

# ATOMIC AND MOLECULAR DATABASES FOR PLANETARY AND TERRESTRIAL APPLICATIONS

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**Abstract.** Characteristics of solar and planetary atmospheres ranging from chemical composition to climate can be accurately measured through spectroscopic remote sensing. Fundamental principles of physics and chemistry can then be applied to interpret the atmospheric observations (with varying degrees of success). The models of planetary atmospheres to simulate the chemistry, radiation fields, and/or dynamics require knowledge of many molecular properties ranging from **photochemical** and kinetic information to atomic and molecular transition parameters. Both the experimental and theoretical efforts require detailed databases of spectral parameters for use in computer simulations. The status of current databases for theoretical models and for microwave and infrared observations will be presented along with an overview of the problems associated with maintaining them.

## OVERVIEW OF DATABASES FOR ATMOSPHERIC RESEARCH

Studies of a planetary atmosphere are undertaken to address important questions such as

- What is its composition?
- What is its weather and climate?
- Do our models based on “fundamental knowledge”
  - a) reproduce what we observe (to within measurement accuracies)
  - b) predict what will happen next

Answering these simply-posed questions proves very difficult because of the complexity of the dynamical processes. For example, characterizing the behavior of climate over time requires the merging of fundamental principles (physics, mathematics and chemistry). As illustrated in the lower part of Fig. 1, the development of intricate theoretical models is performed as an iterative process that is often driven by the experimental observations.

Extensive programs of field observations often are done through the remote sensing by spectroscopic techniques that utilize the full range of the electromagnetic spectrum from the microwave to the ultraviolet. A diverse complement of instrumentation is deployed on a variety of ground-, aircraft-, balloon-borne and space-based platforms (2,3).

