CONFORMATIONAL POLYMORPHISM AND MOLECULAR DYNAMICS OF CRYSTALLINE N-CARBOXYLIC ACIDS

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The IR-spectra for a homologous series of n-carboxylic acids $CH_3(CH_2)_nCOOH$ (n=8-22) are studied in different crystal modifications. Considerable changes in IR-spectra of these substances during polymorphous transformations were discovered: the change of frequencies and forms of the majority of vibrations, the re-distribution of their intencity, "disappearance" of certain bands. The analysis of these changes has shown that during the conversion from one crystal modification into another not only does the packaging of molecules dimers in the crystal change but also their conformation; in particular, the φ angle between planes of the dimeric ring and methylene chain changes. A calculation of frequencies and forms of normal vibrations of planar (φ=0,180^o) and non-planar (φ=10,30,60,90,120,150^o) conformations are performed to explain peculiarities of IR-spectra of different crystal modifications of n-carboxilic acids. The theoretical results agree with the experimental data.