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标题: Experimental and Theoretical Investigations on the Terahertz Vibrational Spectroscopy of Alanine Crystal

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摘要: The terahertz absorption and Raman scattering spectra of an alanine crystal in the range of 0.2-2.6 THz were obtained using terahertz time-domain spectroscopy and low-frequency Raman spectroscopy. The results indicated that there were four vibrational modes in this low-frequency region. Two modes were Raman active whereas the other two were both infrared and Raman active. A theoretical investigation on the periodic structure of alanine was performed using a self-consistent field crystal orbital method based on the B3LYP hybrid density functional. By comparing the experimental and theoretical results, irreducible representations were assigned to the corresponding peaks in the spectra. It was indicated that the vibrational modes in this low-frequency region were mainly torsion or rocking modes involving inter-molecular hydrogen bonds which have been described using schematic representations.

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