Steerochemistry of heterocycles. - V. Stereochemical peculiarities of 1,3-dioxanes and 1,3-dithianes

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Abstract

The stereochemical peculiarities of substituted 1,3-dioxanes and 1,3-dithianes are discussed. The high probability of the existence of flexible conformations in these series, the considerable energy preference of the 5-C-axial position in the chair conformation of 1,3-dioxanes and 1,3-dithianes, and the definite preference of the 2-C-axial position in the chair conformation of 1,3-dithianes as compared with the axial conformations of the cyclohexane type are noted. The PMR spectra of stereoisomeric 2,5-dimethyl-5-isopropyl-1,3-dioxanes, 2-methy-15-isopropyl-1,3-dithianes, and 2,2,5-trimethyl-1,3-dithiane are described, and their configurations and preferred conformations are proved. The results of a study of the epimerization of stereoisomers of substituted 1,3-dioxanes and 1,3-dithianes are examined, and the conformational energies of individual substituents in the 5-position of these cyclic systems are calculated on the basis of this examination. © 1973 Consultants Bureau, a division of Plenum Publishing Corporation.

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