JavaHAWKS

(JAVA HITRAN ATMOSPHERIC WORKSTATION) MANUAL

For MS Windows, UNIX, LINUX, and MAC Operating Systems

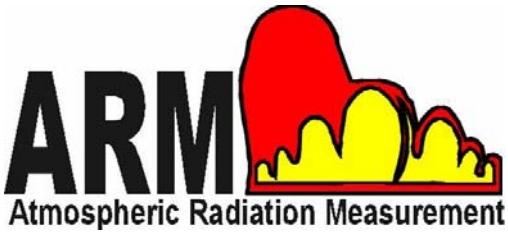
Laurence S. Rothman
Atomic and Molecular Physics Division
Harvard-Smithsonian Center for Astrophysics
60 Garden St, Cambridge MA 02138-1516

John Schroeder and Kuilian Tang
Ontar Corporation
9 Village Way, North Andover MA 01845-2000
USA

September 2004


CENTER • FOR
HARVARD - SMITHSONIAN
ASTROPHYSICS
VE RI
TAS


EOS


ARM
Atmospheric Radiation Measurement


AIR FORCE RESEARCH LABORATORY

This manual is designed to assist the user in easily adapting to the manipulation of the **HITRAN** (*Hi*gh Resolution *Tran*smission) molecular spectroscopic database and associated molecular databases by proper utilization of the JavaHAWKS software package.

1. Software Installation

The software has been written in the Java language so that we can maintain cross-platform performance, and at the same time maintain a single source code. In order to **install** and run the software, you must have a version of the Java runtime environment running on your computer. Java is common on most UNIX computers and many PC and MAC network systems. The installation program will search your computer for Java and will not complete the installation unless a suitable version of Java is installed on your computer. If this is the case, you are advised to consult your system administrator or other computer maintenance personnel about having Java installed on your computer. **We cannot be responsible for assisting you in this task, since most systems administrators have specific requirements that must be met**.

1.1. Installation Files

All installation files for different platforms are distributed via the HITRAN ftp-site (ftp://cfa-ftp.harvard.edu/pub/HITRAN/). These files are: (1) Win_Setup.exe; (2) Linux_Setup.bin; (3) Unix_Setup.bin; (4) MacOS_Setup.bin; (5) MacOSX_Setup.zip and (6) Software-Readme. The first five files are JavaHAWKS installers for different operating systems. The file "Installer of JavaHAWKS for Windows.exe" is for the PC, Linux_Setup is for Linux, Unix_Setup.bin is for any generic Unix system (e.g. Solaris, Linux, Unix, etc), MacOS_Setup.bin is for any Macintosh with operating system from 8.x to 9.x, and MacOSX_Setup.zip is for Macintosh with OS X operating system. Based on the platform one is using, a proper installer should be downloaded from the HITRAN ftp-site. Compared to previous installations of JavaHAWKS, these new installers will greatly simplify the procedures of installing JavaHAWKS on the user's computer, especially for Macintosh users. The Software-Readme file gives the user details about the installation of JavaHAWKS on different platforms and how the user launches the application, which is described below.

1.2. Installation Procedures

Please refer to the introductory paragraph in section 1 about having the Java runtime environment

installed on your computer before proceeding with the installation. It is the user's responsibility to decide which installation file he/she should download from the HITRAN ftp-site based on the platform he/she is using. Please refer to section 1.1 to decide which installer to download. Description of the installation procedures is given below for each of different platforms respectively.

PC Windows

1. Download the installation file "Installer of JavaHAWKS for Windows.exe" from the HITRAN FTP site.
2. Double click the downloaded file to launch the JavaHAWKS installation wizard.
3. Follow the installation procedures step-by-step until finally clicking the "Done" button.

Generic Unix/Linux

1. Download the installation file Unix_Setup.bin or Linux_Setup.bin from the HITRAN ftp-site to a temporary location.
2. Go to the temporary location from the shell.
3. Type in sh Unix_Setup.bin or sh Linux_Setup.bin from the command line and hit return. The JavaHAWKS installation wizard will appear.
4. Follow the installation procedures step-by-step until finally clicking the "Done" button.

Macintosh OS 8.0-9.x

1. Download the installation file MacOS_Setup.bin from the HITRAN ftp-site to a temporary location or to desktop.
2. Double click the downloaded file and a file called installer.bin will be created.
3. Double click the file installer.bin to launch the JavaHAWKS installation wizard.
4. Follow the installation procedures step-by-step until finally clicking the "Done" button.

Macintosh OS X

1. Download the installation file MacOSX_Setup.zip from the HITRAN ftp-site to a temporary location or to desktop.
2. Double click the downloaded file and a file called installer.bin will be created.
3. Double click the file installer.bin to launch the JavaHAWKS installation wizard.
4. Follow the installation procedures step-by-step until finally clicking the "Done" button.

1.3. Launching the JavaHAWKS application

Depending on the platform the user is employing, the way to launch the JavaHAWKS application may

be different. It also depends on how the user chooses to create the application icon during the installation. Following is a general description about how to launch the application for each different platform respectively.

PC Windows

The alternative ways to launch the JavaHAWKS application include the following.

1. If you choose to create an icon on the desktop during the installation, double clicking on the JavaHAWKS icon on the desktop will launch the application.
2. If you choose to create an icon in the **Start** menu during the installation, click the **Start** menu on the tool bar, and then from the **Program** list select JavaHAWKS to launch the application.
3. Locate the directory where JavaHAWKS is located from the command line. Type in JavaHAWKS.exe on the command line and hit return.

Generic Unix/Linux

1. First locate the directory where JavaHAWKS is located from the command line.
2. Type in JavaHAWKS on the command line and hit return.

Macintosh OS 8.0-9.x / OS X

1. If you choose to create an icon on the desktop during the installation, double clicking on the JavaHAWKS icon on the desktop will launch the application.
2. If you choose to create an icon in the **Start** menu during the installation, click the **Start** menu on the tool bar, and then from the Program list select JavaHAWKS to launch the application.

Paths

Put the path to the directory of JavaHAWKS instead of "~" in the Hawks.properties file for LINUX, UNIX, and Macintosh versions.

2. HITRAN and JavaHAWKS

The HITRAN Atmospheric Workstation is the latest version in a series of updates and enhancements to the international standard atmospheric molecular spectroscopic compilation. The database has a plethora of uses, the most prevalent one being as input to high-resolution transmission and radiance modeling codes of the atmosphere. Other examples of applications of HITRAN include laser propagation, hot gaseous source detection, pollution studies, background characterization, remote sensing of the atmosphere, climate assessment, greenhouse gas studies, ozone depletion, and laboratory spectroscopy.

HITRAN has traditionally supplied the necessary input for the molecular absorption part of the total attenuation in Lambert-Beer's law calculations. The other aspects of the attenuation are ascribed to aerosol extinction, continuum absorption, and scattering. The original public edition of the molecular spectroscopic database in a machine-readable form was in 1973 (the AFCRL Atmospheric Absorption Line Parameters Compilation[1]). This first edition was comprised of the seven most infrared-active absorbers in the earth's atmosphere and only covered a spectral range of about 1 to 100 micrometers. In addition, the information for each available transition was essentially limited to the principal parameters: the line position (in vacuum wavenumbers, *i.e*. reciprocal centimeters, cm^{-1}), the intensity of the transition (in $cm^{-1}/(molecule \cdot cm^{-2})$ at 296K), the air-broadened halfwidth (cm^{-1}/atm), and the energy of the lower state of the transition (in cm^{-1}). Knowledge of the parameters at that time was limited, especially for the halfwidth which often simply was given a hard-sphere collision default value.

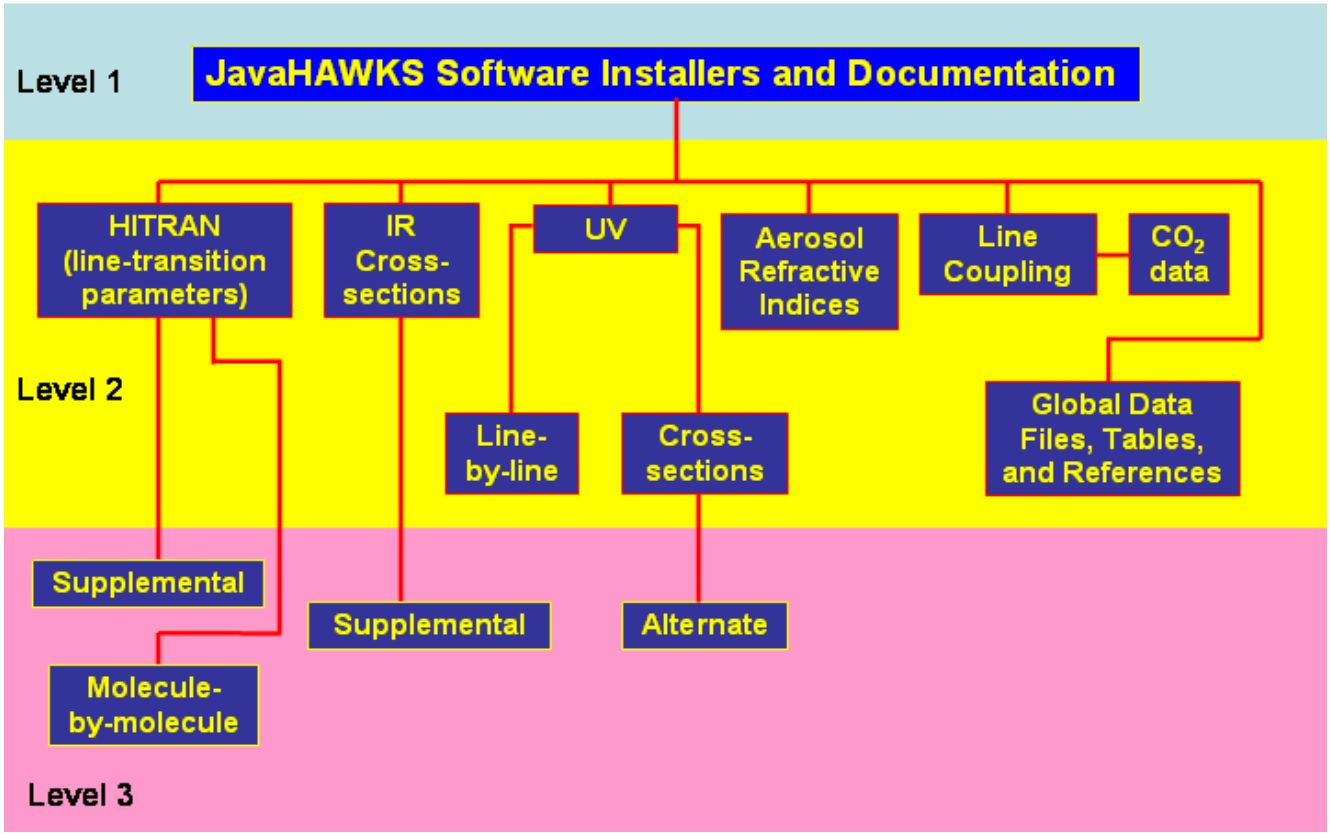
In the intervening decades, the molecular database has been substantially expanded, in terms of spectral coverage, molecular species, added parameters, increased number of molecular bands, and greatly improved accuracy. Details of the various editions and their enhancements are contained in Refs. 2-6. The archival documentation is also contained within the JavaHAWKS software.

The current edition contains 38 different species in the high-resolution portions (see Appendix B), with the inclusion of many of their significant isotopologues as well. The spectral range is from the radio through the ultraviolet (0 to about 60,000 cm^{-1}). From the initial inception of the database, the number of transitions has increased by an order of magnitude to about 1.25 million currently on the HITRAN line-by-line portion.

Another aspect of the development of the spectroscopic molecular database, or HITRAN as it is known, has been the improvement in user access. The initial versions were available on cards (a relic of the past, the cards held 80 characters of information and hence each 80-character HITRAN transition of the early editions was a single record) and on large magnetic tape. Tape became the principal means of distribution, but suffered from many inconveniences: slow sequential access, necessity of reading on mainframes, loss of integrity over time, damage, data corruption, etc. In 1992, HITRAN was made available on CD-ROM. This media enabled a great deal of data to be placed on a small, archival optical disk. More than 3000 copies of the 1992 and 1996 editions have been distributed on CD-ROM as the revolution in the use of personal computers and workstations with attached CD-ROM readers mushroomed in the early '90s. Commencing with the 2000 edition, which is HITRAN version 11.0,

HITRAN has been distributed via an ftp-site at the Harvard-Smithsonian Center for Astrophysics. Information for accessing the ftp-site is provided by completing the request form located in the HITRAN web-site, http://cfa-www.Harvard.edu/HITRAN.

This edition continues the initiative started with the previous HITRAN 1996 by including additional databases of significance. HITRAN itself, the line-by-line portion of the compilation, is now part of a much larger ensemble of tools for modeling. First, the compilation includes HITRAN (significantly updated as always) and several other databases for the "matter" part of the modeling of the interaction of matter and radiation. In addition to HITRAN, the compilation has directories containing cross-section data of heavier species or molecules with very dense spectral features, UV cross-sections and line-by-line parameters, supplemental files (such as for parameters in HITRAN-like format, but consigned to a subordinate folder because they may be better represented for simulation studies in the cross-section files), aerosol indices of refraction, the accompanying HAWKS software and documentation, and algorithms and data for computing line-coupling effects on broadening. The following figure illustrates the file structure of the compilation.



