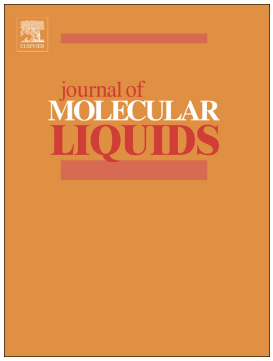

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Inhibited Rotation of Amide Group around C-N bond of Nicotinamide in Different Solvents by ^{1}H DNMR Data

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Present work reports on the influence of solvent nature on the intramolecular rotation barrier of nicotinamide amide group. The values of Gibbs energy of activation are determined at the coalescence temperature. The rotation barrier in vacuum, $CDCl_3$, DMSO and water is estimated by quantum chemistry methods and found to be in good agreement with experimental results. The energy profile of rotation process is shown to be asymmetrical due to lone pair inversion of amide nitrogen.

Ketwords: nicotinamide, rotation barrier, Gibbs energy of activation, transition state, solvent influence

1. Introduction

The amide bonds play a key role in biochemistry. Nucleic acids, proteins as well as significant amount of medicines (e.g. local anesthetics such as lidocaine, articaine, bupivacaine etc.) include the amide bonds into their composition. Nitrogen lone pair donating towards carbonyl group causing partial double bond character of N-C bond is an important peculiarity of amide group. As a consequence of partial double binding in amides, the conformers and rotamers of