Conformational Analysis of 5-Methyl-1,3-oxathiane

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Abstract—Computer simulation of conformational transformations of 5-methyl-1,3-oxathiane at the DFT PBE/3ζ, RI-MP2/λ2, and HF/6-31++G(*d*,*p*) levels of theory has shown that the interconversion between the equatorial (global minimum) and axial *chair* conformers occurs along several independent pathways through five flexible forms. Nine transition states corresponding to different half-*chair* forms, as well as symmetrical and unsymmetrical *boat* conformers, have been localized on the potential energy surface. The free conformational energy of the methyl group has been estimated at 0.9–1.0 kcal/mol by comparison of the calculated and experimental vicinal coupling constants in the ^{1}H NMR spectra.

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