Solvatochromism of Heteroaromatic Compounds: XX.[1] 4(5)-Nitroimidazole

A. I. Vokin, L. V. Sherstyannikova, I. G. Krivoruchka, T. N. Aksamentova, O. V. Krylova, and V. K. Turchaninov

Favorskii Irkutsk Institute of Chemistry, Siberian Division, Russian Academy of Sciences, Irkutsk, Russia

Received May 21, 2001

Abstract - 4(5)-Nitroimidazole in solution is stabilized as the 5-nitro isomer due to formation of hydrogen bond with an aprotic protophilic solvent. Amphiprotic medium favors displacement of the tautomeric equilibrium toward the 4-nitro isomer via formation of a solvate complex where 4-nitroimidazole acts as hydrogen bond acceptor. The observed specific solvatochromic effect in the UV spectrum of 4-nitroimidazole and related heterocyclic nitro compounds is determined by the electronic configuration of the excited π,π^*-state.