HIGH-RESOLUTION SPECTROSCOPY AND ANALYSIS OF THE $\nu_3/2\nu_4$ DYAD OF CF₄

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CF₄ is a strong greenhouse gas of both anthropogenic and natural origin^{*a*}. However, high-resolution infrared spectroscopy of this molecule has received only a limited interest up to now. The public databases only contain cross-sections for this species, but no detailed line list. We reinvestigate here the strongly absorbing ν_3 region around 7.3 μ m. Two new Fourier transform infrared spectra at a 0.003 cm⁻¹ resolution have been recorded: i) a room-temperature spectrum in a static cell with a 5 mb pressure and ii) a supersonic expansion jet spectrum at a 15 K estimated temperature. Following the work of Gabard *et al.*^{*b*}, we perform a simultaneous analysis of both the ν_3 and $2\nu_4$ bands since a strong Coriolis interaction occurs between them, perturbing the ν_3 *R*-branch rotational clusters around J = 20. As in Ref. ??, we also include $\nu_3 - \nu_3$ microwave data in the fit. The analysis is performed thanks to the XTDS and SPVIEW programs^{*c*}. Compared to Ref. ??, the present work extends the analysis up to higher *J* values (56 instead of 32). Absorption intensities are estimated thanks to the dipole moment derivative value of D. Papoušek *et al.*^{*d*} and compare well with the experiment. The rotational energy surfaces for the $\nu_3/2\nu_4$ dyad are also examined in order to understand the distribution of rovibrational levels.

^aD. R. Worton, W. T. Sturges, L. K. Gohar et al., Environ. Sci. Technol. 41, 2184–2189 (2007).

^bT. Gabard, G. Pierre and M. Takami, Mol. Phys. 85, 735–744 (1995).

^cCh. Wenger, V. Boudon, M. Rotger, M. Sanzharov and J.-P. Champion, J. Mol. Spectrosc., 251 102–113 (2008).

^dD. Papoušek, Z. Papoušková and D. P. Chong, J. Phys. Chem. 99, 15387–15395 (1995).