Millenium HITRAN Compilation

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INTRODUCTION

The current edition of the HITRAN molecular absorption compilation has been made available on an anonymous ftp-site located at the Harvard-Smithsonian Center for Astrophysics (**ftp://cfaftp.Harvard.edu/pub/HITRAN**).

The compilation consists of five main folders:
- The traditional line-by-line parameter database
- IR cross-sections
- UV cross-sections and line-by-line parameters
- Aerosol refractive indices
- Tables of globally applicable quantities (partition sums, isotopic abundances, molecular masses, etc), algorithms (for line-coupling corrections), and references to parameters and cross-sections. There is also a high-temperature analog of HITRAN called HITEMP.

Some updates or corrections have been posted since the official release of the archival data in the ftp-site. These improvements are given in the public HITRAN web-site

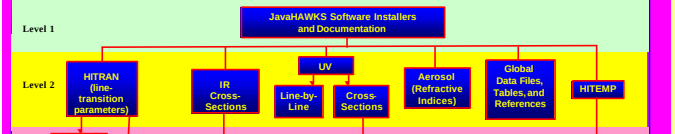
(**http://cfa-www.Harvard.edu/HITRAN**)

and will be incorporated into the next edition.

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 now in preparation.

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 (NLTE) atmospheric dynamics and astrophysics, and improved documentation. The improvements not only will provide increased capabilities for atmospheric transmission/radiance calculations and remote sensing, but will allow access and provide analytical tools for related molecular databases.

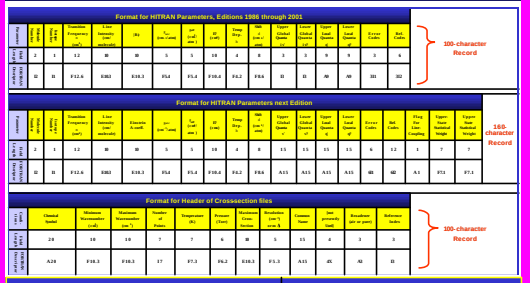
File Structure of HITRAN Compilation



The file structure of the HITRAN compilation is shown here. 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.

Record Formats for HITRAN Line-by-line Parameters and Cross-section Data



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 correspondence 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.

The record length for the cross-section files will remain at a 100-character length, but the headers have been more structured.

Uncertainty Codes used in HITRAN Database

Wavenumber (cm^{-1}) and Pressure-shift (cm^{-1}atm)		Intensity, Halfwidths, and Temperature-dependence	
Code	**Uncertainty Range**	**Code**	**Uncertainty Range**
0	>1. or Unreported	0	Unreported or Unavailable
1	>0.1 and <1.	1	Default or Constant
2	>0.01 and <0.1	2	Average or Estimate
3	>0.001 and <0.01	3	>20%
4	>0.0001 and <0.001	4	>10% and <20%
5	>0.00001 and <0.0001	5	>5% and <10%
6	<0.00001	6	>2% and <5%
		7	>1% and <2%
		8	<1%

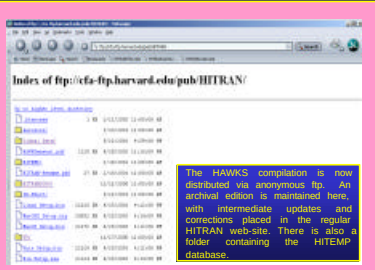
Uncertainty indices are provided for six parameters in HITRAN. There remain some lines from earlier editions with zero or blank for these indices, since this system has been implemented for three parameters in 1986, and now six in 2002.

However, some contributors do not supply this important information, so it is incumbent upon users to consult the references. Unfortunately, the references often do not provide sufficient information for individual transitions.

Sources for these parameters are provided by the reference indices. Links are provided to many of the abstracts.

Current Edition of HITRAN Compilation and HAWKS

The HITRAN web-site (http://cfa-www.Harvard.edu/HITRAN) contains crucial information concerning the current HITRAN compilation, updates to the current edition, and links to relevant meetings and databases.



The HAWKS compilation is now distributed via anonymous ftp. An archival edition is maintained here, with intermediate updates and corrections placed in the regular HITRAN web-site. There is also a folder containing the HITEMP database.

Capabilities for non-LTE Applications and Temperature Conversion of Intensities

Partitions sums, Q(T), have been generated for all isotopologues in HITRAN (about 100). A study was made to determine the best representation over the temperature range of 70K to 3000K, that is, whether the energy levels in HITRAN were a sufficiently large set to use the direct-sum method, or an analytic expression, such as developed by R. McDowell at Pacific Northwest Laboratories, would have to be used. It is important to note that the values include the state-independent degeneracy factors. Details on the methodology are given in Fischer et al, *JQSRT* **82**, 401-412 (2003).

