Ab Initio Conformational Analysis of Tetrahydro-1,3-oxazine

V. V. Kuznetsov

Ufa State Petroleum Technological University, ul. Kosmonavtov 1, Ufa, 450062 Bashkortostan, Russia
e-mail: kuz@anrb.ru

Institute of Molecular and Crystal Physics, Ufa Research Center, Russian Academy of Sciences

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Abstract—Nonempirical RHF/STO-3G and 6-31G(*d*) studies on conformational behavior of tetrahydro-1,3-oxazine showed that interconversion between the axial (global minimum) and equatorial *chair* conformers can follow five independent pathways. The potential energy surface contains seven minima corresponding to *chair* and *twist* conformers, as well as seven transition states having *sofa*, *half-chair*, and *symmetrical* and *unsymmetrical boat* conformations. Additional potential barriers to interconversion, resulting from pyramidal inversion of the nitrogen atom, were also revealed.

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