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Title:Density functional theory studies on molecular structure and vibrational spectra of NLO crystal l-phenylalanine phenylalanium nitrate for THz application
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Abstract:Molecular structure, FT-IR and Raman spectra of l-phenylalanine phenylalanium nitrate have been investigated using density functional theory calculation. The polarizability and hyperpolarizability value of the crystal is also calculated. Natural bond orbital analysis confirms the presence of intramolecular charge transfer and the hydrogen bonding interaction. Simultaneous activation of ring CC stretching modes shows the non-centrosymmetric symmetry. Terahertz time-domain spectroscopy has been used to detect the absorption spectra in the frequency range from 0.05 to 1.3 THz. Theoretically predicted β value exhibits the high nonlinear optical activity.
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