High-Resolution Spectroscopic Database for the NASA Earth Observing System Program

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1. Introduction

The purpose of this project is to develop and enhance the HITRAN molecular spectroscopic database and associated software to support the observational programs of the Earth Observing System (**EOS**). In particular, the focus is on the EOS projects: the Atmospheric Infrared Sounder (**AIRS**), the High-Resolution Dynamics Limb Sounder (**HIRDLS**), Measurements of Pollution in the Troposphere (**MOPITT**), the Tropospheric Emission Spectrometer (**TES**), and the Stratospheric Aerosol and Gas Experiment (**SAGE III**). The data requirements of these programs in terms of spectroscopy are varied, but usually call for additional spectral parameters or improvements to existing molecular bands. In addition, cross-section data for heavier molecular species must be expanded and made amenable to modeling in remote sensing. The effort in the project also includes developing software and distribution to make access, manipulation, and use of HITRAN functional to the EOS program.

During this reporting period, the main contribution of the Principal Investigator has been to coordinate the research and collection of data, and to ensure the quality of data as well as their incorporation into the HITRAN database. The PI also ensures continuing improvement of user access of data for atmospheric modeling, etc., which involves web-site development/maintenance and improvements of HAWKS software. A significant contribution of the PI has been to foster ongoing communications between different research groups throughout the world via conferences/workshops, the HITRAN meeting, and the HITRAN web-site.

2. Data Acquisition and Data Improvement

Table 1 presents a summary of the status of some of the line-by-line and cross-section data that have been or are about to be acquired for the HITRAN database compilation. We highlight below some of the work that is of most significance to the EOS program.

Relevant to **SAGE III**, we have acquired new parameters for the oxygen A band at 13100 cm^{-1} from the group at the Jet Propulsion Laboratory (JPL) headed by Dr. Linda Brown. These data include positions, air- and self-broadened widths, pressure shifts, and intensities. This work has confirmed that the current intensities in HITRAN are good, but suprisingly, the positions of the lines were off and will be updated.

Dr. Brown has also measured H_2O at high-resolution in the 9650 - 11400 cm^{-1} region. Three isotopes were involved, giving new positions, intensities and air-widths and shifts. The air-broadened widths could not be obtained for all the lines that were in the list, so it would be highly desirable to supplement this list with calculated halfwidths where the experiment cannot provide them. In addition, the research group lead by Dr. L. Giver of NASA Ames Research Center has undertaken a measurement program of water vapor above 8000 cm^{-1}. This work has identified numerous problems with line intensities. The work is ongoing, including utilizing the ab initio calculations of Dr. David Schwenke, NASA Ames, to identify lines in HITRAN that were previously not given quantum assignments. Besides now providing lower state energies, this work will facilitate database management (such as affixing calculated halfwidths). We now have the preliminary HITRAN file up on the web, subject to further examination by other collaborators until a consensus is achieved on their reliability. The web-site has provided a forum for data comparisons and analysis. Dr. Giver anticipates having a much larger linelist available by the time of the upcoming HITRAN meeting. We are also collaborating with several other groups independently to evaluate the parameters in this region.

Relevant to **MOPITT** (and other EOS programs), Dr. Brown studied methane in the 900 - 4800 cm^{-1} region. Positions, intensities, with air- and self- widths and shifts added. This large work is, to quote Dr. Brown, “a once-in-a-decade revision”. For carbon dioxide, we have updates in the 4000 - 5000 cm^{-1}, combining the work of JPL with Dr. Giver’s experiments at NASA Ames Research Center, and his published results for band intensities. The group at NASA Ames also has new intensities for overtone bands of CO.

