ISOTOPIC SUBSTITUTION IN POLYATOMIC MOLECULES: COMPARATIVE LINE POSITION AND LINE STRENGTH ANALYSIS OF THE ν_2/ν_4 DYAD OF $^{12}CD_4$ AND $^{13}CD_4$

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A highly accurate ro–vibrational analysis of FTIR spectra (line positions of $^{13}CD_4$ and line strengths of both the $^{12}CD_4$ and $^{13}CD_4$ species) is presented. The high–resolution infrared spectra of both molecules were measured with a Bruker IFS125 HR Fourier transform infrared spectrometer at an optical resolution of 0.003 cm^{-1} and analyzed in the regions of 800–1400 cm^{-1} where the ν_2/ν_4 dyad is located. The number of 901 transitions with $J^{\text{max}} = 23$ were assigned to the ν_4 and ν_2 bands of $^{13}CD_4$. The weighted fit of experimental line positions was made using the Hamiltonian model which takes into account the resonance interactions between the $(0001, F_2)$ and $(0100, E)$ vibrational states. As a result, set of 18 fitted parameters of the $(0001, F_2)$/$(0100, E)$ vibrational states of $^{13}CD_4$ was determined which reproduce the initial 901 experimental ro–vibrational line positions with the $d_{\text{rms}} = 2.59 \times 10^{-4}$ cm^{-1}, which is close to the experimental uncertainty of the recorded spectra. The analysis of 1557 experimental lines of the dyad of $^{12}CD_4$ and 131 lines of the dyad of $^{13}CD_4$ was fulfilled with the Hartmann–Tran profile to simulate the measured line shape and to determine experimental line intensities. Sets of 6/1 varied effective dipole moment parameters of $^{12}CD_4$/$^{13}CD_4$ are determined which reproduce the initial 1557/131 line strengths with the $d_{\text{rms}} = 4.80\%$ and 4.21%.

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