Halo Derivatives of 2,4-Dinitrothiolene 1,1-Dioxides: Synthesis and Structure

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Received February 14, 2001

Abstract—Procedures were developed for preparing representatives of a new type of halonitrothiolene 1,1-dioxides: mono- and dihalo derivatives of 2,2,4-tri- and 2,4-dinitro-3-thiolene 1,1-dioxides. An X-ray diffraction study showed that 2,5-dinitro-2,3-dichloro-3-thiolene 1,1-dioxide molecules exist in the crystal as enantiomeric pairs; the five-membered rings have the *envelope* conformation, with deviation of the sulfur atom from the ring plane; the halogen atom and nitro group at the multiple bond are essentially coplanar with the ring.