Millennium HITRAN Compilation

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Abstract

The current edition of the high-resolution transmission (HITRAN) molecular absorption compilation (HITRAN2000) is available on an anonymous ftp site located at the Harvard-Smithsonian Center for Astrophysics (ftp://cfa-ftp.Harvard.edu/pub/HITRAN). The compilation consists of five main folders: (1) the traditional line-by-line parameter database, (2) aerosol indices of refraction, (3) ultraviolet (UV) cross sections and line-by-line parameters, (4) infrared (IR) cross sections, and (5) software and documentation. There are also extensive tables of partition sums covering a wide temperature range for all the isotopomers in HITRAN, and a high-temperature analog of HITRAN called HITEMP.

Collaborations with many research teams throughout the world have enabled great improvements in providing more accurate parameters, extended spectral coverage, and documentation. Besides the line-by-line absorption parameters, significant progress has been made for pressure-temperature sets of absorption cross sections as well as increased tables of aerosol properties. A new edition of the HITRAN compilation is planned for 2002.

The format of the line-by-line portion of the HITRAN compilation is being expanded to accommodate larger polyatomic molecules, information for non-local thermodynamic equilibrium atmospheric dynamics and astrophysics, and improved documentation. The improvements not only provide increased capabilities for atmospheric transmission/radiance calculations and remote sensing, but allow access and analytical tools for related molecular databases.

Introduction

One of the priorities for the HITRAN project for the Atmospheric Radiation Measurement (ARM) Program continues to be a focus on constituents that impact the radiance codes and simulations of the ARM Program. A major thrust has been to improve the accuracy (and remove any errors) in water-vapor parameters. In the last HITRAN conference, we held a special session on water-vapor parameters. Groups from the United Kingdom, Belgium, France, United States, and Canada were prominent. However, there are differences in the data (mostly at short wavelengths and the visible), and the controversy lingers. As a result of a recent workshop run by National Aeronautics and Space

Administration (NASA) on remote sensing of the atmosphere, a mechanism has been established to deal with situations such as these. A HITRAN steering committee has been setup, consisting of a small number of spectroscopists who have been intimately involved with HITRAN and who represent different spectral regions and molecules in their special expertise. They establish working groups on an ad hoc basis for the evaluation of different sets of data being considered for HITRAN. The steering committee comes from a number of institutions, mostly Europe and the United States, and requires a few days not only to evaluate and validate data, but to cast the consensus data into the appropriate HITRAN format. Documentation of their effort is also required. Some support from NASA has been offered. The logistics for these working groups has to be developed, but there is precedent, for example in the community responsible for chemical reaction rates.

New HITRAN Edition

The file structure of the HITRAN compilation is shown in Figure 1. Supplemental folders are used for line-by-line data such as SF_6 and $ClONO_2$ that are incomplete for many modeling scenarios. The supplemental folder for the IR cross sections contains good, but redundant independent data. The alternate folder for UV cross sections contains data in units of wavelength as observed, in addition to those same data that have been interpolated to a wavenumber grid in the main folder on cross sections. In the future, a folder for collision-induced absorption will be introduced.

The parameter format for HITRAN was originally 80 characters per transition, reflecting the use of paper cards as storage medium. From 1986 through 2001, the format has been 100 characters per transition, allowing several more parameters, but using some mapping codes (for example with the "global quanta" to allow rapid lookup). The new format will be 160 characters per transition. The minimalist approach is still maintained: all parameters are independent. Easily calculated or global parameters such as the partition sum for a molecule are given in separate files or programs.