The PI initiated an *ad hoc* HITRAN meeting at the Ohio State University Symposium on Molecular Spectroscopy in June 1999, where we have proposed a new format for the next edition of HITRAN. Figure 1 illustrates the new format for the line-by-line parameters. We will change the transition-probability squared on previous editions to the Einstein A coefficient, a parameter that will be more useful for non-LTE applications and also a quantity independent of the isotopic abundances and temperature. We are expanding the fields for the vibrational and rotational quantum identifications and foregoing the indexing scheme used in the editions since 1986 (now going back to the ASCII representation of vibrational levels). We have expanded the error indices and the reference indices to include the parameters of self-broadened width, temperature dependence of the air-broadened width, and the pressure shift parameter. A flag will be used for those lines subject to line mixing. An algorithm will be provided in the compilation that computes the line coupling of these lines, while maintaining correct physics, such as detailed balance, etc. We are collaborating on this feature with NASA Langley and the University of Paris to have a methodology that applies for all molecules, is maintainable as new halfwidth data appear, and is transparent to the user. Finally, values for the upper and lower statistical weights of the levels of the transitions will be given.

Forty-three files of near-IR O_2 cross-sections from Dr. Kevin Smith of the Rutherford Appleton Laboratory in the UK have been received. These data will be evaluated against the line-by-line data as well as collision induced absorption (CIA) bands of oxygen to be obtained from the National Institute of Standards and Technology (NIST).

We have a large new set of indices of refraction for aerosols, compiled by Dr. Steve Massie of the National Center for Atmospheric Research (NCAR). These data include: Real and imaginary indices of aqueous HNO_3/H_2O at 220 K from 754 to 4700 cm^{-1} for 35, 45, 54, 63, and 70% HNO_3 by weight; Real and imaginary indices of liquid H_2SO_4/H_2O at 215 K from 499 to 6996 cm^{-1} as a function of the H_2SO_4 concentration by weight; Real indices of liquid H_2SO_4/H_2O from 0 to 16382 cm-1 and imaginary indices from 432 to 5028 cm^{-1} at 12 temperatures (213 to 293K) as a function of the H_2SO_4 concentration by weight; Real and imaginary indices of liquid H_2SO_4/H_2O at 8 temperatures (200 to 300K) from 825 to 4700 cm^{-1}; Real and imaginary refractive indices of organic-based nonvolatile aerosols produced by burning vegetation from 525 to 5000 cm^{-1}. The mixed weed sample indices of Table 2 from the paper by Sutherland and Khanna are tabulated here; Real and imaginary indices of liquid HNO_3/H_2O at room temperature from 250 to 4987 cm^{-1} as a function of the HNO_3 concentration by weight. The concentrations of 3.1, 6.1, 11.8, 22.3, 40.3, and 70% HNO_3 correspond to the molar (M) concentrations of 0.5, 1.0, 2.0, 4.0, 8.0, and 15.7 cited in the Querry and Tyler paper; Real indices of liquid HNO_3/H_2O from 0 to 16382 cm^{-1} and imaginary indices from 432 to 5028 cm^{-1} at 7 tempertatures (213 to 293K) as a function of the HNO_3 concentration by weight; Real and imaginary indices of nitric acid dyhydrate (NAD) at 3 temperature (160 to 190 K) from 700 to 4700 cm^{-1}; Real and imaginary refractive indices of nitric acid trihydrate (NAT) at 160 K from 711 to 4004 cm^{-1}; and Real and imaginary indices of water ice at 9 temperatures (130 to 210 K) from 800 to 4004 cm^{-1}.

3. HAWKS Software Development, Upgrades, and Distribution

A new version of the HAWKS software is being released with the HITRAN2000 compilation. The software is 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 computers. This is a significant improvement because we will only need to maintain a single source and executable code compared to the four versions that are currently maintained. The software will also be distributed via the HITRAN web site in addition to the traditional CD-ROM. A reduced capability version of the JavaHAWKS Software will be implemented on the HITRAN web-site to enable users to query the HITRAN database via the web. An example of one of the many new features now available is the ability to plot cross-section data in the HITRAN compilation as well as line-by-line data, as seen in Figure 2. The software development for this effort is being performed by the Ontar Corporation.

During the period of performance, we purchased a basic iMac computer. This was deemed necessary to develop, test, and evaluate the software for Mac application. The implementation of an easy install has proved more difficult than for PCs or the UNIX workstations. A set of instructions for the user to install HAWKS on the Mac has been written and provided to NASA Goddard Space Flight Center for evaluation.

From 1 May 1999 to the time of this report, approximately 650 copies of the HITRAN compilation have been distributed on CD-ROM. The users are predominantly from the academic community, although most of the government requests have come from NASA.

