# Principal components analysis of infrared spectra of liquid acetylacetone.

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Streszczenie

The spectrum of the absorption index in the Mid-Infrared (MIR) region was determined for intramolecularly hydrogen-bonded liquid acetylacetone from transmission studies. In the MIR region very thin layers with thick nesses of a few micrometers had to be used to obtain reliable data. The keto-enol tautomeric equilibrium in the pure liquid was studied by Principal Components Analysis (PCA) of a set of temperature dependent MIR spectra in the range from 25 to 75 graduate C. Identifications for numerous bands observed in the liquid phase were proposed basing on the results obtained by means of the separation obtained in the loadings plot.

Słowa kluczowe

thin film infrared spectra, acetylacetone, hydrogen bonding, Principal Components Analysis