

Fourier transform near-infrared spectra of N-methylacetamide: dissociation and thermodynamic properties in pure liquid form and in CCl₄ solutions.

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Streszczenie

FT-NIR spectra have been measured for *N*-methylacetamide (NMA) in pure liquid form and in carbon tetrachloride (CCl₄) solutions over temperature ranges of 303-368 K and 283-343 K, respectively. For the pure liquid, the FT-NIR spectra give one band due to a free NH group, at least five bands due to free end NH groups, and at least six bands due to hydrogen-bonded NH groups in the region of the first overtone of the NH stretching mode, demonstrating the potential of FT-NIR spectroscopy for investigating the hydrogen-bonding of NMA. The temperature-dependent spectral changes of NMA in the pure liquid indicate that, with increasing temperature, longer-chain oligomers of NMA dissociate into monomeric and dimeric species. For the CCl₄ solutions, the intensity of a band assigned to the first overtone of the NH stretching mode of the monomeric NMA has been employed to study the degree of dissociation and thermodynamic properties for the dissociation process. Below 4×10^{-3} M, NMA exists completely in the monomer form, and from the absorbance-concentration plot, the molar absorption coefficient of the first overtone of the NH stretching mode has been obtained. The degree of dissociation and dissociation equilibrium constant *K* have been calculated for the solutions at various concentrations, and then they have been employed to evaluate the thermodynamic parameters (ΔH , ΔS and ΔG) for the dissociation of hydrogen-bonded NMA into its monomeric species. The results show that the contribution of the entropy (ΔS) to the standard free energy (ΔG) becomes larger with a reduction in the concentration. It seems very likely that in the dilute solutions shorter-chain oligomers exist predominantly, and they easily dissociate into the monomeric species.

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