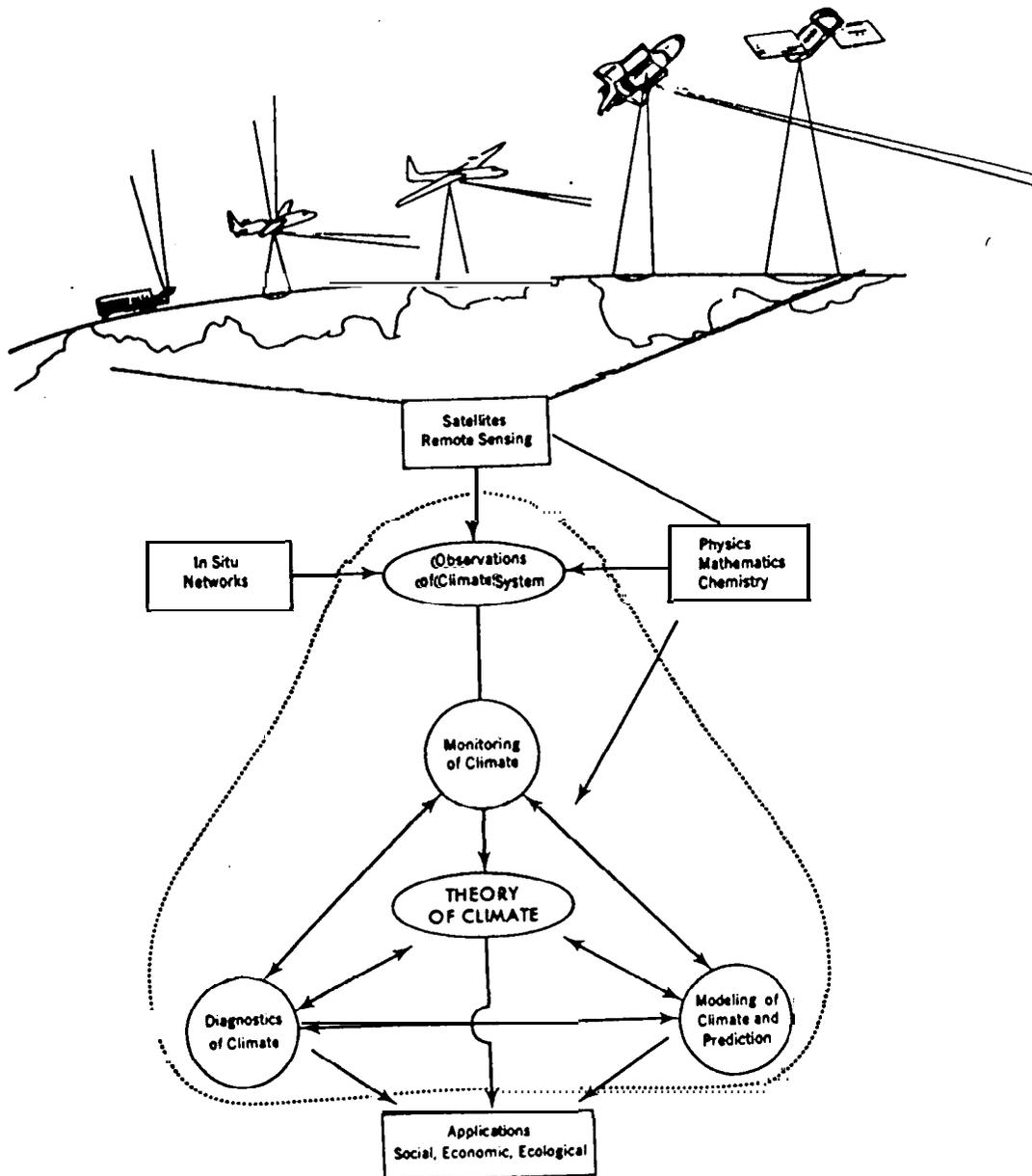


FIGURE 1. Interaction of observations and theoretical modelling of climate (1).

Measurements from these systems then steer the development of models for both atmospheric climate and chemistry. As illustrated in Fig. 2 below (4), within the Earth's atmosphere, there is an labyrinthine scheme of chemical reactions to unravel in order to understand the influence of natural and anthropogenic phenomena on the troposphere and stratosphere.

