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Low temperature investigations of dynamic properties in *L*-leucine – chloranilic acid complex.

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Abstract

Inelastic neutron scattering (INS) and infra-red (IR) spectroscopy methods were used for determination of dynamic structure of *L*-leucine – chloranilic acid complex. A theoretical dynamic pattern calculated by the density functional theory (DFT) method for periodic boundary conditions accompanied the experimental ones. Normal modes in the vibrational spectra were defined and described. The characteristic presence of the Hadži's trio enriched by numerous submaxima is observed in the wavenumber range 3200 - 800 cm^{-1}. Bands assigned to CH_3 torsion vibrations in the leucine cation were observed at 231cm^{-1} and 258 cm^{-1} in the INS spectrum. Temperature-dependent far-infrared spectra in the temperature range 9K - 290K were obtained. Vibrational bands were analyzed as a function of temperature. Activation energies for reorientational motion of CH_3 and CH_2 groups were determined by means of the band shape analysis performed for torsional and twisting vibrations of these groups. The estimated energy is equal to E_a = 2.7 ± 0.2 kJ/mol and E_a = 2.17 ± 0.12 kJ/mol for CH_3 and CH_2 groups, respectively. A phase transition at about 130 K in the *L*-leucine – chloranilic acid complex was observed.

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