PRESSURE DEPENDENT LINE INTENSITY AND CONTINUUM ABSORPTION FOR PURE CO_2: PREDICTIONS BY REQUANTIZED MOLECULAR DYNAMICS SIMULATIONS

H. TRAN, J. M. HARTMANN, *LMD, IPSL, Sorbonne Universite, Ecole Polytechnique, CNRS, Paris, France*; **M. BIRK, C. ROSKE and G. WAGNER**, *Remote Sensing Technology Institute, German Aerospace Center (DLR), D-82234 Wessling, Germany*

We investigate the pressure dependence of the line intensities retrieved from fits, using accurate isolated line shapes, of pure CO_2 spectra predicted using classical molecular dynamics simulations (rCMDS). For that, rCMDS have been carried out, at 296 K and 215 K, for pressure from 0.5 to 1 atm. An accurate ab initio intermolecular potential has been used to represent the CO_2-CO_2 interactions. The usual quadratic speed dependent hard collision model, taking into account the first-order line-mixing, is used to fit the simulated spectra. The results show that the retrieved line intensities linearly decrease with increasing pressure and that this decrease is larger at low temperature, consistently with the experimental results [1]. Quantitatively, at 1 atm and room temperature (resp. 215 K), our predictions show that the retrieved intensity can be up to 2% (resp. 4%) smaller than the intensity obtained at zero pressure. The effect decreases with increasing rotational quantum number. From the spectra fit baselines, a continuum absorption proportional with the square of pressure, is deduced. Our analysis shows that the observed pressure dependent intensity and the continuum are mostly due to incomplete or ongoing collisions, which govern the dipole auto-correlation function at very short times. These collisions transfer a fraction of the intensity from the core region of the line to a broad and weak continuum, and thus reduce its area.

[1] M. Birk et al., Pressure dependent line intensity and continuum absorption for pure CO2: experimental results, this conference