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Experimental and theoretical study of the IR spectrum of $[(CH_2OH)_3CNH_3]_2SiF_6$ crystal.

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Streszczenie

$[(CH_2OH)_3CNH_3]_2SiF_6$, (tris(hydroxymethyl)aminomethane)$_2SiF_6$ crystal, abbreviated as $(TRIS)_2SiF_6$ crystal, exhibits a solid–solid phase transition (PT) at 182 K. The phase transition is connected with reorientational motion of SiF_6^{2-} and $-CH_2OH$ groups. The vibrational infrared spectra of powdered $(TRIS)_2SiF_6$ crystal in Nujol and Fluorolube mulls were studied in the wide range of temperatures, from 320 K to 133 K. A wide region of internal vibrations of the $TRIS^+$ and SiF_6^{2-} ions was investigated. Temperature changes of wavenumber, width, centre of gravity, and intensity of bands were analyzed to clarify the molecular mechanism of the phase transitions. Theoretical calculations were made based on density functional theory (DFT). The calculated normal vibrational modes of the molecules, their frequencies and intensities were compared with those obtained from experimental data.

Słowa kluczowe

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

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