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Stereochemistry of seven-membered heterocycles: XLVI. Synthesis and dynamic 13C 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 13C NMR spectroscopy. Anancomeric displacement of conformational equilibrium toward two nonequivalent twist conformers with close energies was revealed. The relative Gibbs energies ΔG o and enthalpies of formation ΔH o 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.

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