HITRAN IN THE XXIst CENTURY: BEYOND VOIGT AND BEYOND EARTH

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The line-by-line portion of the most recent HITRAN2012 edition[a] contains spectroscopic parameters for 47 gases and associated isotopologues. Continuing the effort of the last five decades, our task has been to improve the accuracy of the existing parameters as well as to add new bands, molecules, and their isotopologues. In this talk we will briefly summarize some of the most important efforts of the past year.

Particular attention will be given to explaining the new development in providing line-shape information in HITRAN. There are two important directions in which the database is evolving with respect to line shapes. The first direction is that, apart from the Voigt profile parameters that were traditionally provided in HITRAN, we are able to add parameters associated with many "mainstream" line shapes, including Galatry, speed-dependent Voigt, and the HT profile[b] recently recommended by IUPAC[c]. As a test case, we created a first complete dataset of the HT parameters for every line of molecular hydrogen in the HITRAN database. Another important development is that in order to increase the potential of the HITRAN database in planetary sciences, experimental and theoretical line-broadening coefficients, line shifts and temperature-dependence exponents of molecules of planetary interest broadened by H_2, He, and CO_2 have been assembled from available peer-reviewed sources. The collected data were used to create semi-empirical models for calculating relevant parameters for every line of the studied molecules in HITRAN.

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[b] N.H. Ngo, et al. "An isolated line-shape model to go beyond the Voigt profile in spectroscopic databases and radiative transfer codes," JQSRT 129, 89–100 (2013).

[c] J. Tennyson, et al. "Recommended isolated-line profile for representing high-resolution spectroscopic transitions," Pure Appl.Chem. 86, 1931–1943 (2014).