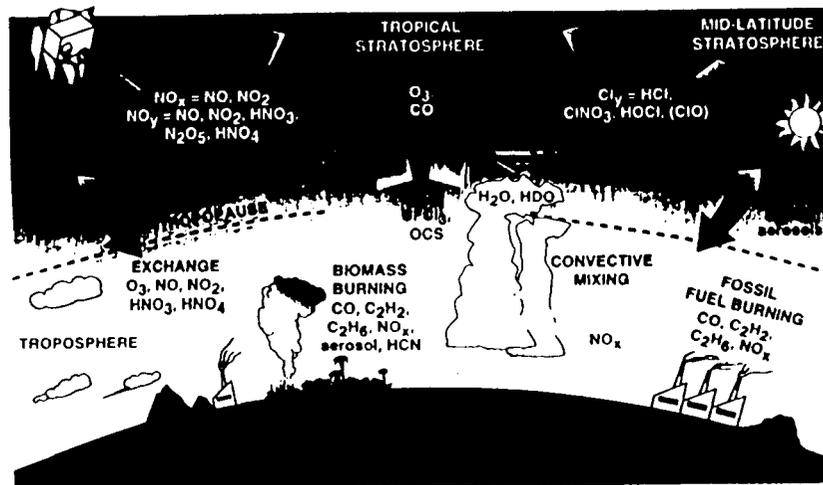


FIGURE 2. Environmental impact of industry, agriculture and biomass burning

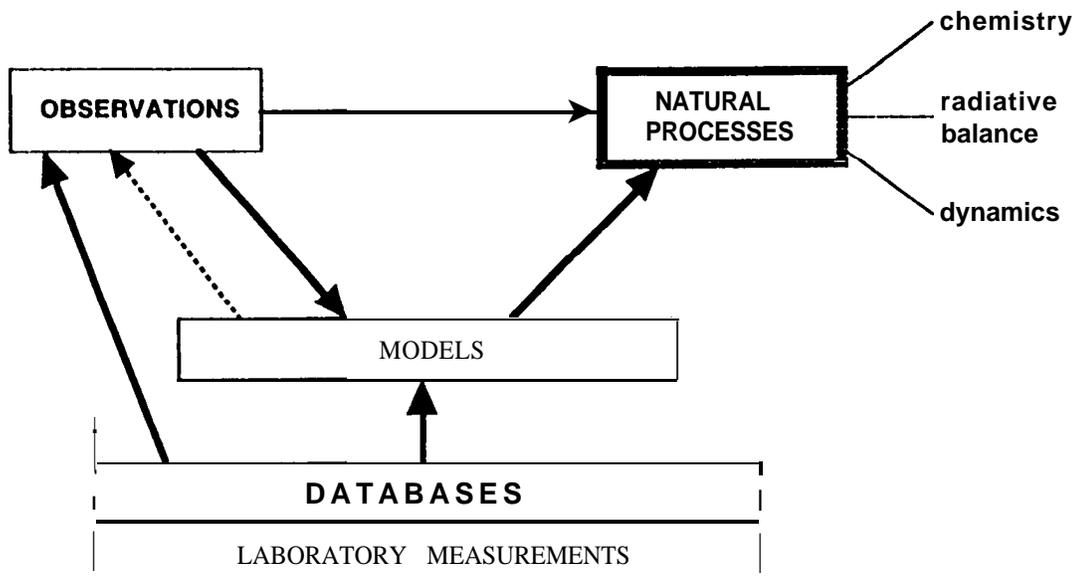
Explaining such chemical mechanisms on a theoretical basis from fundamental principles (5) requires extensive chemical and spectroscopic information. For example, a list of the types of input needed for theoretical calculations was provided by Mark Allen at JPL (6) and is shown in Table 1; these in fact apply to any planetary or solar system body with an atmosphere. Some of the parameters are related to chemical properties such as vapor pressures, and various types of rate constants under different conditions of pressure, temperature and species combinations. The spectroscopic parameters of molecules and atoms are indicated here in the category of "photocross-sections."

TABLE 1 Type of input constants required for theoretical models

<p><b><u>Collisional rate constants</u></b></p> <ul style="list-style-type: none"> <li>• Temperature dependence</li> <li>• Pressure dependence</li> <li>• Nature of third body in recombination reactions</li> <li>• Product species identified</li> <li>• Heterogeneous processes</li> </ul> <p>• <b><u>Photocross-sections</u></b></p> <ul style="list-style-type: none"> <li>• Wavelength dependence</li> <li>• Temperature dependence</li> <li>• Product yields</li> </ul>	<p><b><u>Ion-electron recombination rate constants</u></b></p> <ul style="list-style-type: none"> <li>• Temperature dependence</li> <li>• Product yields</li> </ul> <p><b><u>Electron-neutral collisional rate constants</u></b></p> <ul style="list-style-type: none"> <li>• Temperature dependence</li> <li>• product yields</li> </ul> <p><b><u>Vapor pressures</u></b></p> <ul style="list-style-type: none"> <li>• Temperature dependence</li> </ul>
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Sometimes it seems that the input parameters for such models and observations are regarded as only a minor aspect of very extensive enterprises, but my view is just the opposite. The laboratory measurements are the true foundation of these other endeavors, as depicted in Fig. 4. The acquisition and interpretation of observations require specific atomic and molecular information and also model predictions related to radiative transfer. The models are dependent on the laboratory constants and the guidance from the field measurements. Our ultimate understanding of natural processes through model analysis and observations therefore relies on the availability of laboratory results.



**FIGURE 4.** The dependence of observations and modelling on laboratory results

It is therefore essential that laboratory measurements provide information that is

- complete
- accurate
- organized in convenient form.

This means that experimental results must be available as electronic databases which have been critically reviewed and validated and then thoroughly documented.

