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A tautomerism in 2-amino-7H-purine-6-thiol: Theoretical study using implicit/explicit salvation models

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Abstract

A theoretical study at the B3LYP/6-31++G(d,p) level was performed on the tatumerization of 2-amino-7H-purine-6-thiol into 2-amino-9H-purine-6-thiol. Such a tautomerism can take place *via* three different pathways namely A, B and C. The energetic results associated with the gas phase reveal that pathways A, B and C display a very high activation Gibbs free energy of 47.6, 69.4 and 52.1 kcal/mol, respectively, indicating this process cannot take place in the gas phase. When solvent effects of water are taken into account through a continuum of a uniform dielectric constant, the gas phase activation Gibbs free energies increase to 51.1, 71.9 and 55.4 kcal/mol along pathway A, B and C, respectively, emphasizing long range solute-solvent interactions do not play a key role in the considered tautomerization. The studied process can easily take place by inclusion of three molecules of water in which a significantly reduced activation Gibbs free energy of 24.8 kcal/mol indicates the predominance of short range solute-solvent interactions over the long range ones. Combination of short range and long range solute-solvent interactions lead to an activation Gibbs free energy of 23.6 kcal/mol for tatumerization of 2-amino-7H-purine-6-thiol into 2-amino-9H-purine-6-thiol. This value clearly points out that employing a polar and protic solvent is able to noticeably reduce the barrier of tatomerization.

Keywords: *Tautomerism, purines, DFT, Explicit and implicit solvation models.*

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