

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

**Annual Progress Report for NASA Grant NAG5-8420**

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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.

## **2. Data Acquisition and Data Improvement**

During this performance period, a major focus has been towards the construction of a new archival edition of HITRAN. Due to the expanded format that will be implemented in the next edition, much more management and requirements from contributors is in effect. The current format for the HITRAN database<sup>1</sup> is a 100-character record per transition. This format has been in place since 1986, but it is not quite adequate for the increased demands of remote-sensing algorithms and by the increased accuracy and knowledge of spectroscopic parameters. The new parameters for each line include: the Einstein-A coefficient, the error and references for self-broadened, temperature dependence of halfwidth, and pressure shift parameters. There will also be a flag for treatment of lines with line-coupling parameters and the statistical weights of the upper and lower states of a transition. Table 1 illustrates the new format. Besides attempting to satisfy remote-sensing needs that were not addressed before, such as line-coupling effects, the added documentation and referencing makes maintainability substantially improved. It does require, however, more attention on the part of contributors. The expanded error code indexing is shown in Table 2. The error codes have often not been supplied by contributors in the past; with the referencing of parameters the user should in principal be able to ascertain the quality of the data, albeit with more effort. We have

implemented a user-friendly method of accessing the abstracts of most sources in the software to assist serious users.

Parameter	Field Length	Type	Comment
Molecule number	2	Integer	HITRAN chronological assignment
Isotopomer number	1	Integer	Ordering by terrestrial abundance
Frequency (cm <sup>-1</sup> )	12	Real	Vacuum wavenumber
Intensity	10	Real	cm <sup>-1</sup> /(molecule_cm <sup>-2</sup> ) at 296K
Einstein-A coefficient	10	Real	Revised parameter after 2000 edition
$\gamma$ -air (Lorentzian halfwidth)	5	Real	HWHM at 296K
$\gamma$ -self	5	Real	HWHM at 296K
$E$ (cm <sup>-1</sup> )	10	Real	Lower-state energy
$\eta$	4	Real	Temperature-dependence coefficient of $\gamma$ -air
$\delta$ (cm <sup>-1</sup> )	8	Real	Pressure shift in air
$v$	15	Holerith	Upper-state “global” quanta
$v$	15	Holerith	Lower-state “global” quanta
$Q$	15	Holerith	Upper-state “local” quanta
$Q$	15	Holerith	Lower-state “local” quanta
Error indices	6	Integer	Accuracy of 6 critical parameters
Reference indices	12	Integer	References for 6 critical parameters
Flag for line coupling	1	Holerith	Pointer to line-coupling algorithm
$g$	7	Real	Upper-level statistical weight
$g$	7	Real	Lower-level statistical weight

Table 1. Format for HITRAN Line Transition

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

	8	<1%
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Table 2. Error Code Correspondence for HITRAN

## 2.1 Line-by-line Parameters

For the line-by-line spectroscopic parameters, the most prominent improvements since the last report have been to methane, water vapor, hydroxyl radical, acetylene, nitric oxide, and nitrogen dioxide. These updates have been placed in the sub-page on UPDATES in the HITRAN web-site.

They have been evaluated and verified, but it has been decided to keep the archival edition of HITRAN in the ftp-site unchanged until a new edition is created. Nonetheless, the updates are given as total replacements for the molecule in question in order to simplify the process for users.

A vastly improved line list for methane,<sup>2,3</sup> which will have an impact on the **MOPITT** and many other programs of EOS, was made available in the regular HITRAN web-site. This effort was accomplished in collaboration with L.R. Brown of JPL. The line list represents a fourfold increase in the number of transitions for methane compared to the last edition of HITRAN. The differences are in the 850 to 4810  $\text{cm}^{-1}$  region. Dr. Brown's study includes the three isotopomers in HITRAN ( $^{12}\text{CH}_4$ ,  $^{13}\text{CH}_4$ , and  $^{12}\text{CH}_3\text{D}$ ). The data are far more complete than many species in HITRAN in that they have been prepared with the new format in mind. Inconsistencies had existed in the quantum notation of some bands in the previous HITRAN editions, since contributions from different groups were adhering to different conventions; this has been eliminated and standardized. Having consistent nomenclature is quite important for later processing, such as bringing in observed halfwidths or especially the post calculation of the Einstein-A coefficients, not to mention maintaining the database.

