

Treating CO₂ collisions classically: from pressure effects on spectra to the dissipation of laser-induced alignment

Jean-Michel Hartmann

Laboratoire Interuniversitaire des Systèmes Atmosphériques

Classical Molecular Dynamics Simulations (CDMS) of the translational and rotational motions of a large number of CO₂ molecules in the gas phase will be presented. The latter predict the time evolutions of the center of mass position and velocity as well as the molecular axis orientation and rotational angular momentum of each molecule. These are obtained from an accurate CO₂-CO₂ ab-initio intermolecular potential by numerically solving the purely classical (Newton) equations of motion, thus disregarding all quantum effects.

Starting from knowledge of the molecules positions, orientations and rotational speeds, various spectral properties are then computed without use of any adjusted parameter, and compared with measurements. The first are related to the effects of pressure on pure CO₂ spectra. These include the far infrared roto-translational absorption band due to the collision-induced dipole, light absorption and (Rayleigh) scattering spectra and their far wings as well as line shapes of pressure broadened individual lines and bands. The second are results concerning the collision dissipation of molecules' alignment induced by intense lasers will also be presented and discussed.

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