

MIR and NIR group spectra of *n*-alkanes and 1-chloroalkanes.

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Rok wydania

2015

Czasopismo

Spectrochimica Acta Part A-
Molecular and Biomolecular
Spectroscopy

Numer woluminu

143

Strony

165-171

DOI

10.1016/j.saa.2015.01.134

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Numerous attempts were undertaken to resolve the absorption originating from different parts of alkanes. The separation of the contributions from the terminal and midchain methylene units was observed only in the spectra of solid alkanes at low temperatures. On the other hand, for liquid alkanes this effect was not reported as yet. In this study, ATR-IR, Raman and NIR spectra of eight *n*-alkanes and seven 1-chloroalkanes in the liquid phase were measured from 1000 to 12,000cm⁻¹. The spectra were analyzed by using two-dimensional (2D) correlation approach and chemometrics methods. It was shown that in 2D asynchronous contour plots, constructed from the spectra of *n*-alkanes and 1-chloroalkanes, the methylene band was resolved into two components. These two components were assigned to the terminal and midchain methylene groups. For the first time, the contributions from these two molecular fragments were resolved in the spectra of liquid *n*-alkanes and 1-chloroalkanes. MCR-ALS resolved these spectra into two components that were assigned to the ethyl and midchain methylene groups. These components represent the group spectra that can be used for assignment, spectral analysis and prediction of unknown spectra. The spectral prediction based on the group spectra provides very good results for *n*-alkanes, especially in the first and second overtone regions.

Słowa kluczowe

n-Alkanes, 1-Chloroalkanes, Group MIR/NIR spectra, Spectral prediction, Two-dimensional correlation analysis, chemometrics

Adres publiczny

<http://dx.doi.org/10.1016/j.saa.2015.01.134>

Strona internetowa wydawcy

<http://www.elsevier.com>