Equally important is the vastly improved user interface on the current compilation, JavaHAWKS, that works on UNIX, MAC OS, and MS Windows environments. The features are described in the sections below, and it becomes apparent that the user now has many more functions to examine and process the data on the compilation (or associated external data) than were previously available.

3. Initiating the Operation of JavaHAWKS

Compared to the previous edition of the HITRAN database, the 2004 edition contains files for each individual molecule with the 160-character HITRAN molecular transition format. One major new characteristic of this version of JavaHAWKS is that it works for both the 100-character HITRAN molecular transition format and the upcoming 160-character HITRAN molecular transition format. The corresponding changes to the earlier version of JavaHAWKS, therefore, have been made so that it also works for the 160-character format HITRAN files as well as the 100-character formats HITRAN files. Both the 100-character and 160-character HITRAN molecular transition formats are described in detail and are shown in Appendix D.

Launch the JavaHAWKS application as described in section 1.2. The initial JavaHAWKS screen will then appear:

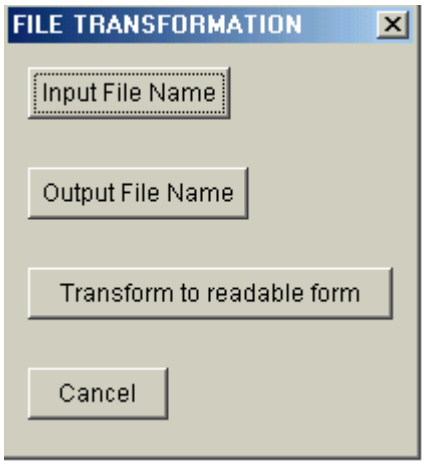
The following options are now available in the menu bar:

The choices produce pull-down screens or dialog boxes. Control is maintained by clicking the left mouse button.

3.1. File Option

By clicking on the FILE option, the user is given the option of performing two different tasks: **Change Format** and **Exit**. The choice, **Change Format**, is an option included for the convenience of allowing a more readable listing of the HITRAN parameters.

3.1.1. Change Format



For the input files with 100-character HITRAN format, the **Change Format** option performs the following two functions: first, it generates a HITRAN-like file with the molecule number in columns 1 and 2 replaced with the corresponding chemical symbol, e.g. 1 in column 2 is replaced by H20. Second, the vibration indices (v′ and v") in columns 68 to 73 are replaced with the notation more familiar to spectroscopists, e.g. 5 1 is replaced by 001-000 for ozone. For the input files with 160-character HITRAN format, **Change Format** works almost the same as working on the 100-character HITRAN format except for a slight difference as described below. Since vibration levels in columns 68 to 97 in files with 160-character HITRAN format are already represented by the corresponding vibration notations, the **Change Format** option needs only to perform the replacement of the molecule number in columns 1 and 2 with the corresponding chemical symbol. Examples of HITRAN-like files generated using SELECT, as described in Section 3.2, are shown below along with the corresponding file generated by the **Change Format** option (the example is for ozone, molecule 3). The changes from one file to the other are highlighted in light blue.

100-Character Format HITRAN-like file:

```
32 1000.003800 1.620E-23 1.498E-02.0706.0908  497.2245 .76 .000000  5  126 819   27 820   005 1 1 1
32 1000.003800 1.620E-23 1.498E-02.0706.0908  497.2245 .76 .000000  5  126 818   27 819   005 1 1 1
31 1000.010100 1.340E-24 1.461E-02.0709.0912 2246.4110 .76 .000000 18  722 914   21 913   005 1 1 1
31 1000.010700 4.800E-24 4.964E-02.0748.1026 2168.1560 .76 .000000 27 1416 215   15 214   455 4 4 1
31 1000.012900 6.440E-24 2.258E-03.0707.0919 1597.2180 .76 .000000 13  428 722   28 721   005 1 1 1
```

160-Character Format HITRAN-like file:

```
32 1000.003800 1.620E-23 1.498E-02.0706.0908  497.2245 .76 .000000           001          000      26 818         27 819   005    1 1 1
32 1000.003800 1.620E-23 1.498E-02.0706.0908  497.2245 .76 .000000           001          000      26 819         27 820   005    1 1 1
31 1000.010100 1.340E-24 1.461E-02.0709.0912 2246.4110 .76 .000000           111          110      22 914         21 913   005    1 1 1
31 1000.010700 4.800E-24 4.964E-02.0748.1026 2168.1560 .76 .000000           003          002      16 215         15 214   455    4 4 1
31 1000.012900 6.440E-24 2.258E-03.0707.0919 1597.2180 .76 .000000           101          100      28 722         28 721   005    1 1 1
```

File generated using the Change Format option:

```
03     2  1000.003800  1.620E-23  1.498E-02 .0706 .0908   497.2245  .76  .000000 001-000          26 819   27 820   005 1 1 1
03     2  1000.003800  1.620E-23  1.498E-02 .0706 .0908   497.2245  .76  .000000 001-000          26 818   27 819   005 1 1 1
03     1  1000.010100  1.340E-24  1.461E-02 .0709 .0912  2246.4110  .76  .000000 111-110          22 914   21 913   005 1 1 1
03     1  1000.010700  4.800E-24  4.964E-02 .0748 .1026  2168.1560  .76  .000000 003-002          16 215   15 214   455 4 4 1
03     1  1000.012900  6.440E-24  2.258E-03 .0707 .0919  1597.2180  .76  .000000 101-100          28 722   28 721   005 1 1 1
```

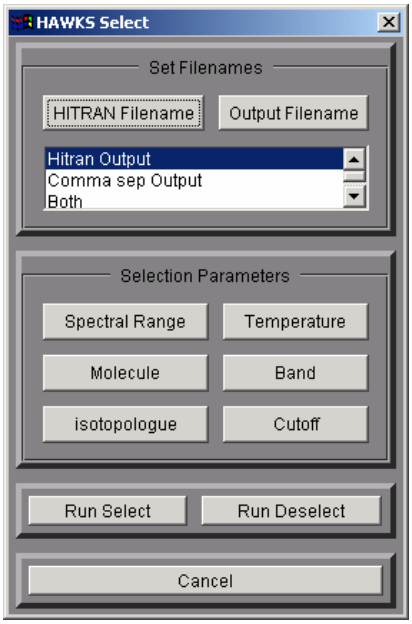
The option is simply run. "Input File Name" is the name of the HITRAN-like file you wish to transform into the new format. "Output File Name" is the name you select for the new file. The action is initiated by selecting "Transform to readable form", and the action is canceled by selection of the "Cancel" option.

3.1.2. Exit

The **Exit** option enables an easy exit from the **JavaHAWKS** software.

3.2. Select Option

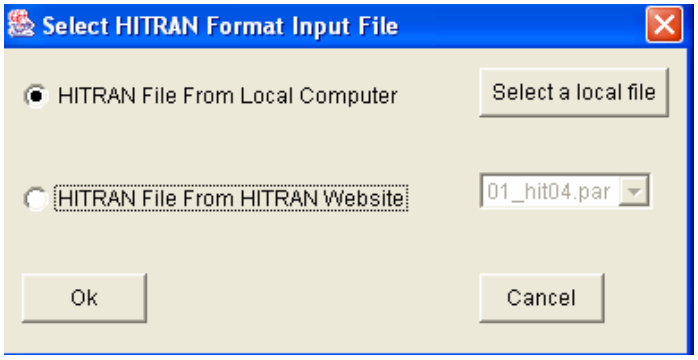
The most important and detailed option screen is **Select**, which contains several choices described below.

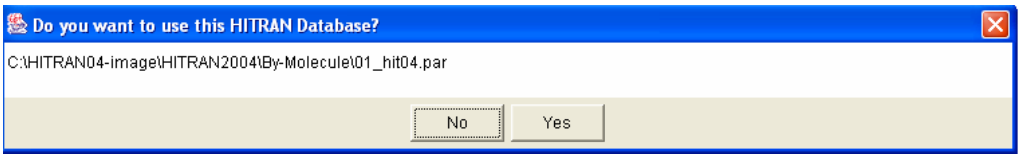


Select is the principal operating program for a detailed manipulation of the HITRAN database, or any files in the HITRAN format. When SELECT is started, a set of default parameters, from your previous run, is retained.

3.2.1. HITRAN Filename

The first choice in the Select screen is HITRAN Filename. Clicking this button will bring up the select file input screen as shown on the right below. There are two choices for the user to bring up a HITRAN-like file. They are HITRAN File From Local Computer and HITRAN File From HITRAN Website. Corresponding to the first choice, there is a button "Select a local file" allowing you to open a HITRAN-like file stored in your local computer by clicking it. Corresponding to the second choice is a pull down menu with all HITRAN files residing in the HITRAN web server listed. These files are either in the 100-character format or in the 160-character format. The user should keep in mind that the speed may be slow if he/she chooses to work with files on the HITRAN website. The speed depends on both the internet access speed and the size of the HITRAN file selected. If a file is selected locally, a dialog box as shown below appears and asks if you wish to open the previously used HITRAN-like file.

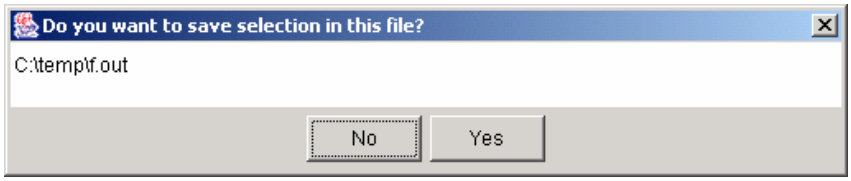




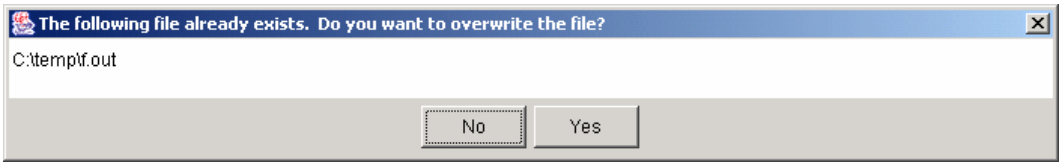
If you answer "no," a second dialog box is displayed which contains standard features for changing drives, browsing paths, or choosing common file types.

3.2.2. Output Filename

The second choice in the **Select** screen is the OUTPUT Filename, which allows the user the option of storing the ASCII output file wherever it is desired. As with the "HITRAN File Name" option, the user is queried regarding the name to use for the new file, and is given the opportunity of changing drives, browsing paths, etc.



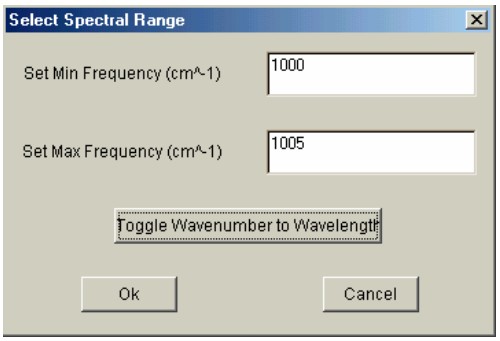
If you answer "No", it will ask you again to locate the place to store the new file. If you answer "yes" and the file the user selects already exists, the dialog below will ask you if you really want to overwrite the existing file.



The Select function allows the user to generate a file in either the standard HITRAN format, or as a comma-separated values file (or both). The format of the latter file is based on the column definitions of the HITRAN database, and is of use to users who want to open the file with a program that delimits the file based on comma separators, e.g. Microsoft Excel®. An example of a comma-separated file, corresponding to the examples shown in Section 3.1.1 above, is given below:

```
3,2,1000.003800, 1.620E-23, 1.498E-02,.0706,.0908,  497.2245, .76, .000000,  5,  1,26 819   ,27 820   ,005, 1 1 1
3,2,1000.003800, 1.620E-23, 1.498E-02,.0706,.0908,  497.2245, .76, .000000,  5,  1,26 818   ,27 819   ,005, 1 1 1
3,1,1000.010100, 1.340E-24, 1.461E-02,.0709,.0912, 2246.4110, .76, .000000, 18,  7,22 914   ,21 913   ,005, 1 1 1
3,1,1000.010700, 4.800E-24, 4.964E-02,.0748,.1026, 2168.1560, .76, .000000, 27, 14,16 215   ,15 214   ,455, 4 4 1
3,1,1000.012900, 6.440E-24, 2.258E-03,.0707,.0919, 1597.2180, .76, .000000, 13,  4,28 722   ,28 721   ,005, 1 1 1
```

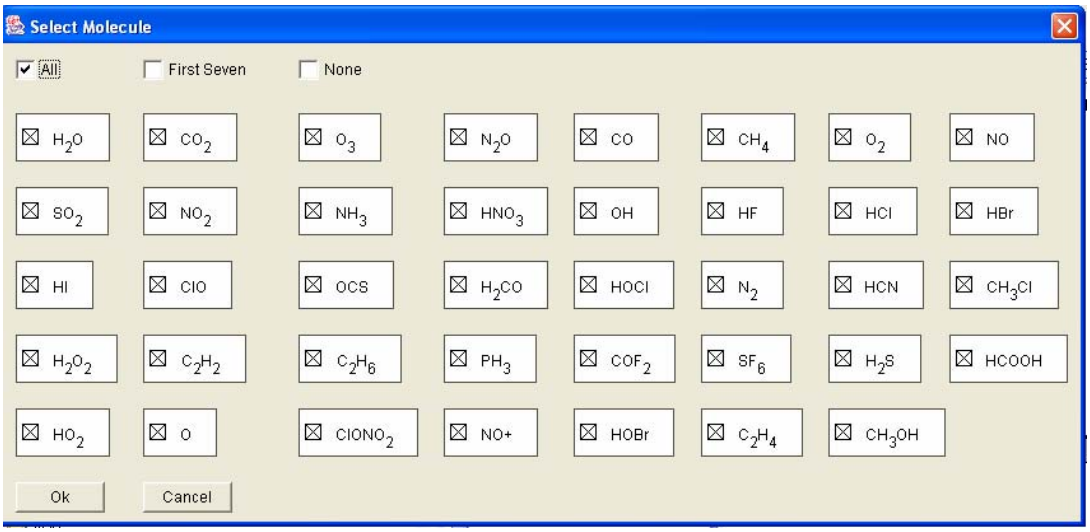
3.2.3. Spectral Range



The third choice in this series is Spectral Range, which allows the user to identify the wavenumber (or wavelength) range of the data being gathered. One can choose the start and end of the selection in either wavenumber (cm^{-1}) or wavelength (μm). This option is the essential choice (necessary and sufficient) in any SELECT procedure.

