HIGH ACCURACY AB INITIO CALCULATIONS OF ROTATION-VIBRATION SPECTRA

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High resolution infra red spectra are recorded with accuracy of 0.001 cm^{-1} or better. However attempting to perform *ab initio* calculations to better than 1 cm^{-1} requires dealing with effects neglected in the standard, non-relativistic, Born-Oppenheimer model. The contribution of corrections to the Born-Oppenheimer approximation via the adiabatic correction (BODC) [1,2] and non-adiabatic correction (both vibrational [2,3] and rotational [4]) are considered. In addition relativistic corrections to electron kinetic energy term [5] and the Coulomb potential (the Gaunt or Breit corrections) [6], and the radiative correction (Lamb shift) [7] have been evaluated. These effects are illustrated using spectra of H_3^+ and water, and the prospects of a complete *ab initio* solution for the spectra of these molecules discussed.

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