Two-dimensional correlation analysis of the second overtone of the ν(OH) mode of octan-1-ol in the pure liquid phase.

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Streszczenie

The temperature-induced variations in Fourier transform near-infrared (FT-NIR) spectra of pure liquid octan-1-ol were studied by two-dimensional correlation analysis. For the first time, the second overtone of the OH stretching band (3*v*(OH)) due to the dimeric species and the splitting of the second overtone of the monomer band arising from the presence of two OH conformers have been observed. Fourier self-deconvoluted (FSD) and second-derivative spectra also confirmed the splitting of the monomer band into two components. It has been demonstrated that positions of the peaks appearing in the two-dimensional contour maps correlating the first- and second-overtone regions can be applied for determination of anharmonicity constants. The results presented in this paper suggest that the rule saying that the less associated species have the stronger overtones holds on going from the first to the second overtones as well.