4. HITRAN Web-site Development

Jim Esmond implemented the HITRAN web-page and re-located it at the Harvard-Smithsonian. After creating the site here, he brought over all the pages from the old commercial server. He updated both the old site and the new one at SAO in preparation for the time when we would be able to completely direct all requests and queries to the SAO site.

Jim made numerous updates to the HITRAN web-site. These improvements included the side-panel links to sub-pages, the update of the sub-page "Latest News" adding, for example, the summary of the fifth Atmospheric Spectroscopy Applications meeting, links to other spectroscopic databases, under the sub-page "Other Spectral Databases", and updates to the sub-page "Relevant Meetings". He placed new HITRAN data on the web with a link for users to access these data. A new simplified request and query form has been designed and implemented on the web. This form not only provides a clearer and more concise questionnaire to HITRAN users, but employs security features that were absent previously. The results are forwarded by e- mail directly to the PI.

Jim Esmond died suddenly on 10 November. His programming talents and assistance with the UV data will be sorely missed. The main web-site work was mostly completed, and the maintenance of the site is being continued with assistance from the Computer Center of the Harvard-Smithsonian. Dr. Kouichi Yoshino in the meantime has hired a post-doc from the UK to carry on the UV data analysis.

5. Collaborations

For the HITRAN project to succeed, a close collaboration with numerous lab and field spectroscopists has been essential. For the present period, we have been particularly involved with Drs. Linda Brown of JPL, Kelly Chance, Kouichi Yoshino, and Thomas Kurosu of the Harvard-Smithsonian Center for Astrophysics, Steve Massie of NCAR, Aaron Goldman of the University of Denver, Jean-Marie Flaud, Victor Dana, Agnes Perrin, Jean-Yves Mandin, and Johannes Orphal of the University of Paris, Prasad Varanasi of SUNY at Stony Brook, Kevin Smith of RAL UK, and Cathy Clerbaux of the Service d'Aeronomie du CNRS France.

6. Meetings, Presentations, and Publications

Several spectroscopic meetings were attended during this period. We attended the 54th Ohio State University Symposium on Molecular Spectroscopy, June 14-18, 1999. It was at that meeting that an *ad hoc* HITRAN database meeting was assembled with principal contributors who were present at the meeting. Following the Ohio State Symposium, we attended the two topical meetings of the Optical Society of America in Santa Barbara CA: *Fourier Transform Spectroscopy: New Methods and Applications*, and *Optical Remote Sensing of the Atmosphere*. These two meetings provided much insight into ongoing and new efforts relevant to the HITRAN program.

In September, L. Rothman attended two meetings in France. He co-chaired the Atmospheric spectroscopy Applications conference in Reims. This meeting, the fifth, takes place every third year, and was created under the auspices of the International Radiation Commission and the Ozone Commision. It covers six areas: 1. Lineshapes, line-coupling, and continua; 2. Atmospheric observations; 3. Experimental Techniques; 4. Laboratory data; 5. Databases; and 6. Non Local Thermodynamic Equilibrium Processes. We presented the invited oral presentation in session 5, as well as 3 poster papers at this meeting. The ASA conference was followed by attendance at the 16th

colloquium on High Resolution Molecular Spectroscopy at Dijon. This is the pre-eminent meeting in spectroscopy in Europe and takes place biennially. We were made aware of several possible deficiencies in HITRAN and potential new modifications that will be made available.

Publications during this period:
"Total Internal Partition Sums for Molecules in the Terrestrial Atmosphere," R.R. Gamache, S. Kennedy, R.L. Hawkins, and L.S. Rothman, *Journal of Molecular Structure* **517/518,** 413-431 (2000).
"HITRAN Partition Functions and Weighted Transition-Moments Squared," A. Goldman, R.R. Gamache, A. Perrin, J.-M. Flaud, C.P. Rinsland, and L.S. Rothman, accepted by the *J. Quant. Spectrosc. and Rad. Transfer*.

