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The Crystal Structure of N,N'-Ditosyl-*p*-phenylenediamine, Density Functional Theory Calculations of Conformations and Hydrogen Bond Motifs in Sulfonamides

Hans Bock*, Norbert Nagel, Christian Näther

Institut für Anorganische Chemie der Universität Frankfurt,
Marie-Curie-Str. 11, D-60439 Frankfurt am Main

Herrn Professor Manfred Eigen gewidmet

Z. Naturforsch. **53 b,** 1389–1400 (1998); eingegangen am 19. August 1998

Sulfonamides, Crystal Structure, N,N'-Ditosyl-*p*-phenylendiamine, Density Functional Theory Calculations

In a study preceeding the investigation of a novel class of inclusion compounds, the low-temperature crystal structure of the host-molecule N,N'-ditosyl-*p*-phenylenediamine has been determined. It crystallizes in the monoclinic space group $P2_1/n$ with two formula units in the unit cell, forming layers of hydrogen-bonded molecules. The essential subunits are rigid phenyl rings and flexible sulfonamide linkages C-N(H)-S(O_2)-C, the conformations of which are discussed by comparison with data from the *Cambridge Structural Database* and based on density functional theory (DFT) as well as semiempirical PM3 calculations for the selected model compounds, N-methyl-methane-, N-methyl-benzene- and N-phenyl-methane-sulfonamide. The torsion angle dependent energy and enthalpy profiles allow estimates of the rotational barriers around the C-S-N-C bonds. In addition, potential hydrogen bonding by the host molecule is discussed in comparison to analogous carbonic acid derivatives.

* Sonderdruckanforderungen an Prof. Dr. H. Bock; E-mail: bock@chemie.uni-frankfurt.de