The fix for  $\text{H}_2\text{O}$  parameters in the 6- $\mu\text{m}$  region was placed in the HITRAN web-site. The current HITRAN edition<sup>1</sup> lacked some bands in this region that existed previously. The error had been caused by a misunderstanding of the files sent by JPL for the last update.<sup>4</sup> Other glitches were fixed in the visible region; these problems pertained to mapping the limited set of references to the larger set for the new format. A study and collaboration is also underway with high-resolution water-vapor parameters generated by the group of Michel Carleer in Belgium. There are numerous sets of independent measurements from different laboratories that are being assessed in the short wavelength region. This region is particularly important for resolving some of the discrepancies in atmospheric radiative budget modeling, for example, as well as serving specifically for **SAGE III**.

A whole new linelist<sup>5</sup> in the UV for the hydroxyl radical (OH) has been acquired for HITRAN. This system, the  $A^2 + C X^2$  electronic bands, were provided by A. Goldman of the University of Denver.

An extensive set of parameters<sup>6</sup> for bands of acetylene,  $\text{C}_2\text{H}_2$ , in the 5- $\mu\text{m}$  region has been posted on the web-site. This linelist has 18 new upper-state levels that are not presently indexed in the '86-format. The far more extensive set of energy levels for this molecule required the development of a more concise labeling with the constraints of ASCII in mind. Table 3 indicates the scope of this correspondence. The effort for acetylene was based on a joint collaboration of the PI with the group at the University of Paris and the group at the University of Reims.<sup>6</sup> Updating the halfwidths and pressure shift parameters of acetylene throughout the database was also undertaken.<sup>6,7</sup>

The collisional broadening parameters and pressure-shift parameters for nitric oxide (NO) have been updated and made consistent throughout the database. There had existed different sets,

sometimes poor, between bands whose line positions and intensities were derived from different laboratories. Algorithms developed at the University of Paris assisted in this endeavor. We have found that developing polynomial expressions for the broadening parameters as a function of rotational level is an excellent method to provide maintainable and consistent values for many molecules in the database, and it is hoped that this method will be adopted. At high values of the rotational quanta, an asymptotic value for the broadening parameter should be used, and for low values of rotation, the detailed structure that might not be well represented by a low-order polynomial can be constructed in the algorithm.

Vibrational level	HITRAN notation $v_1v_2v_3v_4v_5l\pm r$	Vibrational level	HITRAN notation $v_1v_2v_3v_4v_5l\pm r$
Ground state	000000+	$(3_{4+}5_-)^0$	000310-
$\begin{matrix} 1 \\ 5 \end{matrix}$	000011	$(3_{4+}5_-)^2\Pi$	000312 2
3	001000+	$(3_{4+}5_-)^2I$	000312 1
$\begin{matrix} 2+ \\ (4+5)_+^0 \end{matrix}$	010110+	$\begin{matrix} 2+ \\ 5 \end{matrix}$	010011
$\begin{matrix} 1 \\ 4 \end{matrix}$	000101	$(4+3_5)_+^0$	000130+
$(4+5)_+^0$	000110+	$(4+3_5)_-^0$	000130-
$(4+5)_-^0$	000110-	$(4+3_5)^2\Pi$	000132 2
$(4+5)^2$	000112	$(4+3_5)^2I$	000132 1
$\begin{matrix} 2 \\ 5 \end{matrix}$	000020+	$\begin{matrix} 2+ \\ 4 \end{matrix}$	010101
$\begin{matrix} 2 \\ 5 \end{matrix}$	000022	$(2_{4+2}5_+)^0\Pi$	000220+2
$\begin{matrix} 3 \\ 5 \end{matrix}$	000031	$(2_{4+2}5_-)^0$	000220-
$(2_{4+}5)^1\Pi$	000211 2	$(2_{4+2}5)^2\Pi$	000222 2
$(2_{4+}5)^1I$	000211 1	$\begin{matrix} 4 \\ 5 \end{matrix}$	000040+
$(3_{4+}5)_+^0$	000310+	$\begin{matrix} 4 \\ 5 \end{matrix}$	000042

