



## HITRAN/HITEMP has moved to the Harvard-Smithsonian Center for Astrophysics

This HITRAN newsletter marks the first one in the Adobe® PDF (Portable Document File) electronic format and distributed via the HITRAN web-site ([www.HITRAN.com](http://www.HITRAN.com)). We are also making the text portions available as a PDB file for users who have a 3Com Palm® Pilot.

The past year, 1998, has witnessed several significant milestones and changes for the HITRAN database. It was the 25th anniversary of the first public release of the molecular database. This event was celebrated at the conference held in September at Hanscom AFB, which is described elsewhere in this newsletter.



February 1999 marked a change of address for HITRAN with the move of Larry Rothman to the Smithsonian Astrophysical Observatory at Harvard University. This move will make available new and important data to support the increasing needs of the user community. HITRAN will continue to support the requirements of the atmospheric remote sensing and radiative transfer modeling communities, as well as address the needs of anticipated new users. Toward this objective, a major effort is underway for a new database edition, HITRAN2000.

Dr. Rothman will maintain his relationship with the Air Force Research Laboratory through an emeritus position and will continue to provide the molecular, aerosol, and cross-section data used by atmospheric modeling codes, such as MODTRAN and FASCODE.

New information you should add to your mailing list:

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## HITRAN Documentation on the HITRAN Web-site

The HITRAN web-site ([www.HITRAN.com](http://www.HITRAN.com)) continues to be an important method to distribute information related to the database. This newsletter is now being distributed via the web in the Adobe® Portable Document File format. PDF files can be viewed on most computer platforms (e.g., MAC, UNIX, MS Windows) using the appropriate reader. These readers are provided by Adobe at no charge and can be downloaded from their web-site. A link to this site is provided in the HITRAN web-site.

In addition to the newsletter, two other documents, in PDF format, are available via the web-site. The first is the user manual for the HAWKS (HITRAN Atmospheric Workstation) software. The second is a preprint of the article on the HITRAN compilation (*Journal of Quantitative Spectroscopy and Radiative Transfer*, volume 60, pp.665-710 (1998)). The latter is the definitive description of the data contained in the CD-ROM.

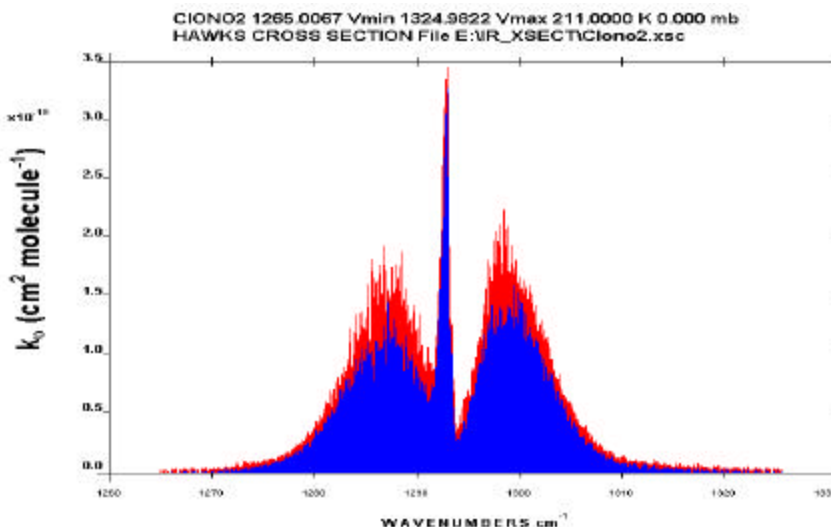
The 1996 HITRAN CD-ROM contained software, called HAWKS, provided to enable users to extract data from the database; sort and merge data in the HITRAN format; plot the data; and perform statistical calculations on the vibrational/rotational bands. In addition, the software allowed the user to read abstracts of technical papers relevant to the line positions, half-widths, and intensities of the molecular data.

A comprehensive user manual is provided with the HAWKS software. It is designed to assist the user in easily adapting to the manipulation of the HITRAN96 molecular spectroscopic database and associated molecular databases by proper utilization of the HAWKS software package. It includes installation instructions for the Windows and UNIX software, and a detailed description of the capabilities of the HAWKS software.

