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.