Table 3. Vibrational quantum-level designation for acetylene in new HITRAN

A significant update of the nitrogen dioxide ( $\text{NO}_2$ ) parameters was accomplished in this period. The update employs the work of the University of Paris for line positions and intensities in the 3- $\mu\text{m}$  region.<sup>8</sup> There has also been a thorough update of the air-broadened halfwidths, the self-broadened halfwidths, and the temperature-dependence of the air-broadened halfwidth. The latter was accomplished uniting the work of the Paris group with the groups at NASA Langley Research Center and at JPL.<sup>9</sup> Numerous bookkeeping details had to be checked and corrected in creating the

overall file, which is now available in the HITRAN web-site and will be part of the next edition of HITRAN.

We discuss later in this report some of the line-by-line data that are close to being ready for inclusion into HITRAN.

## 2.2 Cross-sections

It should first be remarked that the improved header format for the cross-sections has already been implemented. The cross-section data compliment the HITRAN line-by-line data. They have been established to cover molecules whose spectra are so dense as to make a line-by-line transition representation either extremely difficult or impractical from the user's standpoint. Table 4 presents the list of species and spectral coverage for the infrared bands in HITRAN (some additional semi-redundant, but independent data are preserved in a sub-directory). There are also similar sets for the UV region, shown in Table 5. A discussion of the cross-sections was given in the previous annual report for this grant.

Two new data sets have recently been obtained. They are for chlorine nitrate ( $\text{ClONO}_2$ ) and dinitrogen pentoxide ( $\text{N}_2\text{O}_5$ ). The measurements were made at the high-resolution laboratory at the DLR in Germany by M. Birk and G. Wagner and reported on in the last HITRAN Conference.<sup>10</sup> The manipulation and casting into HITRAN form was performed by J. Schroeder and K. Tang of the Ontar Corp. The files for  $\text{N}_2\text{O}_5$  represent a significant improvement to the HITRAN compilation and will totally replace the older data which had a very poor resolution grid. These data cover the prominent band regions of 699 to 799 and 1199 to 1279  $\text{cm}^{-1}$ . For chlorine nitrate, we split the DLR data into 2 spectral regions (740-840 and 1250-1330  $\text{cm}^{-1}$ ). The bands in the spectral range 1680 to 1790  $\text{cm}^{-1}$  from the former Rutherford Appleton Lab data<sup>11</sup> will be retained. The size of the cross-section files has grown rapidly, even with the efficient method used to store the data in HITRAN.

## 2.3 Aerosol Indices of Refraction

A very extensive tabulation for various aerosol indices of refraction has been compiled and submitted to the HITRAN project by S. Massie of the National Center for Atmospheric Research. The sets were summarized in a previous report, and a more complete table is given in both the HITRAN web-site and ftp-site.



