Elementorganische Verbindungen mit *o*-Phenylenresten, XXXI [1]. Charge-transfer-Komplexe von 2,3,7,8-Tetrakis(methylthio)chalkogenanthrenen mit 7,7,8,8-Tetracyanchinodimethan und Tetracyanethen

Organometalloidal Compounds with *o*-Phenylene Substituents, Part XXXI [1]. Charge-transfer Complexes of 2,3,7,8-Tetrakis(methylthio)chalkogenanthrenes with 7,7,8,8-Tetracyanoquinodimethane and Tetracyanoethene

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Z. Naturforsch. **53 b,** 1316–1322 (1998); eingegangen am 3. Juli 1998

2,3,7,8-Tetrakis(methylthio)thianthrene and -selenanthrene/7,7,8,8-Tetracyanoquinodimethane, 2:1 Charge-Transfer Complexes, Donor/Acceptor/Donor Units; 2,3,7,8-Tetrakis(methylthio)thianthrene/Tetracyanoethene, 2:1 Charge-Transfer Complex, Columnar Structure; MNDO Calculations

The title compounds are prepared by slow evaporation of dilute solutions of the components. 2,3,7,8-Tetrakis(methylthio)thianthrene and -selenanthrene give isostructural 2:1 complexes with 7,7,8,8-tetracyanoquinodimethane (TCNQ) built up by donor/acceptor/donor units in which the TCNQ molecule is inserted into the cavity formed by two of the folded, oppositely arranged chalcogenanthrene molecules. These units are connected to chains by S···S contacts via the methylthio groups. From 2,3,7,8-tetrakis(methylthio)thianthrene and tetracyanoethene again a 2:1 complex is obtained, however, with a columnar structure in which two donor stacks are slightly interlinked by an acceptor stack thus forming a structure with alternating donor and acceptor molecules. The molecules are arranged in such a way that an optimum overlap of the HOMOs of the donors and the LUMOs of the acceptors, all of which are of π-type character according to MNDO calculations, is secured.

* Sonderdruckanforderungen an Prof. Dr. G. Klar.