High-Resolution Stimulated Raman Spectroscopy and Analysis of the ν₁/ν₅, ν₂ and ν₃ Bands of C₂H₄

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High-resolution stimulated Raman spectra of the ν₁/ν₅, ν₂ and ν₃ bands of C₂H₄ have been recorded and analyzed by means of the tensorial formalism developed in Dijon and Reims for X₂Y₄ asymmetric-top molecules [1,2].

For the ν₁/ν₅ bands, a total of 689 lines were assigned and fitted as a dyad including Coriolis coupling constants. We obtained a global root mean square deviation of 4.39 x 10⁻³ cm⁻¹. The nearby 2ν₂ band, extrapolated from ν₂, was included in the analysis. However, no interaction parameter involving it could be fitted. The analysis is quite satisfactory, although some parts of ν₅ are not well reproduced, probably indicating some yet unidentified resonances. This region is indeed quite dense, with many interacting dark states that cannot be included at present [3].

Part of the ν₅ band, compared to the simulation.

For the ν₂ band, a total of 191 lines were assigned and fitted. We obtained a global root mean square deviation of 1.86 x 10⁻³ cm⁻¹.

For the ν₃ band analyzed in interaction with ν₆, a total of 1895 lines were assigned and fitted. We obtained a global root mean square deviation of 1.29 x 10⁻³ cm⁻¹. Both of these last analyses lead to very satisfactory synthetic spectra compared to experimental ones [4].