In practice, the databases for spectroscopic remote sensing have been driven by what is needed to perform radiative transfer calculations (5) in order to compute synthetic spectra for comparison with observed spectra. The bulk of the activity has involved the infrared and microwave regions. The databases have been tailored to include specific knowledge of the molecular line parameters associated with the interaction of the electromagnetic radiation with molecules and atoms. The type of parameters required are:

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 TABLE 2 DATABASE LINE PARAMETERS FOR REMOTE SENSING  
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Rotation-vibration transition position (wavelength, frequency)

Transition intensity  
 or cross sections (for unresolvable bundles)  
 including pressure-induced continua

Line shape parameters  
 Half-widths  
 Pressure-induced frequency shifts  
 Line-mixing parameters

Parameters to describe how these vary with temperature and pressure  
 Transition lower state  
 Temperature coefficients for widths, shifts, line-mixing

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The accuracies required depend on the application. The state-of-the-art results in experimental values are  $0.0001 \text{ cm}^{-1}$  for infrared positions, 3% for intensities, 3% of line widths,  $\approx 20\%$  pressure-induced frequency shifts and 15- 30% for line mixing coefficients. Generally, the most important parameter for quantitative atmospheric observations is the intensity; errors in the laboratory values extrapolate directly on a one-to-one basis into the atmospheric observations.

As described by the prior speaker, the line positions and intensities found in a database are obtained by **modelling** a sampling of **laboratory** measurements with quantum mechanics to provide predicted values for several thousand transitions connected with a vibration-rotation band. In some cases, models fail to converge to the accuracy of the laboratory data and also to the accuracy required by the applications. In these cases, tedious and time-consuming empirical tabulations of line parameters are obtained from laboratory spectra. Some molecules **give rise** to unresolved bundles of transitions so that the "line-by-line" approach can not be applied. In these cases, experimental absorption coefficients are used rather than intensities. For line shape parameters, theoretical models based on quantum mechanics are often inadequate, and so the community must rely on limited experimental values of a few hundred transitions extrapolated by arbitrary schemes to the tens of thousands of transitions associated with a specific molecule.

The more public databases of molecular parameters (7, 11-17) that are utilized by applications are summarized in Table 3 below. The year of the most recent release is shown before the name, and a web site is given with the name of the database. The overall summary of region covered in cm<sup>-1</sup>, number of species, number of transitions, and the references are indicated. The Appendix contains individual summaries of the contents of these databases by molecule and spectral region. Three of these (HITRAN, GEISA and the JPL catalog) have existed because they receive long-term funding to provide for specific types of applications.

TABLE 3. SPECTROSCOPIC DATABASES OF MOLECULAR PARAMETERS

DATABASE* and WEBSITES		region* cm <sup>-1</sup>	number of species	millions of transitions	Ref.
1996	JPL catalog <a href="http://spec.jpl.nasa.gov">http://spec.jpl.nasa.gov</a>	0 - 330	331 "entries"	1.5	14
1997	SAO-rotational <a href="http://firs-www.harvard.edu/dir/sao92">http://firs-www.harvard.edu/dir/sao92</a>	10- 1600	49	0.5	16
1997	GEISA <a href="http://ara01.polytechnique.fr">http://ara01.polytechnique.fr</a>	0-22,600	50	0.7	13
1996	HITRAN <a href="http://www.hitran.com">http://www.hitran.com</a>	0-22,600 -58300	46	1.0	11
1996	HITEMP	0- 23,000?	3 or 4 ?	2.3 +	12
1995	ATMOS	0-10,000	49	0.8	15
1996	JPL VUV Reference Data <a href="http://remus.jpl.nasa.gov/jpl97">http://remus.jpl.nasa.gov/jpl97</a>	Vis-UV	≈ 65	cross sections	7
1993	Hanst Digitized IR Spectra	500-4000	250	lab spectra	177

\*JPL is the Jet Propulsion Laboratory "entries" indicate that different isotopes and bands of a species are classified as a different species

SAO is the Smithsonian Astrophysical Observatory

GEISA is Gestion et Etude des Information Spectroscopiques Atmospheriques

HITRAN is High resolution Transmission; ATMOS is Atmospheric Trace Molecule Spectroscopy; Vis-WV = visible and ultra-violet.

one wavenumber = 1 cm<sup>-1</sup>; 5000 cm<sup>-1</sup> = 2 μm and 1000 cm<sup>-1</sup> = 10 μm

