Propwerties of hexasubstituted benzenes with one or two nitro groups. Dielectric, DSC, X-ray and Raman studies.

Autorzy

Hubert A. Kołodziej

Kazimierz Orzechowski

Roman Szostak

Piotr Freundlich

Tadeusz Głowiak

Salvatore Sorriso

Rok wydania

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Streszczenie

Selected hexasubstituted benzenes containing one or two nitro groups and chlorine atoms or methyl groups have been studied in the solid state by means of dielectric, differential scanning calorimetry (DSC), X-ray and Raman techniques. Unknown phase transitions at 223 and 412 K were found in pentachloronitrobenzene (PCNB), and the existence of a rotational phase above 223 K was confirmed with the help of dielectric measurements. In the case of 1,3-dinitrotetramethylbenzene (1,3-DNTMB) and 1,3-dinitrotetrachlorobenzene (1,3-DNTCB) permittivity dispersion in a low-frequency range has not been detected which was interpreted as a lack of rotatory phases in these compounds. No rotational phase in compounds with the angle between the aromatic ring and nitro group planes equal or close to 90° has been found. The crystal structure of 1,3-DNTCB was determined. 1,3-DNTCB crystallizes in $P2_1/c$ space group with $Z = 4$ molecules in a unit cell. DSC data for the studied crystals are quoted for the temperatures from 305 K to the melting point. Low-frequency Raman spectra of the studied compounds are presented and discussed.

Słowa kluczowe

Dielectric study, DSC study, X-ray crystallography, Raman spectroscopy, Substituted benzene

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