

Quantum chemical description of the ability to form peptide bonds

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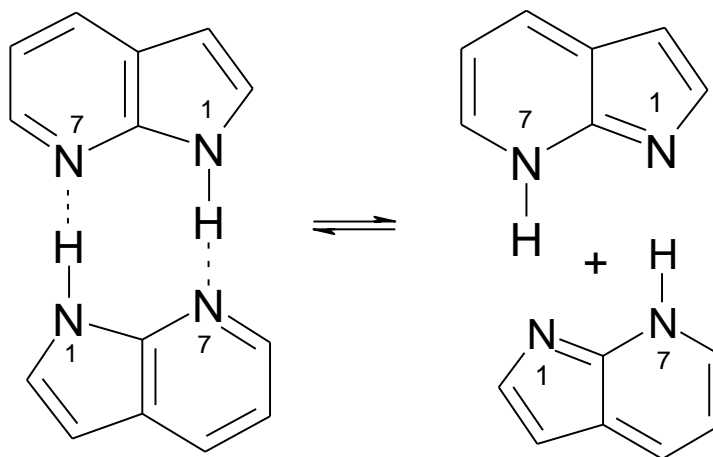
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One of the most popular areas of modern molecular science is the study of the electronic structure and reactivity of biologically active compounds by the modern method of quantum chemistry-the theory of density functional (DFT). The researches of Professor Jumber Kereselidze's in this area is are very successful and topical. In particular, a formula was constructed for the propensity of amino acids to form a peptide bond.

$$K_p = \frac{\Delta q \cdot R_{NH} \cdot R_{CO}}{P_{NH} \cdot P_{CO} \cdot \Delta E^\#}$$

Where Δq is the difference between the charges of carbon and nitrogen atoms of the peptide bond, R_{NH} , R_{CO} and P_{NH} , P_{CO} are the lengths and orders of NH and CO bonds. $\Delta E^\#$ is the activation energy for the formation of peptide bonds.



$$\nu = \frac{c}{\lambda} = c\bar{\nu} = 3 \cdot \frac{10^{10} \text{ cm}}{\text{sec}} 3300 \text{ cm}^{-1} = 10^{14} \text{ sec}^{-1},$$
$$t = \frac{1}{\nu} 10 \cdot 10^{-15} \text{ sec} = 10 \text{ femtosec}$$