SOME COMPLEX PRESSURE EFFECTS ON SPECTRA FROM SIMPLE CLASSICAL MECHANICS

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I will first recall how [the two Newton's equations, 1rst year of university] one can very easily compute the rotational and translational classical dynamics of an ensemble of linear molecules interacting through an (input) pair-wise intermolecular potential. These Classical Molecular Dynamics Simulations (CMDS), which provide the time dependence of the positions and axis-orientations of gas phase molecules, are then used to calculate a number of pressure effects manifesting in absorption and scattering spectra. The cases of CO2, O2 and N2 will be considered, systems for which fully quantum approaches are intractable, and comparisons with measured data will be made, free of any adjusted parameter. I will show that, with a few input ingredients from literature (molecule geometry, electric multipoles, polarizabilities, ...) an no adjusted parameter, excellent agreements with various measurements are obtained. Examples will be given for: (1) Collision induced absorption (due to the interaction induced dipole) ; (2) The far wings of absorption (due to the dipole) and light scattering (due to polarizability) bands ; (3) The broadening and shapes (with their deviations from the Voigt profile) of individual absorption lines for both "free" and spatially tightly confined gases. If times allows, additional demonstrations of the interest of CMDS will be given by considering line-mixing effects and the relaxation of laser-kicked molecules.