Table 4. Summary of Molecules Represented by IR Cross-section Data in HITRAN

Molecule	Common Name	Temperature Range (K)	Pressure Range (Torr)	Number of P,T sets	Spectral Coverage (cm <sup>-1</sup> )
SF <sub>6</sub>	Sulfur hexafluoride	180-295	20-760	32	925-955
ClONO <sub>2</sub>	Chlorine nitrate	213-296	0	2	740-840
		213-296	0	2	1240-1340
		213-296	0	2	1680-1790
CCl <sub>4</sub>	Carbon tetrachloride	208-297	8-760	32	750-812
N <sub>2</sub> O <sub>5</sub>	Dinitrogen pentoxide	233-293	0	4	555-600
		233-293	0	4	720-765
		233-293	0	4	1210-1275
		233-293	0	4	1680-1765
HNO <sub>4</sub>		268	0.7	1	770-830
CCl <sub>3</sub> F	CFC-11	201-296	40-760	55	810-880
		201-296	40-760	55	1050-1120
CCl <sub>2</sub> F <sub>2</sub>	CFC-12	190-296	7.5-760	52	850-950
		190-296	7.5-760	52	1050-1200
CClF <sub>3</sub>	CFC-13	203-293	0	6	765-805
		203-293	0	6	1065-1135
		203-293	0	6	1170-1235
CF <sub>4</sub>	CFC-14	180-296	7.5-761	55	1250-1290
C <sub>2</sub> Cl <sub>2</sub> F <sub>3</sub>	CFC-113	203-293	0	6	780-995
		203-293	0	6	1005-1232
C <sub>2</sub> Cl <sub>2</sub> F <sub>4</sub>	CFC-114	203-293	0	6	815-860
		203-293	0	6	870-960
		203-293	0	6	1030-1067
C <sub>2</sub> ClF <sub>5</sub>	CFC-115	203-293	0	6	955-1015
		203-293	0	6	1110-1145
		203-293	0	6	1167-1260
CHCl <sub>2</sub> F	HCFC-21	296	1	1	785-840
CHClF <sub>2</sub>	HCFC-22	181-297	0-764	29	760-860
		181-296	0-761	34	1070-1195
		253-287	0	3	1274-1380
CHCl <sub>2</sub> CF <sub>3</sub>	HCFC-123	253-287	0	3	740-900
		253-287	0	3	1079-1450
CHClF <sub>2</sub> CF <sub>3</sub>	HCFC-124	287	0	1	675-1430
CH <sub>3</sub> CCl <sub>2</sub> F	HCFC-141b	253-287	0	3	700-1500
CH <sub>3</sub> CClF <sub>2</sub>	HCFC-142b	253-287	0	3	650-1475
CHCl <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub>	HCFC-225ca	253-287	0	3	695-1420
CClF <sub>2</sub> CF <sub>2</sub> CHClF	HCFC-225cb	253-287	0	3	600-1500
CH <sub>2</sub> F <sub>2</sub>	HFC-32	203-297	0-750	17	995-1236
		203-297	0-750	17	1385-1475
CHF <sub>2</sub> CF <sub>3</sub>	HFC-125	287	0	1	700-1500
CHF <sub>2</sub> CHF <sub>2</sub>	HFC-134	203-297	0-750	9	600-1700
CFH <sub>2</sub> CF <sub>3</sub>	HFC-134a	190-296	20-760	69	1035-1340
		203-297	0-750	9	580-630
CF <sub>3</sub> CH <sub>3</sub>	HFC-143a	203-297	0-750	9	750-1050
		203-297	0-750	9	1100-1500
CH <sub>3</sub> CHF <sub>2</sub>	HFC-152a	253-287	0	3	840-1490

  

