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A Mathematical Theory for Vibrational Levels Associated with Hydrogen Bonds

We propose an alternative to the usual time–independent Born–Oppenheimer approximation that is specifically designed to describe molecules with Hydrogen bonds. In our approach, the masses of the Hydrogen nuclei are scaled differently from those of the heavier nuclei, and we employ a specialized form for the electron energy level surface. Consequently, anharmonic effects play a role in the leading order calculations of vibrational levels for symmetric molecules. For non-symmetrical molecules, the different vibrational modes appear at different orders of approximation.