Two versions of the manual are provided on the CD-ROM in the DOCUMENT directory in a PKZIP executable file format. The first, called HAWKS\_WP.EXE, contains the manual in the Corel WordPerfect® format. The second, called HAWKS\_PS.EXE, contains the manual in an Adobe Postscript® format. A user can expand these files by copying them into the desired directory on his hard disk and typing the file name. A document file and several linked image files will be generated for the former, while a large Postscript file will be produced for the latter. Unfortunately, neither of these is particularly easy to read and print. Consequently, a third version is available on the HITRAN web page in the Adobe Acrobat® (PDF) format. The document, along with a reader, can be easily downloaded. Those users who wish to make a printed copy of the manual are encouraged to use this version.

## New HAWKS Software

A major upgrade of the HAWKS software is nearing completion. The 1996 HITRAN CD-ROM included two versions of the HAWKS software, one for systems using MS Windows (3.1, 95, 98, and NT), and a second version for SUN Solaris 2® and SUN OS 4®. (There is a slightly updated version of HAWKS.EXE located in the web-site.) On the 1996 CD-ROM, there is no version for other operating systems such as MAC, VAX, or other UNIX computers, although generic software is provided that can be compiled and run. The generic software lacks some of the more user-friendly features of the Windows versions.



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The new software is being written in the JAVA programming language and will be a complete cross-platform application. That is, the same executable code will run on a PC, UNIX workstation, and Macintosh computer. This is a significant improvement because we will only need to maintain a single source and executable code compared to the several versions we currently maintain. We will thus have greatly reduced difficulties with version control.

In addition to the capabilities of the current HAWKS, the new software will have new options for writing files, and will let the user select and plot cross-section data.

We have tested the software on PC, UNIX, and MAC platforms and are encouraged by the results. The Java version is slower than the older C software, because of the nature of Java. The speed difference as of March 1999 is about a factor of five. However, over the past year, the speed of Java has increased by approximately a factor of three, and the speed is just at the limit of acceptability. We anticipate that a combination of increased processor speeds and improvements to Java will shortly make the speed more than adequate for most users.

The new software is also designed to run over the web. Toward the end of 1999 users will be able to select and download HITRAN data via the web using the new software. The software will be distributed via the HITRAN web-site, so users are encouraged to check the web-site from time to time for its availability.

### **Twenty-fifth Anniversary HITRAN Database Conference**

On 23-25 September 1998, the fifth in a series of conferences on the HITRAN molecular database and related issues was held at the Air Force Research Laboratory at Hanscom AFB, Massachusetts. This meeting celebrated the 25<sup>th</sup> anniversary of the first public release of HITRAN (on magnetic tape) in 1973. The keynote speaker was Prof. Richard Goody, former director of the Planetary and Applied Physics Department at Harvard University, and now Professor Emeritus at Harvard. His book, "Atmospheric Radiation, Vol. I Theoretical Basis," published in 1963, had a seminal impact on the creation of the HITRAN database.



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There were five sessions: 1) Molecules and Cross-sections; 2) Line-mixing; 3) Databases; 4) Aerosols; and 5) Applications. In addition to invited papers on these subjects, there was also a poster session. The abstracts of the oral and poster presentations can be viewed in the HITRAN web-site using a link in the page "Latest News." At the conclusion of the meeting, an open panel session was held to summarize the findings of the conference and to formulate the priorities and future direction of the next HITRAN edition. Some of the more significant decisions were: the methodology to parametrize line-mixing (line-coupling), the substitution of the Einstein-A coefficient for the current transition-moment squared, and an increase in the number of parameters describing an individual transition.

Line-coupling produces an apparent distortion in the half-widths of some densely packed lines. This effect can cause a pronounced effect on atmospheric remote sensing. Attempts had been made on a past HITRAN database (the edition of 1986) to parametrize line-coupling for key carbon dioxide Q-branches that were being used for retrievals. However, the simple first-order theory employed at the time gave rise to great errors in some simulations. Jean-Michel Hartmann (University of Paris) and co-workers have now come up with a scheme that satisfies many previous problems: it can be adapted to many absorbing species, minimizes the amount of data that has to be stored, is quite maintainable when changes are made to other related parameters on the database, minimizes changes to subsequent modeling codes, and minimizes risks of misuse.

