

Fourier transform infrared and Raman spectroscopy in the study of phase transitions in dipyrazolium iodide triiodide : experimental and theoretical analysis.

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Streszczenie

The paper presents the Infrared and Raman spectra of the powdered $[C_3N_2H_5]^+2[I- \cdot I_3^-]$ crystal at the temperature intervals of 11–270 K, covering two low-temperature phase transitions: discontinuous at 182/188 K (cooling/heating) and continuous at 254 K. The research shows that the vibrational states of the pyrazolium cations change significantly during discontinuous phase transition (III $\rightarrow$ II), while the continuous nature of successive structural transformation is more subtle and displays an insignificant change in the temperature coefficient of numerous vibrations during the II $\rightarrow$ I PT at 254 K. The spectacular changes at Raman spectra above 188 K confirm a huge rebuilding of inorganic network from $[I- \cdot I_3^-]$ to $[I_4^{2-}]$. Additionally, a complete geometry optimization was carried out in the solid state in order to obtain minimum structures and bonding properties. The theoretical results correspond well with the experimental data. Moreover, the infrared spectrum in harmonic approximation was calculated, and a comparative vibrational analysis was performed. CRYSTAL09 vibrational results appear to be in a good agreement with the experimental ones

Słowa kluczowe

Polyhalides, phase transition, Infrared, Raman

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