Theoretical Studies on the Tautomeric Properties of Diamino-5-formamidopyrimidines

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The results of theoretical geometry prediction of formamidopyrimidine(fapy)-adenine and fapy-guanine tautomers are presented. Among 54 potential tautomeric structures of fapy-adenine the most stable structure corresponds to the diamino-keto isomer. The solvent effect has insignificant influence on the fapy-adenine tautomers succession. The fapy-guanine has 172 potential isomers. There are three most stable tautomers of this guanine derivative, which may exchange the order depending on the polarity of the environment. In vapour the most probable is the 4-enol-6-keto-diamino tautomer, while in water environment the 4,6-diketo-diamino isomer is dominant. A more polar solvent stabilises more polar fapy-guanine tautomers.

The geometric parameters and point-atomic charges corresponding to most probable tautomers are also supplied.

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