

°. There are numerous publications devoted to the synthesis of halogenobutadienes containing atom of chlorine. They possess a broad spectrum of useful properties: they are employed as monomers for the preparation of valuable polymers and copolymers resistant to heat, light, chemical corrosion, etc. and they show algicidal, bactericidal fungicidal activities[1]. A number of halogenobutadienes manifest high antitumour activity. However, there are a few reports on the crystal structures of nitrobutadiene compounds[2,3]. It is the first publication about single crystal structure of 1,1,3-tris(arylthio)nitrobutadiene derivative.

The title compound, (I), was synthesized from 2-nitropentachlorobutadiene and benzyl mercaptan[4]. It is noted that, our spectroscopic data are in accordance with reported by this article but apparently, title compound is not a 1,1,4-substituted, but a 1,1,3-substituted regioisomer instead. This indication was proven by X-Ray analysis newly. Crystallographic analysis was carried out and the results are presented in this paper.

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Keyword: single-crystal structure analysis; sulfur compounds; synthetic organic chemistry

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NBO Analysis – A Useful Tool on Interpretation of Results of Crystal Structure Determination.

Eva Scholtzová^a, Pavel Mach^a, Vratislav Langer^b.

^a*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, SK-845 36 Bratislava, Slovak Republic.* ^b*Environmental Inorganic Chemistry Department of Chemical and Biological Engineering, Chalmers University of Technology, SE-41296 Göteborg, Sweden.*

E-mail: uacheva@savba.sk

General picture of crystal structure of compounds, especially of molecular crystals, can be appropriately complemented by means of Natural Bond Orbital (NBO) analysis, which provides a detailed view on the electronic structure of compounds. NBO analysis is based on a method for optimal transformation of a given wavefunction into a localized form, corresponding to the one-center (“lone pair”) and two-center (“bond”) elements of the Lewis structure picture [1]. NBO analysis provides information on localization of the individual Natural Atomic Orbitals (NAOs), degree of delocalization of the electronic structure, resonance structures, charge balance, bond orders (Wiberg indices) and other useful information on electronic structure of a compound. This method has been successfully applied in our works on several crystal structures of push-pull olefins [2-4], where the charge balance, possible and preferred resonance structures and Wiberg indices have been analysed. The contribution of lone pairs of respective atoms to electronic density of a bifunctional monophenol

[5], pyrazoline chromophore [6], fluoroquinolone [7] and imidazol[2, 1/b]thiazoles [8] (Fig. 1) and deviations from the expected bond orders in those compounds have been analyzed. NBO analysis revealed the impact of electronic redistribution to geometrical parameters in these molecules. It was found that the electronic delocalization caused shortening of the respective single bonds and/or elongating of some double bonds, when compared to typical bond lengths in the crystal structures of similar compounds.

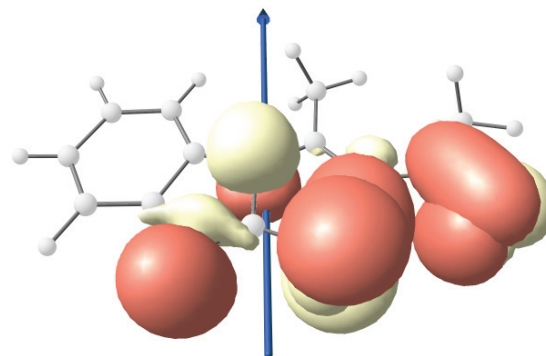


Fig. 1 The contributions of lone pairs of respective atoms to the electronic structure of 2-acetyl-3-methylbenzo[d]imidazol[2, 1/b] thiazole. The arrow represents the direction of total dipole moment.

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Hindered Rotation in N-(Acyloxy)-4-methylthiazole-2(3H)-thiones.

Ingrid Svoboda^a, Hartmut Fuess^a, Uwe Bergstraesser^b, Sabine Altermann^b, Jens Hartung^b. ^a*Department of Materials Science University of Technology Darmstadt, Germany.* ^b*Department of Organic Chemistry, TU Kaiserslautern, Germany.*

E-mail: svoboda@tu-darmstadt.de

Dynamic processes associated with a topological exchange of substituents in mixed anhydrides composed of carboxylic and cyclic thiohydroxamic acids were unexpectedly slow at ~298 K [1]. At ~320 K signal coalescence occurred for anhydrides derived from cyclic thiohydroxamic acid N-hydroxy-4-methylthiazole-2(3H)-thione and β-disubstituted carboxylic acids. At temperatures significantly above this point, fast exchange of diastereotopic substituents was evident from averaged