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Geometric structure of 2-phenyl-1,3-dithia-5,6-benzocycloheptene 1-oxide

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Abstract

Two-dimensional nuclear Overhauser effect spectroscopy (2D NOESY) was used to determine proton-proton distances for the chair conformer of 2-phenyl-1,3-dithia-5,6-benzocycloheptene 1-oxide in CD2Cl2 in the system CS2-CDCl3. Changing the solvent by a more polar changes the molecular conformation. As a result, the dipole moment may also be affected, and this should be taken into account in analysis of solvent effects on thermodynamic parameters of the conformational equilibrium.

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