

КРАТКИЕ СООБЩЕНИЯ

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INTERMOLECULAR HYDROGEN BONDING BETWEEN N-SUBSTITUTED CAPROAMIDES AND TETRAHYDROFURAN

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The results are reported of a study of hydrogen bonding between various N-substituted caproamides and tetrahydrofuran as an O-electron donor by means of FTIR spectroscopy. The spectroscopic characteristics for N—H...O hydrogen bonded complexes are given. The B3LYP functional with 6-31G** basis set has been used to calculate the structural parameters of the studied hydrogen bonded complexes. It can be assumed that both inductive and steric effects play an important role in the stability of these hydrogen bonded complexes.

Key words: hydrogen bonding, N-substituted caproamide, tetrahydrofuran, DFT.

INTRODUCTION

Hydrogen bonding has a great importance in chemistry and biology. Numerous theoretical and experimental studies have been devoted to hydrogen bonding [1—3]. Knowledge of N—H...O interactions of N-substituted amides contributes to a better understanding of the structure of polypeptides and proteins. [4]. In our laboratory, during continuous and extensive research of N-substituted amides and their interactions in solutions, N—H...O, [5—8] hydrogen bonded complexes were investigated using IR techniques. The application of the B3LYP density functional with various basis sets can provide reasonable information about the geometry and energy of different hydrogen bonded complexes [9, 10]. In the present work, we investigated the N—H...O interactions of newly synthesised N-alkyl caproamides in order to provide better insight into the nature of the hydrogen bonding of secondary amides.

EXPERIMENTAL

Various N-monosubstituted caproamides (NsCA) of general formula $\text{CH}_3(\text{CH}_2)_4\text{CONHR}$, wherein R is *n*-propyl, *n*-butyl, *sec*-butyl, *iso*-butyl, *tert*-butyl, and *n*-pentyl (NPrC, NBuC, NsBC, NiBC, NtBC, NPeC), were synthesised by Schotten-Baumann reaction, by acylation of the corresponding amines with alkyl chloride. The purity of these N-monosubstituted amides was checked by GC and mass spectrometry. Based on the GC results all the samples used in this work had purities 99.2 % or better. Tetrahydrofuran was obtained from commercial sources (Fluka, > 97 %) and was used without further purification.

In order to avoid self-association, amide concentrations in carbon tetrachloride solutions were below $0.003 \text{ mol} \cdot \text{dm}^{-3}$. The concentration of tetrahydrofuran varied between $0.25 \text{ mol} \cdot \text{dm}^{-3}$ and $1 \text{ mol} \cdot \text{dm}^{-3}$.

Infrared spectra were obtained using a Thermo-Nicolet Nexus 670 instrument. A DTGS detector was employed in IR measurements. Samples were placed in 1—5 cm (IR) UVIRASIL cells and the measurements were performed at 298 K. The reported frequencies and half-widths were reproducible