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MH. Linelists

Monday, June 22, 2015 – 1:30 PM

Room: B102 Chemical and Life Sciences

Chair: Shanshan Yu, California Institute of Technology, Pasadena, CA, USA

MH01 **1:30 – 1:45**

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.

This work has been supported by NASA Aura Science Team Grant NNX14AI55G and NASA Planetary Atmospheres Grant NNX13AI59G.

[a] L.S. Rothman, et al. "The HITRAN 2012 molecular spectroscopic database," JQSRT 130, 4–50 (2013).

[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).

MH02 **1:47 – 2:02**

HITRANonline: A NEW STRUCTURE AND INTERFACE FOR HITRAN LINE LISTS AND CROSS SECTIONS

CHRISTIAN HILL, LAURENCE S. ROTHMAN, IOULI E GORDON, ROMAN V KOCHANOV, PIOTR WCISLO, *Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*; JONAS WILZEWSKI, *Department of Astronomy, Harvard University, Cambridge, MA, USA*.

We present **HITRAN***online*, an online interface to the internationally-recognised HITRAN molecular spectroscopic database[1], and describe the structure of its relational database backend[2].

As the amount and complexity of spectroscopic data on molecules used in atmospheric modelling has increased, the existing 160-character, text-based format has become inadequate for its description. For example, line shapes such as the Hartmann-Tran profile[3] require up to six parameters for their full description (each with uncertainties and references), data is available on line-broadening by species other than "air" and "self" and more than the current maximum of 10 isotopologues of some molecules (for example, CO_2) can be important for accurate radiative-transfer modelling. The new relational database structure overcomes all of these limitations as well as allowing for better data provenance through "timestamping" of transitions and a direct link between items of data and their literature sources.

To take full advantage of this new database structure, the online interface **HITRAN***online*, available at www.hitran.org, provides a user-friendly way to make queries of HITRAN data with the option of returning it in a customizable format with user-defined fields and precisions. Binary formats such as HDF-5 are also supported. In addition to the data, each query also produces its own bibliography (in HTML and BibTeX formats), "README" documentation and interactive graph for easy visualization.

1. L. S. Rothman *et al.*, *JSQRT* **130**, 4-50 (2013).
2. C. Hill, I. E. Gordon, L. S. Rothman, J. Tennyson, *JQSRT***130**, 51-61 (2013).
3. N. H. Ngo, D. Lisak, H. Tran, J.-M. Hartmann, *JQSRT* **129**, 89–100, (2013); erratum: *JQSRT* **134**, 105 (2014).

This work has been supported by NASA Aura Science Team Grant NNX14AI55G and NASA Planetary Atmospheres Grant NNX13AI59G.