

## NUMERICAL EVALUATION OF HARTMANN-TRAN LINE PROFILE USE IN SYNTHETIC, NOISY SPECTRA

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Although the Voigt profile (VP) has long been used as a standard spectroscopic line profile, more stringent demands in high-resolution spectroscopy now require the application of other profiles that account for physics not captured by the VP. The Hartmann-Tran Profile (HTP) [1] was recommended by an IUPAC task group to be a standard for high-resolution spectroscopy because it parameterizes higher-order physical effects, is computationally efficient, and reduces to the VP and other widely used profiles as limiting cases [2]. As advanced line profiles such as the HTP are adopted by more researchers to model or predict absorption spectra, it is important to understand the limitations that data quality has on the ability to retrieve physically meaningful parameters from least-squares fits of assumed profiles to measurements with finite signal-to-noise ratio (SNR). In this work, synthetic, noisy spectra were simulated using the HITRAN Application Programming Interface (HAPI) [3] across a range of parameters, SNR, and spectral sampling interval. The HTP was fit to these spectra to determine how simulated conditions affect fitted parameter uncertainty and correlations between parameters. We also investigated under what circumstances and constraints the parameters derived from fitting the HTP adequately model the full HTP.

1. Tran, H., N. Ngo, and J.-M. Hartmann, Efficient computation of some speed-dependent isolated line profiles. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 2013. 129: p. 199-203.
2. Tennyson, J., et al., Recommended isolated-line profile for representing high-resolution spectroscopic transitions (IUPAC Technical Report). *Pure and Applied Chemistry*, 2014. 86(12): p. 1931-1943.
3. Kochanov, R.V., et al., HITRAN Application Programming Interface (HAPI): A comprehensive approach to working with spectroscopic data. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 2016. 177: p. 15-30.