Presentations during this period:
"HITRAN2000," Fifth Atmospheric Spectroscopy Applications Conference, Reims, France (September 1999). (Invited)
"Line Parameter and database Needs for non-LTE Modeling and Remote Sensing," Paper FO2, Fifth Atmospheric Spectroscopy Applications Conference, Reims, France (September 1999).
"UV Spectral Data for HITRAN2000," Paper EP7, Fifth Atmospheric Spectroscopy Applications Conference, Reims, France (September 1999).
"HAWKS (HITRAN Atmospheric Workstation)," Fifth Atmospheric Spectroscopy Applications Conference, Reims, France (September 1999).
"HITRAN and HITEMP," Atmospheric Transmission Workshop, US Army Night Vision Directorate, Fort Belvoir, Virginia (September 1999).

7. Future Effort

A major effort is going into preparing for the upcoming HITRAN meeting. This conference will take place at the Harvard-Smithsonian Center for Astrophysics in Cambridge Massachusetts, 19-21 June 2000. Drs. Kelly Chance and William Parkinson have agreed to assist in the local committee. We have put up a registration form on the web and put an emphasis on poster presentations. We will construct the agenda of oral and poster presentations after the deadline of 17 April. We have reserved the Phillips Auditorium at the SAO, and the rotunda beneath the old telescope for poster presentations. Accommodations have been obtained at Lesley College dormitories and at the Best Western hotel nearby.

A great deal of effort has been extended into improving and expanding the quality and usefulness of the cross-section data in HITRAN. From laboratories in the UK, France, and the US, we have acquired many new sets of temperature-pressure data for "heavy" molecular species. A process of conversion to appropriate units and to the slightly new HITRAN format for cross-sections is underway. More importantly, we have begun a validation program to eliminate duplicate but inferior data present on prior editions of HITRAN and to correct some typographical errors in some of the sets. Some data will be relegated to a sub-directory of the IR cross-sections, called "supplemental".
The Ontar Corp is processing and making graphical evaluations of the cross-sections.

New Data above 20000 cm^{-1}

The last edition of the HITRAN compilation extended spectral coverage into the ultraviolet region with the addition of line-by-line parameters for the oxygen Schumann-Runge system and cross-section data for nitrogen dioxide and sulfur dioxide. We now propose to expand the data coverage in this spectral region with the addition of data for major atmospheric absorbers such as ozone, additional coverage of band systems of oxygen, and several trace species that impact ongoing atmospheric remote sensing experiments.

For the upcoming edition of the database, HITRAN2000, we anticipate adding high-resolution cross-sections for several molecular band systems: O_3, OClO, BrO, H_2CO, ClO, and NO_2. In addition, there will be line-by-line data for O_2, NO, and OH. The spectra of these gases have applications to a number of programs, including the ESA Global Ozone Monitoring Experiment (GOME)[2] and the NASA EOS (Earth Observing System) program.[3].

For O_3, the Hartley-Huggins bands at temperatures between 203 to 293K in the region of about 237 to 407nm will be included. We propose to use an algorthm to generate the Chappuis and the Wulf bands, similar to the procedure adopted in the LOWTRAN band-model code. For O_2, we will add the Herzberg band systems I, II, and III, and the Herzberg continua from the observations made by the Harvard-Smithsonian Center for Astrophysics and the University of Reims. The latter constituents will benefit remote-sensing retrievals of the Stratospheric Aerosol and Gas Experiment (**SAGE III**) of NASA, for example. We will also be extending the coverage of the hydroxyl radical, OH, to include the A $^2E^+$ 7 X ^2A_i band system. These latter data will be included in the HITEMP database as well.

The choice of other molecules to include for HITRAN2000 is based upon current needs for the analysis of satellite- and ground-based measurements of the atmosphere. The European Space Agency's Global Ozone Monitoring Experiment (GOME), for example, can measure BrO, OClO, SO_2, H_2CO, and H_2O as well as O_3 and NO_2. These trace gases will be measured by future satellite instruments including SCHIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY), OMI (Ozone Measuring Instrument), GOME-2, and OMPS. While the choices of cross sections used in the analysis of field measurements is currently evolving, HITRAN2000 includes spectra that have been demonstrated to provide reasonable fitting.