Molecule	Band System	Spectral Range (cm <sup>-1</sup> )	Temperatures
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			(K)
N <sub>2</sub> O	( <sup>1</sup> A <sup>-</sup> , <sup>1</sup> )? 7 <sup>1</sup> +	44925 - 58956	296
SO <sub>2</sub>	<sup>1</sup> B <sub>2</sub> 7 <sup>1</sup> A <sub>1</sub>	41691 - 58452 45455 - 50505	213 295
O <sub>3</sub>	<sup>1</sup> B <sub>2</sub> 7 <sup>1</sup> A <sub>1</sub> (Hartley-Huggins) <sup>1</sup> B <sub>1</sub> 7 <sup>1</sup> A <sub>1</sub> (Chappuis) (Wulf)	24570 - 42190	203 - 293
H <sub>2</sub> CO	<sup>1</sup> A <sub>1</sub> 7 <sup>1</sup> A <sub>1</sub>	27391 - 33311	223, 293
BrO	A <sup>2</sup> <sub>3/2</sub> 7 X <sup>2</sup> <sub>3/2</sub>	25756 - 32013	228, 298
OCIO	<sup>2</sup> A <sub>2</sub> 7 <sup>2</sup> B <sub>1</sub>	20992 - 41228	228
ClO	A <sup>2</sup> <sub>3/2</sub> 7 X <sup>2</sup> <sub>3/2</sub>	32000 - 37700	220
NO <sub>2</sub>	<sup>2</sup> B <sub>1</sub> 7 <sup>2</sup> A <sub>1</sub>	17540 - 32260	213 - 298

Table 5. UV Cross-sections for HITRAN

### 3. HAWKS Software Development, Upgrades, and Distribution

Work continued on improving the HAWKS (HITRAN Atmospheric Workstation) software for the next HITRAN edition. It has been written in the Java language for cross-platform applicability. In addition to features described in the last report, several new ones have been added. Many documents related to HITRAN, such as earlier articles, have been made into pdf files and incorporated into HAWKS. A pull-down menu has been added that allows users to bring up related databases, such as the JPL submillimeter catalog or the Harvard-SmithsonianCenter databases of UV cross-sections. One can also access the ftp-site of the HITRAN database itself, rather than using a CD-ROM or storage on one's system. The Ontar Corporation, under the direction of J. Schroeder, have performed this task, as well as been highly involved with all aspects of database management.

The Ontar Corp has also gathered many of the scores of references and citations invoked by and made their abstracts available in the software. This feature is a valuable resource for the database and for future development.

### 4. HITRAN Web-site Development

The HITRAN web-site ([cfa-www.harvard.edu/HITRAN](http://cfa-www.harvard.edu/HITRAN)) continued to be updated during this period of performance. The AHITRAN UPDATES@ sub-page includes corrections as discovered by users and new data that has been validated since the current edition. The "FAQ" sub-page has additional frequently asked questions and our solutions, garnered from the many e-mails sent into the PI. The web-site includes links to relevant conferences, and in particular to the

upcoming HITRAN conference in June as well as the Atmospheric Spectroscopy Applications conference in August.

The ftp-site ([cfa-ftp.harvard.edu/pub/HITRAN/](ftp://cfa-ftp.harvard.edu/pub/HITRAN/)) for the HITRAN compilation was established during the last period. There are security issues that have prevented a few users from accessing the site. Generally the problem has been that the machines the users are using are not properly registered with a nameserver. We have solved this problem by allowing users to also access the server that contains the compilation via regular internet while protecting our site.

## **5. Collaborations**

The development of HITRAN relies on cooperation and collaboration with the whole spectroscopic community. As can be seen from the description of data in this report, we have continued to develop these connections. In this period in particular, the generous contributions of groups in Belgium are to be noted. We are also working closely here with scientists in the Atomic and Molecular Physics Division: K. Chance and K. Yoshino especially for updating and improving the UV portion of the compilation. Linda Brown of JPL provided much data in very complete HITRAN format (even anticipating the next expanded format). Aaron Goldman of the University of Denver also provided much data, as did Steven Massie of NCAR for the aerosols. We have a strong collaboration with Victor Dana and Jean-Yves Mandin of the University of Paris, providing us with accurate high-resolution parameters for trace gas species. Curtis Rinsland and Mary Ann Smith of NASA Langley Research Center and their colleagues at the College of William and Mary, D. Chris Benner and V. Malathy Devi, are also close collaborators. Robert Gamache at the University of Massachusetts, Lowell has been working on the partition sums and other molecular aspects of the database.

