex materials have been studied for such properties as semiconductivity or superconductivity. The synthesis of new CT materials using trimeric perfluoro-orthophenylene mercury (Hg3) as electron acceptor compound was done first by Haneline and Gabaï [1]. A series of studies of CT materials containing Hg3 and tetrathiafulvalene (TTF) or dithieno thiophene (DTT) as an electron donor compounds was carried out by different methods. Co-crystalzation with TTF gave a larger variety of co-crystals than with DTT, producing three polymorphs and one pseudopolymorph. One pot crystal growth of TTF and Hg3 in a 1:1 mixture of solvents dichloromethane (DCM) and dichloroethane (DCA) has led to the formation of TTF polymorphs 1 and 2 with same 1:1 donor acceptor ratio [Hg3·TTF] as well a pseudopolymorph [Hg3·TTF·DCA] 3 that contains the solvent DCA in the asymmetric unit. Slow evaporation in a 1:1 mixture of dichloromethane and carbon disulfide was used to obtain the previously reported CT [(Hg3)2·TTF] (4)1. By slow evaporation as well in pure dichloromethane was obtained the CT material [Hg3·DTT·DCM] 5. All these five CT co-crystals contain mixed donor acceptor stacks, however only in 3, 4 and 5 these stacks are parallel to each other. In the packing of 1 and 2 these stacks are in herringbone arrangement. Polymorphs 1 and 2 differ in crystal shape and color. Contacts Hg···S shorter than the sum of the Van Der Walls radii were observed in the five CTs materials reported, however only 1, 2, 3, and 5 have extended short donor acceptor molecular associates. Moreover only 3, and 5 has these extended donor acceptor associates along one direction.

[1] Haneline, M. R.; Gabbaï, F. P., TTF and TCNQ adducts of trimeric perfluoro-ortho-phenylene mercury. Comptes Rendus Chimie 2004, 7, (8–9), 871-876.

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