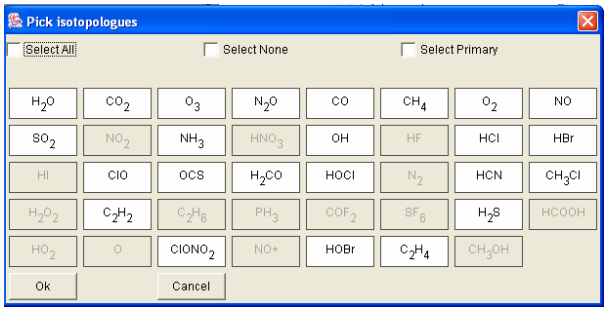
3.2.4. Molecule

The fourth optional choice in the **Select** screen is Molecule, which gives the user the option of including All the available molecules within the spectral range defined, the First 7 molecules (coinciding to the original HITRAN), or None. None is provided as a convenient button to allow the user to subsequently select various specific assortments of molecules; hence this choice is probably the most frequently employed.

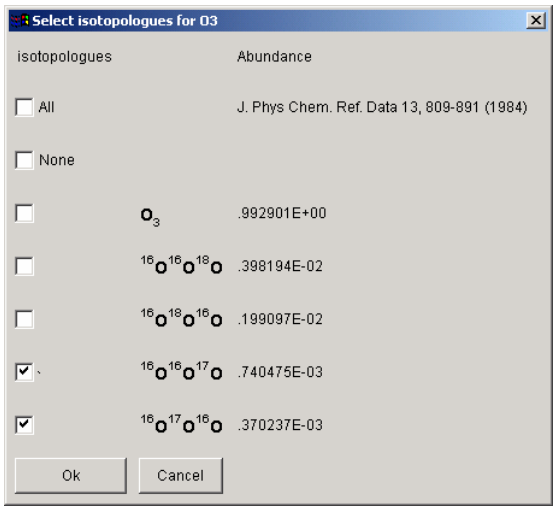


3.2.5. Isotopologue

The fifth optional choice in the **Select** screen is Isotopologue, which gives the user the option of retaining all of the available isotopologues of a given selected molecule or selecting individual isotopologues to include in the output. Isotopologues are molecular entities that differ only in isotopic composition (for example $^{16}O^{12}C^{16}O$ and $^{16}O^{13}C^{16}O$) and isotopomers are molecular entities that have the same isotopic atoms, but arranged in different positions (for example $^{16}O^{16}O^{18}O$ and $^{16}O^{18}O^{16}O$).



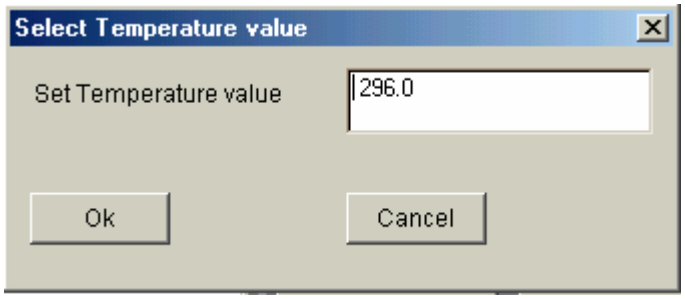
In the following example, the user has previously selected ozone as at least one of the molecules. When the Isotopologue box is clicked on the ozone box, the screen at right appears (Select Isotopologues for O_3). In this example, one has chosen the odd assortment of the pair with ^{17}O. Thus one can choose all of the isotopologues for a molecule (a typical choice, therefore the default) or specific sets of isotopologues, useful in some laboratory cell experiments. Of course, in the spectral range selected, there may not exist any data for some isotopologues.



The actual values of isotopic abundances used in HITRAN are given in the second column in the isotopologue selection box. These values enable the user to re-normalize the intensities, for example where the output is to correspond to a laboratory absorption experiment with enhanced isotopic mixtures.

3.2.6. Temperature

The sixth optional choice is Temperature, which lets the user set the desired temperature for the chosen set of lines. The present allowable range of temperatures is 70K to 3000K. The parameters in a HITRAN transition that depend on temperature, namely the intensity of the line and the halfwidths, are given at a standard reference of 296K. Being an atmospheric database, many transitions that are appropriate for high temperatures are liable to be missing, a fact that the user should consider. This is particularly true in spectral regions where a molecule may have many "hot" bands originating from a low vibrational state. However, the temperature option is necessary for line files such as HITEMP, since the intensities in HITEMP line files are also given at the standard 296K and must be converted through the temperature option to the required temperature.

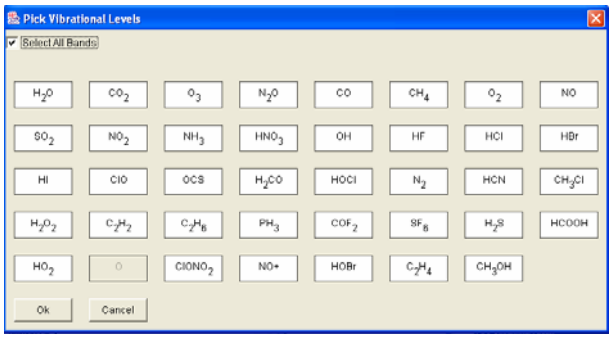


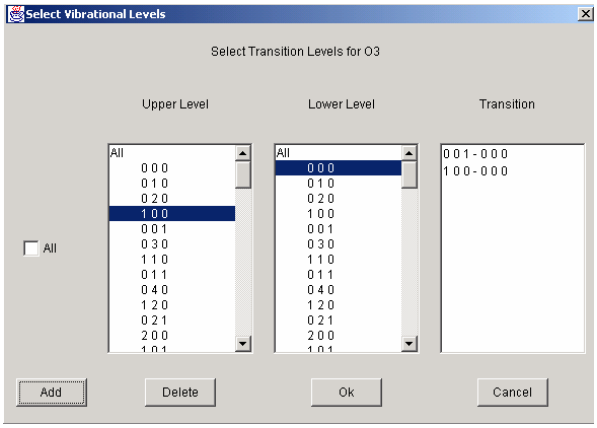
Another caveat is that the partition sums used in SELECT necessary to perform the temperature conversion may have errors at the higher temperatures, noticeable in the case of species with many very low vibrational states such as HNO_3. Nevertheless, we believe these errors are quite tolerable for most applications.

3.2.7. Band

The seventh optional choice in the **Select** screen is Band, which brings in the VIB LEVEL SELECTION screen, allowing the identification of vibrational levels for a specific molecule. This powerful feature allows the user to select individual vibrational bands from the input database file by highlighting a quantum level from the UPPER LEVEL box and one from the LOWER LEVEL box. The user then depresses the **Add** button to include his selection. This procedure can be repeated to obtain a series of bands. In addition, one can choose ALL as either the upper or lower level. In this

manner, it is possible to search the database for all transitions originating from one particular lower level to ALL possible upper levels. If a transition was highlighted by mistake, a button **Delete** is provided to delete the choice from the UPPER-LOWER box. In this case one highlights the transition not to be considered in the search and clicks on the delete button. When the selection of bands is complete, the user clicks on OK. The default for the Band option is ALL transitions.





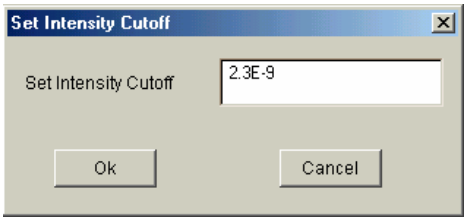
NOTE: The use of the Band option should be considered very carefully. It should only be employed by those users thoroughly familiar with the manipulation of various vibrational transitions for specific molecules.

By clicking on a specific molecule (the example above is for O_3) the Vibrational Selection for O_3 screen appears. The user can now select upper level and lower level vibrational transitions for the given molecule. In the example above for O_3, the transitions for ν_1 and ν_3 have been chosen. After highlighting the upper and lower levels, the user presses the **Add** button. If a level has been incorrectly added, it can be highlighted and removed by pressing the **Delete** button.

The current version of JavaHAWKS has added some new vibration levels for three classes of molecules compared to the old version. Class 3, which includes molecules NO, OH and ClO, has added new vibration levels from level 21 to 24; class 7, which includes molecule C_2H_2, has added new vibration levels from level 11 to 28; new vibration levels from level 44 to 48 are added for class 10, which includes molecules CH_4, HNO_3, CH_3Cl, C_2H_6, SF_6, HCOOH, $ClONO_2$, and C_2H_4. Users who have used the last version of JavaHAWKS may also notice some changes in the vibration notations for class 7 (molecule C_2H_2).

3.2.8. Cutoff

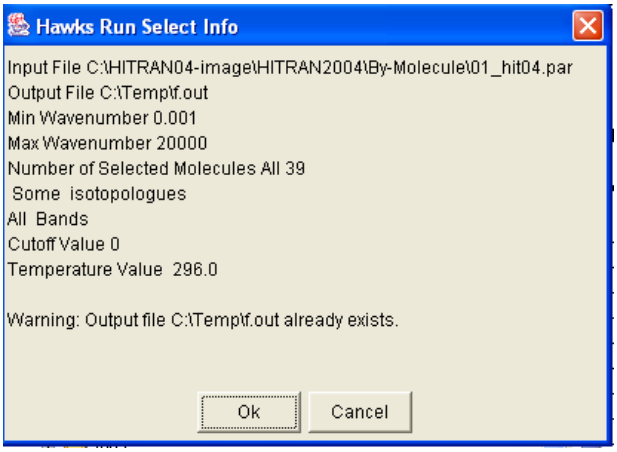
The eighth optional choice in the **Select** screen is Cutoff, which gives the user the option of eliminating lines below a specified intensity. To implement, one types in the threshold intensity in exponent notation. JavaHAWKS will convert the exponent to a 3-digit value even if one number is typed in, *e.g.* 2.3E-9 becomes 2.3e-009. There are some transitions in HITRAN, and many in HITEMP, whose intensities (given at the standard 296K) are less than the single precision allowed by most compilers. In that case Cutoff can be used to eliminate them from the selected output.

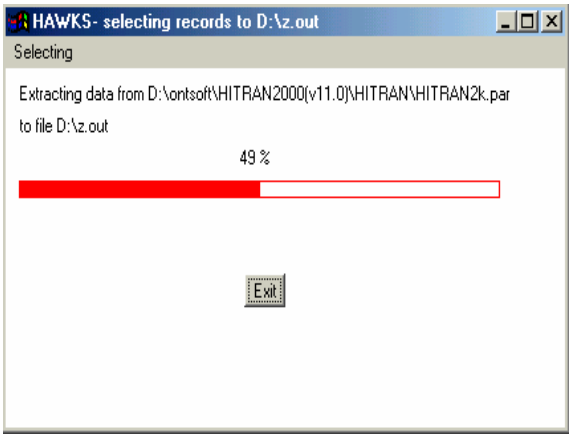


NOTE: This Cutoff option can be used to limit the dynamic range, but one generally does not know, a priori, what the overall effect on simulations that use the output file will be. Therefore, this option, as with the choice of Band, is probably only useful to very experienced users of the database. Since the plotting package (see Section 3.6) allows control of the minimum plotted intensity, this cutoff option does not need to be used for that purpose.

3.2.9. RUN SELECT

The ninth choice in the **Select** option is RUN SELECT, which when activated, will produce an outline of the chosen case to run, as shown in the following example. This box is provided as a rough check for the user to verify his/her choices. If the output file already exists, a warning message will appear on this box.





