

Stereochemistry of seven-membered heterocycles: XLVI. Synthesis and dynamic ^{13}C NMR spectroscopy of spiro[cyclohexane-1,4'-[3,5] dioxabicyclo[5.1.0]octanes]. DFT calculations of structurally related formaldehyde and acetone acetals

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Abstract

Spiro[cyclohexane-1,4'-[3,5]dioxabicyclo[5.1.0]octanes] were synthesized, and their conformational behavior was studied by dynamic ^{13}C NMR spectroscopy. Anancomeric displacement of conformational equilibrium toward two nonequivalent twist conformers with close energies was revealed. The relative Gibbs energies ΔG° and enthalpies of formation ΔH° of twist and chair-like conformers with endo and exo orientation of the three-membered ring of structurally related formaldehyde and acetone acetals were calculated in terms of the density functional theory at the B3LYP/6-31G(d,p) level. Like spiro-cyclohexane analogs, they were shown to have a non-chair conformation. © 2007 Pleiades Publishing, Ltd.

<http://dx.doi.org/10.1134/S1070428007120196>
