Conformational Analysis of 4,4-Dimethyl-1,3-dioxane

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Abstract—The potential energy surface of 4,4-dimethyl-1,3-dioxane molecule was analyzed in terms of the density functional theory at the PBE/cc-pVDZ and B3PW91/aug-cc-pVDZ levels. Eight energy minima were revealed with account taken of enantiomeric structures, the corresponding transition states were found, and the most probable *chair–chair* conformational isomerization pathways were proposed.

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