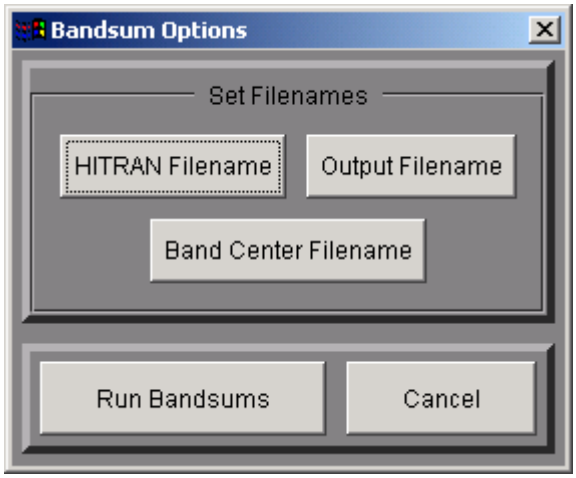
By clicking on the OK button the Select program will begin its operation. As the program is searching the database to select the desired lines, a window is displayed with a "thermometer" which indicates the progress of the selection process.

3.2.10. RUN DESELECT

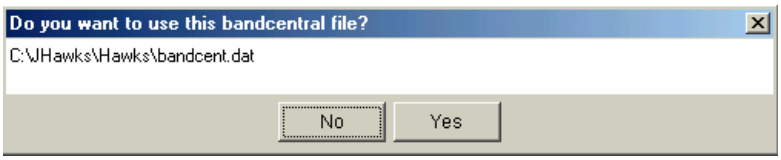
The RUN DESELECT option is provided to the user to perform the inverse operation on the HITRAN database to Select. The concept here is to allow an editing feature for subtracting old or unwanted bands from a database and leaving the skeleton database to which one subsequently may add new or replacement data. One proceeds with the same selection criteria as one would in a normal Select procedure. The current version of this software extends the deselecting function to both isotopologues and bands, which was not the case in earlier versions of the software. In addition, in older versions of this software the choice of spectral interval was ignored: the initial database being "deselected" is taken in full. However, that **IS NOT THE CASE** with the current version. **Only lines between the initial and final wavenumber (wavelength) will be given in the resulting output file.** One should note that ample disk space needs to be considered in the general case of deselecting a few bands of a molecule from the HITRAN database. The resulting database that is written may very well be almost the same size as the original.

3.3. Band Stats Option

The **Band Stats** option runs the Bandsum program on a given file of data, or on the entire HITRAN database, for one or more molecules. The output gives: the number of lines for every band of each isotopologue; the minimum and maximum wavenumber, *J* values, line intensities, broadening parameters, line shift; sum of the line intensities; and additional spectroscopic statistics of use for in-depth analysis. At the end of the output, a new section called Summary of Missing Bands is attached. Information contained in each line of this section includes the missing upper and lower vibrations for a specific molecule and isotopologue. This is a new feature to the previous version of JavaHAWKS. The program accessed by selecting the **Band Stats** option from the main menu will give the dialog box as shown here.



The HITRAN Filename and **OUTPUT Filename** options are used in the same way as described above in Sections 3.2.1, and 3.2.2 for the **Select Option**. Selecting the **Band Center Data** options brings up the dialog box that is used to select a file of band centers for each isotopologue of every molecule. Bandstats will work for both the 100- and 160-character line formats.

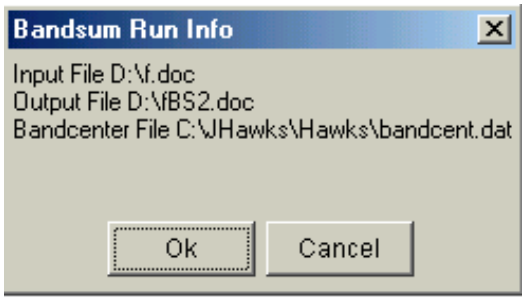


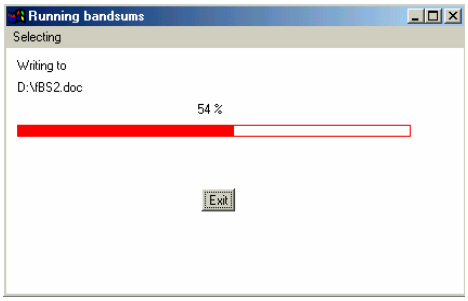
The following bandcent input file example is for the new 160-character format:

```
1  161 '          0 0 1' '          1 0 0'     98.877   7
1  161 '          0 0 1' '          0 2 0'    604.300   7
1  161 '          0 3 0' '          0 2 0'   1515.163   7
1  161 '          0 2 0' '          0 1 0'   1556.8804
1  161 '          0 1 0' '          0 0 0'   1594.7498
1  161 '          1 0 0' '          0 1 0'   2062.306
1  161 '          0 0 1' '          0 1 0'   2161.183
1  161 '          0 3 0' '          0 1 0'   3072.046   7
1  161 '          0 2 0' '          0 0 0'   3151.6302  5
1  161 '          1 1 0' '          0 1 0'   3640.245   7
1  161 '          1 0 0' '          0 0 0'   3657.0532 21
```

Users will probably employ the default file either "Bandcent_Newformat.dat" or "Bandcent_Oldformat.dat" located in the HAWKS folder under JavaHAWKS. Advanced users may want to edit these files to tailor them to specific molecules being investigated.

The program is executed by selecting the **RUN BAND SUM** option. An ASCII table, with the filename selected with the **OUTPUT Filename** option, is created. A summary dialog box and a pair of "thermometer" boxes are displayed to indicate the status of the calculation.





The output statistics are as follows and are printed in one single line:
***V*o Iso V′ ← V″ *V*min - *V*max #lines ΣS Smin Smax J″max gmin gmax J″min E″min E″max gsmin gsmax nmin nmax shiftmin shiftmax**

where *V*o is the bandcenter in cm^{-1}, Iso is the shorthand code for the isotopologue, V′ is the upper-state

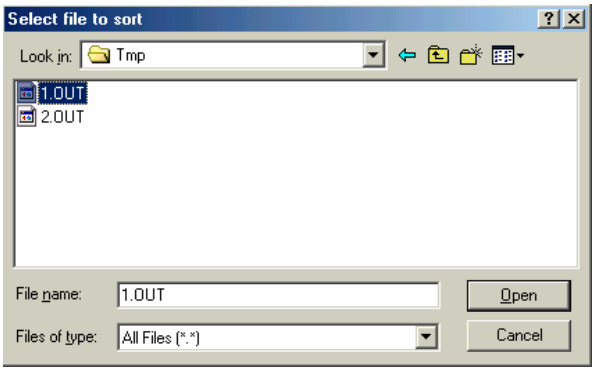
vibrational band quanta, V″ is the lower-state vibrational band quanta, V_{min} is the minimum wavenumber found for the band (rounded down to the nearest integer wavenumber), V_{max} is the maximum wavenumber found for the band (rounded up to the nearest integer wavenumber), #lines is the number of transitions found for the band, ΣS is the sum of intensities in the band, S_{min} is the minimum intensity in the band, S_{max} is the maximum intensity in the band, J''_{max} is the maximum lower-state rotational quantum value found. On the second line for the band, g_{min} is the minimum value of air-broadened halfwidth, g_{max} is the maximum value of air-broadened halfwidth, J''_{min} is the minimum lower-state rotational quantum value found, E''_{min} is the minimum lower-state energy, E''_{max} is the maximum lower-state energy, gs_{min} is the minimum value of self-broadened halfwidth, gs_{max} is the maximum value of self-broadened halfwidth, n_{min} is the minimum value of the temperature-dependence coefficient, n_{max} is the maximum value of the temperature-dependence coefficient, $shift_{min}$ is the maximum value of self-broadened halfwidth, is the minimum value of the pressure-shift, and $shift_{max}$ is the maximum value of the pressure-shift.

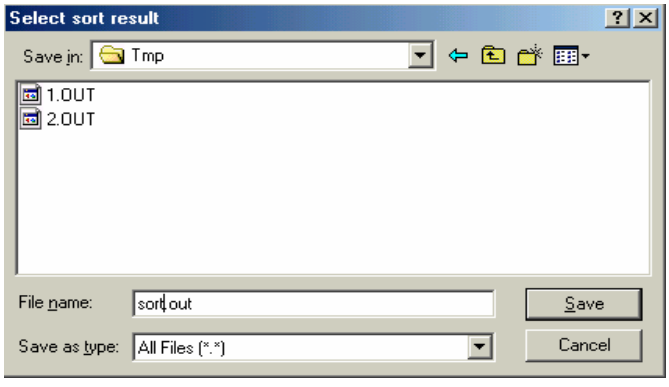
If you request a band in the bandcent.dat input file that is not found in the HITRAN-like file, the output will indicate zero lines, and pre-set extrema will be given for the ranges (50000 for the minima, and 0 for the maxima). On the other hand, if a band exists in the HITRAN file that was not requested in the bandcent.dat file, a summary is indicated at end of the output to inform you that you may want to add this band to your search.

3.4. Sort Option

The **Sort** option allows the user to sort by wavenumber of a HITRAN-like file (the field defined by positions 4 through 15), or to merge numerous individual HITRAN-like files into a single file.

3.4.1. Sort





When choosing the **Sort** option the user is asked to identify the physical location of the particular file to be sorted as displayed in the following dialog box on the left above.

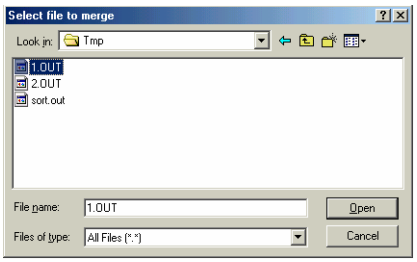
Next the user is asked to identify the name and location for the sorted result as shown in the dialog box to the right above.

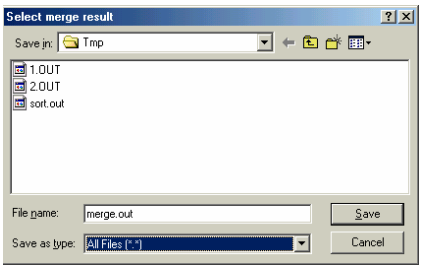
Before running Sort, users may select the sorting type by going into the SORT TYPE window from the Sort pull-down menu of the main window. There are two sort types provided: Sort by Wave Number and Sort by Quantum Number. When Sort by Wave Number is selected, the current version of JavaHAWKS queries the wavenumber first, and, if necessary, then queries in the order of molecule number, isotopologue number, intensity and so on, the other parameters in a transmission line. When Sort by Quantum Number is selected, unlike Sort by Wave Number, the current JavaHAWKS only queries three other parameters in addition to the quantum numbers. They are the molecule number, isotopologue number and wavenumber in the order that may be queried.

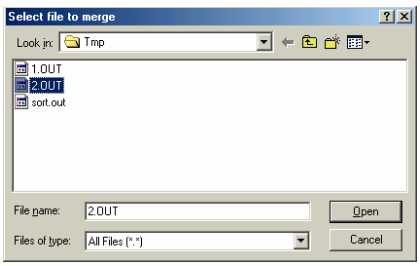
If the querying finds that two lines compared are identical, one line was discarded in the last version of JavaHAWKS. However, this is not the case of the current version of JavaHAWKS. In the current version, if two lines are identical, the second of the two lines encountered is not deleted but flagged with a "*" at its end. Users can conveniently use this feature to find out if there are any duplicated lines in a HITRAN-like file. Users may also need to remember that the sorted file with duplicated lines in it cannot be used as a normal HITRAN data file.

3.4.2. Merge

The second choice in the **Sort** pull-down screen is **Merge**. The **Merge** option allows the user to merge two or more separate HITRAN-like files into one file and gives the user the option of sending this merged file to whatever location is desired. The following screens will appear asking the user to identify files to be merged:







Click on the CANCEL button to end the selection of files being merged. A new dialog box will now appear (at the right above) directing the naming of the file containing the merged results.

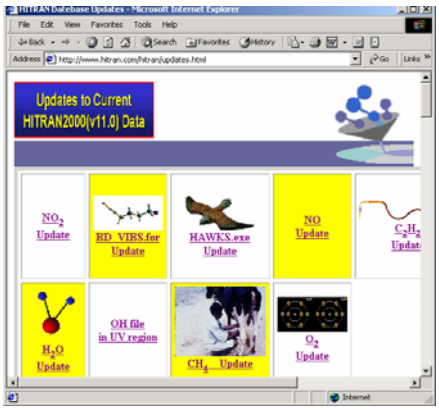
NOTE: Merge will also sort the resulting file, if (and only if), the lines in the individual HITRAN files are already in order of increasing wavenumber. If there is an identical line existing in more than one file to be merged (that is there is an overlap between files), this line will be duplicated but flagged at its end with a "*" except the first one in the merging resulting file. Users may need to remember that the merged file with duplicated lines in it can not be used as a normal HITRAN data file.

3.5. Internet Option

The **Internet** option has been added to the main menu bar in the latest version of JavaHAWKS. This option allows users to interact with the outside world through the Internet by providing access to the HITRAN database and other data sources. There are five choices under the Internet option. They are HITRAN Website, HITRAN FTP Site, JPL Submillimeter Data, Cologne Spectroscopy Data, and CfA UV Xsection Data.

