

**GENERATING COMPLETE SETS OF BEYOND-VOIGT LINE-SHAPE  
PARAMETERS FOR THE HITRAN DATABASE:  
DATASET STRUCTURE, TEMPERATURE-DEPENDENCIES,  
LINE-SHAPE MODEL**

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The accurate characterization of collision-perturbed spectral lines from many molecular systems requires a profound understanding of the beyond-Voigt effects that influence the spectrum <sup>1</sup>. These effects are described by eight essential spectral line-shape parameters: pressure broadening and shift ( $\gamma_0$  and  $\delta_0$ ), their speed dependencies ( $\gamma_2$  and  $\delta_2$ ), the real and imaginary parts of the complex Dicke parameter ( $\tilde{\nu}_{opt}^r$  and  $\tilde{\nu}_{opt}^i$ ) and the complex line-mixing coefficient ( $y^r$  and  $y^i$ ). Accurate knowledge of the temperature dependencies of these parameters is crucial for spectroscopic investigations of terrestrial <sup>2</sup> and extraterrestrial <sup>3</sup> atmospheres.

In my presentation, I will focus on the methodology employed to establish an extensive dataset of beyond-Voigt spectral line-shape parameters <sup>4</sup>. I will discuss interpolation and extrapolation schemes of the *ab initio* data to provide entries for the entire datasets in the HITRAN database <sup>5</sup>. I will introduce the double-power-law (DPL) temperature-dependence model <sup>6</sup>, which offers a universal, straightforward, and accurate structure for each of the six line-shape parameters. I will discuss a new beyond-Voigt line-shape profile recommended for the HITRAN database.

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<sup>4</sup>[doi:10.1016/j.jqsrt.2020.107477](https://doi.org/10.1016/j.jqsrt.2020.107477), P. Wcisło, F. Thibault, N. Stolarczyk, H. Jóźwiak, M. Ślowiński, M. Gancewski, K. Stankiewicz, M. Konefał, S. Kassi, A. Campargue, Y. Tan, J. Wang, K. Patkowski, R. Ciuryło, D. Lisak, R. Kochanov, L.S. Rothman, I.E. Gordon, *JQSRT*, **260**, 107477, (2021).

<sup>5</sup>[doi:10.1016/j.jqsrt.2021.107949](https://doi.org/10.1016/j.jqsrt.2021.107949), I.E. Gordon *et al*, *JQSRT*, **277**, 107949, (2022).

<sup>6</sup>[doi:10.1016/j.jqsrt.2019.106676](https://doi.org/10.1016/j.jqsrt.2019.106676), N. Stolarczyk, F. Thibault, H. Cybulski, H. Jóźwiak, G. Kowzan, B. Vispoel, I.E. Gordon, L.S. Rothman, R.R. Gamache, P. Wcisło, *JQSRT*, **240**, 106676, (2020).