## **6. Meetings, Presentations, and Publications**

This project is tasked to conduct a biennial conference on issues relating to the HITRAN database. A first circular was sent out via e-mail for the meeting to be held 12-14 June 2002 at the Harvard-Smithsonian Center for Astrophysics in Cambridge Massachusetts. The local committee is chaired by the PI, L.S. Rothman, and includes Drs. K. Chance, T. Kurosu, and W. Parkinson. We plan to have invited and contributed talks and poster sessions. The latter have been very successful in the past for promoting workshop-type discussions. These discussions and panels are essential in forming a consensus for the standardization of the data, establishing definitions of various quantities, and for providing direction for future measurement programs. We are in the planning stage for special sessions. Emphasis is always on applications for remote sensing and for spectroscopic data that enhance the capabilities of radiance algorithms. A book of abstracts will be prepared from the meeting, and made available on the web-site as with the proceedings from previous HITRAN meetings. At this time we have many key people pre-registered. Titles of presentations assembled so far can be viewed in the HITRAN web-site. A second circular is being prepared, which will be sent out via e-mail to the HITRAN mailing list (about 5000); additional notices will be sent to the EOS and ARM communities in general.

We have obtained some limited funding from the NASA Upper Atmosphere program to invite members of the HITRAN Advisory Board who are not US government employees. This

board is tasked to oversee and create sub-panels of researchers in specific areas for updating HITRAN. For example, when one has several independent and highly qualified groups measuring the same parameters for a high-priority molecule (water, for example), we need an evaluation of the data and a decision of what goes into a HITRAN update. This issue was highlighted at the NASA Remote Sensing Workshop held in San Diego October 2001. A summary of the meeting will be presented by K. Jucks at the upcoming HITRAN conference.

In March, the PI attended and made a poster presentation at the Atmospheric Radiation Measurement (ARM) science team annual meeting, held in Atlanta.

During the month of May, the PI was an invited professor at the University of Paris, where he worked with the group of Prof. V. Dana. The group includes Dr. J-Y. Mandin and D. Jacquemart. The latter will defend his thesis this May, and is a candidate for post-doc on the HITRAN project.

In June, the PI organized and chaired a session on spectroscopy at the DOD annual atmospheric transmission meeting that was held at Hanscom AFB.

The PI gave an invited talk at the NASA Remote Sensing Workshop that was held in San Diego in October. This meeting was particularly effective for the development of HITRAN.

The PI also participated in NASA Peer Review panel for the Upper Atmosphere program that took place outside Washington at the end of October (it had been delayed due to events of 9-11).

*Publications during this period:*

“The spectrum of acetylene in the 5- $\mu$ m region from new line parameter measurements,” D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, J.J. Plateaux, D. Décatoire, and L.S. Rothman, *JQSRT* (in press, 2002).

*Presentations during this period:*

“A New Edition of the HITRAN Database,” ARM Science Team Meeting, Atlanta, Georgia (March 2001)

“A New Edition of HITRAN,” 24<sup>th</sup> Annual Review of Atmospheric Transmission Models, Hanscom Air Force Base, Massachusetts (June 2001).

“HITRAN’2001: Status of the Spectroscopic Database Compilation,” NASA Workshop on Spectroscopic Needs for Atmospheric Sensing, San Diego, California (October 2001).

## **7. Future Effort**

Other line-parameter data that will soon be made available include bands of N<sub>2</sub>O, HCN, CH<sub>3</sub>Cl, HOCl, H<sub>2</sub>O<sub>2</sub>, and numerous UV data sets that are mostly being developed at the Atomic and Molecular Physics Division at the SAO.

We have completed an update for nitrous oxide (N<sub>2</sub>O). Two bands in the 10- $\mu$ m region were obtained from the Free University of Brussels, but based on work performed at the University of Paris.<sup>12</sup> The bands that were replaced in HITRAN had very poor intensities, so this update should significantly improve some simulations. The other update is the  $\nu_2$  band at 17  $\mu$ m; K. Jucks of SAO assisted with this effort, which was based on data from a joint program of the National Research Council of Canada and NASA.<sup>13</sup>

We continue to evaluate new data on water vapor in the near IR through visible region that has come from a collaboration of laboratories directed out of the University College London supported by the European Space Agency.