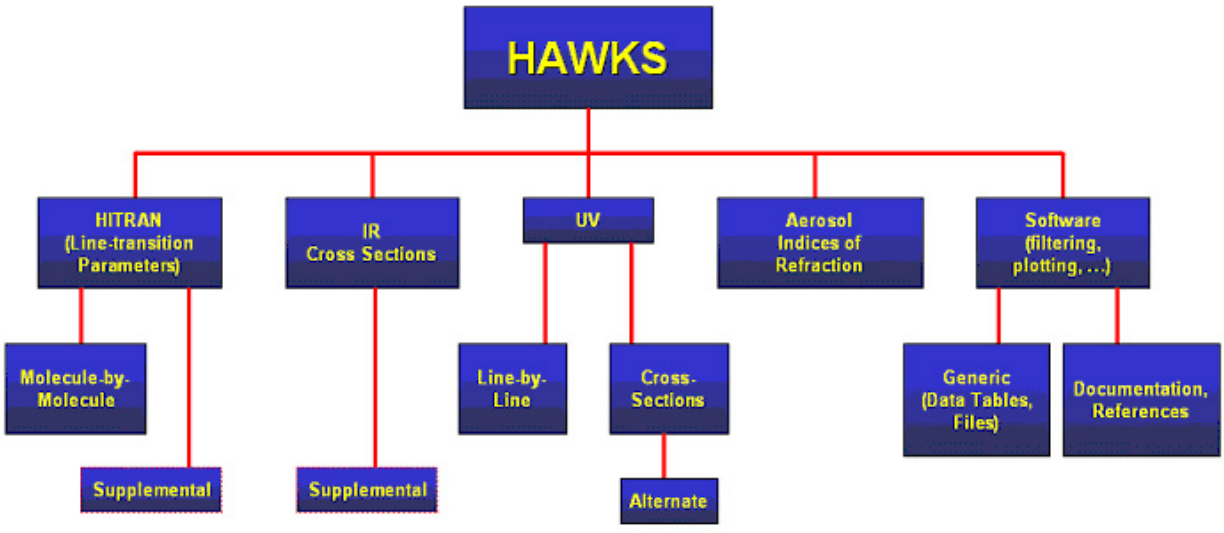
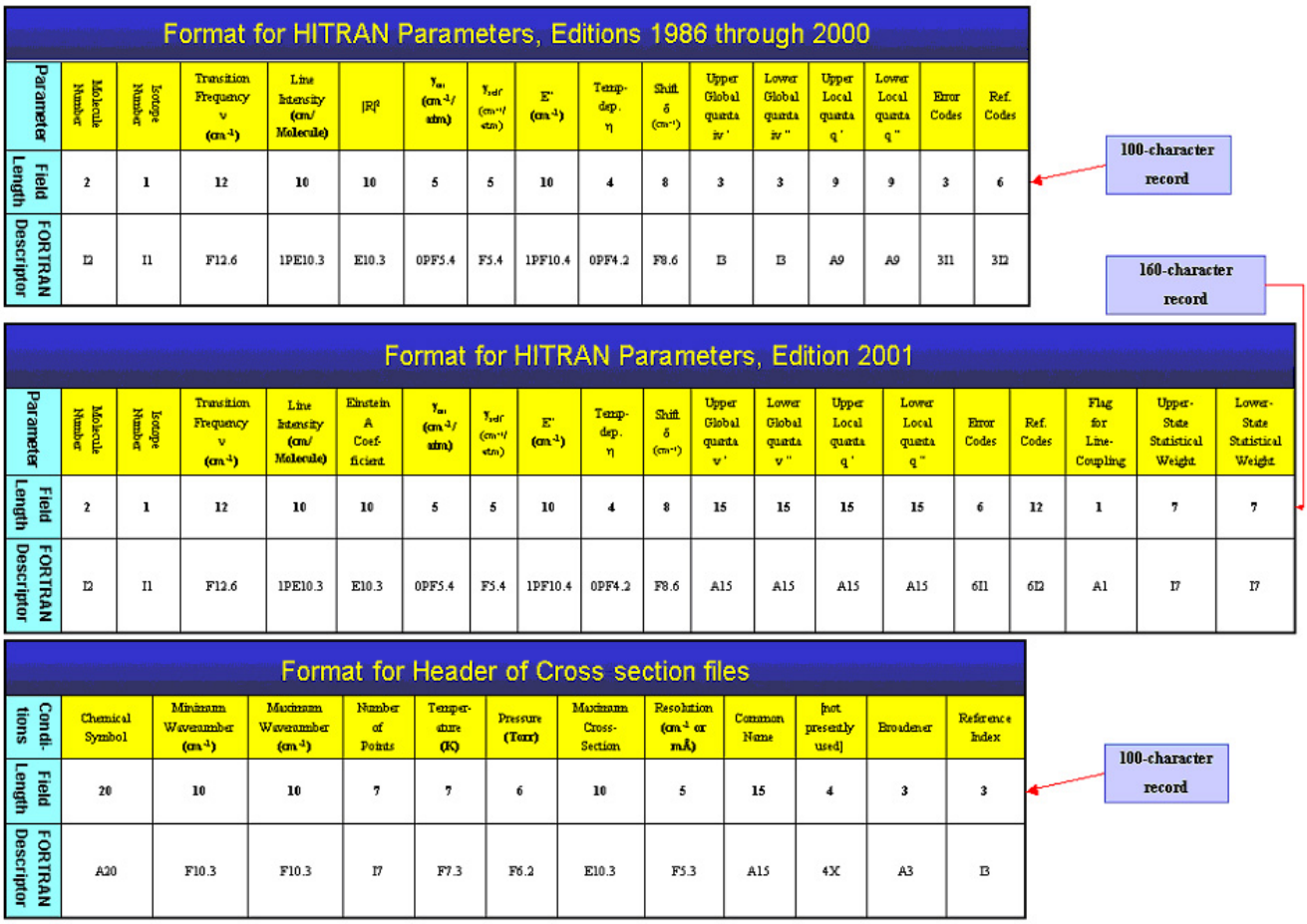