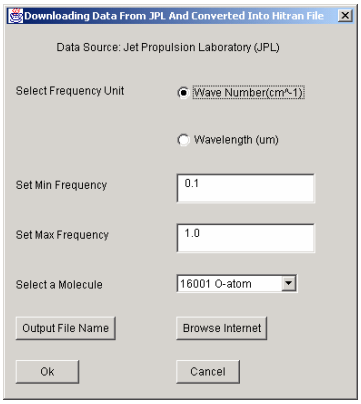
3.5.1 HITRAN Website

When the HITRAN Website is selected under the **Internet** Option, JavaHAWKS will start the internet connection and bring users directly to the updates webpage of the HITRAN website (http://www.hitran.com/hitran/updates.html). From this page, you can get the most recent JavaHAWKS software as well as the most recent HITRAN updates.



3.5.2 HITRAN FTP Site

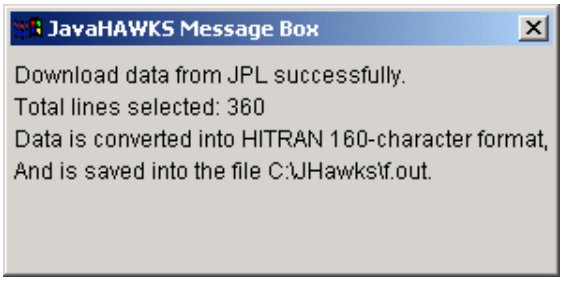
When the HITRAN FTP Site is selected under the **Internet** option, JavaHAWKS will start the internet connection and bring users to the location to download archival HITRAN files in the HITRAN FTP site.



3.5.3 JPL Submillimeter Data

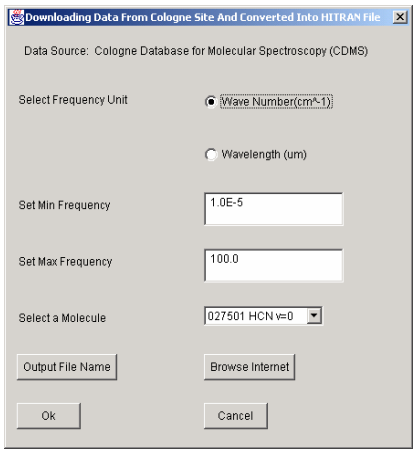
The third choice under the **Internet** option is JPL Submillimeter Data. This choice will lead you to access to JPL (Jet Propulsion Laboratory)

submillimeter catalog,[7] download a JPL catalog file from the database and then convert the downloaded data into a HITRAN format file. Selection of this item will bring in a screen called Downloading Data From JPL and Converting Into HITRAN File, which lets you set up the downloading parameters. The parameters include wavenumber units (in wavenumber or in wavelength), minimum wavenumber, maximum wavenumber and the molecule you are interested in. The Output File Name button will ask you to specify a location to save the converted data. Pressing the Browse Internet button will initialize the data downloading over the internet and then the conversion to a HITRAN format file. This reformatting includes converting the line intensities to the HITRAN units and standard of 296K, changing the vibrational notation, and converting the JPL error bars to the HITRAN system. Since the JPL catalog does not contain information about collision-broadening, these parameters are left blank in the conversion to the HITRAN-like file. A file with the data in its original format will also be saved under the current JavaHAWKS working directory.



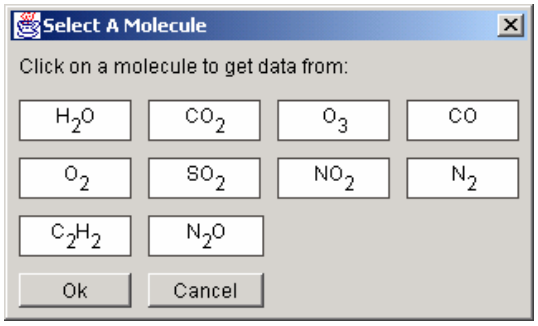
Users should keep in mind that downloading data over the internet might fail if there is an internet connection problem or if the host of the data source has shut down its server. JavaHAWKS provides a window message for you, letting you know if it has successfully downloaded the data. If it is successful, a window message comes up telling you how many lines you have downloaded and where you have saved the converted file. Otherwise, a message of internet connection failure shows up. Depending on the user's internet connection speed, the download process may be slow.

3.5.4 Cologne Spectroscopy Data



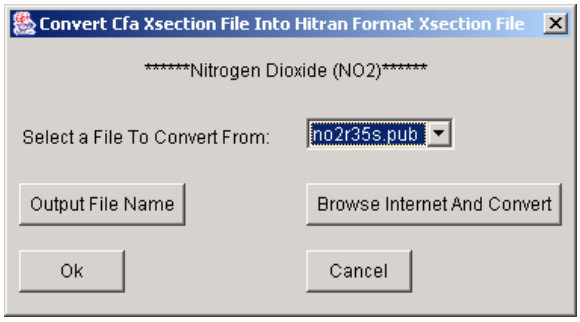
The fourth choice under the **Internet** option is Cologne Spectroscopy Data. This choice will give you access to the CDMS (Cologne Database for Molecular Spectroscopy[8]) files, download a CDMS file from the database and then convert the downloaded data into a HITRAN format file. Selection of this item will bring in a screen called Downloading Data From Cologne Site And Converting Into HITRAN File, which lets you set up the downloading parameters. The procedures to download and convert the CDMS data are same as those to download and convert the JPL data described in section 3.5.3.

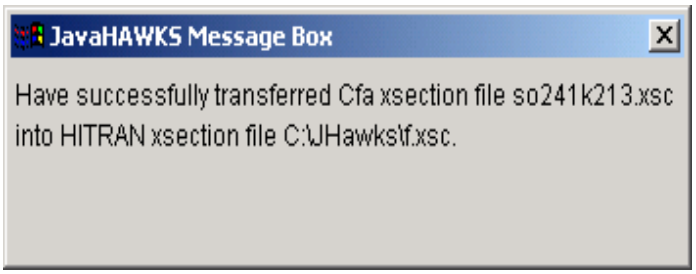
3.5.5 CfA UV Xsection Data



The fifth choice under the **Internet** option is CfA UV Xsection Data. This choice allows you to download UV cross-section data from the molecular database at the Harvard-Smithsonian Center for Astrophysics (CfA) and to convert the data to a file with the HITRAN cross-section file format. Selecting this choice will bring up a screen listing those molecules with available UV cross-section data files.

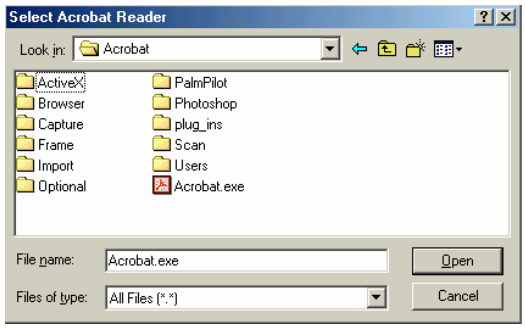
More than one UV cross-section data file exists for each molecule in the molecular database at the CfA. Clicking on the molecule that you are interested in will bring up the next screen, which allows you to select one of the UV cross section data files. Specify the location you want to save the converted cross section file in HITRAN format. Clicking the Browse And Convert button will complete the process of data downloading and converting. The CfA absorption cross-section data are listed linearly in wavelength; the conversion to HITRAN format has created a grid linear in wavenumber. Again, downloading data over the internet may fail if there is an internet connection problem or if the host of the data source has shut down its server. A message box will come up, indicating success or failure of the downlaod.





3.6. Reference Option

The next pull-down screen is Reference. It contains three separate options: Molecule, Wavenumber, and Xsection, for obtaining information on references utilized in creating the database. If you are using **JavaHAWKS** for the first time, these three options will be "grayed" out. The reference files are in the Adobe portable document format (pdf). Java is unable to search for the appropriate reader; you must point the **JavaHAWKS** software to the correct location of either the Adobe reader or Adobe Acrobat. You do this by selecting the "Acrobat Reader" in the dialog box shown below. You may wish to



consult your system administrator if you cannot find the reader, or are uncertain of how to proceed. Copies of the reader can be obtained from Adobe by using the link contained in the HITRAN web-site under the documentation sub-page.

After the reader has been selected, the "Molecule", "Wavelength", and "Xsection" options will be active.

3.6.1. Molecule

The first option, Molecule, allows the user to address the molecular reference table utilized by the HITRAN database for identifying the series of references for the line position, line intensity, and air-broadened halfwidth. Selection of this option will open the Adobe reader with the corresponding molecule pdf file. From links in this reference table, you can obtain the abstracts relating to the HITRAN parameters (such as line positions, line intensity and air-broadened halfwidth) of a line stored in HITRAN database.

3.6.2. Wavenumber

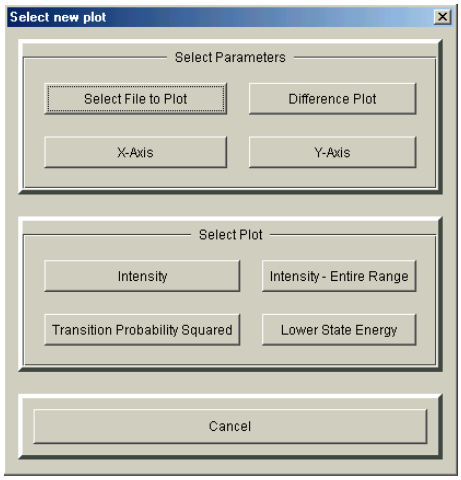
This feature is yet to be implemented in the **JavaHAWKS** software. It will be added in a future version.

3.6.3. Xsection

The third option in the Reference pull down screen is Xsection. Selection of this option will open the Adobe reader with the corresponding cross-section references.

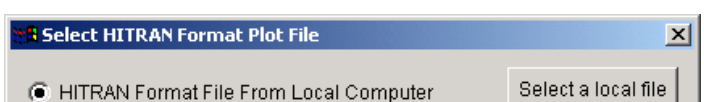
3.7. Plot Option

The sixth optional screen is Plot. The JavaHAWKS Plot screen has two selections: "Plot Line by Line", which allows the user to plot the "Intensity", "Transition Probability Squared" in the 100-character format ("Einstein-A coefficient" in the 160-character format), or "Lower State Energy" from HITRAN-like files as a function of wavenumber; and "Plot Xsection", which allows the user to plot the cross-section data as a function of wavenumber. Selecting "Plot Line by Line" will display the screen shown here. This screen is divided into sections. The upper section, Select Parameters, is used to open

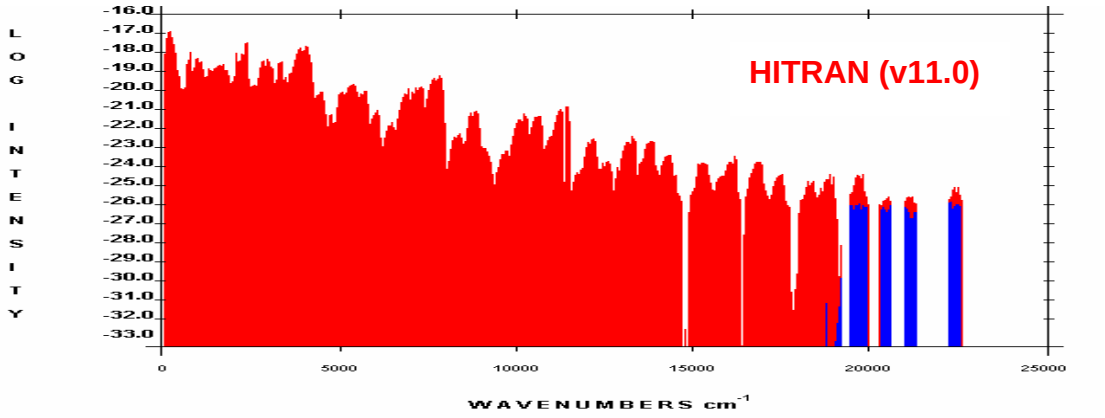


the file to be plotted, set the X- and Y-axes, and make difference plots. Difference plots are discussed below in Section 3.7.1. The second section of the pull-down window, Select Plot, determines what will be plotted, for example the intensity of the lines (the most common usage) or the lower state energy. Both the X-axis and Y-axis have autoscaling, so that the user can immediately create a plot by selecting one of the options in the second section.

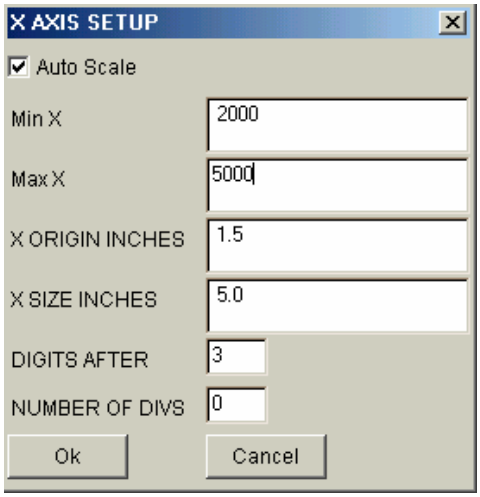
When the button Select File to Plot is clicked, the screen on the left will appear, asking you if you want to plot a file stored in your local computer or a HITRAN file from the HITRAN web server. The user should keep in mind that plotting a file residing on the HITRAN web server may take some time. This is especially true if the user use a modem to access the internet. The resulting plot will be a stick plot. In general, when there is a high density of lines in the spectral interval, the plot displayed on the screen will have **blue** and **red** lines. This is to indicate the maximum and minimum value in each channel. Typical computer monitors have less than 2000 horizontal and vertical pixels. However, the data may have many thousands of data points. Consequently, the data have been placed in bins corresponding to the number of display channels. The red and blue lines are used to indicate the maximum and minimum value in each display channel. One can easily expand the X-axis to see individual lines.



