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Tautomeric design of *ortho*-hydroxyheterocyclic *Schiff* bases.

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Streszczenie

The article reports on the synthesis and crystallographic and theoretical studies on various heterocyclic derivatives of *ortho*-hydroxy *Schiff* bases. The prevailing of one of the two (enolimine – OH and ketoamine – NH) tautomeric forms has been stated in studied compounds depending on the substitutes in heterocyclic formation, the nitrogen and carbon atoms of the imine group. A specific situation has been shown in (1*E*)-1-(5-chloro-2-hydroxy-3-nitrophenyl)ethanone oxime compound. The potentials on the proton transfer of the hydrogen bridges in these compounds have been found out. Grounded on the obtained potential curves the influence of the protonation on nitrogen in the pyridoxal derivative of the studied *ortho*-hydroxy *Schiff* bases has been analysed. The most efficient method of the impact (by means of various substitutes) on the intramolecular tautomeric equilibrium in *ortho*-hydroxy *Schiff* bases has been presented.

Słowa kluczowe

Tautomeric equilibrium, hydrogen bonding, Schiff-base, Pyridoxal and oxime

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