

Accepted Manuscript

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PII: S2210-271X(17)30445-0
DOI: <https://doi.org/10.1016/j.comptc.2017.10.007>
Reference: COMPTC 2646

To appear in: *Computational & Theoretical Chemistry*

Received Date: 31 August 2017
Revised Date: 17 October 2017
Accepted Date: 17 October 2017



Please cite this article as: E.D. Raczyńska, Quantum-chemical studies on the favored and rare isomers of isocytosine, *Computational & Theoretical Chemistry* (2017), doi: <https://doi.org/10.1016/j.comptc.2017.10.007>

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Quantum-chemical studies on the favored and rare isomers of isocytosine

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Abstract: Quantum-chemical calculations have been performed for twenty-one favored and rare isomers of neutral isocytosine in two extreme media, in the gas phase {B3LYP/6-311+G(d,p)} and in aqueous solution {PCM(water)//B3LYP/6-311+G(d,p)}. In aqueous solution, the most aromatic hydroxy-amino form, favored in the gas phase, becomes a rare form, and less delocalized amino-oxo forms predominate. Monoprotonation of the favored isomers leads also to two different forms, the N1-protonated hydroxy-amino cation in the gas phase, and the N1-protonated amino-oxo cation in aqueous solution. Electron delocalization for the solvated isocytosine isomers is parallel to that observed for the isolated molecules. However, aromaticity is not the main factor that influences isomeric stabilities. Geometric and energetic results for neutral isocytosine isomers, compared to those for other pyrimidine bases (uracil and cytosine), show interesting similarities in electron delocalization and important differences in energetic stabilities. Some parallelism in energetic parameters exists for amine-imine and enamine-imine conversions, and separately for amide-iminol and keto-enol ones.

Keywords: Isocytosine, Electron delocalization, Energetic stabilities, Monoprotonation, Proton affinity, DFT and PCM(water)/DFT studies

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