The current edition of HITRAN uses a parameter, the weighted transition-moment squared. This parameter is similar to the line intensity on the database, but is independent of temperature and isotopic ratio, and was added to the database initially for the purpose of aiding codes concerned with non-local thermodynamic equilibrium conditions. From the discussion at the meeting, as well as recent user feedback, we have decided that it would serve the community better to replace this parameter with the Einstein-A coefficient. This will also require the addition of the statistical weights for the upper and lower states of each transition.

Regrettably, the time has come again to alter the HITRAN transition format. Part of this change has been necessitated by the need for larger fields for some of the current parameters, such as the descriptors for the quantum identifications. We have more energy levels (such as in the case of CO<sub>2</sub> in the High Temperature database, HITEMP) or the need for greater values of rotational quanta for heavy molecules. Another issue is the request of several users to add new parameters, such as broadening by other foreign gases with the corresponding dependence on temperature.

### **Intermediate HAWKS Updates**

The HITRAN web-site is being utilized for placing corrections, updates, and occasionally new data. Users should go to the sub-page called **Database Updates**. There is a slightly newer version of the MS-WINDOWS HAWKS software located there (HAWKS.EXE version number 1.1). If you use this software frequently, we recommend that you use the updated version.

We have also placed on this sub-page some files that were inadvertently omitted from the 1996 CD-ROM. One of these files is called MOLPARAM.TXT. This file contains general information specific to all the isotopomers in HITRAN, such as statistical weights, the partition sum at 296K, isotopic abundance as used by HITRAN, and molar mass. MOL.DAT and ABUN.CMN, which are only required by some of the generic software on the CD-ROM, have also been resurrected on the web-site. Some of the other generic files have also been updated and uploaded to the web-site.

A year after the release of HITRAN96, two HITRAN-type files were deposited on the web. A file, called **38\_HIT97.par**, is a compilation of parameters for ethylene (C<sub>2</sub>H<sub>4</sub>) in the spectral range 701 to 3242 cm<sup>-1</sup>. This molecule is new to HITRAN. The second file, **19\_HIT97.par**, represents a complete upgrade and replacement of carbonyl sulfide (OCS). The data are far more extensive in the IR than the older data set existing in HITRAN.

The HAWKS96 CD-ROM includes two tar (compressed) files of the HAWKS software, one for SUNOS and the other for SUN Solaris. The Solaris version will work properly up through version 2.5, but will not work for Solaris 2.6. Since we are committed to developing the cross-platform JAVA software, there are no plans to update the old software. The zApp motif windows manager file needed for the UNIX operation of HAWKS can be found in the HITRAN web-site; it was not included in the CD-ROM.

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## HITRAN Special Issue in the *JQSRT*

The 1998 November issue (volume 60, no. 5) of the *Journal of Quantitative Spectroscopy and Radiative Transfer (JQSRT)* was developed to the HITRAN database and related issues. The lead article is the description of the current HITRAN molecular database and its associated software and data compilation (cross-sections, indices of refraction, etc.). There are also articles in this Special Issue that describe the efforts behind some of the key components of the current HITRAN database. The authors report on progress, new available data, and imminent plans for the future of HITRAN. This journal is an excellent reference source for atmospheric molecular spectroscopy and associated topics. We owe our gratitude to the editor of *JQSRT*, Prof. Prasad Varanasi of the State University of New York at Stony Brook, for the encouragement he has provided in promoting focused volumes for spectroscopy and atmospheric physics in this journal.

## Acknowledgements

The HITRAN project is currently supported by the NASA Earth Observing System (EOS) and the Atmospheric Radiation Measurement (ARM) program of the Environmental Sciences Division, Office of Biological and Environmental Research, US Department of Energy. The effort toward the development of the compilation owes an enormous gratitude to the extensive international cooperation of laboratories and government agencies that has made this project successful.



## HITRAN Advocacy

With the move of the HITRAN project from the AFRL to SAO, we are looking for new sources of support. There is a great deal of data that users would like to have added to the compilation that does not fit within the goals of the EOS and ARM programs. The program is looking for additional sponsors. Any suggestions would be appreciated.