

The Appearance of Conformational Mobility of Behenic Acid in IR Spectra

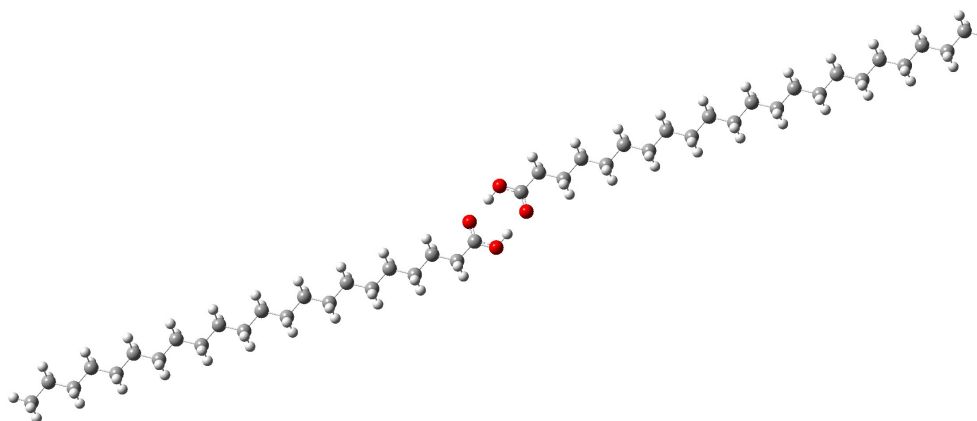
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In the last time the interest in investigation of structure and dynamics of the long chain aliphatic compounds (of the highest members of homologous series, particularly) appeared again [1].

In wide temperature interval (11-330 K) IR absorption spectra of the carbonic acid $\text{CH}_3(\text{CH}_2)_{20}\text{COOH}$ (behenic acid, kC_{22}) were measured. The changes revealed in the spectra at the temperature increasing can be explained by the assumption about the conformational mobility of the molecules in the sample. The modeling of the structure and vibrational spectra of conformers of $\text{CH}_3(\text{CH}_2)_{20}\text{COOH}$ molecule have been carried out to confirm this assumption. These conformers were differed by the orientation of carboxylic group and by the orientation of fragment including carboxylic group and the closest CH_2 group relatively to the remaining part of the plane carbonic frame of alkyl radical (AR). Also the modeling of the $\text{CH}_3(\text{CH}_2)_{20}\text{COOH}$ molecules H-bond dimer, in which the AR carbonic frames and dimer ring are lying in the same plane, was performed.



Using density functional method (B3LYP/6-31G) [2] the energies, structures, dipole moments and polarizabilities of conformers of the $\text{CH}_3(\text{CH}_2)_{20}\text{COOH}$ molecule with different orientation angles and of the H-bond dimer were calculated. The force fields were built and the frequencies of normal vibrations with intensities in IR spectra were calculated for all mentioned above quantum molecular systems. On the basis of the analysis of the calculated and measured IR spectra the authors made a conclusion about the conformational mobility of the molecules in $\text{CH}_3(\text{CH}_2)_{20}\text{COOH}$ carbonic acid sample.

[1] H-W. Li, H.L. Strauss, R.G. Snyder. J. Phys. Chem. A 108 (2004) 6629-6642.

[2] Frisch J., Trucks G.W., Schlegel H.B. et al., Gaussian03, Revision B.03; Gaussian, Inc., Pittsburgh PA, 2003.