Instrumental line shape function for molecular line parameters retrieval, from high resolution Fourier transform spectra, for terrestrial or planetary atmospheric remote sensing

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MOTIVATION
The physico-chemistry of planetary atmospheres, and particularly the Earth’s one, have been among the main subjects of studies over the last years. For this purpose, remote sensing measurements by means of spectroscopic techniques have been established as an indispensable tool. In spite of the improved Fourier Transform Spectrometers (FTS), and the advances in computational facilities, one requires the accurate knowledge of involved line parameters: positions, transition intensities, pressure-broadened halfwidths, pressure-induced frequency shifts and their temperature-dependence. In particular, the collisional broadening parameters have a crucial influence on the accuracy of spectra calculations and on the reduction of remote sensing data.

In laboratory spectroscopy, measurements of positions, intensities and other parameters of lines are in general long, very difficult, tedious and even impossible for weak, blended, large, or superposed lines. That is why it is impossible to have theoretical models which permit calculating parameters. But models are reliable only if they are built up using correct data concerning line parameters. The correct data are obtained using adequate line profile (Lorentz, Voigt, Rautian), accordingly to experimental conditions (temperatures, pressures of absorbing gas and of buffer ones), and taking into account instrumental parameters for modeling a “realistic” adequate line profile (Lorentz, Voigt, Rautian, Dicke, …) according to experimental conditions (temperature, pressures of absorbing gas and of buffer ones), and taking into account instrumental parameters for modeling a “realistic” Instrumental Line Shape.

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If many lines (i) of diverse molecules (j) in different mediums (k) are considered:

\[ I_{\text{LS}}(\sigma) = \sum_{i,j,k} A_{ij} \sigma_{ij} \cdot \left( 1 - \frac{\cos^2(\sigma \cdot \text{FWHM})}{\sigma^2} \right) \]

where \( I_{\text{LS}}(\sigma) \) is the instrumental line shape, \( A_{ij} \) are the line intensities, \( \sigma_{ij} \) are the line widths, and FWHM is the full width at half maximum. The observed line intensity is given by

\[ I_{\text{obs}}(\sigma) = \int_{-\infty}^{\infty} I_{\text{LS}}(\sigma) \cdot I_{\text{model}}(\sigma) \, d\sigma \]

where \( I_{\text{model}}(\sigma) \) is the theoretical line shape.

The ILS is FT [I_{\text{obs}}(\sigma) = \sum_{i,j,k} A_{ij} \sigma_{ij} \cdot \left( 1 - \frac{\cos^2(\sigma \cdot \text{FWHM})}{\sigma^2} \right)] = q(\sigma) only.

For the ILS, it is a convolution of line shape and line profile, where the line shape is the instrumental line shape and the line profile is the theoretical line shape.

The instrumental line shape is defined according to Beer-Lambert’s law:

\[ I(\sigma) = e^{-\frac{\sigma^2}{2 \sigma_0^2}} \]

where \( I(\sigma) \) is the intensity at the wavenumber \( \sigma \), \( \sigma_0 \) is the line width at half maximum, and \( e \) is the base of the natural logarithm.

The theoretical line shape is defined as

\[ I(\sigma) = \int e^{-\frac{\sigma^2}{2 \sigma_0^2}} \cdot I_{\text{model}}(\sigma) \, d\sigma \]

where \( I_{\text{model}}(\sigma) \) is the theoretical line shape.

The ILS is obtained by a convolution of the theoretical line shape and the line profile:

\[ I_{\text{LS}}(\sigma) = I_{\text{model}}(\sigma) * I(\sigma) \]

where \( * \) denotes the convolution operator.

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