Conformational Analysis of Stereoisomers of 2,4-Dimethyl-5-isopropyl-1,3,2-dioxaborinane

V. V. Kuznetsov

Ufa State Aviation Technical University, Ufa, 45000 Russia
e-mail: kuzmaggy@mail.ru
Ufa State Petroleum Technological University, Ufa, Russi

Received August 4, 2012

Abstract—The investigation of conformation conversions of *cis*- and *trans*-isomers of 2,4-dimethyl-5-isopropyl-1,3,2-dioxaborinane using *ab initio* quantum-chemical approximation HF/6-31G(d) and the hybrid DFT-method PBE/3z showed that the routes of the transformations presuppose an equilibrium between sofa conformers with the different orientation of substituents at the atoms C^4 and C^5 of the ring that convert into each other through transition states corresponding to the equatorial and axial conformations of the 2,5-*twist* form. Based on experimental data of ^1H NMR spectra and calculated vicinal spin-spin coupling constants the quantitative conformational composition of *cis*- and *trans*-isomers was established and also the ΔG^o value of the conformation equilibrium was determined.

DOI: 10.1134/S1070428013020206