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Title:Low-frequency vibrational modes of glutamine

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Abstract:High-resolution terahertz absorption and Raman spectra of glutamine in the frequency region 0.2 THz-2.8 THz are obtained by using THz time domain spectroscopy and low-frequency Raman spectroscopy. Based on the experimental and the computational results, the vibration modes corresponding to the terahertz absorption and Raman scattering peaks are assigned and further verified by the theoretical calculations. Spectral investigation of the periodic structure of glutamine based on the sophisticated hybrid density functional B3LYP indicates that the vibrational modes come mainly from the inter-molecular hydrogen bond in this frequency region.

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