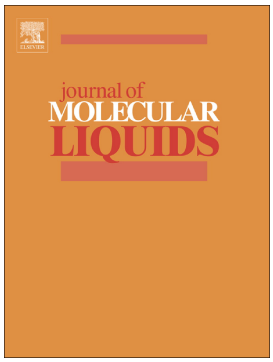

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Multiple dynamics of aroylhydrazone induced by mutual effect of solvent and light - spectroscopic and computational study

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Abstract

The structural identification of aroylhydrazone derived from nicotinic acid hydrazide and 2-hydroxy-5-nitrobenzaldehyde was performed in solvents of different polarities (DMSO, acetone, methanol, ethanol) by spectroscopic (NMR, UV-Vis, IR, Raman) and computational methods. In acetone solution *N*'-(2-hydroxy-5-nitrophenylmethylidene)-3-pyridinecarbohydrazide (**1**) adopted the most stable ketoamino form (form I-*E*, –CO–NH–N=C–) stabilised by intramolecular H-bonds. However, in polar protic solvents (MeOH, EtOH) the equilibria between neutral hydrazine molecule in I-*E* form and deprotonated molecule in I-*Z* form was immediately observed, while continuous conversion of I-*E* to I-*Z* was recorded during time in DMSO when solution was kept in dark. However, when solution was exposed to UV light, an isomerisation to form III-*E* in equilibrium with III-*Z* (–CO–NH–NH–C=C–) occurred in all solvents. The tautomeric and isomeric interconversion was most pronounced in DMSO solution, and is consequence of mutual effect of solvent and light. All findings acquired by experimental methods were in excellent agreement with those obtained by DFT computational methods.

Keywords: aroylhydrazones, tautomerism, *cis-trans* isomerism, spectroscopic methods, computational study