

Wechselwirkungen in Molekülkristallen, 155 [1, 2].

Kristallzüchtung und Strukturbestimmung des Radikalkation-Salzes

[Tetrahydrotetrathiafulvalenium^{•⊕}][AlCl₄[⊖]]

Interaction in Molecular Crystals, 155 [1, 2]. Crystallization and Structure Determination of the Radicalcation Salt [Tetrahydrotetrathiafulvalenium^{•⊕}][AlCl₄[⊖]]

Hans Bock^a, Andreas Seibel^a, Mark Sievert^a und Zdenek Havlas^b

^a Institut der Anorganischen Chemie der Universität Frankfurt, Marie-Curie-Str. 11, D-60439 Frankfurt am Main, Bundesrepublik Deutschland

^b Institut für Organische und Biochemie der Tschechischen Akademie der Wissenschaften, Flemingovo nam 2, CZ-11610 Prag, Tschechische Republik

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Professor Dieter Seebach gewidmet

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Hexathia-dispiro[4.0.4.4]decane, Tetrahydrotetrathiafulvalenium Radical Cation Salt, DFT Calculations

The dark red tetrahydrotetrathiafulvalenium radical cation has been generated 20 years ago by iodine oxidation of hexathia-dispiro[4.0.4.4]decane and characterized in solution by its temperature-dependent ESR spectrum. Here we report the single crystal growth of its tetrachloroaluminate salt as well as its low temperature structure determination, which proves the C=C double bond to be elongated to 140 pm length and one molecular half to be twisted by 7°. The assumed slight cyanine type distortion is supported by structural comparison with tetrakis(dimethylamino)ethene dication salts and with the 1:3 complex of tetrahydrotetrathiafulvalene mercury dichloride. Unrestricted Density Functional Theory calculations predict both the spin as well as the positive charge to be distributed predominantly within the π molecular center {S₂C=CS₂}.