Figure 1. File structure of HITRAN compilation.

The record length for the cross section files will remain at a 100-character length, but the headers have been more structured. The field structure is shown in Figure 2.



Format for HITRAN Parameters, Editions 1986 through 2000

Parameter	Molecule Number	Isotope Number	Transition Frequency ν (cm⁻¹)	Line Intensity (cm/Molecule)	|R|²	γair (cm⁻¹/atm)	γself (cm⁻¹/atm)	E'' (cm⁻¹)	Temp-dep. η	Shift δ (cm⁻¹)	Upper Global quanta iv'	Lower Global quanta iv''	Upper Local quanta q'	Lower Local quanta q''	Error Codes	Ref. Codes
Field Length	2	1	12	10	10	5	5	10	4	8	3	3	9	9	3	6
FORTRAN Descriptor	I2	I1	F12.6	1PE10.3	E10.3	0PF5.4	F5.4	1PF10.4	0PF4.2	F8.6	I3	I3	A9	A9	3I1	3I2

100-character record

160-character record

Format for HITRAN Parameters, Edition 2001

Parameter	Molecule Number	Isotope Number	Transition Frequency ν (cm⁻¹)	Line Intensity (cm/Molecule)	Einstein A Coef-ficient	γair (cm⁻¹/atm)	γself (cm⁻¹/atm)	E'' (cm⁻¹)	Temp-dep. η	Shift δ (cm⁻¹)	Upper Global quanta v'	Lower Global quanta v''	Upper Local quanta q'	Lower Local quanta q''	Error Codes	Ref. Codes	Flag for Line-Coupling	Upper-State Statistical Weight	Lower-State Statistical Weight
Field Length	2	1	12	10	10	5	5	10	4	8	15	15	15	15	6	12	1	7	7
FORTRAN Descriptor	I2	I1	F12.6	1PE10.3	E10.3	0PF5.4	F5.4	1PF10.4	0PF4.2	F8.6	A15	A15	A15	A15	6I1	6I2	A1	I7	I7

Format for Header of Cross section files

Condi-tions	Chemical Symbol	Minimum Wavenumber (cm⁻¹)	Maximum Wavenumber (cm⁻¹)	Number of Points	Temper-ature (K)	Pressure (Torr)	Maximum Cross-Section	Resolution (cm⁻¹ or mÅ)	Common Name	[not presently used]	Broadener	Reference Index
Field Length	20	10	10	7	7	6	10	5	15	4	3	3
FORTRAN Descriptor	A20	F10.3	F10.3	I7	F7.3	F6.2	E10.3	F5.3	A15	4X	A3	I3

100-character record

Figure 2. Formats for line-by-line parameters and cross section data.

Water-Vapor Absorption Parameters

There is an urgent need to improve the absorption parameters for water vapor in the HITRAN database. The high-resolution H_2O parameters in the HITRAN database are a combination of theoretical calculations, fitting to observations, and direct laboratory observations. These parameters include the line position, the intensity, the collision-broadened half width, and its temperature dependence. Some of these data are based on older works, especially in the near IR and visible portions of the spectrum.

The HITRAN program has initiated a research effort to compare, evaluate, and validate the various data. There are now several sources of new, high-quality data that cover different spectral regions. There is also spectral overlap among these independent data. Several sources under consideration are listed in Table 1.

