New Edition of HITRAN Database

L. S. Rothman and K. Chance
Harvard-Smithsonian Center for Astrophysics
Cambridge, Massachusetts

J. Schroeder
Ontar Corp.
North Andover, Massachusetts

A. Goldman
University of Denver
Denver, Colorado

Introduction

The goal of this effort is to provide the Atmospheric Radiation Measurement (ARM) community with an archival database of spectroscopic parameters that serve as input to atmospheric radiation modeling codes. The high-resolution transmission (HITRAN) compilation includes molecular spectroscopic parameters for simulating absorption and radiance by gases in the atmosphere, infrared (IR) cross sections for gases with dense spectra, aerosol indices of refraction, and associated software to enable ARM users to easily extract information relevant to their problems.

New Edition of HITRAN Compilation

A new edition of the HITRAN molecular spectroscopic database was made available on the internet in December 2000. This new edition contains five major areas: line-by-line spectroscopic parameters (conventional HITRAN), IR absorption cross sections, UV line-by-line and absorption cross sections, management software, and aerosol indices of refraction. All of these aspects have been significantly improved and expanded upon since the last HITRAN edition (Rothman et al. 1998). The file structure of the new compilation is given in Figure 1.

The most prominent changes to the line-by-line portion of the HITRAN compilation since the previous public edition (Rothman et al. 1998) are highlighted in Table 1.

Comments on the improvement for water vapor will be discussed in the next section. A major update has been accomplished for methane (Fejard et al. 2000; Ouardi et al. 1996). The number of transitions and the completion of parameters for this gas has more than quadrupled since the 1996 edition. A study was initiated by the Earth Observing System (EOS) program on the oxygen atmospheric *A*-band parameters at 760 nm for HITRAN by Brown and C. Plymate (2000). These new data have been

