

Wechselwirkungen in Molekülkristallen, 166 [1, 2].

Polyiod-Moleküle $I_2C=CI_2$, $(IC)_4S$, $(IC)_4NH$, $(IC)_4N-CH_3$ und HCl_3 : Strukturbestimmung nach Kristallzüchtung oder durch

Dichtefunktionaltheorie-Berechnung

Interaction in Molecular Crystals, 166 [1, 2]. Polyiodo Molecules $I_2C=CI_2$, $(IC)_4S$, $(IC)_4NH$, $(IC)_4N-CH_3$ and HCl_3 : Structure Determination Following Crystallization or by Density Functional Theory Calculation

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Tri- and Tetraiodo-Substituted Carbon Compounds, Density Functional Theory Calculations

The structures of tri- and tetraiodo-substituted carbon compounds are determined either experimentally by X-Ray Structure Analysis or, because crystallization of tetraiodothiophene could not be achieved, approximated by Density Functional Theory optimization of structural data from a donor/acceptor complex. The structures show noteworthy details such as a second polymorph of tetraiodoethene crystallized by sublimation or herringbone crystal packing patterns of tetraiodopyrrole derivatives. All molecular geometries are discussed and compared based on relativistic density functional theory calculations with 6-31G* basis sets including iodine pseudopotentials. They reproduce even finer structural details due to van der Waals repulsion of the bulky iodo substituents. Natural Bond Orbital (NBO) charge distributions suggest positive partial charges at all iodine centers with the strongest polarization $C^{\delta-} \rightarrow I^{\delta+}$ in HCl_3 , which contains well over 97% iodine.