Table 1. Sources under evaluation for water-vapor parameter updates.

Data	Source
HITRAN2000	FTP-site – Rothman et al. (2001)
FTS analysis	Univ. Libre de Bruxelles/Univ of Reims – Carleer et al. (1999)
ICLAS measurements	Univ. of Paris – Picqué et al. (2002)
European Space Agency (ESA) water database	RAL/Univ. College London – Belmiloud et al. (2000)
FTS observations	NASA Ames – Giver et al. (2000)
FTS measurements	State Univ. New York – Varanasi (2002)
FTS measurements	Ohio State Univ./Univ. Giessen – (Winnewisser, private communication)
FTS measurements	Jet Propulsion Lab. – Brown and Toth (2000)
Ab Initio calculations	NASA Ames Research Center- Schwenke (1998)
Complex calculations of halfwidths	Univ. Massachusetts – Gamache (2002)
Calculations of pure-rotation bands	Smithsonian Astrophysical Observatory – (Jucks, private communication)
Isotopomers	Univ. of Paris – Camy-Peyret et al. (1999)

The issues of weak water-vapor lines is a major factor in deficiencies of spectroscopic linelists. Figure 3a illustrates in a compressed form the lines of water vapor that are currently available in HITRAN in the visible region 13000 to 25000 cm^{-1}. These lines include corrections from Giver et al. (2000) and new data from Brown and Toth (2000). New linelists have been recently generated. The so-called ESA water database (Belmiloud et al. 2000) has shown detailed differences in intensities with HITRAN. However, this database (a portion shown in Figure 3b) is constructed of lines based on observations for the stronger decades of intensities, coupled with calculations for the weaker lines. Figure 3c is from the lines list of a joint effort with groups in Belgium and France (Carleer et al. 1999), using a very long-path absorption cell yielding a large dynamic range in intensities. It can be seen that many more lines as well as bands are contained in this list compared with the current HITRAN. Figure 4 shows a ratio of individual lines intensities with HITRAN. This type of plot, however, can be slightly misleading since it gives equal weight to all lines, not distinguishing between strong lines (which are generally in good agreement) and weak lines.

In Figure 5 are similar plots showing comparisons of observations made by the group of Varanasi (2002) with both HITRAN96 (Rothman et al. 1998) and the current HITRAN (Rothman et al. 2001) in the longer wavelength region. The improvement resulting from the incorporation of the results of Toth (1998) are clearly seen, but much improvement is still needed.

In the troposphere, the values assumed for the air-broadened halfwidths in the HITRAN database impact the radiation budget calculations as much as the intensities. With current FTS analysis procedures, one usually obtains self-consistent values of halfwidths with the intensities. However, different methods have been employed, and the quality of the halfwidths obtained can have large errors or be missing from many unobserved or blended lines. Calculational schemes for collision broadening with molecules larger than diatomic are very involved. However, the calculations made by Gamache (2002) have begun to be successful for water vapor. Figure 6 shows the spread of values for the air-broadened Lorentzian halfwidth (halfwidth at half maximum) for two bands in the visible region. The plots show the