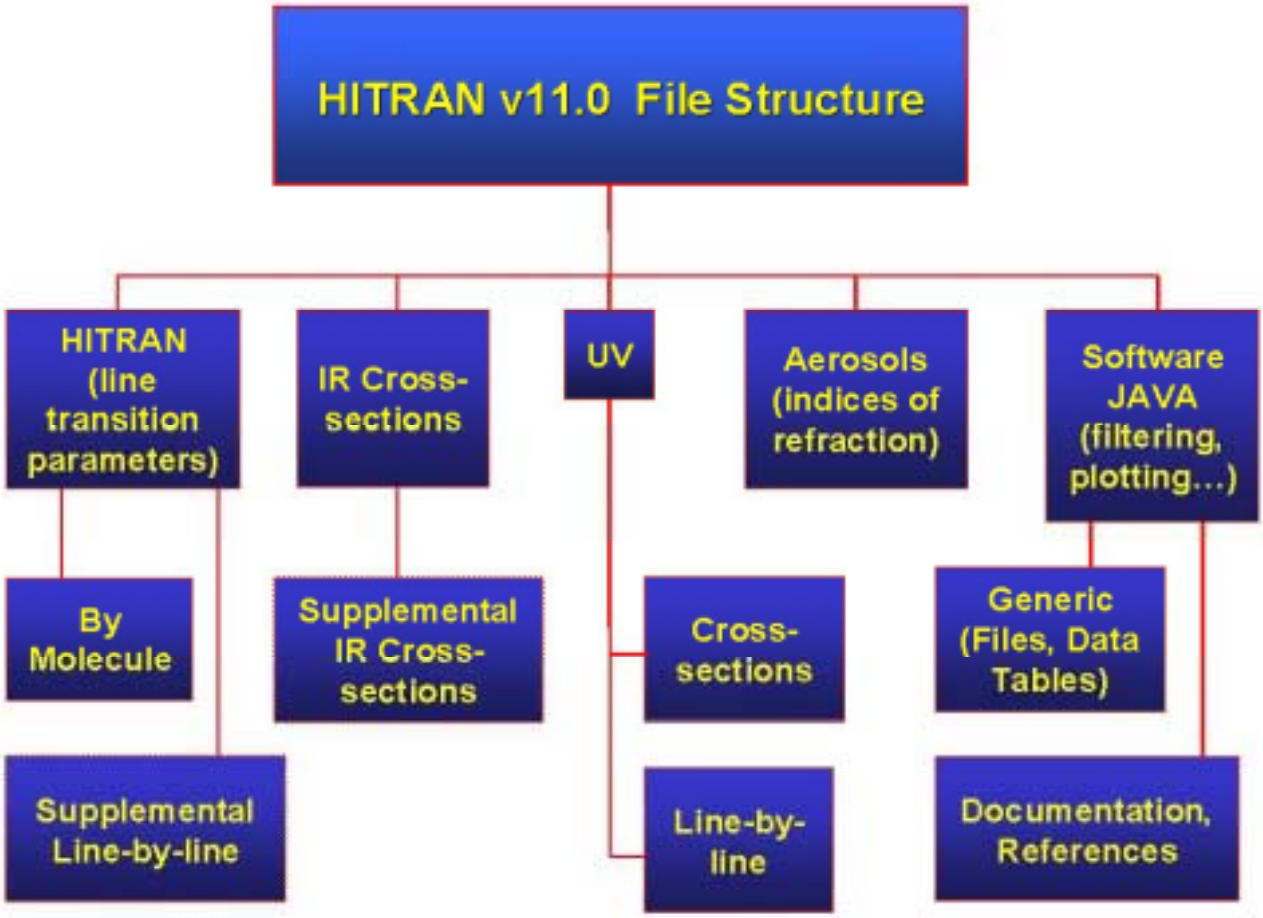

Figure 1. HITRAN version 11.0 file structure.

implemented in HITRAN as well as improved intensities for the band at 1.27μm, work performed at National Institute for Standards and Technology (NIST) by Lafferty et al. (1998) and corroborated by independent observations in the United Kingdom (UK) (Smith and Newnham 1999).

The IR cross sections included in the HITRAN compilation have been greatly expanded. Twenty-seven gases are now included and, in most cases, there are many pressure-temperature sets for each gas, which enables quite good quantitative simulations using the standard line-by-line radiation codes. A summary of these gases can be found in Rothman and Živkovic´-Rothman (2000). They have been assembled from high-resolution laboratory efforts.

The software accompanying the new edition of HITRAN has now been made to be platform independent and has new functionality for plotting.

Table 1. Highlights of New Line-by-line Data for HITRAN	
Molecule	**Enhancement**
H_2O	8000-23000 cm^{-1} region (L. P. Giver et al.)
H_2O	9600-11400 cm^{-1} region (L. R. Brown et al.)
H_2O	500-2820 cm^{-1} region (R. A. Toth)
CH_4	500-5500 cm^{-1} region (L. R. Brown)
O_2	Atmospheric A-band at 760 nm (L. R. Brown)
O_2	$a^1\Delta$ band at 1.27 μm (Lafferty et al.)
NO	Overtone bands (2-0),(3-1) (V. Dana et al.)
NH_3	3-μm and 5 to 7-μm revision (L. R. Brown)
HNO_3	Improved hot bands in 11-μm region (A. Goldman)
OH	Improved intensities (A. Goldman)
HBr	Pure rotation and fundamental(A. Goldman et al.)
HI	Pure rotation and fundamental(A. Goldman et al.)
OCS	Fundamentals (Fayt et al.)
C_2H_2	600-870 cm^{-1} region (hot bands) (V. Dana et al.)
H_2S	ν_1 and ν_3 plus combination bands (L. R. Brown)
HO_2	Pure rotation (K. Chance)
C_2H_4	New to HITRAN (Pine et al.)

Water Vapor Parameters

New water vapor parameters are among the many updates to HITRAN for enhanced capabilities of atmospheric radiation modeling. These data have been incorporated in the .94-μm region (Brown et al. 2001) and in the 6-μm region (Toth 1993). However, there are many more new data and analyses taking place for water vapor, especially in the near-IR and visible regions.

A resolution between the data of different groups in the shortwave region (Schermaul et al. 2000; Giver et al. 2001) requires a careful validation program for assimilation into the next version of HITRAN. Whereas the UK group, which has produced a line-list for the European Space Agency, claims that the Giver et al. corrections to HITRAN96 have, in some cases, actually produced a larger error; preliminary laboratory work in the United States indicates otherwise.[(a)] We are also about to update the HITRAN water vapor transitions in this region with improved calculations for the halfwidths where laboratory observations have been unattainable.

(a) S. Adler-Golden, Spectral Sciences, Inc., private communication (2000).

Plots obtained using the HITRAN plotting software for the longwave and shortwave regions that have been updated are shown in Figures 2 through 4.

