Competitive intra- and intermolecular interactions in secondary Mannich bases.

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Rok wydania

2010

Czasopismo

Journal of Molecular Structure

Numer woluminu

976

Strony

290-296

DOI

10.1016/j.molstruc.2010.03.076

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The secondary Mannich base 2-(N-cyclohexylaminomethyl)-4-methyl-phenol (1) was synthesized. The crystal structure was determined whereby linear chains through NH···O hydrogen bonds were detected between molecules containing typical chelate rings with intramolecular OH···N hydrogen bonds, as in the traditionally studied tertiary Mannich bases. The N···O distance appeared much shorter, i.e. 2.614 and 2.601 Å in the two conformers in the chain, in comparison to tertiary Mannich bases [1]. Extensive experimental and theoretical studies on aggregation in solution and in the gas phase (by DFT B3LYP/6-31+G(d,p) calculations) were undertaken. It was shown self-aggregation is weak even in weakly polar CCl4 solvent. Up to the concentration 0.3 mol/dm3, as follows from dipole moment and average molecular weight investigations, there are only monomers of structure resembling those detected in the solid state. The experiments at higher concentrations as well as theoretical calculations proved the postulate that the specific strong intramolecular hydrogen bond found in the solid state of secondary Mannich bases results from intermolecular interactions.

Słowa kluczowe

Secondary Mannich bases, DFT calculations, Strength of hydrogen bond, crystal structure, Anharmonicity

Adres publiczny

https://doi.org/10.1016/j.molstruc.2010.03.076

Strona internetowa wydawcy

http://www.elsevier.com