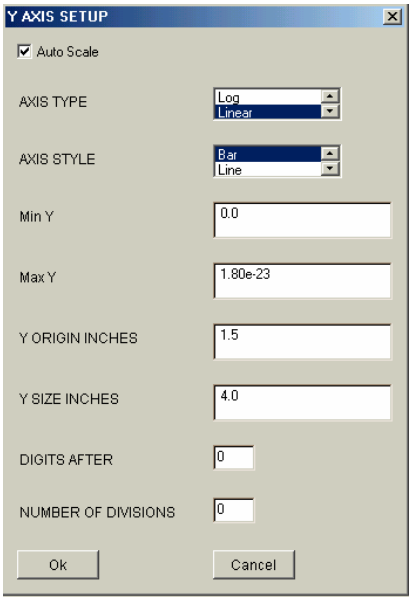
The first step is to select the file, e.g. HITRAN2K.par, and parameter, e.g. intensity, to plot.



The X- and Y-axes can be manually adjusted using the appropriate dialog box.



The user is provided different methods of defining the X axis for the given plot. If Auto Scale is chosen, the program will control the setting of the maximum and minimum for the X axis. When turning off the Auto Scale option, one is required to enter real numbers in the Min X and Max X boxes. The X ORIGIN allows one to set the distance from the left of the screen to the X axis. X SIZE allows modification of the size of the X axis. These latter two options are very useful for those who have large display screens. DIGITS AFTER is the number of digits after the decimal point for the axis values, and NUMBER OF DIVS is the number of divisions (marked off by tick marks) over the entire axis.



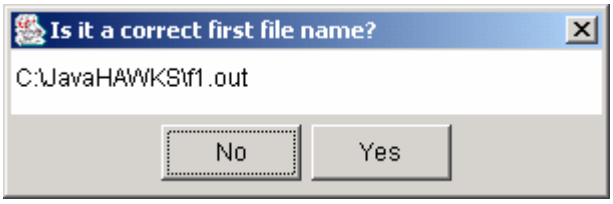
For the Y axis, the user is provided similar methods of defining the axis for the given plot, with two additions, "Axis Type", and "Axis Style". Axis Type allows the user to plot the Y-values in either a linear or log scale. For log plots, one enters the value in exponential format, for example 1.5e-23 (**remember to turn off Auto Scale first**). For "Axis Style" the user can select either a Bar plot (a histogram plot equal to the parameter being plotted at the corresponding wavenumber) or a Line plot (a "connect the dots" plot).

Proceeding clockwise, the first optional form of plotting the results is by Intensity vs wavenumber. The second optional form of plotting is by Transitional Probability-Squared or Einstein-A coefficient (depending upon whether the HITRAN file being plotted is 100-character format or the new 160-character format) vs wavenumber. The third optional form of plotting is the Lower State Energy. The final form of plotting is the Intensity-Entire Range of the applicable wavenumber. This latter choice over-rules the X-axis wavenumber selection and plots over the entire range of data in the opened file.

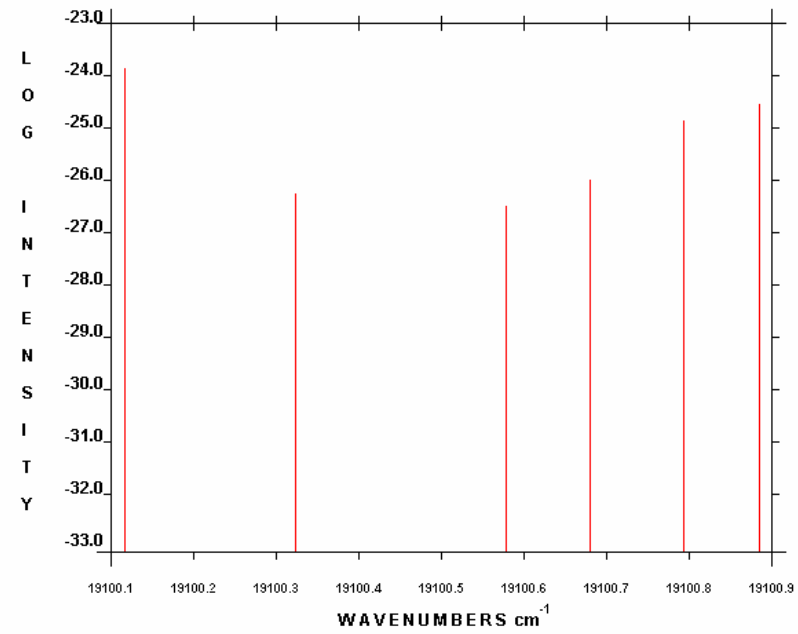
A typical plot (intensity vs wavenumber) of a HITRAN file is shown above.

3.7.1 Difference Plot

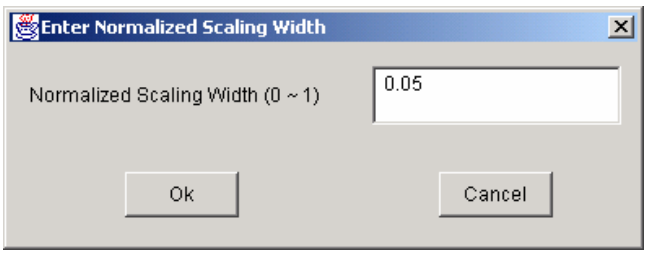
This option lets the user take the difference of two spectral plots. This can be a useful tool to determine small shifts in wavenumber (or line strength) between two files. The following screen is displayed when the **Difference Plot** option is selected:



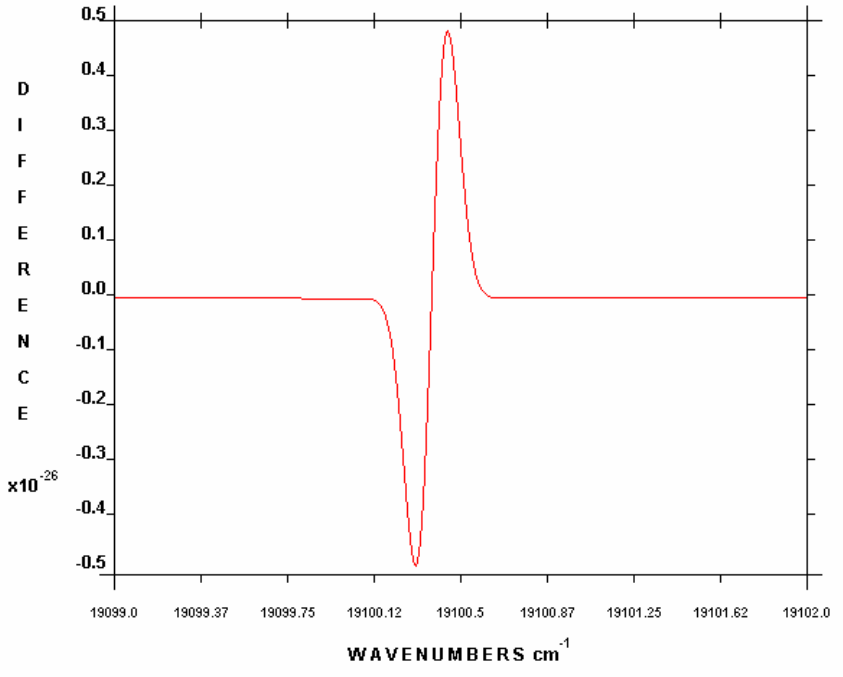
After selecting the first file, the user is prompted to select the second file (the second file is subtracted from the first). We will use f1.out and f2.out as an example to show how Dif file works. A stick plot of f1.out is shown below:



The second file (f2.out) is identical to the first except that the line at 19100.3239 cm^{-1} has been shifted to 19100.43239cm^{-1}. After the two files have been selected, the user is prompted to input a normalized scaling width, which is a value between 0 and 1 (see the figure on left). We have arbitrarily chosen a Doppler line shape to broaden the lines for subtraction. This is not an attempt to simulate a spectroscopic feature, but simply a means chosen to

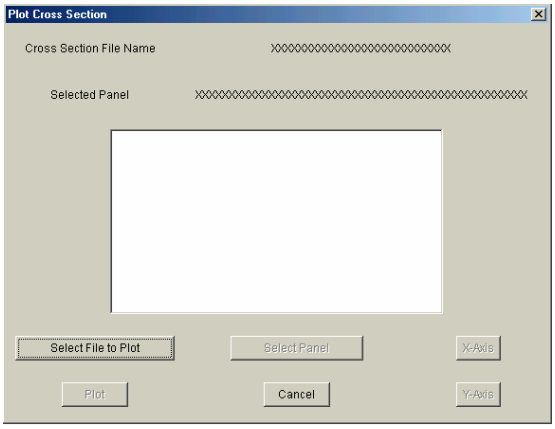


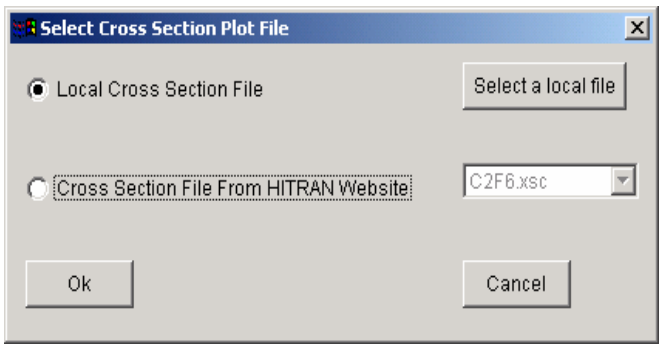
enable reasonable subtraction of lines. We used 0.5 in the current example with the resulting difference plot shown below.

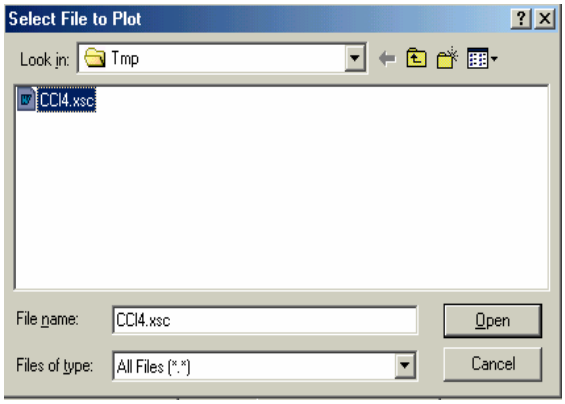


3.7.2. Plotting Cross-Section Data

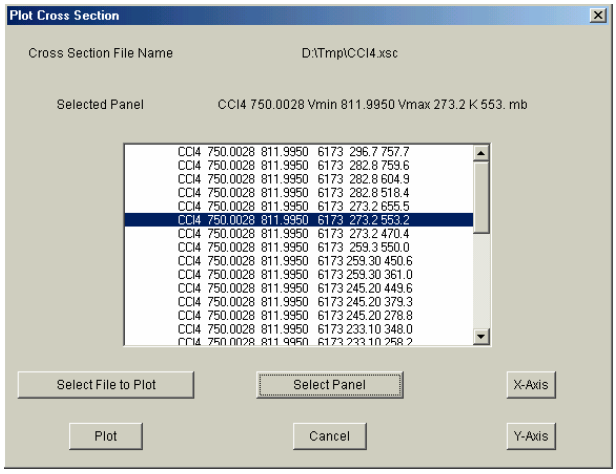
The HITRAN cross-sections files can be displayed on the screen and printed as a hard copy by using the "Plot Xsect" option from the "Plot" menu. HITRAN cross-section files have the extension *.xsc; however any file of the same format can be displayed using this option. The cross-section files are organized into a series of temperature/pressure sets (or panels), which are described in Ref.5. The user is presented a series of dialog boxes after selecting the "Plot Xsect" option to select the desired file and panel. The first dialog box is shown on the left, with the choice to select a file to plot. The user should depress the "Select File to Plot" option to select a cross section file to plot. Like the "Plot Line by Line" option, the user has the choice to plot either a file stored in the local computer or a file residing on the HITRAN web server, as shown on the left below. If the user chooses to plot a local file, a file dialog box will appear as shown on the right below.

