CONVERGENCE AND ISOTOPIC STUDIES OF METHANE SPECTRA BY GLOBAL VARIATIONAL CALCULATIONS

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A detailed convergence study for the methane spectra is presented both for vibrational and rotational degrees of freedom as well as for intensities [1]. Vibration-rotation calculations are carried out using the variational normal mode approach with a full account of the symmetry. The various numerical tests and comparisons in this study suggest that our PES and DMS[2,3] are currently the most accurate ones in all available observed energy range and that variational calculations are now converged within the error margins of these surfaces. Isotopic effects in methane IR spectra under H→D and ^{12}C→^{13}C substitutions will be also discussed[4,5]. In Particular, we will focus on the state/polyad and band correspondence for symmetry breaking $T_d \to C_{3v}$ and $T_d \to C_{2v}$ substitutions.

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