The particular set of molecular and atomic species that are required depends on the application. An example of the molecules for remote sensing of the earth's atmosphere is indicated below in Fig. 5. This graphic is taken from the web site for the HITRAN (High Resolution Transmission) database (1 1). It shows the molecules for which there are line parameters incorporated as a function of wavelength. The most extensive information are parameters of the most abundant species like water, carbon dioxide, ozone, nitrous oxide and methane. The graph stops at 20 microns, but in fact the HITRAN list also extends through the microwave region as well. While the wavelength coverage is extensive, all parameters of all molecules in all regions are not equally well characterized, In general, the longer wavelength regions are much better determined in terms of degree of completeness and overall accuracies because there have been extensive usage of the region between 2.5 to 1000 microns by field experiments; also quantum mechanical models are more likely to reproduce the observed spectra in the rotational and fundamental regions. At wavelengths smaller than 2.5 microns, the compilations are generally incomplete even for the more abundant species like methane and inaccurate (for some of the bands of water).

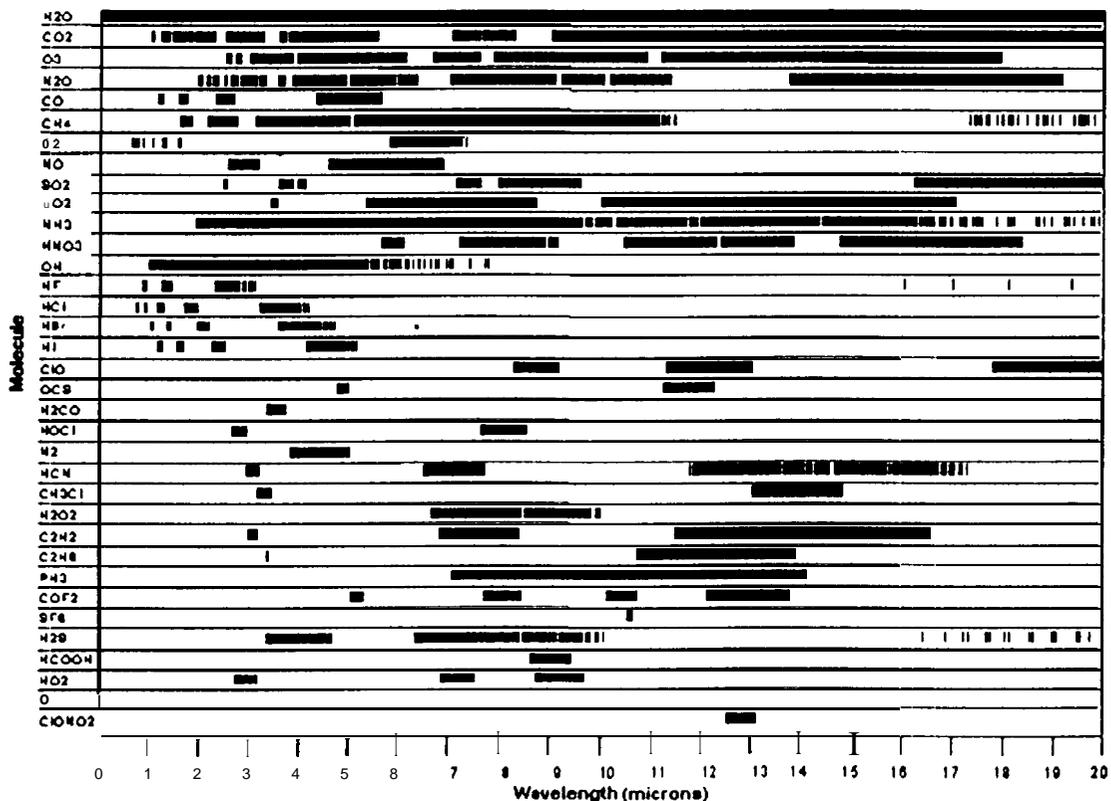


FIGURE 5. A summary of the 1996 HITRAN database between 20 and 0.1 microns

HITRAN started in the early 1970's as the AFGL (Air Force Geophysical Laboratory) compilation and funded by the Department of Defense so that the transmission of the earth's atmospheric could be understood, It has been revised and improved every two to four years by collecting new research funded by groups such as NASA and NSF. In the past, the database organizers have also been able to support specific laboratory research in order to obtain improvements. This compilation has been the mainstay for atmospheric remote sensing.