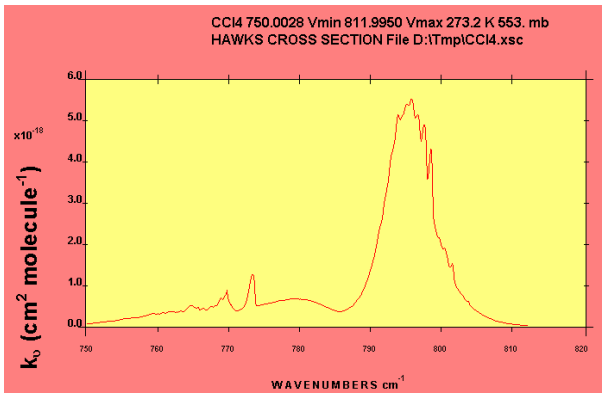






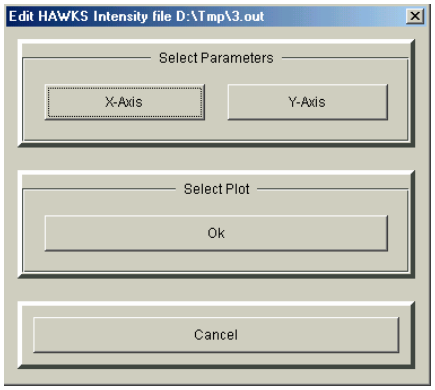
Next the user should select the temperature/pressure, i.e. panel, of interest by highlighting the panel in the display window (shown in the left figure below), and depressing the "Select Panel" option. Finally, depress the "Plot" option to display the figure, shown below to the right.





The user can access editing features, identical to those of the line-by-line display, by selecting the "Plot" option in the upper left hand corner of the screen.

3.7.3. Edit Plot and Print Plot



After a plot is displayed on the screen, a "Plot" option is available in the upper left hand corner of the screen. This allows the user to: "Redraw" the plot, "Print" the plot, "Edit" the plot, and "Exit" or return to the main screen.

The **Edit Plot** option allows the user to change the plot parameters. Selecting this option brings up the previously shown

X axis and Y axis dialog boxes. The X axis and Y axis choices have the same functions as described above.

A hard copy of the plot displayed on the screen can be made by using the "Print" options.

3.8. Help Option

The eighth optional pull down screen is **Help**. This option gives the user informative help on all of the molecules stored in the database as well as pertinent information on the structure and uses of the HITRAN database. A complete informative package of information on all of the molecules and isotopologues is provided within the **Help** pull-down menu. You can find historical documentation about the HITRAN database, from earliest HITRAN documentation (1973) to the most recent documentation. This informative package consists of pdf files and users can open them with Acrobat Reader to find relevant information.

3.8.1. About

Another choice in the **HELP** section is About, which is a standard statement describing the construction of the **JavaHAWKS** program for the HITRAN database.

4. Acknowledgments

The contributors to the spectroscopy of this effort are too numerous to cite here. We urge users of **JavaHAWKS** to consult the references contained on all transitions updated since 1986, and we apologize for any omissions or oversights that may have been made.

The current effort for the HITRAN compilation has been supported by the NASA Earth Observing System (EOS), grant NAG5-8420; the NASA Upper Atmospheric Research Satellite (UARS) program; the Atmospheric Radiation Measurement (ARM) program of the Biological and Environmental Research Program (BER), US Department of Energy, Grant No. DE-FG02-00ER62930; the Air Force Research Laboratory, Hanscom AFB; and internal funding from the Smithsonian Institution.

5. References

1. R.A. McClatchey, W.S. Benedict, S.A. Clough, D.E. Burch, R.F. Calfee, K. Fox, L.S. Rothman, and J.S. Garing, "AFCRL Atmospheric Absorption Line Parameters Compilation," AFCRL-TR-0096 (1973).

2. L.S. Rothman and R.A. McClatchey, "Updating the AFCRL Atmospheric Absorption Line Parameters Compilation," *Appl. Opt.* **15,** 2616 (1976); L.S. Rothman, "Update of the AFGL Atmospheric Absorption Line Parameters Compilation," *Appl. Opt.* **17,** 3517 (1978); L.S. Rothman, "AFGL Atmospheric Absorption Line Parameters Compilation: 1980 Version," *Appl. Opt.* **20,** 791 (1981); L.S. Rothman, R.R. Gamache, A. Goldman, J.R. Gillis, A. Barbe, L.R. Brown, R.A. Toth, J.-M. Flaud, and C. Camy-Peyret, "AFGL Atmospheric Absorption Line Parameters Compilation: 1982 Edition," *Appl. Opt.* **22,** 2247 (1983); L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN Database: 1986 Edition," *Appl. Opt.* **26,** 4058 (1987).

3. L.S. Rothman, S.A. Clough, R.A. McClatchey, L.G. Young, D.E. Snider, and A. Goldman, "AFGL Trace Gas Compilation," *Appl. Opt.* 17, 507 (1978); L.S. Rothman, A. Goldman, J.R. Gillis, R.H. Tipping, L.R. Brown, J.S. Margolis, A.G. Maki, and L.D.G. Young, "AFGL Trace Gas Compilation: 1980 Version," *Appl. Opt.* **20,** 1323 (1981); L.S. Rothman, A. Goldman, J.R. Gillis, R.R. Gamache, H.M. Pickett, R.L. Poynter, N. Husson, and A. Chedin, "AFGL Trace Gas Compilation: 1982 Version," *Appl. Opt.* **22,** 1616 (1983).

4. L.S. Rothman, R.R. Gamache, R.H. Tipping, C.P. Rinsland, M.A.H. Smith, D.Chris Benner, V.Malathy Devi, J.-M. Flaud, C. Camy-Peyret, A. Perrin, A. Goldman, S.T. Massie, L.R. Brown, and R.A. Toth, "The HITRAN Molecular Database: Editions of 1991 and 1992," *J. Quant. Spectrosc. and Rad. Transfer* **48,** 469 (1992).

5. L.S. Rothman, 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.V. Chance, K.W. Jucks, L.R. Brown, V. Nemtchinov, and P. Varanasi, "The HITRAN Molecular Spectroscopic Database and HAWKS (HITRAN Atmospheric Workstation): 1996 Edition," *J. Quant. Spectrosc. and Rad. Transfer* **60,** 665-710 (1998).

6. 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, J. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *J. Quant. Spectrosc. and Rad. Transfer* **82,** 5-44 (2003).

7. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S..P Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalogue," *J. Quant. Spectrosc. and Rad. Transfer* **60,** 883-890 (1998).

8. H.S.P. Müller, S. Thorwirth, D.A. Roth, and G. Winnewisser, "The Cologne Database for Molecular Spectroscopy, CDMS," *Astronomy & Astrophysics* **370,** L49-L52 (2001).

APPENDIX A. Directories and Files in HITRAN (v11.0)

HITRAN (v12.0) contains the directories and files listed below with their sizes.

Directory of **\Hitran04**

HITRAN-Readme.pdf	22,517
HAWKSmanual.pdf	~1,132,830
Win_Setup.exe	29,501,946
Linux_setup.bin	20,448,010
Unix_Setup.bin	20,448,010
MacOS_Setup.bin	20,487,680
MacOSX_Setup.zip	20,037,001
Aerosols	<DIR>
Global_Data	<DIR>
HITRAN2004	<DIR>
IR-XSect	<DIR>
Line-Coupling	<DIR>
UV	<DIR>

Directory of **\Hitran04\Aerosols**

Aerosol-Readme.pdf	19,761
DowningandWilliams.dat	16,412
h2so4T183.biermann	413,406
h2so4T200.niedziela	161,550
h2so4T188.biermann	515,023
h2so4T210.niedziela	195,737
h2so4T193.biermann	616,640
h2so4T220.niedziela	298,298
h2so4T203.biermann	718,257
h2so4T230.niedziela	127,363
h2so4T213.biermann	819,874
h2so4T240.niedziela	264,111
h2so4T215.biermann	616,640
h2so4T260.niedziela	298,298
h2so4T223.biermann	616,640
h2so4T280.niedziela	264,111
h2so4T233.biermann	1,023,108
h2so4T300.niedziela	195,737
h2so4T253.biermann	1,023,108
h2so4T263.biermann	515,023
h2so4T273.biermann	1,327,959
h2so4T293.biermann	1,531,193
hno3T213.biermann	515,021
hno3T223.biermann	616,638
hno3T233.biermann	718,255
hno3T253.biermann	718,255
hno3T263.biermann	515,021
hno3T273.biermann	1,023,106
hno3T293.biermann	1,023,106
ice130.clapp	139,956
ice140.clapp	139,998
ice150.clapp	139,998
ice160.clapp	139,914
ice170.clapp	139,830
ice180.clapp	139,662
ice190.clapp	139,914
ice200.clapp	139,914
ice210.clapp	139,914
Kou_etal.dat	30,046
nad160.niedziela	85,506
nad180.niedziela	85,588
nad190.niedziela	85,506
Norman_etal.dat	279,165
norman-indices.dat	308,232
PalmerandWilliams.dat	32,966
QuerryandTyler.dat	278,447
Remsberg.dat	27,464
Richwine_etal.dat	20,544
Shettle.dat	39,702
SteeleandHamill.dat	1,800
SutherlandandKhanna.dat	8,113
Timmermans.dat	12,154
Tisdale_etal.dat	321,060
Toon_etal.dat	29,984
Warren.dat	34,262

Directory of **\hitran04\Global_Data**

ref-table2004.pdf	367,716
molparam.txt	6,544
parsum.dat	8,359,118
bandcent.dat	157,021
TIPS_2003.zip	118,711

Directory of **\hitran04\HITRAN2004**

By-Molecule	<DIR>
Supplelmental	<DIR>
HITRAN04.par	280,983,978

Directory of **\hitran04\HITRAN2004\By-Molecule**

By-Molecule-Readme.pdf	65,626
01_hit04 par	10,237,752
02_hit04 par	10,191,906
03_hit04 par	50,459,922
04_hit04 par	7,749,270
05_hit04 par	725,274
06_hit04 par	40,733,280
07_hit04 par	1,041,336
08_hit04 par	16,569,360
09_hit04 par	6,294,186
10_hit04 par	16,884,126
11_hit04 par	4,711,608
12_hit04 par	43,928,892
13_hit04 par	6,864,426
14_hit04 par	17,334
15_hit04 par	99,306
16_hit04 par	209,466
17_hit04 par	130,572
18_hit04 par	1,171,260
19_hit04 par	3,227,040
20_hit04 par	437,724
21_hit04 par	2,636,712
22_hit04.par	19,440
23_hit04.par	688,986
24_hit04.par	5,041,278
25_hit04.par	16,326,522
26_hit04.par	569,754
27_hit04.par	769,338
28_hit04.par	1,909,980

29_hit04.par	11,437,362
31_hit04.par	3,367,656
32_hit04.par	4,018,896
33_hit04.par	6,286,248
34_hit04.par	324
36_hit04.par	195,372
37_hit04.par	705,996
38_hit04.par	2,102,436
39_hit04.par	3,223,638

Directory of **\hitran04\HITRAN2004\Supplemental**

30_hit04.par	3,709,962
35_hit04.par	5,216,238

Directory of **\hitran04\IR-XSect**

IRCrossSection-Readme.pdf	59,383
C2F6_IR00.xsc	15,598,934
CCl4_IR00.xsc	2,018,175
CFC-11_IR00.xsc	16,717,448
CFC-113_IR00.xsc	55,692
CFC-114_IR00.xsc	1,496,952
CFC-115_IR00.xsc	777,852
CFC-12_IR00.xsc	21,401,118
CFC-13_IR01.xsc	745,414
CFC-14_IR01.xsc	3,898,920
ClONO2_IR04.xsc	23,732,873
HCFC-123_IR00.xsc	1,868,640
HCFC-124_IR00.xsc	669,629
HCFC-141b_IR00.xsc	1,920,354
HCFC-142b_IR00.xsc	1,984,920
HCFC-21_IR00.xsc	51,306
HCFC-22_IR01.xsc	13,926,811
HCFC-225ca_IR00.xsc	2,060,502
HCFC-225cb_IR00.xsc	2,346,000
HFC-125_IR00.xsc	592,824
HFC-134_IR00.xsc	6,703,434
HFC-134a_IR00.xsc	19,833,114
HFC-143a_IR00.xsc	4,572,846
HFC-152a_IR00.xsc	1,707,582
HFC-32_IR00.xsc	3,813,440
HNO4_IR04.xsc	204,879
N2O5_IR04.xsc	889,440
SF5cf3_IR04.xsc	1,347,810
SF6_IR00.xsc	1,328,960
Supplemental	<DIR>

Directory of **\hitran04\IR-XSect\Supplemental**

CFC-11-92_IR00.xsc	319,464
CFC-12-92_IR00.xsc	690,336
ClONO2-96_IR00.xsc	73,950

Directory of **\hitran04\Line-Coupling\CO2**

Data_Q	<DIR>
Soft_Q	<DIR>
Test_Q	<DIR>
LineCoupling-Readme.txt	43,511

Directory of **\hitran04\UV**

Line-by-line	<DIR>
Cross-sections	<DIR>

Directory of **\hitran04\UV\Line-by-line**

07_UV04.par	1,785,240
13_UV04.par	174,798

Directory of **\hitran04\UV\Cross-sections**

BrO_UV04.xsc	110,224
H2CO-UV04.xsc	925,836
N2O-UV00.xsc	143,230
NO2-UV00.xsc	571,264
NO3_UV04.xsc	176,266
O2-O2_UV04.xsc	154,960
O3-UV04.xsc	356,676
OClO_UV04.xsc	1,387,768
SO2-UV00.xsc	2,377,764