The improvement of quantitative spectroscopy in the UV and its cataloguing in HITRAN will substantially improve the state of global measurements of these gases. Improvements are intended to include FTS-based measurements of cross sections and their temperature dependences for the complete set of molecules included in HITRAN2000, as well as extension to other species. These might include, for example, OBrO and NO_3, and line-by-line UV parameters for ClO. Tables 2 and 3 illustrate some of the constituents that will be in HITRAN.

References

1. 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. Chance, K. 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).

2. K.V. Chance, J.P. Burrows, and W. Schneider, “Retrieval and molecule sensitivity studies for the Global Ozone Monitoring Experiment and the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY, *Proc. S.P.I.E., Remote Sensing of Atmospheric Chemistry* **1491,** 151-165 (1991).

3. M.D. King, D.D. Herring, and D.J. Diner, “The Earth Observing System (EOS): A space-based program for assessing mankind’s impact on the global environment,” *Opt.Photon.News* **6,** 34-39 (1995).

Table 1. Agenda for Data Acquisition for the HITRAN Compilation

	Agenda for HITRAN with files in hand	Status and Program Plans
1 H_2O	Have replacement in hand (8000cm^{-1} to end) from L. Giver (available on the web).	Ken Jucks retrieving water vapor concentrations from rotational lines, 150 - 500 cm^{-1}, found that Coudert's latest calculations, especially for $\Delta K = 3$, reduced systematics (intensities). Positions also can be improved using Coudert's data (good to .0001 cm^{-1}). Need permission from Jean-Marie Flaud to use data. Problem with intensity unit conversion of lines in near-IR and visible found by Giver et al. Linda Brown has new measurements in near-IR. Isotopic water-vapor parameters due from line-list of Bob Toth, JPL late 2000 in region 500 to 8000 cm^{-1}.
2 CO_2		Obtain update in 3-µm region from D.C.Benner. Update intensities of hot bands at 5687.17 (00031-10002) and 5584.39 (00031-10001) measured by NASA Ames group. Fix Herman-Wallis factor measured by J Henningsen, Denmark in the 1.575 µm-band. Examine position discrepancy reported by R. Sams, PNL in the 2300 cm^{-1} region.
3 O_3		Below is a summary of the changes recommended for the air-broadened widths, the air-broadened shifts, and the n(air) coefficient. 1. ν_2 band. Adopt the mean value of n(air) = 0.53 ±0.08. Adopt the mean air shift of -0.0008 cm^{-1}/atm at 296 K. These values are from the Malathy Devi et al. article. 2. ν_1 band. Adopt the mean value of n(air) = 0.67 ±0.07. Adopt the mean air shift of -0.0007 cm^{-1}/atm at 296 K. These values are from Smith et al., *JMS* **182,** 239-259 (1997). 3. $\nu_1+\nu_2+\nu_3$ band. Adopt a mean air shift of -0.004 ±0.004 cm^{-1}/atm at 296 K. This value comes from Table IV of Smith et al., *JMS* **164,** 239-259 (1994). 4. $3\nu_3$. Adopt a mean air shift of -0.008 ±0.003 cm^{-1}/atm at 296 K. This value also comes from Table 4 of Smith et al. *JMS* **164,** 239-259 (1994). These are modest changes. Of course, we could introduce the individual measurement values, but the mean values should be OK for this round. They are better than doing nothing. There will be other updates based on GEISA 1997 and possibly other studies, for example at the University of Reims, France. NASA Langley recommends that the other parameters remain at the HITRAN defaults.
4 N_2O		New, improved line-list to come from Bob Toth, JPL late in 2000. Will cover the region 500 to 8000 cm^{-1}. Perturbed lines are corrected.
5 CO		NASA Ames update based on new electric dipole-moment function, will improve intensities.
6 CH_4		The vibrational notation seems to be reversed, that is, upper and lower levels reversed, for all lines of CH_3D. Waiting for files from Linda. Consulting with NASA Langley re halfwidths. For CH_3D, Linda has in the 900 to 3200 cm^{-1} positions, intensities and air- and self- widths and shifts.
7 O_2	Replacing old data with JPL file above 11483 cm^{-1}	Small problems with oxygen A-band (see Schermaul et al, *JQSRT* **61,** 62 (1999)).
8	Replaced old data with new $\Delta v = 2$ bands	Fix hyperfine notation in pure rotation.

