Investigation of phase transitions in liquid crystal 12BBAA using window clustering of infrared spectra.

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The k-means cluster analysis has been applied to the temperature-dependent infrared spectra of 4-bromobenzylidene-4′-dodecyloxyaniline (12BBAA). This method appears to be particularly sensitive to the tracking of the melting process of alkyl chains. 12BBAA may form a variety of phases including: isotropic liquid, smectic A, crystalline smectic B and crystal phase. Clustering methods are helpful tool for detection of phase transitions, but do not provide information on the structural changes due to the phase transitions. For this reason, window clustering analysis method has been proposed. Multivariate data has been divided into small spectral windows, and then cluster analysis has been applied for each data window. This approach allows to reduce the dimensionality of large data set, while reveals the spectral characteristic of given phase associated with various regions of spectra.

Słowa kluczowe

Infrared spectroscopy, Phase transition, Machine learning Clustering analysis, Window analysis, Liquid crystals, 12BBAA

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