Multispectrum fit of non-Voigt lineshape in the H_2O v_2 band

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A new fitting tool for analysis of multiple molecular absorption spectra utilizing a microwindow-based line-by-line-approach has been developed. It's capabilities include the choice of numerous different line shape models, from a simple Voigt to more sophisticated models like a speed-dependent Galatry including line-mixing. A comfortable manual mode as well as a fully automatic mode have been implemented including various quality assessment procedures like the monitoring of correlation coefficients or the supply of useful information e.g. needed for filecuts (single spectrum residuals) [1].

As a first application the new tool is used to re-analyze water vapor absorption spectra in the 1250-1750 cm^{-1} range [1,2]. The measurements include pure water as well as water+air-mixture measurements and cover a wide range of column densities. The total air pressure and partial pressure ranges were 50-1000 mb and 0.001-5 mb, respectively.

Whereas the original analysis was based on single spectrum fits applying the Voigt procedure, in the present multispectrum fit the speed-dependent Voigt lineshape was used. The advantages of a multispectral analyis approach as well as the need for consideration of narrowing effects is illustrated by the presentation of differences in residuals as well as resulting line parameters for selected transitions. As indicated in [3] opaque as well as non opaque lines could be fitted with the speed-dependent Voigt while the pure Voigt yields to narrow opaque lines.

[1] M. Birk, G. Wagner, *Journal of Quantitative Spectroscopy and Radiative Transfer* **2012**, *113*, 889.
[2] L. H. Coudert, G. Wagner, M. Birk, Yu. I. Baranov, W. J. Lafferty, J.-M. Flaud, *Journal of Molecular Spectroscopy* **2008**, *251*, 339.
[3] G. Wagner, M. Birk, S. A. Clough, „Undiscovered errors of Voigt profile beyond tiny w-shaped residuals", *International Symposium on Molecular Spectroscopy – 68th Meeting, Columbus (OH)* **2013**