

Rovibrational analysis and line intensity measurements of the $\nu_7 + \nu_8$ band of ethylene ($^{12}\text{C}_2\text{H}_4$) by high-resolution Fourier transform infrared spectroscopy

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Ethylene is a simple hydrocarbon that is of atmospheric and astrophysical interest. It is a tropospheric pollutant that acts as one of several precursors to the formation of ground-level ozone. It has also been detected in the atmospheres of Jupiter, Saturn and Neptune and in Titan, one of Saturn's moons. Accurate rotation-vibration parameters and knowledge of line positions and intensities are needed in the detection and monitoring of ethylene in the atmosphere. As part of our ongoing FTIR investigation of ethylene and its isotopic variants, determination of the upper state rovibrational constants and line intensity measurements of the A-type $\nu_7 + \nu_8$ combination band of $^{12}\text{C}_2\text{H}_4$ in the 1820–1950 cm^{-1} region were performed (see Figure 1). The present study aims to contribute to the limited but growing body of knowledge on ethylene line positions and intensities.

Four high-resolution FTIR absorbance spectra were collected and recorded at a spectral resolution of 0.0063 cm^{-1} and at an ambient temperature of 296 K in the 1.628×10^{-4} – 8.954×10^{-4} atm vapor pressure range. The resultant spectrum was used in the rovibrational analysis. A rather straightforward rovibrational analysis of the unperturbed lines of the band was carried out using a standard A -reduced Watson's Hamiltonian in I' representation. The final fit with a rms deviation of 0.000653 cm^{-1} included a total of 391 infrared transitions. The rovibrational constants determined for the excited state consisted of the three rotational constants, the band center, all five quartic and two sextic centrifugal distortion

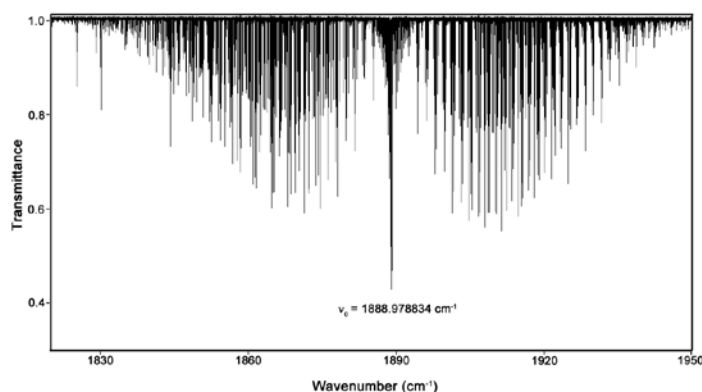


Figure 1. An overview of the FTIR absorption spectrum of the $\nu_7 + \nu_8$ combination band of $^{12}\text{C}_2\text{H}_4$ in the 1820–1950 cm^{-1} region

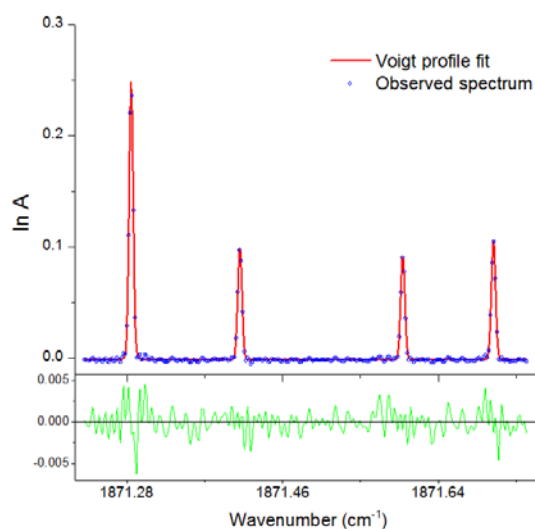


Figure 2. Part of peak fitting analysis performed ($p = 4.569 \times 10^{-4}$ atm) with the corresponding residuals in the lower panel

parameters. These constants were used to generate line positions and assignments which in turn were used, along with the experimental parameters, for the line intensity calculations.

Extraction of the line positions and intensities in the spectral region of all four high-resolution absorbance spectra of $^{12}\text{C}_2\text{H}_4$ was done using a peak fitting analysis that implemented the Levenberg–Marquardt algorithm. Each peak was fitted to a Voigt profile which accounts for the effects of both Doppler and collisional broadening. A total of 123 line intensities were measured. Figure 2 illustrates the quality of the peak fitting analysis that was performed in one of the high-resolution spectra. The bottom panel of Figure 2 gives the residual plot. Overall, the experimental fit was satisfactory with the % error between measured and calculated line intensities within $\pm 6\%$ for all 123 lines.