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Evaluation of different parameterizations of temperature dependences of the line-shape parameters based on ab initio calculations: Case study for the HITRAN database HUBERT JOZWIAK, NIKODEM STOLARCZYK, Nicolaus Copernicus University, Torun, Poland, FRANCK THIBAULT, Universite de Rennes 1, Rennes, France, HUBERT CYBULSKI, Kazimierz Wielki University, Bydgoszcz, Poland, GRZEGORZ KOWZAN, Nicolaus Copernicus University, Torun, Poland, BASTIEN VISPOEL, University of Namur, Namur, Belgium, IOULI E. GORDON, LAURENCE ROTHMAN, Harvard-Smithsonian Center for Astrophysics, Cambridge, ROBERT GAMACHE, University of Massachusetts Lowell, PIOTR WCISLO, Nicolaus Copernicus University, Torun, Poland — Proper description of the temperature dependence of the line-shape parameters is essential for the spectroscopic studies of both terrestrial and extraterrestrial atmospheres. Here, we use ab initio collisional line-shape calculations for several molecular systems to compare the four temperature ranges (4TR) representation, adopted in the HITRAN database in 2016, with the double-power-law (DPL) representation. Besides the collisional broadening and shift parameters, we consider the most important beyond Voigt line-shape parameters, i.e., the speed dependence of broadening and shift parameters, and real and imaginary parts of the complex Dicke parameter. We demonstrate that not only does the DPL give better overall approximation of the temperature dependencies, but it also requires fewer parameters than the 4TR. We recommend the usage of DPL representation, and present DPL parametrization for Voigt and beyond-Voigt line profiles that will be adopted in the HITRAN database.

Hubert Jozwiak
Nicolaus Copernicus University, Torun, Poland

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