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

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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 at two temperatures (145 and 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 Dijon[a] and a program suite called $D_{2h}TDS$ (now part of the XTDS/SPVIEW spectroscopic software[b] was proposed to calculate their high-resolution spectra. 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 103 and 51 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 0.54×10^{-3} cm^{-1} and 0.36×10^{-3} cm^{-1}, respectively. The figures below shows the stimulated Raman spectrum of the ν_2 and ν_3 bands of $^{13}\text{C}_2\text{H}_4$, compared to the simulation at 296 K.

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[a]Raballand W, Rotger M, Boudon V, Loëte M. J Mol Spectrosc 2003;217:239–48.

[b]Wenger Ch, Boudon V, Rotger M, Champion JP, Sanzharov M. J Mol Spectrosc 2008;251:102–13.