Vibrational spectroscopic, optical and thermal properties of a deuterated ferroic crystal, $[(CH_2OD)_3CND_3]_2SiF_6$—An experimental and theoretical study.

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$[(CH_2OD)_3CND_3]_2SiF_6$ ferroic crystal, abbreviated as D-$(TRIS)_2SiF_6$ crystal was investigated. Optical (linear birefringence) and thermal (differential scanning calorimetry, DSC) measurements indicated a solid–solid phase transition (PT) of the first order at 185 K. The vibrational infrared spectra of powdered D-$(TRIS)_2SiF_6$ crystal in Nujol and Fluorolube mulls were studied in the wide range of temperature, from 308 K to 133 K. The temperature changes of wavenumber, width, centre of gravity position and intensity of the bands were analyzed to clarify the molecular mechanism of the phase transition and the contribution of SiF_6^{2-} and CH_2OD groups to the PT. A wide range (4000–400 cm^{-1}) of internal vibrations of the $DTRIS^+$ and SiF_6^{2-} ions was investigated and the assignment of the observed infrared absorption bands was discussed. Raman spectra of the crystal at room temperature (RT) were recorded and discussed in relation to the structure of isostructural $(TRIS)_2SiF_6$ crystal in the range (4000–400 cm^{-1}). Theoretical calculations were made based on density functional theory (DFT). The calculated normal vibrational modes of the molecules, their intensities and frequencies were compared with those obtained from experimental data.

Słowa kluczowe

D-(TRIS)2SiF6, phase transition, IR spectra, Raman spectra, DFT calculation, DSC measurements

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