

HIGH-RESOLUTION STIMULATED RAMAN SPECTROSCOPY AND ANALYSIS OF ν_2 AND ν_3 BANDS OF $^{13}\text{C}_2\text{H}_4$ USING THE D_{2h} TOP DATA SYSTEM

A. ALKADROU, M. ROTGER, *Groupe de Spectrométrie Moléculaire et Atmosphérique, UMR 7331 CNRS-Université de Reims Champagne-Ardenne, Reims, France*; **D. BERMEJO**, *Instituto de Estructura de la Materia, CSIC, Serrano 123, 28006-Madrid, SPAIN*; **V. BOUDON**, *Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Université de Bourgogne, France*

High resolution stimulated Raman spectra of $^{13}\text{C}_2\text{H}_4$ in the regions of the ν_2 and ν_3 Raman active modes have been recorded at room temperature (296 K) based on the quasi continuous-wave (cw) stimulated Raman spectrometer at Instituto de Estructura de la Materia (CSIC) in Madrid. A tensorial formalism adapted to X_2Y_4 planar asymmetric tops with D_{2h} symmetry has been developed in Dijon¹ and a program suite called $D_{2h}TDS$ (now part of the XTDS/SPVIEW spectroscopic software²) was proposed to calculate their high-resolution spectra³. The effective Hamiltonian operator, involving a polyad structure, and transition moment (dipole moment and polarizability) operators can be systematically expanded to carry out global analyses of many rovibrational bands. A total of 172 and 65 lines corresponding to ν_2 and ν_3 Raman active modes have been assigned and fitted in frequency with a global root mean square deviation of $2.0 \times 10^{-4} \text{ cm}^{-1}$. and $2.3 \times 10^{-4} \text{ cm}^{-1}$, respectively. The figure below shows the stimulated Raman spectrum of the ν_2 band of $^{13}\text{C}_2\text{H}_4$, compared to the simulation at 296 k.

¹[doi:10.1016/s0022-2852\(02\)00038-3](https://doi.org/10.1016/s0022-2852(02)00038-3), W. Raballand, M. Rotger, V. Boudon, M. Loëte, *J. Mol. Spectrosc.*, **217**, 239–248 (2003).

²[doi:10.1016/j.jms.2008.01.011](https://doi.org/10.1016/j.jms.2008.01.011), Ch. Wenger, V. Boudon, M. Rotger, M. Sanzharov, J.-P. Champion, *J. Mol. Spectrosc.*, **251**, 102–113 (2008).

³[doi:10.1016/j.jqsrt.2004.11.012](https://doi.org/10.1016/j.jqsrt.2004.11.012), Ch. Wenger, W. Raballand, M. Rotger, V. Boudon, *J. Quant. Spectrosc. Radiat. Transf.*, **251**, 102–113 (2008).