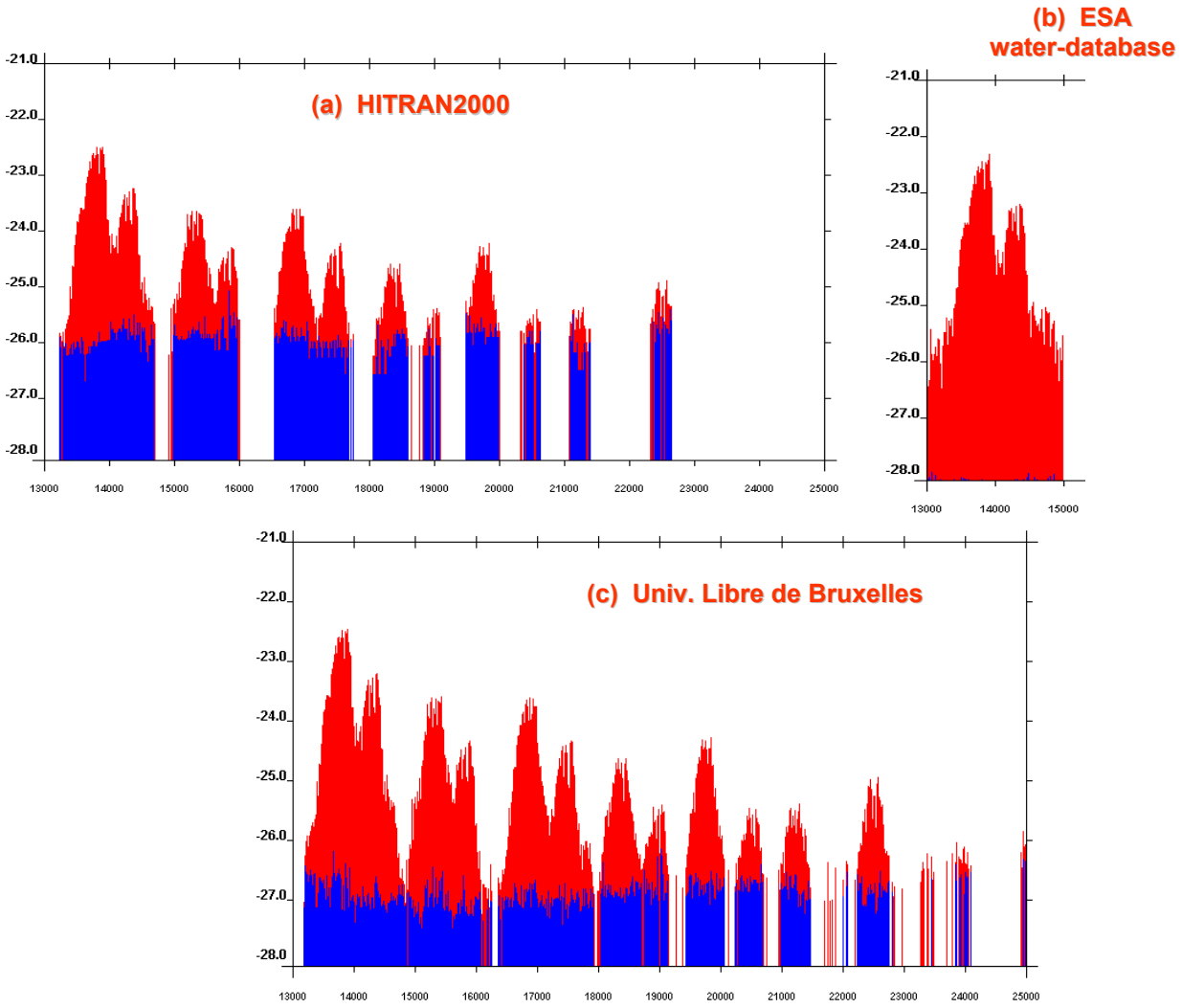


Figure 3. (a) Water-vapor lines in shortwave region in HITRAN (Rothman et al. 2001), (b) ESA water database (Belmiloud et al. 2000), and (c) water-vapor database from University Libre of Brussels (ULB) consortium (Carleer et al. 1999).

calculation, the measurements of Grossman and Browell (1989), and the halfwidths given in the ESA (Belmiloud et al. 2000) (called RAL in the plot) and ULB (Carleer et al. 1999) linelists. The points are plotted for convenience in terms of the total rotational number J added to the difference of the K_a and K_c quantum numbers.

The HAWKS compilation is now distributed via anonymous ftp (ftp://cfa-ftp.Harvard.edu/pub/HITRAN) or via the Internet with password, shown in Figure 7: (http://cfa-www.Harvard.edu/HITRAN/hitrandata/). An archival edition is maintained here, with intermediate updates and corrections placed in the regular HITRAN Web site. There are also folders containing partition sums at one-degree intervals from 70K to 3000K and the HITEMP database.

