Recent results on the modelling of isolated line shapes

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Atmospheric observation is mainly based on the solar radiation transmitted by the atmosphere or on the thermal radiation emitted by the Earth surface and by the atmosphere. The analysis of the measured data, mostly done through the so-called "inversion" procedures, requires the knowledge of the intrinsic spectroscopic parameters of absorption lines (positions, intensities,...). The collisions between the molecules also have to be considered as their effects yield a modification of the line shape for most of the atmospheric physical conditions (pressure, temperature).

It is now well known that the widely used Voigt profile does not well describe the measured absorption shapes of molecular gases. For an isolated optical transition, this is due to the neglect of the collision-induced velocity changes and of the speed dependences of the collisional parameters. Examples of the influence of these non-Voigt effects on the extraction of spectral line parameters from laboratory measured spectra as well as on atmospheric spectra analysis will be presented. A short review on different models used to fit measured spectra will be also given. Recent theoretical line-shape models developed in our group will be presented. In contrast with existing empirical models ([1] and references therein) where model parameters are adjusted to measured spectra, our *ab initio* approaches are directly based on independent classical molecular dynamics simulations. Examples will be given for the case of H_2, H_2O and CO_2 showing very good agreement between measured spectra and our predictions [2-6]. The latter are then used as a benchmark to choose the “proper” simplified line-shape model to fit measured spectra. Futures works and experimental needs for correct determinations of line parameters will be also discussed.

[1] J.-M. Hartmann, C. Boulet, D. Robert, “Collisional effects on molecular spectra. Laboratory experiments and models, consequences for applications”. Amsterdam: Elservier, **2008**.
[2] H. Tran, J.-M. Hartmann, F. Chaussard, M. Gupta, *J. Chem. Phys.* **2009**, *131*, 154303.
[3] N. H. Ngo, H. Tran, R. R. Gamache, *J. Chem. Phys*. **2012**, *136*, 154310.
[4] N. H. Ngo, H. Tran, R. R. Gamache, D. Bermejo, J.-L. Doménech, *J. Chem. Phys.* **2012**, *137*, 064302.
[5] H. Tran, N. H. Ngo, J.-M. Hartmann, R. R. Gamache, D. Mondelain et al, *J. Chem. Phys.* **2013**, *138*, 034302.
[6] J.-M. Hartmann, H. Tran, N. H. Ngo, X. Landsheere, P. Chelin et al, *Phys. Rev. A* **2013**, *87*, 013403.