AB INITIO CLASSICAL DYNAMICS SIMULATIONS OF $CO_2$ LINE-MIXING EFFECTS IN INFRARED BANDS

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*Ab initio* calculations of line-mixing effects in $CO_2$ infrared bands are presented and compared with experiments. The predictions were carried using requantized Classical Dynamics Molecular Simulations (rCDMS) based on an approach previously developed and successfully tested for $CO_2$ isolated line shapes[b]. Using classical dynamics equations, the force and torque applied to each molecule by the surrounding molecules (described by an *ab initio* intermolecular potential) are computed at each time step. This enables, using a requantization procedure, to predict dipole and isotropic polarizability auto-correlation functions whose Fourier-Laplace transforms yield the spectra. The quality of the rCDMS calculations is demonstrated by comparisons with measured spectra in the spectral regions of the $3\nu_3$ and $2\nu_1 + 2\nu_2 + \nu_3$ Infrared bands[c].

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[b] J.-M. Hartmann, H. Tran, N. H. Ngo, *et al.*, *Phys. Rev. Lett. A* **87** (2013), 013403.

[c] H. Tran, C. Boulet, M. Snels, S. Stefani, *J. Quant. Spectrosc. Radiat. Transfer* **112** (2011), 925-936.