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Spectroscopic studies of the intramolecular hydrogen bonding in o-hydroxy Schiff bases, derived from diaminomaleonitrile, and their deprotonation reaction products

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Key words

diaminomaleonitrile, Schiff bases, ¹H, ¹³C, and ¹⁵N NMR, ATR-FTIR, X-Ray, intramolecular hydrogen bond, deprotonation.

Abstract

The structural study of five Schiff bases derived from diaminomaleonitrile (DAMN) and 2-hydroxy carbonyl compounds was performed using ¹H, ¹³C and ¹⁵N NMR methods in solution and in the solid state as well. ATR-FTIR and X-Ray spectroscopies were used for confirmation of the results obtained by NMR method. The imine obtained from DAMN and benzaldehyde was synthesized as a model compound which lacks intramolecular hydrogen bond. Deprotonation of all synthesized compounds was done by treating with tetramethylguanidine (TMG). NMR data revealed that salicylidene Schiff bases in DMSO solution exist as OH forms without intramolecular hydrogen bonds and independent on the substituents in aromatic ring. In the case of 2-hydroxy naphthyl derivative, the OH proton is engaged into weak intramolecular hydrogen bond. Two of imines (salDAMN and 5-BrsalDAMN) exist in DMSO solution as equilibrium mixtures of two isomers (A and B). The structures of equilibrium mixture in the solid state have been studied by NMR, ATR-FTIR and X-Ray methods.

The deprotonation of three studied compounds (salDAMN, 5-BrsalDAMN, and 5-CH₃salDAMN) proceeded in two different ways: deprotonation of oxygen atom (X form) or of

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