MODELING VIBRATIONAL STRUCTURE USING HARMONICALLY-COUPLED MORSE OSCILLATORS: A GLOBAL DESCRIPTION OF THE C-H STRETCHES IN METHYL RADICAL AND ITS DEUTERATED ISOTOPOMERS

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Methyl radical has been the subject of numerous theoretical and experimental studies over the past 50 years, including several studies fitting force constants to experimental data. Only recently have high-resolution gas phase data become available for most of the stretches of all four isotopic species: CH_3, CH_2D, CHD_2, and CD_3. A harmonically-coupled Morse oscillator model, developed by Halonen and Child[a] for tetrahedral molecules, is used to describe the set of high resolution data for the first time. In this picture, each C-H (or C-D) stretch is modeled as a Morse oscillator and the interactions between the local mode stretches are modeled as harmonic interactions. The C-H and C-D stretches differ only by analytic G-matrix element terms thus making this a three parameter model that describes each of the three stretches for all four isotopic species, where the parameters are the Morse oscillator dissociation energy (D), the range parameter (a), and the harmonic potential coupling constant.

[a] L. Halonen and M. S. Child *Mol. Phys.* **46**, 239 (1982).