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Investigation of Far-IR Phonon Modes of Nucleic Acids XIAOWEI LI, University of Virginia, BORIS GELMONT, University of Virginia, MARIA BYKHOVSKAIA, Lehigh University, TATIANA GLOBUS, University of Virginia, DWIGHT WOOLARD, US Army Research Laboratory — We have performed the normal modes analysis of two nucleic acid molecules using AMBER in Cartesian coordinate space. The computational method that couples the normal modes of macromolecules with absorption spectra in the very far IR region (2-300cm^{-1}) is demonstrated. The calculated absorption spectrum of homopolymer poly[C]-poly[G] RNA shows good correlation with experimental result as well as with the modeling spectrum based on the normal mode analysis using JUMNA & LIGAND in internal coordinate space. The positions of resonance frequencies in the absorption spectrum of homopolymer poly[A]-poly[T] DNA modeled by AMBER are very similar to those observed in the experiment. These encouraging results demonstrate the capability of the normal mode analysis to predicate the optical characteristics of macromolecules in terahertz gap. This work builds the foundation for future application of submillimeter-wave spectroscopy technology in the identification and characterization of DNA and RNA molecules.

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