Russian Journal of General Chemistry 2006 vol.76 N7, pages 1117-1122

Quantum-chemical study of the structure and reactivity of 4,5-dihydropyrazol-5-ones and their thio and seleno analogs: VIII. Solvation effects and tautomerism of 4,5-dihydropyrazol-5-ones and their thio and seleno analogs

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Abstract

The effect of hydration on the stability of tautomeric forms of 1-methyl-4,5-dihydro-1H-pyazol-5-one, 1-methyl-4,5-dihydro-1H-pyrazole-5- thione, and 1-methyl-4,5-dihydro-1H-pyrzole-5-selone was analyzed by nonempirical quantum-chemical methods at different theory levels. The results of calculations by all these methods, including density functional theory, with two types of models (continuum and discrete) showed stronger stabilization of the NH tautomers of all the examined heteropyrazolones in water, as compared to their CH and XH tautomers. The strongest stabilization effect is reached in the calculation of discrete complexes in terms of the self-consistent reaction field model. The degree of differentiation of the stability of tautomeric forms considerably decreases when electronic correlation is taken into account, whereas the use of polarization functions on hydrogen atoms in addition to polarization functions on heavy atoms almost does not affect the position of the tautomeric equilibrium. © Pleiades Publishing, Inc., 2006.

http://dx.doi.org/10.1134/S107036320607019X