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Stereochemistry of seven-membered heterocycles: XLVII. Synthesis, NMR, XRD, and theoretical investigation of monosulfoxides of (Z)-4,7-dihydro- 1 λ 4,3-dithiepine series

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Abstract

By oxidation of (Z)-4,7-dihydro-1,3-dithiepines with meta-chloroperbenzoic acid the corresponding 4,7-dihydro-1 λ 4,3-dithiepine 1-oxides were synthesized in ~85% yield. A complete assignment of signals in the ¹H and ¹³C NMR spectra of the compounds obtained was established. According to XRD analysis the seven-membered heterocycles crystallized in conformations chair or boat. The calculations by DFT method in the B3LYP/6-31G(d,p) version showed the possibility of conformational equilibrium of these forms in the gas phase. © 2010 Pleiades Publishing, Ltd.

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