Conformational state of β-hydroxynaphthylamides: Barriers for the rotation of the amide group around CN bond and dynamics of the morpholine ring.

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Three β-hydroxynaphthylamides (morpholine, pyrrolidine and dimethylamine derivatives) have been synthesized and their conformational state was analyzed by NMR, X-ray and DFT calculations. In aprotic solution the molecules contain intramolecular OHO hydrogen bonds, which change into intermolecular ones in solid state. The energy barriers for the amide group rotation around the CN bond were estimated from the line shape analysis of (1)H and (13)C NMR signals. A tentative correlation between the barrier height and the strength of OHO bond was proposed. Calculations of the potential energy profiles for the rotations around CC and CN bonds were done. In case of morpholine derivative experimental indications of additional dynamics: chair-chair 'ring flip' in combination with the twisting around CC bond were obtained and confirmed by quantum chemistry calculations.

Słowa kluczowe

β-Hydroxynaphthylamides, Amide group rotation, Intramolecular hydrogen bond, Conformational isomerism, solvent effects, DNMR

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