FREQUENCY ANALYSIS OF BINARY MIXTURES INVOLVING HYDROGEN BONDS

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In molecular dynamics, geometry optimization and energy calculation ignore the constant vibrations of nuclei in molecules. In equilibrium state, there is some regularity in these vibrations and the molecules can be identified from their characteristic spectra. Theoretically calculated vibrational frequencies are used in characterizing molecular potential surfaces. They can be used to determine the nature of a stationary point obtained by geometry optimization. In geometry optimization procedure, the final equilibrium structure will correspond to a minimum on the potential energy surface or it may represent a saddle point. The frequency calculations provide a means of identification for stable but higly reactive short lived molecules by the appearence of a single infrared line. With the help of statistical mechanics, calculated normal mode vibrational frequencies provide information on thermodynamical properties of stable molecules such as reaction entropies and equilibrium isotope effect. Calculated vibrational frequencies are used to correct experimental thermodynamical data at absolute zero and to evaluate zero-point vibrational energies. The true energy of the system is obtained by adding the zero-point energy to the predicted total energy. The polarizability and hyper-polarizability can also be predicted by these frequency calculations.