Solvent Effect on the Tautomeric Equilibria of 2- and 4-hydroxypyridines and Their Sulphur Analogues.

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Abstract

The tautomeric equilibria of 2- and 4-hydroxypyridines and their sulphur analogues were investigated at the HF/6-31 G+d level of theory. The potential energy surface of the tautomerization process is explored, critical points are well identified, and a correlation effect on the energetic of the process is computed at the MP2 level. Similarities and differences in the geometric features of the transition states of the 2- and 4-hydroxy derivatives are pointed out. The effect of replacing oxygen by sulphur on the geometries and energies of the tautameric equilibria are discussed. Solvent effects on the studied tautomerization processes are carefully examined using the self-consistent reaction field model (SCRF). Results of the present work elaborate on the known chemistry of pyridines and phenols.