NO		
9 SO_2		Agnes Perrin and Jean-Marie Flaud in process of improving bands.
10 NO_2		Use French algorithm for air-broadened widths, use a mean value for self-broadening (use for all lines) 1. Temperature-dependence n=1 (from 10 lines of Malathy Devi) 2. Fix up $<_1+<_3$ region, obtain from French.
11 NH_3		Inversion lines of ammonia missing, especially around 24 Ghz extending to 40 GHZ. Lines currently end at about .5cm^{-1}. See JPL catalog, P.Pracna, Czech Republic, and Linda. (Discussion with Ed Pearson, 5 May 1999 concerning these problems.). Brown has studied three regions: 1200 - 2100 cm^{-1} positions and intensities, 3000 - 3600 cm^{-1}, and 0.- 5300 cm^{-1} applying new air widths from V. Nemtchinov (now at JPL).
12 HNO_3	Created file to be substituted into HITRAN.	11-µm recommendation for HITRAN 96 as discussed in Goldman's invited talk in ASA Reims 96, it is better to remove the two hot bands $<_5+<_9-<_9$ and $3<_9-<_9$, and add the new hot band $<_5+<_9-<_9$; halfwidths appear incorrect (he uses .05 and .11); check error and reference indices.
13 OH	New file from A. Goldman	New high-temperature line parameters from Aaron Goldman (replace equivalent bands). Vibration indices need correcting, and reference indices need updating .
14 HF		
15 HCR		Make revision of positions with collaboration from Rinsland at NASA Langley.
16 HBr	New files of pure rotation and fundamental from A. Goldman	Update per article in *JQSRT* Special Issue.
17 HI	New files of pure rotation and fundamental from A. Goldman	Update per article in *JQSRT* Special Issue.
18		Rinsland will have update.

CRO		
19 OCS	Changes have been made	Refine references of new Fayt data
20 H_2CO		
21 HOCR	Done, unless Jean-Marie Flaud has improvements for minor parameters.	Reformat, add new reference, add halfwidths, etc, (replacement).
22 N_2		Need pressure induced continuum.
23 HCN		
24 CH_3CR		Need pure rotation lines (E.Pearson). Need for bands at 1000 cm^{-1} and 13-1500 cm^{-1} (communication from Jim Wray, jgwiz@yahoo.com).
25 H_2O_2	All done except vibration notation--decide on notation for N and J. Check with Kelly Chance for halfwidth.	Reformat, add new reference, add halfwidths, etc, (replacement); Vibrational identifications are weird (consult with Kelly Chance).
26 C_2H_2	Replace main isotope in $<_5$ region with Dana-Mandin file	Band ($2<_5^2 - <_5^1$) ~729 cm^{-1} missing "e" and "f" identification (non-unique assignments)--Same thing for band [$(<_4+ <_5)^2 - <_4^1$] ~ 731 cm^{-1}.

27 C_2H_6		Can we employ set of programs from Blass, U. Tennessee? Goldman can scale Daunt's data, and Rinsland can use Pine's measurements to improve PQ^3 region.
28 PH_3		Linda has predictions from Tarrago.
29 COF_2		
30 SF_6	Move all lines to supplemental directory.	Essential hot bands lacking in line-by-line files.
31 H_2S		Linda sending new files of 2.7- and 4-µm bands..
32 HCOOH		Goldman can improve.
33 HO_2	Replacement for pure rotation, check reference indices.	Halfwidths need to be be .107 rather than a generic 0.05 [Nelson and Zahnhiser, *JMS* **166**, 273-279 (1994)].
34 O		
35 CRO	Move all lines to supplemental directory.	Essential hot bands lacking in line-by-line files.