Tables of partition sums at 1K intervals from 70 to 3000K are given in the ftp-site. A file, MOLPARAM.txt, contains global isotopologue information, such as the degeneracy factors, the partition-sum value at the standard 296K, and other constants.

This work is necessary for the formulation of the Einstein-A coefficient and for software that does a rapid interpolation for temperatures in the range noted above.

Additional Datasets in HITRAN Compilation

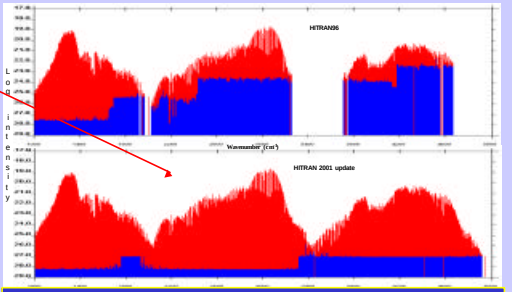
- Tables of Aerosol Refractive Indices (see Massie and Goldman, *JQSRT* **82**, 413-428 (2003).
- IR and UV Absorption Cross-sections
- Access to JPL sub-millimeter catalog
- Access to Cologne sub-millimeter Database
- Access to SAO UV Cross-sections
- Links to related databases in HITRAN web-site

HITRAN Data Assimilation

Highlighted Updates to HITRAN line-by-line Portion Since Last Edition

Molecule	Spectral Region / Bands	Parameters	Source
H_2O	9600 – 11400 cm^{-1}	Positions, intensities,halfwidths	L.R. Brown et al
	8000 – 9600, 11400 - 22000 cm^{-1}	Intensities (units massage)	L.P. Giver et al
	500 – 2800 cm^{-1}	Positions, intensities,halfwidths	R.A. Toth
CH_4	500 – 5500 cm^{-1}	Positions, intensities, halfwidths	L.R. Brown et al
O_3	1.27 μm (a^1 band)	Intensities	W.J. Lafferty et al
	0.76 μm (A-band)	Positions	L.R. Brown
NO	Overtones (2-0, 3-1)	Positions, intensities	J-Y.Mandinet al
	?.v = 2 bands, (1-0, 2-1) bands	Halfwidths	Chackerian et al, J-Y.Mandin et al
NO_2	3 μm (algorithms for halfwidths throughout)	Positions, intensities, halfwidths	V. Dana, J-Y. Mandin et al
NH_3	0 – 3700 cm^{-1} (new data in 3, 5-7μm regions, halfwidths throughout)	Positions, intensities,halfwidths	L.R. Brown et al
HNO_3	11 μm (hot bands)	Positions, intensities	A. Goldman et al
OH	All bands of the main isotopologue	Positions, intensities	A. Goldman et al
HBr	Fundamental	Positions, intensities	M.T. Coffey et al
HI	Pure-rotation, fundamental	Positions, intensities	A. Goldman et al
OCS	Extensive (many bands,isotopologues)	Positions, intensities,halfwidths	A. Fayt , L.R. Brown
C_2H_2	1248-1415 cm^{-1}	Positions, intensities	J. Vander Auwera
	1?, and 5-μm region (many new bands)	Positions, intensities,halfwidths	D. Jacquemartet al
H_2S	Fundamentals and combination band	Positions, intensities	L.R. Brown et al
C_2H_6	New Species	Positions, intensities, halfwidths	I. Caouet et al, W. Blass et al; A. Pine et al; P. Varanasi

Details given in Rothman et al, *JQSRT* **82**, 5-44 (2003)



Graphical example (from JavaHAWKS plotting routine) of CH_4 transitions in HITRAN96 (upper plot) and new linelist (lower plot). Besides a higher dynamic range and more bands, the new linelist has far better quality and a more complete set of parameters and references.

