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Quantum-chemical studies of the structure and reactivity of Pyrazol-5-ones and their Thio and Seleno analogs: V. effect of electron correlation on tautomerism and acidity of 1-Methylheteropyrazolones

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Abstract

The relative stability of tautomeric forms of 1-methyl-substituted heteropyrazolones (O, S, Se) and their gas-phase acidity were estimated by DFT calculations with various basis sets and methods of geometry optimization. The electron correlation effects make an appreciable contribution to the Gibbs free energies of their tautomers and anions, especially those containing the heavy atoms. The qualitative pattern of tautomerism in pyrazolones is essentially similar to that obtained by semiempirical and nonempirical RHF calculations: The most stable is the CH form. For hetero analogs, consideration of electron correlations effects increases the relative stability of SH (SeH) forms. The series of relative acidity of the compounds depending on the heteroatom is preserved (Se ≥ S ≫ O).

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