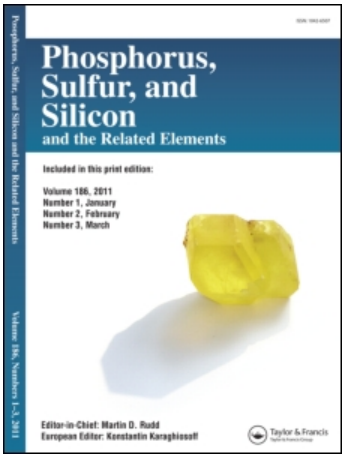

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AN ESCA STUDY OF THE ELECTRONIC STRUCTURE OF TETRATHIONAPHTHALENE AND TETRATHIOTETRACENE: TWO PLANAR AROMATIC BIS-DISULFIDES WITH SEMICONDUCTING PROPERTIES

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AN ESCA STUDY OF THE ELECTRONIC STRUCTURE OF TETRATHIONAPHTHALENE AND TETRATHIOTETRACENE : TWO PLANAR AROMATIC BIS-DISULFIDES WITH SEMICONDUCTING PROPERTIES.

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High resolution X-ray photoelectron spectra have been obtained for two planar aromatic bis-disulfides : tetrathionaphthalene (Fig. 1, N° 1) and tetrathiotetracene (Fig. 1, N° 2).

By looking not only at the outer shells forming the valence band, but also at C1s and S2p core levels and their shake-up satellites, we are able to give a detailed picture of the electronic structure of these two compounds in relation with their molecular geometry.

In particular, a complete description is given for the disulfide group bonding with zero CSS/SSC dihedral angle to an aromatic system. The various atomic contributions to molecular orbitals in the C-S bonds have been explored.

We have found that low-energetic core-level shake-up satellites, indicating the excitation of a valence electron to an unoccupied molecular state, occur easier in this C-S bond region. As such an excitation is needed in the mechanism of conductivity, we conclude that the molecular orbitals involved in the C-S bond must play a determining role in the electron conduction by these organic solids. The participation of sulfur 3d orbitals in this phenomenon is also discussed in relation with formal atomic charges in the molecule.

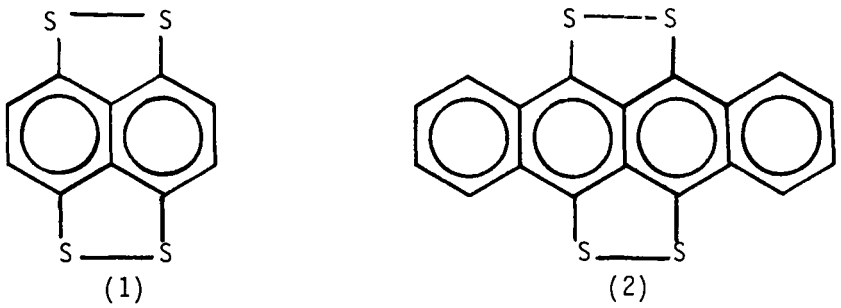

Fig. 1 : Schematic molecular structure of tetrathionaphthalene (1) and tetrathiotetracene (2).