Wechselwirkungen in Molekülkristallen, 154 [1 - 3]. Wirt/Gast-Einschlußverbindungen von N,N'-Ditosyl-*p*-phenylendiamin-Derivaten: Die Kristallstrukturen von N,N'-Di(4-nitro-benzosulfuryl)-*p*-phenylendiamin und seinen Wasserstoffbrücken-Addukten mit Cyclopentanon, Cyclohexanon, Tetrahydrofuran, N,N-Dimethylformamid- sowie Pyridin

Interactions in Molecular Crystals, 154 [1 - 3]. Host/Guest-Inclusion Compounds of N,N'-Ditosyl-*p*-phenylenediamine Derivatives: The Crystal Structures of N,N'-Di(4-nitro-benzosulfuryl)-*p*-phenylenediamine and its Hydrogen-Bonded Adducts with Cyclopentanone, Cyclohexanone, Tetrahydrofurane, N,N-Dimethylformamide as well as Pyridine

Hans Bock*, Norbert Nagel, Peter Eller

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

Herrn Professor Manfred Eigen gewidmet

Z. Naturforsch. **54 b,** 501–514 (1999); eingegangen am 26. Oktober 1998

N,N'-Di(4-nitro-benzosulfuryl)-*p*-phenylenediamine, Inclusion Compounds, Hydrogen Acceptor Guest Molecules, Crystal Growth, Structures

Based on preceeding investigations on the crystallization and structures of 13 inclusion compounds with a variety of guest molecules in the host matrix of N,N'-Ditosyl-*p*-phenylenediamine, the crystal structures of N,N'-Di(4-nitro-benzosulfuryl)-*p*-phenylenediamine and the five hydrogen bond acceptor molecules cyclopentanone, cyclohexanone, tetrahydrofurane, N,N-dimethylformamide, and pyridine are reported and discussed. In all of the host/guest aggregates formed, the planes of the (4-nitro)phenyl substituents are more strongly twisted out of the p-phenylene plane than in the guest-free host crystal structure, substantiating the importance of optimum conformation of the sulfonamide backbone. The dominant interactions, however, are the hydrogen bonds from the donor host to the acceptor guest, which prevent the usual formation of (sulfonamide···sulfonamide) hydrogen bond motifs in the host lattice. A pecularity is found in the 4:1 stochiometry of the pyridine inclusion compound of N,N'-di(4-nitro-benzosulfuryl)-*p*-phenylenediamine.

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