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Stereochemistry of 1,3-dithia-5,6-benzocyclohepte-e-s-oxides

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Abstract

According to dynamic 13C NMR spectroscopy trans-2-R-(R=Ph, Me, Et, Pri)-5,--benzocycloheptene-1-oxides at -60°C in CDCl 3 exist as an equilibrium mixture of the chair and boat forms with the substituents in the equatorial position. Unsubstituted (R=H) compound has in addition a boat form with an axial sulfinyl group, whereas for Bu t derivative conformational equilibrium is anancomerically shifted to the boat structure. X-ray study of trans-2-isopropyl--,3-dithia-5,6- benzocycloheptene-1,3-dioxide displays a chair form with equatorial alkyl substituent and axial-equatorial SO-moieties.

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Keywords

Dynamic 13C NMR spectroscopy, Sulfoxides of seven-membered dithioacetals, X-ray crystallography