However, for some applications, the standard HITRAN database has proved incomplete. A portion of the information about the HITRAN database given in the Appendix is repeated below in Table 4 to illustrate this point. For example, for observations involving gases at high temperatures tend to see very weak transitions which are difficult to measure in the lab and predict by the standard models. To provide some knowledge for these situations, a second database call HITEMP (12) was formed which duplicates and extends the information in the normal HITRAN compilation for water, carbon dioxide and carbon monoxide. As seen in Table. 4, rather than having 50 thousand transitions of water in HITRAN, there are over a million water transitions in HITEMP. The disadvantage is that the accuracies of the parameters in the HITEMP prediction vary widely, and in many cases the calculated intensity may be off an order of magnitude. However, if the user is observing "extra lines" in new remote sensing data or is interpreting low resolution spectra, the HITEMP list may be more useful. Alternatively, users interested in obtaining accurate chemical concentrations from high resolution data require the few (or the few thousand) transitions with very accurate intensities that can be found in HITRAN.

TABLE 4. COMPARISON OF NUMBER OF TRANSITIONS IN 1996

Mol #.	Species	HIT RAN	HITEMP
1	H <sub>2</sub> O	49,444	1,174,009
2	c o,	60,802	1,032,259
3	o,	275,133	0
4	N <sub>2</sub> O	36,174	0
5	c o	4,477	113,022
6	CH <sub>4</sub>	46,032	0

A second public database (13) is GEISA (Gestion et Etude des Information Spectroscopiques Atmospheriques). It was started in the 1980's to support remote sensing of the planets. As seen in the appendix, its selection of included species contains species like GeH<sub>4</sub>, AsH<sub>3</sub>, C<sub>2</sub>N<sub>2</sub> and HC<sub>3</sub>N. These molecules are well below the detection limit for terrestrial observations, but they are abundant enough to be detected in the outer planets. Unfortunately, the GEISA organizers were unable to sustain funding for planetary studies. Later, the database became oriented toward for terrestrial research as well, in a sense duplicating the efforts of HITRAN. However, the revisions of the GEISA database have generally been

released on different years compared to HITRAN, and this alternation has provided users with faster access to improvements. Table 5 below (18) compares differences between 1996<sub>HITRAN</sub> and 1997<sub>GEISA</sub>; the underlined species indicates that new laboratory studies are being included. It shows that a great deal of new information (involving 11 different species) became available in just one year after the 1996<sub>HITRAN</sub> compilation was released. It demonstrates that we need to update and release our databases more frequently.

**TABLE 5. SUMMARY OF DIFFERENCES: HITRAN 96 VS GEISA 97**

(for molecules in common)  
Underlined molecules have been updated for GEISA97 edition