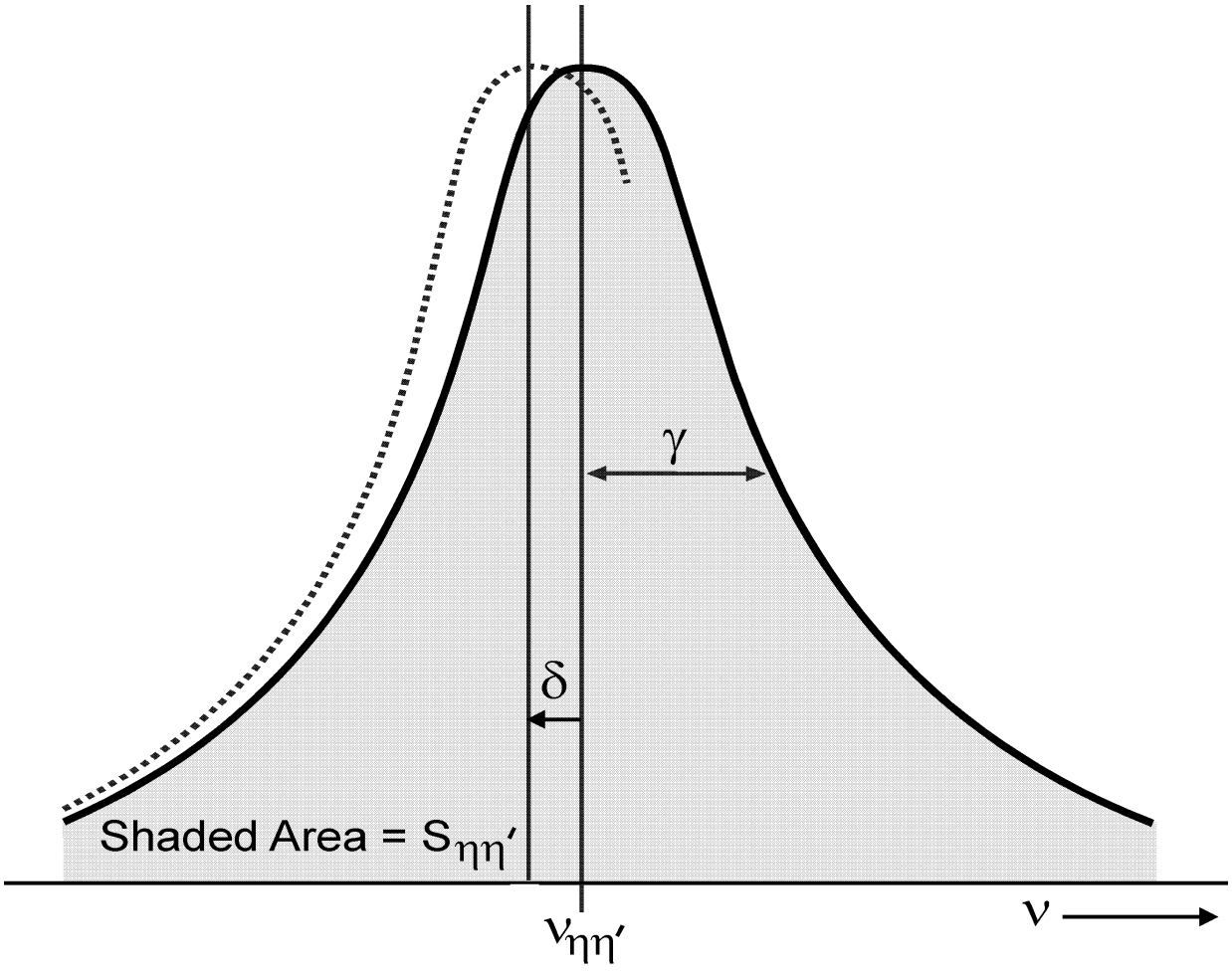
APPENDIX B. HITRAN (v12.0) Molecules with Associated Indices

HITRAN Molecule Number	Molecule Chemical Symbol	Number of trans-itions	HITRAN Molecule Number	Molecule Chemical Symbol	Number of trans-itions
1	H_2O	63197	21	HOCl	16276
2	CO_2	62913	22	N_2	120
3	O_3	311481	23	HCN	4253
4	N_2O	47835	24	CH_3Cl	31119
5	CO	4477	25	H_2O_2	100781
6	CH_4	251440	26	C_2H_2	3517
7	O_2	6428	27	C_2H_6	4749
8	NO	102280	28	PH_3	11790
9	SO_2	38853	29	COF_2	70601
10	NO_2	104223	30	SF_6	22901
11	NH_3	29084	31	H_2S	20788
12	HNO_3	271166	32	HCOOH	24808
13	OH	42373	33	HO_2	38804
14	HF	107	34	O	2
15	HCl	613	35	$ClONO_2$	32199
16	HBr	1293	36	NO^+	1206
17	HI	806	37	HOBr	4358
18	ClO	7230	38	C_2H_4	12978
19	OCS	19920	39	CH_3OH	19899
20	H_2CO	2702			

This table gives the HITRAN numbering scheme for the molecular species on various line-by-line portions of **JavaHAWKS**. Shaded areas are for molecules relegated to the "supplemental" folder.

APPENDIX C. Schematic of Fundamental Spectroscopic Parameters of a Line Transition in HITRAN.

The dotted line refers to a perturbed transition (with a negative pressure-shift δ).



APPENDIX D. Formats for Line-by-line Parameters and Cross-section Headers

"1986-2001" line parameter format:

M	I	ν	S	R	γ_{air}	γ_{self}	E"	n	δ	iv'	iv"	q'	q"	ier	iref
I2	I	F12.6	E10.3	E10.3	F5.4	F5.4	F10.4	F4.2	F8.6	I3	I3	A9	A9	3I1	3I2

10 20 30 40 50 60 70 80 90

"2002+" line parameter format:

M	I	ν	S	A	γ_{air}	γ_{self}	E"	n	δ	v'	v"	Q'	Q"	ierr	iref	*	g'	g"
I2	I1	F12.6	E10.3	E10.3	F5.4	F5.4	F10.4	F4.2	F8.6	A15	A15	A15	A15	6I1	6I2	A1	F7.1	F7.1

10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160

Note: **v'** and **v"** are ASCII representations of upper and lower global quanta; ***** is flag for line coupling; **g'** and **g"** are upper and lower statistical weights.

"2000" Cross-section Header format:

Chemical symbol	Wavenumber Min	Wavenumber Max	No. Pts.	Temp [K]	Press [Torr]	Max X-section	Res.	Common Name	Not used	Br	Re No
20	10	10	7	7	6	10	5	15	4	3	3

10 20 30 40 50 60 70 80 90

Note: **Chemical Symbol** is right adjusted; **Res**. is resolution in cm^{-1} for FTS measurements, and in milli-Angstroms for grating measurements in the UV (xxxmÅ), and **Br** indicates any broadening gas, such as air.

Example of 100-character HITRAN line-transition format.

Mol/Iso	ν_{ij}	S_{ij}	R_{ij}	γ_{air}	γ_{self}	E"	n_{air}	δ_{air}	iv'	iv"	q'	q"	ierr	iref
21	800.451076	3.197E-26	6.579E-05	.0676	.0818	2481.5624	.78	.000000	14	6		P 37	465	2 2 1
291	800.454690	9.724E-22	1.896E-02	.0845	.1750	369.6303	.94	.000000	9	1	341619	331519	000	4 4 1
291	800.454690	3.242E-22	2.107E-03	.0845	.1750	369.6303	.94	.000000	9	1	341519	331419	000	4 4 1
121	800.455380	1.037E-22	1.657E-03	.1100	.0000	530.3300	.75	.000000	32	14	46 640	45 540	000	4 4 1
121	800.455380	1.037E-22	1.657E-03	.1100	.0000	530.3300	.75	.000000	32	14	46 740	45 640	000	4 4 1
101	800.456743	1.680E-23	1.659E-04	.0670	.0000	851.0494	.50	.000000	2	1	45 244 0-	44 143 0-	301	6 6 1
101	800.457045	1.710E-23	1.689E-04	.0670	.0000	851.0469	.50	.000000	2	1	45 244 1-	44 143 1-	301	6 6 1
101	800.457310	1.740E-23	1.718E-04	.0670	.0000	851.0442	.50	.000000	2	1	45 244 2-	44 143 2-	301	6 6 1
121	800.457760	4.726E-23	4.614E-03	.1100	.0000	920.0900	.75	.000000	32	14	502922	492822	000	4 4 1
121	800.457760	4.726E-23	4.614E-03	.1100	.0000	920.0900	.75	.000000	32	14	502922	492722	000	4 4 1
24	800.465942	9.792E-27	6.063E-04	.0754	.1043	1341.2052	.69	.000000	8	3		R 13	425	2 2 1
121	800.466160	1.061E-22	2.720E-03	.1100	.0000	632.1200	.75	.000000	32	14	471236	461136	000	4 4 1
121	800.466160	1.061E-22	2.720E-03	.1100	.0000	632.1200	.75	.000000	32	14	471136	461036	000	4 4 1
35	800.472900	3.878E-26	6.919E-04	.0686	.0871	629.0354	.76	.000000	2	1	1814 4	1713 5	455	5 5 1
101	800.473083	1.270E-23	1.254E-04	.0670	.0000	851.0095	.50	.000000	2	1	45 244 0+	44 143 0+	301	6 6 1
101	800.474860	1.210E-23	1.195E-04	.0670	.0000	851.0064	.50	.000000	2	1	45 244-1+	44 143-1+	301	6 6 1
31	800.475500	1.680E-24	3.617E-05	.0653	.0890	1092.4340	.76	.000000	2	1	51 547	50 248	002	1 1 2
291	800.476220	9.597E-22	6.010E-03	.0845	.1750	361.9747	.94	.000000	9	1	341420	331320	000	4 4 1
291	800.476220	3.199E-22	6.010E-03	.0845	.1750	361.9747	.94	.000000	9	1	341520	331420	000	4 4 1
101	800.476937	1.160E-23	1.145E-04	.0670	.0000	851.0037	.50	.000000	2	1	45 244-2+	44 143-2+	301	6 6 1
101	800.484334	1.740E-23	2.153E-05	.0670	.0000	106.0760	.50	.000000	2	1	8 4 4-1+	9 3 7-1+	301	6 6 1

Example of 100-character HITRAN line-transition format.

FORTRAN Format (I2,I1,F12.6,1P2E10.3,0P2F5.4,F10.4,F4.2,F8.6,2I3,2A9,3I1,3I2) corresponding to:					
Mol	I2	Molecule number	***E″***	F10.4	Lower state energy in cm^{-1}
Iso	I1	Isotopologue number (1= most abundant, 2= second most abundant, etc.)	n_{air}	F4.2	Coefficient of temperature dependence of air-broadened halfwidth
ν_{ij}	F12.6	Wavenumber in cm^{-1}	δ_{air}	F8.6	Air-broadened pressure shift of line transition in cm^{-1}/atm @ 296K
S_{ij}	E10.3	Intensity in cm^{-1}/(molecule x cm^{-2}) @ 296K	**iv′, iv″**	2I3	Upper-state global quanta index, lower-state global quanta indices
R_{ij}	E10.3	Weighted transition moment-squared in Debyes	**q′, q"**	2A9	Upper-state local quanta, lower-state local quanta
γ_{air}	F5.4	Air-broadened halfwidth (HWHM) in cm^{-1}/atm @ 296K	**ierr**	3I1	Uncertainty indices for wavenumber, intensity, and air-broadened halfwidth
γ_{self}	F5.4	Self-broadened halfwidth (HWHM) in cm^{-1}/atm @ 296K	**iref**	3I2	Indices for table of references corresponding to wavenumber, intensity, and halfwidth

Example of 160-character HITRAN line-transition format.

FORTRAN Format (I2,I1,F12.6,1P2E10.3,0P2F5.4,F10.4,F4.2,F8.6,2A15,2A15,6I1,6I2,A1,2F7.1) corresponding to:					
Mol	I2	Molecule number	δ_{air}	F8.6	Air-broadened pressure shift of line transition in cm^{-1}/atm @ 296K
Iso	I1	Isotopologue number (1= most abundant, 2= second most abundant, etc.)	**v′, v″**	2A15	Upper-state global quanta, lower-state global quanta
ν_{ij}	F12.6	Wavenumber in cm^{-1}	**q′, q″**	2A15	Upper-state local quanta, lower-state local quanta
S_{ij}	E10.3	Intensity in cm^{-1}/(molecule x cm^{-2}) @ 296K	**ierr**	6I1	Uncertainty indices for wavenumber, intensity, air- and self-broadened halfwidths, temperature-dependence, and pressure shift
A_{ij}	E10.3	Einstein-A coefficient	**iref**	6I2	Indices for table of references corresponding to wavenumber, intensity, air- and self-broadened halfwidths, temeperature-dependence, and pressure shift
γ_{air}	F5.4	Air-broadened halfwidth (HWHM) in cm^{-1}/atm @ 296K	Flag	A1	Flag (*) for lines supplied with line-coupling algorithm
γ_{self}	F5.4	Self-broadened halfwidth (HWHM) in cm^{-1}/atm @ 296K	***g′***	F7.1	Upper-state statistical weight
E″	F10.4	Lower state energy in cm^{-1}	***g″***	F7.1	Lower-state statistical weight
n_{air}	F4.2	Coefficient of temperature dependence of air-broadened halfwidth			