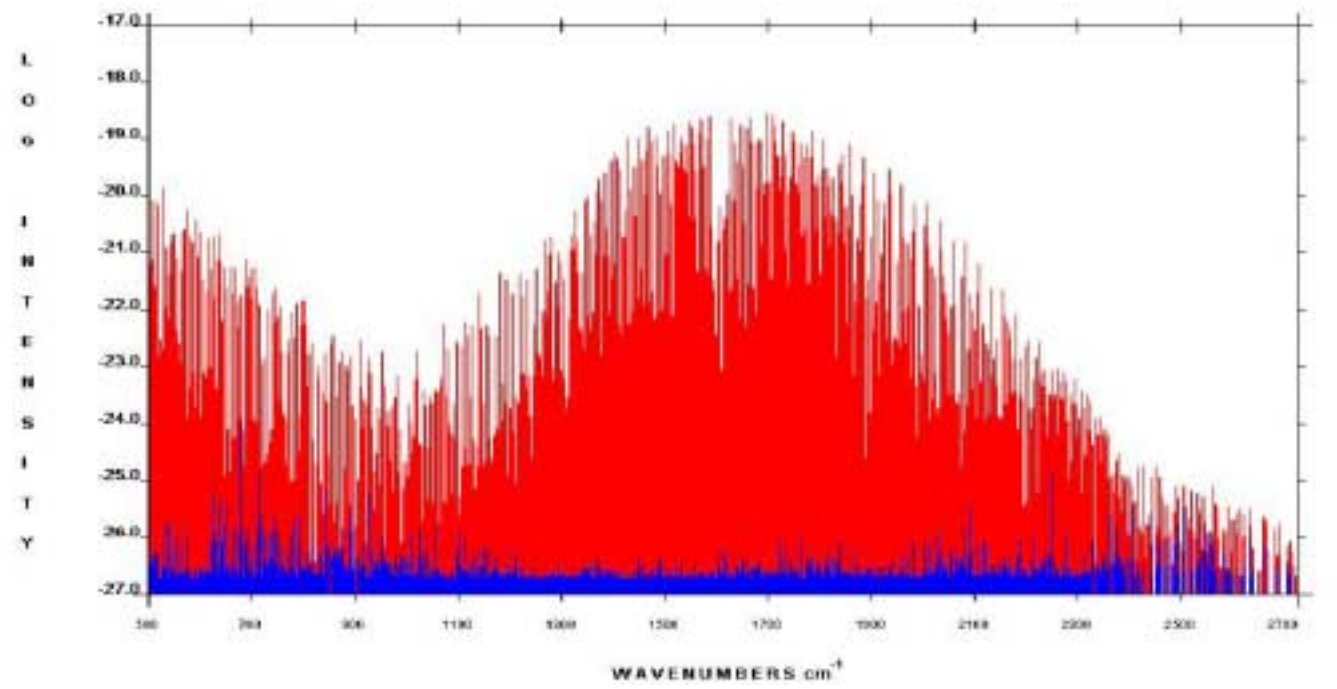

Figure 2. Example of new line-by-line parameters for water vapor, 500 to 2700 cm^{-1}.

