

## **Quantum-Chemical Studies of the Structure and Reactivity of Pyrazol-5-ones, Their Thio and Seleno Analogs. I. Nonempirical and Semiempirical Calculations of the Structure of Some 1,3- And 1,4-Substituted 2-Pyrazolin-5-ones**

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### **Abstract**

Energies for various tautomeric forms of pyrazolones substituted in the 1, 3 and 4 positions, and for a series of their protonated and deprotonated forms are calculated by the nonempirical STO-3GF and semiempirical CNDO/2 methods. Analysis of the effect of electronic and spatial structure of the substituents on the stability of the tautomeric forms, the energies of frontier orbitals, and the effective atomic charges is performed. The calculated characteristics were applied to explanation and prediction of some aspects of reactivity of pyrazolones.

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