NO_2		
36 NO^+		
37 HOBr	Bring file from Supplemental directory.	
38 C_2H_4	Changes have been made Files are on web.	
	IR-Cross-sections	
	Make separate files for each molecule (break up old 92 files)	
	Remove some old duplicate molecule files (old Denver/NCAR data, CFC-11, CFC-12, HCFC-22, CCl_4, and only 1240-1340cm^{-1} $ClONO_2$)	
	New IR-Cross-sections from Kevin Smith, RAL, UK ; format for HITRAN	
	HCFC files from Clerbeaux, format for HITRAN	
	CFCs from SUNY	Reformat and work with Prasad Varanasi
	UV-Cross-sections and line-by-line parameters	
	O_3, H_2CO, BrO, OClO, and NO_2 from SAO	Work with Kelly Chance; Obtain UV Herzberg system bands from K. Yoshino, SAO.
	New SO_2 , O_2, NO from SAO (coalesce UV SO_2)	Work with Kouichi Yoshino
	ClO, OH from Denver	Work with Aaron Goldman

Table 2. UV Cross-sections Represented in HITRAN (Highlighted data already present in HITRAN96)

Molecule	Band System	Spectral Range (cm^{-1})	Temperatures (K)
N_2O	(^{1}A0 $^1E^-$, ^{1}))? 7 $\tilde{X}$ $^1E^+$	44925 - 58956	296
SO_2	$\tilde{C}$ $^1B_2$ 7 $\tilde{X}$ $^1A_1$	41691 - 58452 45455 - 50505	213 295
O_3	$^1B_2$ 7 $\tilde{X}$ $^1A_1$ (Hartley-Huggins) $^1B_1$ 7 $\tilde{X}$ $^1A_1$ (Chappuis) (Wulf)	24570 - 42190	203 - 293
H_2CO	^{1}A0 7 $\tilde{X}$ $^1A_1$	27391 - 33311	223, 293
BrO	A 7 X	25756 - 32013	228, 298
OClO	$\tilde{A}$ $^2A_2$ 7 $\tilde{X}$ $^2B_1$	20992 - 41228	228
ClO	B 7 X ^2A_i	32000 - 37700	220
NO_2	$\tilde{A}$ $^2B_1$ 7 $\tilde{X}$ $^2A_1$	17540 - 32260	213 - 298

Table 3. UV Line-by-line Data Represented in HITRAN (Highlighted data already present in HITRAN96)

Molecule	Band System	Spectral Range (cm^{-1})
O_2	B $^1E_u^-$ 7 X $^3E_g^-$ (Schumann-Runge) A $^3E_u^+$ 7 X $^3E_g^-$ (Herzberg I) c $^1E_u^-$ 7 X $^3E_g^-$ (Herzberg II) AN ^{3})$_u$ 7 X $^3E_g^-$ (Herzberg III)	44606 - 57028 37000 - 41600 36400 - 41600 36400 - 41600
OH	A $^2E^+$ 7 X ^2A_i	31000 - 36000
NO	A $^2E^+$, B ^2A_r , C ^{2}A , D $^2E^+$ 7 X ^2A_i ((, $, *, , -bands)	44300 - 62500

Figure 1. Formats for Line-by-line Portion of HITRAN and for Cross-sections.

1986-1996 line-parameter format

```
M I       νηη′     Sηη′     Uηη′        gair  gself    E0     n      d    iv′iv″     q′      q″  ierr iref
1234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
         1         2         3         4         5         6         7         8         9         100
```

"2000" line parameter format:

```
M I       νηη′     Sηη′     Aηη′       gair  gself    E0    n      d           v′             v″              q
1234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012
         1         2         3         4         5         6         7         8         9         100       1
      q″       ierr     iref    * g′g″
345678901234567890123456789012345678901234567890
       2         3         4        150
```

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

"2000" Cross-section Header format:

```
  Chemical Symbol     Minimum   Maximum    #    Temp  Press    Max    Res.  Common Name    Unused Ref
                         Wavenumber       Pts    K    Torr   X-sect                             No.
1234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
         1         2         3         4         5         6         7         8         9         100
```

Note:

Chemical Symbol: Right adjusted

Res.: Resolution in cm^{-1} for FTS measurements, and in milli-Angstroms for grating measurements in the UV (xxxmA)

Figure 2. Example of Plotting Capabilities in the new JavaHAWKS Software Interface.