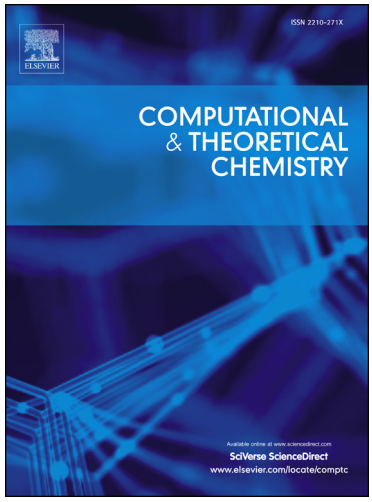

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Catalytic effect of water, water dimer, or formic acid on the tautomerization of nitroguanidine

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Abstract

We have investigated the reaction mechanisms and kinetics of water, water dimer, or formic acid catalyzed gas-phase isomerization of α–nitroguanidine to β–nitroguanidine by means of high level theoretical methods and transition state theory. The potential energy surface profile has been characterized at the CCSD(T)/6-311++G(2df,2pd)//M06-2X-D3/6-311++G(3df,3pd) level with zero-point energy correction. The calculations indicate that incorporation of water, water dimer, or formic acid molecule into the reactant α–nitroguanidine can noticeably reduce the energy barrier. The reductions are found to be small for water and most significant for formic acid. Most importantly, the kinetics calculations show that the rate constants for the water, water dimer or formic acid assisted reactions are about 14, 14 or 19 orders of magnitude larger than those for the uncatalyzed reaction, respectively. These results suggest that formic acid should play a larger role than both water and water dimer on isomerization of α–nitroguanidine to β–nitroguanidine

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