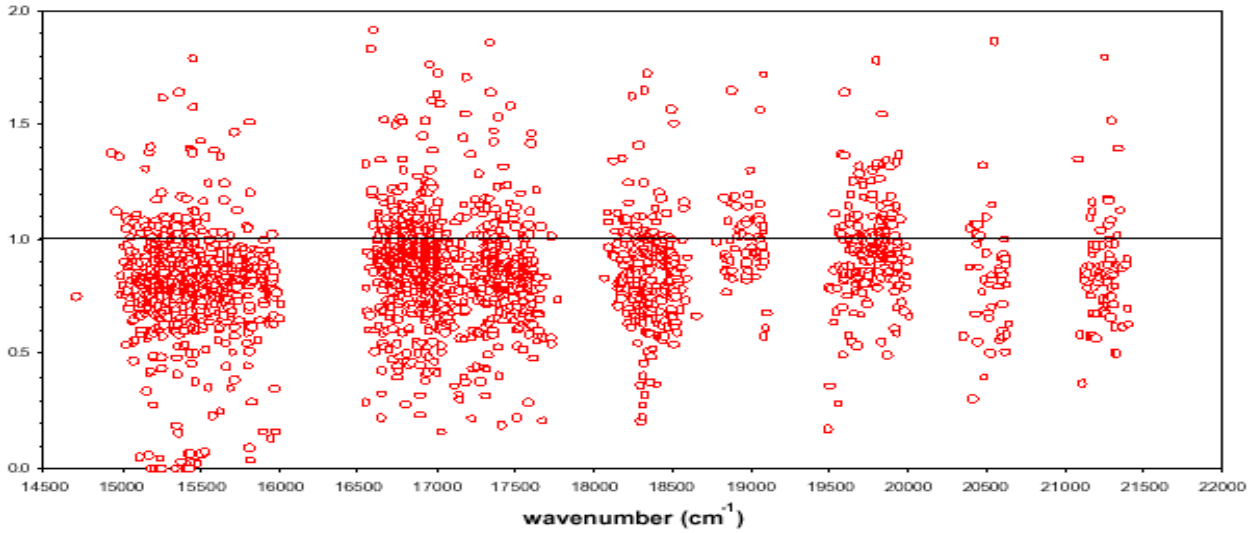


Figure 4. Comparison of absorption cross sections from ULB (Carleer et al. 1999) with HITRAN96 (Rothman et al. 1998).

Access to Data

Figure 8 shows the homepage for HITRAN. The sub-page "HITRAN UPDATES" contains files of parameters that are updates, corrections, or entirely new data that have been acquired since the official edition of HITRAN. The new or improved data are in the process of validation, but have been deemed sufficiently important to applications to warrant access by the scientific community.

The Web site also provides access and links to related databases and relevant spectroscopic conferences. A request and questionnaire form provides feedback to the user for access passwords.

Conclusion

The Upper Atmospheric Program of NASA is assisting the HITRAN Validation Committee. The panel is comprised of an international group of experts covering the molecules, parameters, and spectral range in HITRAN. The group sets priorities and establishes ad hoc sub-groups to compare, validate, and make recommendations for updating the HITRAN database. The next meeting will take place at the upcoming biennial HITRAN Conference, June 12-14, 2002. The activity of the advisory board and the work of the ad hoc panels are crucial to the future of HITRAN. In the case of water vapor, it is essential that the ad hoc committee review the sources listed in Table 1 as well as other credible efforts and make the recommendations and procedures for incorporating the data that will best improve the efforts of modelers.

The new HITRAN edition is anticipated to come out in the summer of 2002.