Species	Region	v	I	γ	References
H2O	2v2-v2 lines of H <sup>16</sup> OD and v2 band of isotope 182 from ATMOS molecular line list in the region 8.9 - 5.7pm (not included in HITRAN)	•	"	•	GEISA92 ATMOS line list
<u>CO2</u>	In the 4.3 μm region, lines of <sup>18</sup> O <sup>13</sup> C <sup>18</sup> O are included in GEISA as well as weak intensity lines of the other isotopes	•	•	•	F
<u>O2</u>	The 2 regions, 5.6 - 4.3pm (bands 2v1, v1+v3, 2v3) and .53 - 3.6 μm [bands v1+2v2, 2v2+v3, 3v3-v2, and (v1+2v2+v3)-v21 have been updated	•	*	*	Barbe et al. Gamache et al.
<u>N2O</u>	The entire 19 - 16pm region has been reworked. This includes 11 bands (band v2+v3-v2 new band)	•	*	*	Weber et al.
CO	In the whole spectral range 2929-1.18 μm transitions with v'' ≥ 9 are present in GEISA (v'' ≤ 1 in HITRAN)	•	*	*	GEISA92
<u>CH4</u>	New predictions in the regions 11 - 5pm and 5.2- 2.8pm	*	*	*	Brown et al. Champion et al.
<u>NO</u>	New spectroscopic line parameters for <sup>14</sup> N <sup>16</sup> O in the region from microwaves to 1.07 μm	•	*	*	Brown et al. Goldman et al.
PH3	GEISA whole content in the region 561.6-4.1 pm is different from HITRAN	•	*	*	GEISA86 GEISA52
<u>HNO3</u>	3v9-v9 and v5+v9-v9 bands present in HITRAN% have been replaced by new data for band v5+v9-v9 in the region 12.6-10.53 μm	•	*	*	Goldman et al. Perrin et al.
<u>OH</u>	New data for the whole content of <sup>16</sup> OH in the region from the microwaves to 2.4 μm	•	*	*	Goldman et al.
<u>OCS</u>	Region 20.4 -2.4 μm entirely updated. Two new isotopes, <sup>16</sup> O <sup>12</sup> C <sup>33</sup> S and <sup>16</sup> O <sup>12</sup> C <sup>34</sup> S	•	*	*	Brown et al. Favt et al.
<u>C2H6</u>	The v9 band in the region 13 - 11 μm. The new isotope <sup>12</sup> C <sup>13</sup> CH6 band v12 in the region 13.7 - 10.9 μm	•	*	*	Weber et al.
<u>CH3D</u>	New list for the triad v3, v5, v6 in the region 11.8 - 5.7 μm (Independent molecule in GEISA; isotope of CH4 in HITRAN).	•	*	*	Brown et al.
HCN	The whole content in the 1.7 - 0.5 μm region	•	•	•	GEISA92
N2	The whole content in the 5 - 3.8 μm region	•	•	•	GEISA92
<u>H2O2</u>	The whole content with new predictions in the 4 μm and 2.7 μm regions	•	•	•	Perrin et al. Gamache et al.
<u>H2S</u>	New predictions in the 4 μm and 2.7 μm regions	•	*	*	Brown et al.

One important set of parameters on HITRAN is the scheme to indicate a range of accuracies for the positions, intensities and air-broadened widths and the sources of the data (listed as accuracy and reference indicators in Table 6). An accuracy index code appears with each transition in the database to provide users with embedded information about the data quality. This should be adopted by others.

Now, applications that implement new technology beyond the state-of-the-art inevitably find that the standard databases are lacking; new species are observed or accuracies of important parameters like line intensity are too poor. For example, the ATMOS experiment (9,10,3) flew a high resolution interferometer on the space shuttle to record atmospheric and solar occultation spectra. Its investigators realized that the data to be acquired would contain features of species not already compiled in the standard databases and so they fixed the problem by creating their own specialized databases (15 and see the appendix). Investigators at SAO (**16**) (Smithsonian Astrophysical Observatory) faced a similar situation, and that database is also summarized in the appendix. Kelly Chance and Ken **Jucks** at SAO provided the overview of the their database (20) shown in Table 7 below; their philosophy statements succinctly summarize what **all** of us are trying to do when we turn to “customizing”. We start with the best available at the time (from HITRAN, **GEISA**, JPL CATALOG) and then do our own laboratory studies as **needed**. Our improvements are then feed back into the public databases. Much of what we do is to rehash existing information, but we make those changes that are important for our particular field experiment,

**TABLE 7 THE SAO MOLECULAR SPECTROSCOPY DATABASE**

Philosophy behind database:

- To construct the most accurate database for analyzing FIRS-2 data.
- Keep database **as** up to **date as possible**.
- Cover **the** FIRS-2 spectrometer spectral range: 10-1600 cm<sup>-1</sup>.
- Provide **HITRAN** with future **updates** in the far-infrared.

Sources of data in SAO database.

- **HITRAN96**
- JPL **Submillimeter** and **Microwave Catalogue**
- Pseudo **lines** for **cross section** data from **HITRAN96** and other sources (**G.C. Toon, U. Giessen, SAO**).
- **Best current** laboratory **data**.

