Inelastic and quasielastic neutron scattering and IR and R spectroscopic studies of 1,2,4,5-tetracyanobenzene(TCNB)-1,2,4,5-tetramethylbenzene(durene) complex.

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Streszczenie

The infrared and Raman spectra for durene, tetracyanobenzene and their 1 : 1 complex were studied. Simultaneously the neutron scattering experiments (INS and QENS) were performed. A detailed analysis of the modes assigned to the methyl groups vibrations were analyzed based on the simulated frequencies and intensities by using the GAUSSIAN-03 and auntie-CLIMAX programs. A good agreement between calculated frequencies and INS experimental ones was found. Moreover the calculations generate, with a quite high accuracy, the observed lattice phonons below 70 cm^{-1}. The QENS studies have shown that the activation energy for the 120° CH_3 jumps equal to 49 ± 13 meV for durene and 35 ± 12 meV for the complex confirming that the complexation leads to a decrease of the potential barrier for the methyl group rotations.

Słowa kluczowe

INS, QENS, IR, Raman spectroscopies, Tetracyanobenzene, Durene

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