The plans continue for an enhanced format for HITRAN that will include new parameters for each line: the Einstein-A coefficient, the error and references for self-broadened, temperature dependence of halfwidth, and pressure shift parameters. We had a student from the University of Massachusetts work during the summer on partition sums for all of the molecular species and their isotopomers. We have completed all but three of the species. The values are given at one-degree intervals from 70K to 3000K and are now in the HITRAN ftp-site. The student, J. Fischer, did an excellent job. He evaluated different methods for each isotopomer (nearly 200). The methods included direct sum and analytical. We chose the method that produced the most accurate values. Prof. R. Gamache is now using these partition sums to implement the algorithm for producing Einstein-A coefficients for HITRAN.

We are collaborating with the group at NASA Langley and R. Hawkins at AFRL to update the CO<sub>2</sub> parameters based on energy level observations in the 3- $\mu$ m region and new intensity observations by NASA Ames. This effort requires a whole new global fit of the energy levels, and then a calculation of all carbon dioxide parameters for a self-consistent set.

We are expecting to receive new parameters for carbon monoxide from NASA Ames. These data as well as the CO<sub>2</sub> improvements are expected to impact **MOPITT**, **TES**, etc. However, new data have recently been published from other groups on the higher overtones of CO that we have begun to evaluate.

Vastly improved line positions and intensities for bands of HCN have been obtained from A. Maki (formerly of NBS).<sup>14</sup> The group at NASA Langley will soon have new improved values for the halfwidths; however, in the interim, we are using new algorithms provided by M.A.H. Smith of NASA to update the halfwidths (air and self) and the temperature-dependence parameter.

The availability of the halfwidth and temperature-dependence parameters has improved a great deal. In the early editions of HITRAN, one would often have no information for some molecules, so that the average value of 0.05 cm<sup>-1</sup>/atm was adopted for the air-broadened halfwidth, no value was given for the self-broadened halfwidth, and the hard-sphere collisional value of 0.5 was adopted for the temperature dependence coefficient. The current situation, with all the species presently in HITRAN, is illustrated in Table 6. Some of the extrema are perhaps misleading since some bands of a species may have these parameters, while other bands may still possess old default values. Improvement and completeness of these parameters must be one of the HITRAN goals for remote sensing.

Table 6. Range of Parameters in HITRAN for Air- ( $\gamma_{air}$ ) and Self-broadened ( $\gamma_{self}$ ) Halfwidths, Temperature Dependence of Air-broadened Width ( $\eta$ ), and Pressure-shift ( $\delta$ ).

Molecule	$\gamma_{air}$		$\gamma_{self}$		$\eta$		$\delta$	
	Min.	Max.	Min.	Max.	Min.	Max.	Min.	Max.
1. H <sub>2</sub> O	0.0023	0.1099	0.	0.7048	0.28	0.97	-0.0312	0.0212
2. CO <sub>2</sub>	0.0554	0.0949	0.0523	0.1279	0.49	0.78	-0.00372	0.

