Quantum-Chemical Study of 1,3-Dioxane Complexes with Two Water Molecules

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Abstract—Methods PM3, RHF/6-31G(d), and MP2/6-31G(d)//RHF/6-31G(d) were used in calculation of the energy of formation of five 1,3-dioxane complexes with two water molecules formed through hydrogen bonds. The study of the conformational properties of the most stable associate revealed two routes of the *chair–chair* conformation isomerization. It was shown that the difference between the minima on the potential energy surface in this gase increased, and the barriersto the interconversion decreased as compared to the calculated values for the isolated molecule of 1,3-dioxane.

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