Partial List of Parameters being Analyzed and Prepared

Molecule	Update	Source	Molecule	Update	Source
H_2O	Visible and near-IR	(see below)	H_2CO	Pure rotation; 5-10 μm region	JPL catalog; Perrin et al
	Pure rotation	Jucks	HOCl	Pure rotation and ?, band	Flaud et al
	Isotopologues	Carny Peyret et al	HCN	New bands and update	Maki; NASA Langley for halfwidths
CO_2	Line positions	Tashkun et al; Benner et al; Ding et al	CH_3Cl	?, region; halfwidths	Brown; Bouanich
	Intensities	Devi; Giver; Henningsen; Teffo; Miller	H_2O_2	Pure rotation and ?, band	Perrin et al
O	Many band systems	Ozone article; Reims	C_2H_4	?, +?, region	Vander Auwera et al
N_2O	Intensities (10μm & 17 μm)	L. Daumont et al, J.W.C. Johns et al; Toth?	C_2H_6	Q-branch	Rinsland
CO	Intensities of overtones	Dana; NASA Ames; others	PH_3	Replacement plus new band system	Kleiner et al
CH_4	Tetradecad region (< 2 μm)	Brown et al, *JQSRT* **82** (2003)	COF_2	Replacement 5-μm region	Brown
O_3	$^{16}O^{17}O$ A-band	Carny Peyret	H_2S	Halfwidths	Sumpf
HNO_3	11-μm region	Flaud et al	HCOOH	Pure rotation, ?, region	JPL catalog; Perrin et al
OH	Pure rotation (isotopologues)	JPL catalog	CH_3OH	New molecule for HITRAN	Li-Hong Xu
OCS	Band intensity update	?, band - Vander Auwera	BrO	New molecule for HITRAN	
			CH_3Br	New molecule for HITRAN	

The *Tions*: Acquisition, Evaluation, Validation, Verification, and Documentation

In the early years of the HITRAN database, life was simple. There were few sources of quality, high-resolution parameters to choose from. In fact, default values were often chosen for whole ranges of parameters. For example, 0.05 cm^{-1}atm for air-broadened halfwidth or 0.5 for the temperature-dependence coefficient of halfwidth. The situation for many of the molecular bands has now become one of bringing together several sources of experimental and theoretical results.

An organization is being used to facilitate rapid acquisition of data into the archive that will have the confidence of users. It is also intended to encourage producers of data to contribute. A HITRAN Advisory Group has been established consisting of international representatives with expertise in different regions of the spectrum and different types of molecules.

Ad hoc panels are assembled by this group as determined by priorities. Members of the panels are those involved in taking the high-resolution data and also theorists if necessary. The goals of the panels are to evaluate and validate different data sets, and to propose a final set, with documentation, to the Advisory Group.

Program for Improving 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 halfwidth, and its temperature dependence. Some of these data are based on older works, especially in the near infrared and visible portions of the spectrum.

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 of the sources under consideration are listed here.

The HITRAN program has initiated a research effort to compare, evaluate, and validate the various data.

Water line lists that are being evaluated

HITRAN2000
ULB (Univ. Libre de Bruxelles, Univ of Reims – Carleer et al)
ICLAS measurements (Univ. of Paris -Picqué et al)
ESA water database (Univ. College London – Tennyson et al)
NASA Ames (Giver et al)
SUNY (Varanasi)
Ohio State Univ./Univ. Giessen (Winnewisser et al)
JPL (Toth)
RAL (Smith et al)
Ab Initio calculations (NASA Ames - Schwenke)
CRB (Complex Robert-Bonamy calculations of halfwidths – Gamache)
SAO (Jucks)

References
- L.S. Rothman, A. Barbe, D.C. Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, V. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *J.Quant.Spectrosc.Radiat.Transfer* **82**, 5-44 (2003).
- D. Belmiloud , R. Schermaul, K. Smith, N.F. Zobov, J.W. Brault, R.C.M. Learner, D.A. Newnham, and J. Tennyson, "New Studies of the Visible and Near-Infrared Absorption by Water Vapour and some Problems with HITRAN," Sixth Biennial HITRAN Database Conference, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, 19-21 June 2000.
- L.R. Brown and R.A. Toth, "Laboratory Spectroscopy to Support EOS: Water Line Parameters near 0.94 μm (940 nm) For SAGEIII," Sixth Biennial HITRAN Database Conference, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, 19-21 June 2000.
- M. Carleer, A. Jenouvrier, A.C. Vandaele, P.F. Bernath , M.-F. Mérienne , R. Colin, N.F. Zobov, O.L. Polyansky, J. Tennyson, and V.A. Savin, "The Near Infrared, Visible, and Near Ultraviolet Overtone Spectrum of Water," *J.Chem.Phys.* **111**, 2444-2450 (1999).
- D.W. Schwenke, "New H_2O Rovibrational Line Assignments," *J.Mol. Spectrosc.* **190**, 397-402 (1998).

Summary

The HITRAN compilation for the new millenium takes advantage of the technologies providing improved and more extensive data, as well as the media distribution. The means for assimilating and validating improved data will be refined.

In the future, the compilation will have:
- Improved Accuracy
- More Molecular Species
- Inclusion of Weaker Lines
- Higher-temperature Capabilities
- Implementation of Line-coupling
- Collision-Induced-Absorption
- Web-based Software

The current effort has been funded by the NASA Earth Observing System (EOS), grant NAG5-8420; the Air Force Research Laboratory, Hanscom AFB; and internal