VIBRATIONAL SPECTROSCOPY OF TRANSFER RNA OF E.COLI: EXPERIMENT AND MODELING

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The molecular structure of the entire transfer RNA (tRNA) molecule of E. coli was simulated and the associated THz vibrational spectra was derived theoretically. The molecular structure was optimized using the potential energy minimization and molecular dynamical (MD) simulations. Solvation effects (water molecules) were also included explicitly in the MD simulations. A parallel experimental study of tRNAs of E. coli was also conducted in the spectral range 0.3-0.75 THz using FTIR spectroscopy. Samples were prepared in the form of water solutions (suspension) with the concentrations in the range 0.01-1 mg/ml. The calculated THz signature of the tRNA of E. coli reproduces many features of measured spectra.