Quantum-Chemical Study of the Structure and Reactivity of Pyrazol-5-ones and Their Thio and Seleno Analogs: VI.[1] Tautomeric and Acid–Base Properties of 3-Methyl-1-phenyl-4,5-dihydropyrazol-5-one, 3-Methyl-1-phenyl-4,5-dihydropyrazole-5-thione, and 3-Methyl-1-phenyl-4,5-dihydropyrazole-5-selenone

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Abstract - The relative stabilities of tautomeric forms of 3-methyl-1-phenylpyrazol-5-one and its 5-thioxo and 5-selenoxo analogs, as well as their acid–base properties in the gas phase, were estimated in terms of nonempirical calculations and density functional theory. According to the results of both calculation methods, the CH tautomer of 3-methyl-1-phenylpyrazol-5-one is the most stable. The stabilities of the XH and CH forms of its heteroanalogs (X = S, Se) are comparable; the relative stability of the SeH (SH) tautomers increases when thermal corrections, zero-point energy, and electron correlation effects are taken into account. The two methods indicate increase in the gas-phase acidity of the title compounds on variation of the heteroatom in the series O < S < Se and fairly similar basicities of the oxygen and sulfur analogs.