HIGH-RESOLUTION SPECTROSCOPY AND PRELIMINARY GLOBAL ANALYSIS OF C–H STRETCHING VIBRATIONS OF C_2H_4 IN THE 3000 AND 6000 CM^{-1} REGIONS

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Ethylene is a naturally occurring compound in ambient air that affects atmospheric chemistry and global climate. The C_2H_4 spectrum is available in databases only for the 1000 and 3000 cm^{-1} ranges. In this work[a], the ethylene absorption spectrum was measured in the 6030-6250 cm^{-1} range with the use of a high resolution Bruker IFS 125HR Fourier-spectrometer and a two-channel opto-acoustic spectrometer with a diode laser. As a secondary standard of wavelengths, the methane absorption spectrum was used in both cases. A preliminary analysis was realized thanks to the tensorial formalism developed by the Dijon group that is implemented in the XTDS software package[b]. We considered the two combination bands $\nu_5 + \nu_9$ and $\nu_5 + \nu_{11}$ as an interacting dyad. Parameters for the ν_9/ν_{11} dyad were fitted simultaneously from a re-analysis of previously recorded supersonic expansion jet FTIR data, while parameters for the $v_5 = 1$ Raman level were taken from literature. More than 600 lines could be assigned in the 6030-6250 cm^{-1} region (and also 682 in the 2950–3150 cm^{-1} region) and effective Hamiltonian parameters were fitted, including Coriolis interaction parameters. The dyad features are globally quite well reproduced, even if there are still problems at high J values.

[a] M. A. Loroñno Gonzalez *et al., J. Quant. Spectrosc. Radiat. Transfer*, **111**, 2265–2278 (2010).

[b] Ch. Wenger, V. Boudon, M. Rotger, J.-P. Champion and M. Sanzharov, *J. Mol. Spectrosc.*, **251**, 102–113 (2008).