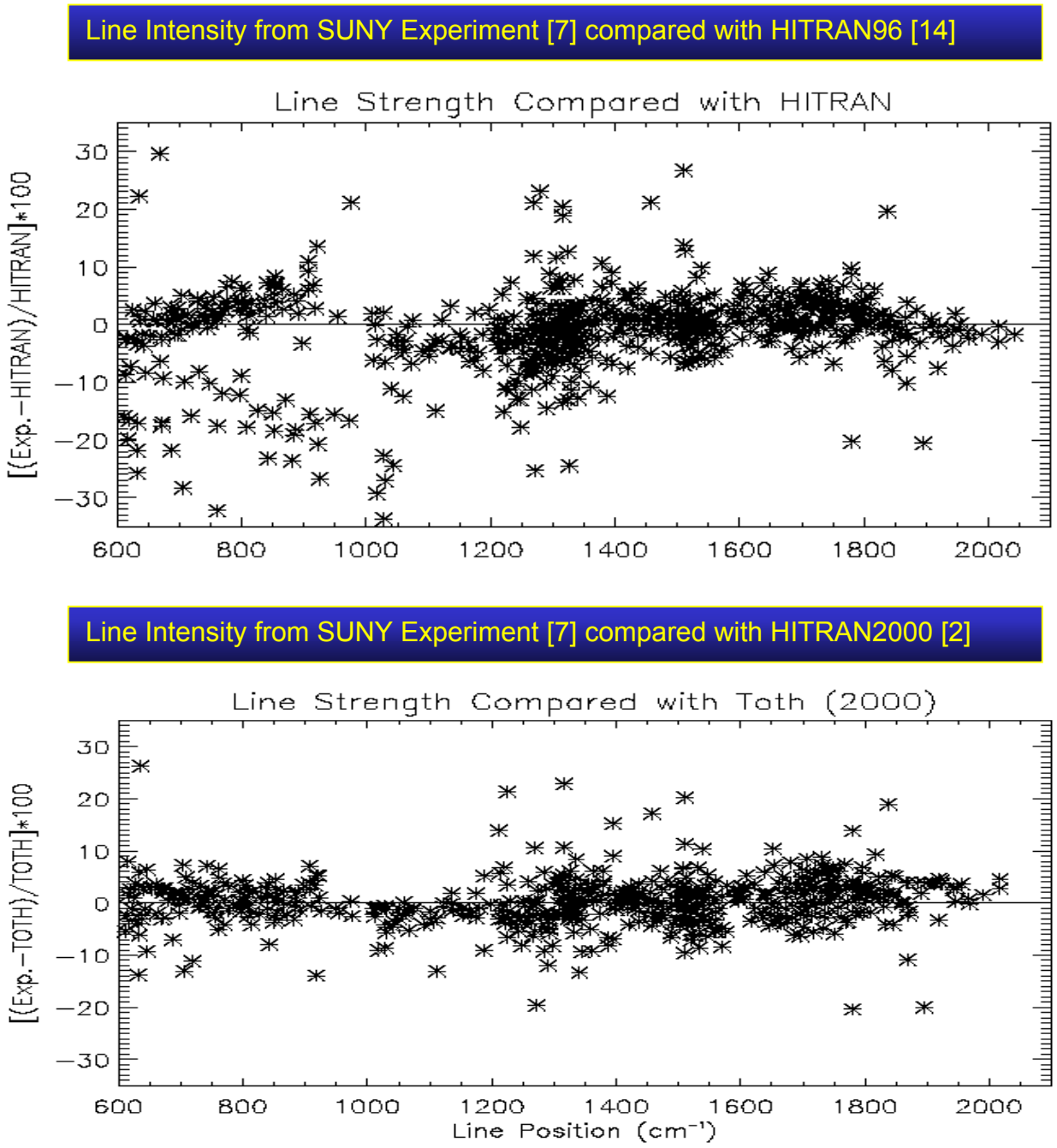


Figure 5. Comparison of line intensities between State University of New York (SUNY) (Varanasi [2002]) and (a) HITRAN96 (Rothman et al. 1998) and (b) HITRAN2000 (Rothman et al. 2001).

