Conformational Analysis of 5-Bromo-5-nitro-1,3-dioxane

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Abstract—Conformational analysis of 5-bromo-5-nitro-1,3-dioxane has been performed by computer simulation in terms of HF/pVDZ, hybrid DFT PBE/3ξ, and RI-MP2/λ2 quantum chemical methods. The global minimum on the potential energy surface corresponds to the *chair* conformer with axial nitro group, and the other two minima have been identified as *chair* conformer with equatorial nitro group and 2,5-*twist*. All transition states on the route of conformational transformations of the title molecule have been revealed.

Keywords: 5-bromo-5-nitro-1,3-dioxane, potential energy surface, conformer, energy minimum, transition state

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