High-Resolution Stimulated Raman Spectroscopy and Analysis of the ν_1/ν_5, ν_2 and ν_3 Bands of C_2H_4

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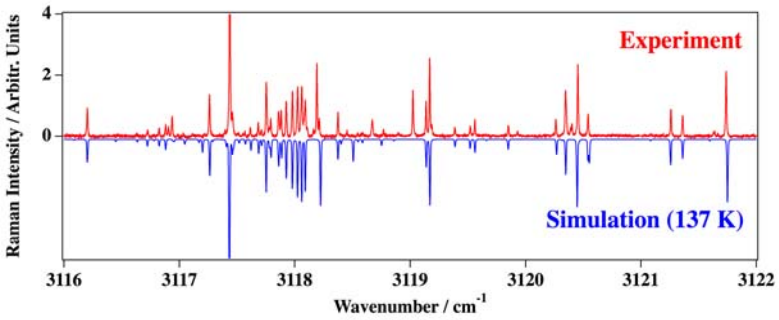
High-resolution stimulated Raman spectra of the ν_1/ν_5, ν_2 and ν_3 bands of C_2H_4 have been recorded and analyzed by means of the tensorial formalism developed in Dijon and Reims for X_2Y_4 asymmetric-top molecules [1,2].
For the ν_1/ν_5 bands, a total of 689 lines were assigned and fitted as a dyad including Coriolis coupling constants. We obtained a global root mean square deviation of 4.39 x 10^{-3} cm^{-1}. The nearby $2\nu_2$ band, extrapolated from ν_2, was included in the analysis. However, no interaction parameter involving it could be fitted. The analysis is quite satisfactory, although some parts of ν_5 are not well reproduced, probably indicating some yet unindentified resonances. This region is indeed quite dense, with many interacting dark states that cannot be included at present [3].



Part of the ν_5 band, compared to the simulation.

For the ν_2 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 ν_3 band analyzed in interaction with ν_6, 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].

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[4] A. Ballandras, M. Cirtog, M.A. Loroño, M.-T. Bourgeois, M. Rotger, D. Bermejo, R. Z. Martínez, J. L. Doménech, V. Boudon, *JRS* **2013**, in press.