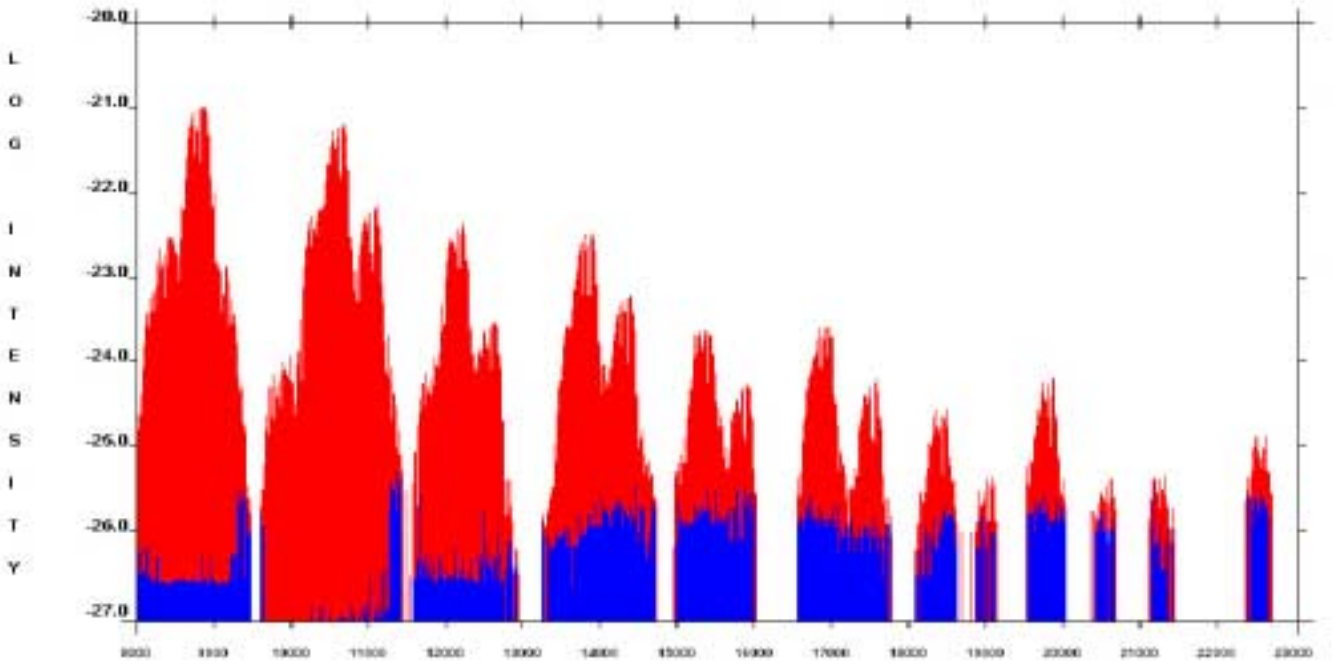

Figure 3. Example of new line-by-line parameters for water vapor, 8000 to 23,000 cm^{-1}.

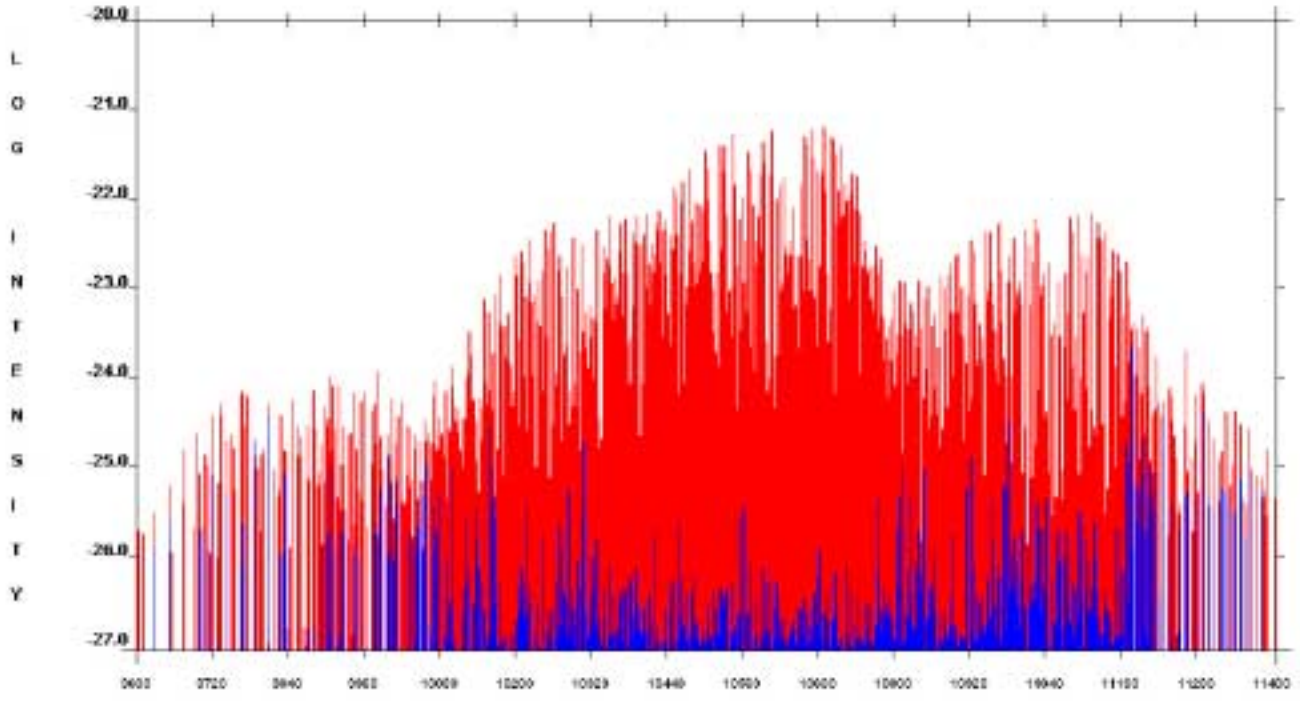

Figure 4. Expansion of plot for new line-by-line parameters for water vapor, 9600 to 11,400 cm^{-1}.

