Conformational Analysis of 2-Isopropyl-5-methyl-5-methoxymethyl-1,3,2-dioxaborinane

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Abstract—Study of conformational transformations of 2-isopropyl-5-methyl-5-methoxymethyl-1,3,2-dioxaborinane using DFT approximation PBE/3ζ and the second order perturbation theory method RI-MP2/λ2 revealed beside the interconversion route *sofa–sofa* through a transition state corresponding to 2,5-twist form a number of local minima due to internal rotation of isopropyl and methoxymethyl substituents in *sofa* conformers. Over 88% of the molecules of the studied compound are present in a *sofa* form with the equatorially oriented CH_2OCH_3 group.

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