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NON-VOIGT LINE-SHAPE ANALYSIS OF H₂ SPECTRA FOR THE HITRAN DATABASE.

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A proper interpretation and modeling of accurate molecular spectra, at certain pressure/temperature ranges, require the non-Voigt line-shape effects to be incorporated. Therefore, for a more reliable representation of molecular spectra in the HITRAN database¹, both the Dicke narrowing and speed-dependent effects have to be considered. We demonstrate how to determine and store the line-shape parameters for the case of self-perturbed molecular hydrogen, for which the non-Voigt effects are especially pronounced.

We performed a detailed line-shape analysis of the recent high-quality H₂ spectra² recorded with cavity ring-down spectrometers and optical feedback cavity-enhanced absorption spectrometer, showing the possible solutions to the problems of strong numerical correlations between the parameters and their temperature dependences. Note that the previous line-shapes models, which reproduce the H₂ spectra better than the simple phenomenological profiles, are computationally ineffective. Therefore for the purpose of the HITRAN database we developed a new technique allowing the Hartmann-Tran profile³ to be adopted for the H₂ spectra analysis. Finally we

¹[doi:10.1016/j.jqsrt.2013.07.002](https://doi.org/10.1016/j.jqsrt.2013.07.002), L.S. Rothman, I.E. Gordon, Y. Babikov, A. Barbe, et al., *J. Quant. Spectrosc. Radiat. Transfer.*, **130**, 4-50, (2013).

²[doi:10.1016/j.jms.2014.03.022](https://doi.org/10.1016/j.jms.2014.03.022), S. Kassi, A. Campargue, *J. Mol. Spectrosc.*, **300**, 55-59, (2014); [doi:10.1016/j.jms.2014.03.010](https://doi.org/10.1016/j.jms.2014.03.010), Y. Tan, J. Wang, C.-F. Cheng, X.-Q. Zhao, A.-W. Liu, S.-M. Hu, *J. Mol. Spectrosc.*, **300**, 60-64, (2014).

³[doi:10.1016/j.jqsrt.2013.06.015](https://doi.org/10.1016/j.jqsrt.2013.06.015), H. Tran, N.H. Ngo, J.-M. Hartmann, *J. Quant. Spectrosc. Radiat. Transfer.*, **129**, 199-203, (2013).

demonstrate the use of the new relational structure of the HITRAN database⁴ and the HITRAN Application Programming Interface (HAPI)⁵ for the case of H₂ spectra.

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⁴[doi:10.1016/j.jqsrt.2013.04.027](https://doi.org/10.1016/j.jqsrt.2013.04.027), C. Hill, I.E. Gordon, L.S. Rothman, J. Tennyson, *J. Quant. Spectrosc. Radiat. Transfer.*, **130**, 51-61, (2013).

⁵[doi:10.5281/zenodo.17719](https://doi.org/10.5281/zenodo.17719), R.V. Kochanov, I.E. Gordon, L.S. Rothman, C. Hill, J. Wilzewski, P. Wcisło, HITRAN Application Programming Interface (HAPI) - Beta version, Zenodo (2015).