An update is close to completion for the intensities in the far-IR region, and there is an ongoing analysis of data to replace the old parameters between 3000 and 8000 cm^{-1}.

Summary

The format for the line-by-line portion of HITRAN will soon be increased to accommodate extra parameters, namely the Einstein-A coefficient, the upper- and lower-level statistical weights of the transitions, a flag for lines with significant line-mixing, and references and error codes for three more parameters (the self-broadened width, the temperature-dependence of the air-broadened width, and the pressure shift of the line). Algorithms will be provided for the line-coupling correction to lines as well as improved partition sums for all species.

The HITRAN compilation can now be accessed via anonymous ftp. Users need only fill out the request form located in the HITRAN Web site for instructions (http://CfA-www.Harvard.edu/HITRAN). Database updates are ongoing and can be downloaded from this site. In the future, it is planned to allow operation on the entire database using interactive JAVA software resident on the Web site.

Biennial conferences focusing on the molecular database are held and the proceedings of the most recent conference can be viewed on the Web site.

Corresponding Author

Laurence S. Rothman, LRothman@CfA.Harvard.edu, (617) 495-7474

References

Brown, L. R., R. A. Toth, and M. Dulick, 2001: Line Parameters of Water from 9600 to 11400 cm^{-1}. *J. Mol. Spectrosc.* Submitted.

Brown, L. R., and C. Plymate, 2000: Experimental Line Parameters of the Oxygen *A* Band at 760 nm. *J. Mol. Spectrosc.*, **199,** 166-179.

Fejard, L., J.-P. Champion, J. M. Jouvard, L. R. Brown, and A. S. Pine, 2000: The intensities of methane in the 3-5 μm region revisited. *J. Mol. Spectrosc.*, **201,** 83-94.

Giver, L. P., P. Pilewski, W. J. Gore, C. Chackerian, P. Varanasi, R. S. Freedman, and R. Bergstrom, 2001: Uncertainties in the Line Intensities in the 1130 nm Band of Water Vapor. *ARM Science Team Meeting Proceedings*, March 19-23.

Lafferty, W. J., A. M. Solodov, C. L. Lugez, and G. T. Fraser, 1998: Rotational line strengths and self-pressure-broadening coefficients for the 1.27-μm, $a^1\Delta_g$ - XΣg, ν = 0 - 0 band of O_2. *Appl. Opt.* **37,** 2264-2270.

Ouardi, O., J. C. Hilico, M., Loëte, and L. R. Brown, 1996: The hot bands of methane between 5 and 10 μm. *J. Mol. Spectrosc.*, **180,** 311-322.

Rothman, L. S., C. P. Rinsland, A. Goldman, S. T. Massie, D. P. Edwards, J.-M. Flaud, A. Perrin, C. Camy-Peyret, V. Dana, J.-Y. Mandin, J. Schroeder, A. McCann, R. R. Gamache, R. B. Wattson, K. Yoshino, K. Chance, K. Jucks, L. R. Brown, V. Nemtchinov, and P. Varanasi, 1998: The HITRAN Molecular Spectroscopic Database and HAWKS (HITRAN Atmospheric Workstation): 1996 Edition. *J. Quant. Spectrosc. and Rad. Transfer*, **60,** 665-710.

Rothman, L. S., and M. Živkovic´-Rothman, 2000: Atmospheric Molecules. *Atomic and Molecular Data and their Applications*, eds. K. A. Berrington and K. L. Bell, AIP Conference Proceedings **543,** 92-103.

Schermaul, R., R.C.M. Learner, D. A. Newnham, J. Ballard, N. F. Zobov, D. Belmiloud, and J. Tennyson, 2000: The water vapor spectrum in the region 8600-15000 cm^{-1}: Experimental and theoretical studies for a new spectral line database II: Linelist construction. *J. Mol. Spectrosc.* Submitted.

Smith, K. M., and D. A. Newnham, 1999: Near-infrared absorption spectroscopy and cross sections of oxygen and nitrogen gas mixtures. Paper DP18, *Proceedings of Atmospheric Spectroscopy Applications*, Reims.

Toth, R. A., 1993: *JOSA* **B 10,** 2006-2029.