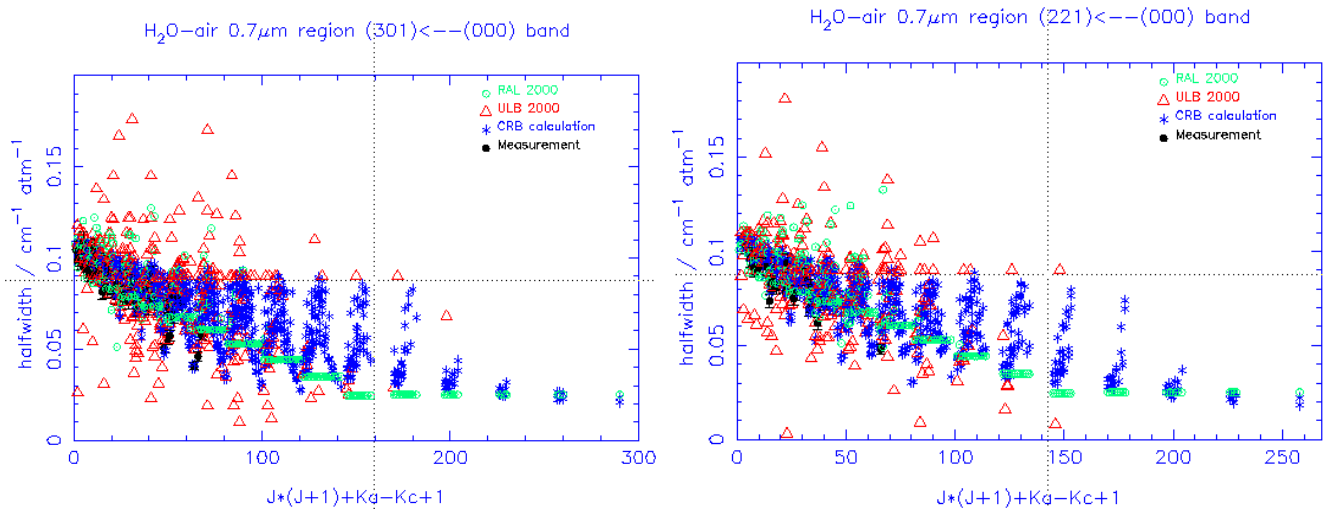


Figure 6. Comparison of air-broadened halfwidths for two H_2O bands in the 0.7-μm region.

Figure 7. Internet site for acquisition of official HITRAN compilation.

Acknowledgments

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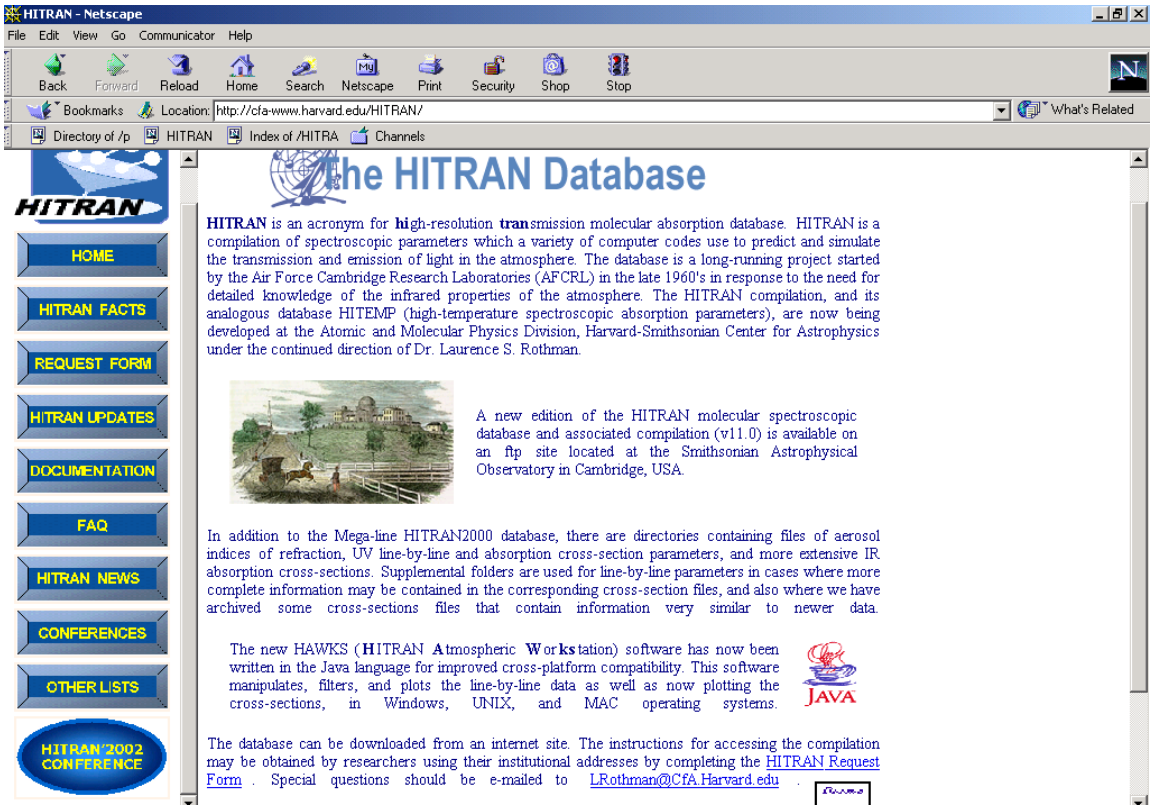

Figure 8. The HITRAN Web site.

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