

Make Tautomerism Great Again: New Challenges and New Possibilities

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Prototropic tautomerism is one of the most important phenomena in organic chemistry despite the relatively small proportion of molecules in which it can occur. Tautomers are the chameleons of chemistry, capable of changing by a simple change of environment from an apparently established structure to another not perhaps till then suspected, then back again when the original conditions are restored, and of doing this in an instant: intriguing, disconcerting, perhaps at times exasperating¹. It therefore becomes vital to know and/or to predict which tautomer is the major one, since not only structure but chemical properties are bound up with this.

Although currently this field of research is considered mainly as fundamental one, it gives a lot of opportunities for useful applications.

In the present lecture a historical overview of the concept of the tautomerism and methods for investigations of tautomeric systems will be given. Fundamental processes, both structural and environmental, affecting the tautomerism will be discussed. Several tautomeric systems will be considered from the viewpoint of the applicability of the tautomerism and proton transfer: excited state proton transfer, tautomerism in the drug design (curcumin solubility case), tautomeric metal binding ligands (red shift upon complexation), tautomeric vs zwitterionic proton cranes as prototypes of molecular switches and motors.

References:

¹ Taylor, P.J.; van der Zwan, G.; L. Antonov, L. Tautomerism: Introduction, History, and Recent Developments in Experimental and Theoretical Methods. Tautomerism Methods and Theories. (Ed.: L. Antonov), Wiley-VCH, Weinheim, Germany, 2013, pp. 1–24