3. <b>O<sub>3</sub></b>	0.0494	0.0836	0.0809	0.1119	— 0.76 —		— 0. —	
4. <b>N<sub>2</sub>O</b>	0.0686	0.0974	0.0	0.127	0.64	0.82	— 0. —	
5. <b>CO</b>	0.04	0.0789	0.046	0.0878	— 0.69 —		— 0. —	
6. <b>CH<sub>4</sub></b>	0.0000	0.0987	0.0137	0.2045	0.1300	1.07	-0.0328	0.017967
7. <b>O<sub>2</sub></b>	0.0279	0.0601	0.0274	0.059	0.63	0.74	-0.009	0.0
8. <b>NO</b>	0.041	0.0687	0.0	0.076	0.5	0.71	-0.004	0.0
9. <b>SO<sub>2</sub></b>	0.1	0.152	0.0	0.4	0.5	0.75	— 0. —	
10. <b>NO<sub>2</sub></b>	0.063	0.067	— 0. —		— 0.5 —		— 0. —	
11. <b>NH<sub>3</sub></b>	0.0531	0.11	0.0585	0.6603	0.45	0.95	— 0. —	
12. <b>HNO<sub>3</sub></b>	— 0.11 —		0.	0.73	— 0.75 —		— 0. —	
13. <b>OH</b>	0.04	0.095	— 0. —		0.5	0.66	— 0. —	
14. <b>HF</b>	0.01	0.105	0.	0.7295	0.22	1.	-0.029	0.012
15. <b>HCl</b>	0.005	0.0984	0.0221	0.264	0.05	0.76	-0.0129	0.001
16. <b>HBr</b>	0.015	0.123	0.05	0.1378	— 0.5 —		— 0. —	
17. <b>HI</b>	— 0.05 —		0.01	0.12	— 0.5 —		— 0. —	
18. <b>ClO</b>	0.085	0.093	— 0. —		0.5	0.75	— 0. —	
19. <b>OCS</b>	0.07	0.1092	0.	0.1685	0.3	0.9	— 0. —	
20. <b>H<sub>2</sub>CO</b>	0.107	0.108	— 0. —		— 0.5 —		— 0. —	
21. <b>HOCl</b>	— 0.06 —		— 0. —		— 0.5 —		— 0. —	
22. <b>N<sub>2</sub></b>	0.0314	0.053	0.0314	0.053	— 0.5 —		— 0. —	
23. <b>HCN</b>	0.0819	0.1566	— 0. —		— 0.5 —		— 0. —	
24. <b>CH<sub>3</sub>Cl</b>	0.08	0.1238	— 0. —		— 0.5 —		— 0. —	
25. <b>H<sub>2</sub>O<sub>2</sub></b>	— 0.1 —		— 0. —		— 0.5 —		— 0. —	
26. <b>C<sub>2</sub>H<sub>2</sub></b>	0.04	0.1158	0.0812	0.1969	— 0.75 —		-0.001	0.0
27. <b>C<sub>2</sub>H<sub>6</sub></b>	— 0.1 —		— 0. —		— 0.5 —		— 0. —	
28. <b>PH<sub>3</sub></b>	— 0.075 —		— 0. —		— 0.5 —		— 0. —	
29. <b>COF<sub>2</sub></b>	— 0.0845 —		— 0.175 —		— 0.94 —		— 0. —	
30. <b>SF<sub>6</sub></b>	— 0.05 —		— 0.08 —		— 0.65 —		— 0. —	
31. <b>H<sub>2</sub>S</b>	0.08	0.15	— 0.17 —		— 0.75 —		— 0. —	
32. <b>HCOOH</b>	— 0.1 —		— 0. —		— 0.75 —		— 0. —	
33. <b>HO<sub>2</sub></b>	— 0.107 —		— 0. —		0.5	0.67	— 0. —	
34. <b>O</b>	— Not Applicable —							
35. <b>ClONO<sub>2</sub></b>	— 0.14 —		— 0.8 —		— 0.5 —		— 0. —	
36. <b>NO<sup>+</sup></b>	— 0.06 —		— 0. —		— 0.5 —		— 0. —	
37. <b>HOBr</b>	— 0.06 —		— 0. —		— 0.67 —		— 0. —	
38. <b>C<sub>2</sub>H<sub>4</sub></b>	— 0.087 —		— 0.09 —		— 0.82 —		— 0. —	

Note: “zero” as minimum value means “no value given”; ClONO<sub>2</sub> and SF<sub>6</sub> are in supplemental line-files; ranges indicate extremes for some bands, others may be defaults or blank

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