Russian Journal of General Chemistry 2007 vol.77 N9, pages 1628-1634

Quantum-chemical study of the structure and reactivity of pyrazol-5-ones and their thio and seleno analogs: X. 1-methylpyrazol-5-one and its thio and seleno analogs in H-complex formation reactions in the gas phase and in solutions

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Abstract

The effects of specific solvation and self-association of chalcogenpyrazol-5-ones are assessed using nonempirical quantum-chemical, density functional theory (DFT), and MP2 second-order perturbation theory methods. The formation of H-complexes with water, methanol, and DMSO stabilizes all tautomeric forms, the NH tautomers of all hetero analogs being the most affected. The NH tautomers form with water 1:2 complexes which reveal cooperativity. The complexes of chalcogenpyrazolones with DMSO are more stable than the respective complexes with water, and, therewith, the extra stabilization in continuum is less pronounced than in the case of hydration. Quantitatively, the effects of tautomer self-association compare with the effects of interaction of chalcogenpyrazolones with proton-donor solvents.

http://dx.doi.org/10.1134/S1070363207090228