

ON THE BASICITY OF CONJUGATED NITROGEN HETEROCYCLES IN DIFFERENT MEDIA

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Conjugated nitrogen heterocyclic compounds containing one or more nitrogen atoms in their ring(s) are very common in nature, research and technology. Almost all N-heterocycles are basic compounds and often the basicity is essential to the properties of these compounds. The basicity of N-heterocyclic compounds in water has been extensively studied but in non-aqueous media the situation is the opposite – the basicity data is scarce and often inconsistent.

In this fundamental work we explored the relationship between the structure and solvent effects on the basicity of a large selection of conjugated heterocyclic nitrogen bases in different media: the polar aprotic solvent acetonitrile, the polar protic solvent water and the gas phase [1]. The gas-phase basicity is predominantly determined by the ability of a molecule to disperse the excess positive charge over a large number of atoms. In solution the situation is less clear. It was found that the fusion of an additional benzene ring does not always lead to an increase in basicity in solution: its effect can be either basicity increasing or decreasing, depending on the ring size, number and position of nitrogen atoms and medium.

Altogether experimentally determined pK_a values for 30 simple N-heterocyclic compounds in acetonitrile and calculated gas-phase basicity values were presented. A correlation between the measured pK_a values in acetonitrile and in water suggests that these two different solvents exert a similar effect on the basicity of the studied heterocycles.

References

1. M. Lõkov, S. Tshepelevitsh, A. Heering, P.G. Plieger, R. Vianello, I. Leito, 2017, *Eur. J. Org. Chem.*, 30, 4475-4489.



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