Line-by-line parameters of self- and foreign-broadened CH_2F_2 ro-vibrational transitions in the 8.3 μm region and the dissociation energy of $(CH_2F_2)_2$

N. Tasinato[a], A. Turchetto[a], P. Stoppa[a], A. Pietropolli Charmet[a], and S. Giorgianni[a]

[a] Dipartimento di Scienze Molecolari e Nanosistemi, Università Ca' Foscari Venezia, Calle Larga S. Marta 2137, I-30123 Venezia, Italy.

Over the past years, CFCs were extensively used as refrigerants and fire extinguishers. Therefore, they accumulated in the atmosphere where they catalytically destroy the stratospheric ozone molecules and contribute to the global warming. For these reasons they have been banned by the Montreal Protocol since 1996, and HCFCs and HFCs, having shorter atmospheric lifetimes, have been proposed as replacement gases. In particular, HFCs have appeared as the most convenient choice due to the absence of chlorine. On the other hand, all of these compounds are potential greenhouse gases, as they strongly absorb the infrared radiation in the atmospheric window around 9 μm. Difluoromethane (CH_2F_2, HFC-32) and its mixture with CF_3CH_3, CF_3CH_2F and CF_3CHF_2 is widely used as refrigerant. Because of the commercial applications, the atmospheric concentration of CH_2F_2 has increased rapidly since 1990s and its abundance was 3 pptv in 2005.

In the present work, the line-by-line parameters of several CH_2F_2 ro-vibrational lines have been determined in the spectral region around 8.3 μm within the atmospheric window. The observed spectral lines belong to the ν_7 fundamental which corresponds to the rocking of the CH_2 chromofore. The spectra have been acquired at room temperature by means of a tunable diode laser spectrometer and perturbing CH_2F_2 by a range of collisional partners (N_2, O_2, He, Ne, Ar). From the analysis of the spectral line shapes, transitions frequencies, self- and foreign-broadening coefficients and line intensities have been derived.

From the obtained foreign broadening collisional cross sections, the dissociation energy of the $(CH_2F_2)_2$ dimer has been retrieved according to the Lin - Seaver - Parmenter relationship [1]. This value, experimentally determined, has been compared to that obtained according to *ab initio* calculations carried out at the DFT level. In particular, B3LYP, M05-2X, B97-D and CAM-B3LYP functionals have been employed in conjunction with different basis sets of double- and triple-zeta quality. From these calculations the structural and spectroscopic properties of the dimer have been simulated and compared with the available experimental data.

[1] H.-M. Lin, M. Seaver, K. Y. Tang, C. S. Parmenter, J. Chem. Phys. **1979**, *70*, 5442.