A third public database is the Jet Propulsion Laboratory catalog for the Submillimeter, Millimeter and Microwave Spectral region (14). This database started in the 1980's to support astrophysics observations in the frequency range between 0 and 10,000 GHz; it continues to exist because of funding from NASA. Their database contains both atomic and molecular species; a summary is given in the appendix (19). One major difference between the JPL catalog and HITRAN or GEISA is that while the other two compilations assemble finished predictions from many different researchers, the JPL organizers gather reported laboratory measurements from many available sources and then perform their own quantum mechanical analyses in order to make the predictions for their database.

Because these three databases were started at different times and for different purposes, they have different selections of formats, parameters and units, A comparison of the parameters in the three lists is shown below. Some choices are dictated by the fact that these lists are intended as input into computer calculations rather than being reading material for human eyes. For example, the molecules and their isotopes are given identity numbers rather than names, and these become array indices in various standing software routines. Some parameter fields like the vibrational quantum numbers are rarely used in the calculations and so they are abbreviated by indices that require a lookup table to interpret. If line shape information is included, it is assumed to be air- and self-broadening values for terrestrial applications. Those applications that involve other planets must customize that portion of the lists for their own needs.

TABLE 6 COMPARISON OF INCLUDED PARAMETERS FOR THREE DATABASES

PARAMETER	HITRAN	GEISA	JPL-cat
molecule number	X	X	X
isotope number	X	X	
frequency	X	X	X
absolute error in frequency			X
lower state energy	X	X	X
intensity	X	X	X
transition probability squared	X	~X	
air-broadened widths	X	X	
self-broadened widths	X	X	
temperature dependence (air-width)	X	X	
pressure shifts (air-width)	X		
vibrational quanta	X	X	X
rotational quanta	X	X	X
accuracy range indicators	X	~X	
reference indicators	X		



In general, the burning of trees and vegetation (i. e. biomass burning) generates high concentrations of some species that are not usually detected by routine atmospheric remote sensing. Interestingly, these include organic species such as acetic acid ( $\text{CH}_3\text{OOH}$ ), methanol ( $\text{CH}_3\text{OH}$ ), formic acid ( $\text{HCOOH}$ ) and formaldehyde ( $\text{H}_2\text{CO}$ ) for which the databases have few or no parameters in the infrared. For the remote sensing of wildfires and forest fires, new information is required (22, 23). For example, Table 7 below shows some of the molecules and corresponding spectral intervals that are already being used to monitor the emissions. For the usual species on the left, the compilations do not contain enough hot bands. For the formic acid, a less desirable wavelength is utilized because no parameters are compiled for the other stronger fundamental bands. For the acetic acid and methanol, investigators must resort to low resolution cross sections available just at room temperature (such as the **Hanst** and **Hanst** collection). Other spectral regions for the new molecules could be utilized to achieve better measurements and currently unknown features could be identified perhaps as species detections if complete spectroscopic information were accessible.

TABLE 7. Species seen in spectra of biomass burnings (see Ref. 23)

**Table 2. The Spectral Regions Used to Retrieve Concentrations Reported in This work**

Molecule	Spectral Regions or Peaks	Molecule	Spectral Regions or Peaks
$\text{H}_2\text{O}$	3020.0 -3007.1	$\text{CH}_3\text{COOH}$	1176
$\text{CO}_2$ and CO	2242.7 -2210.9	$\text{CH}_3\text{OH}$	1033.3
$\text{CO}_2$	737.01-727.92	$\text{CH}_2\text{O}$	2782.7 -2777.3
$\text{CO}_2$	2252.8- 2239.9 <sup>a</sup>	$\text{HCOOH}$	1107.4 >1102.7
Co	2055.8-2049.5 <sup>b</sup>	NO	1913.4 -1911.0
$^{13}\text{CO}$	20622-2061.7 <sup>b</sup>	NO	1907.1- 19(M.1)
c o	2179.7, 2176.2, 2172.8 <sup>b</sup>	NO	.1903 .8-19023
$\text{CH}_4$	3020.0 -3007.1	NO	1901.1 -1899.9
$\text{CH}_4$	2997.3 -2976.1	NO	1906.9 -1899.5
$\text{CH}_4$	1306.7 -1299.0	$\text{NO}_2$	1599.s -1597.7
$\text{C}_2\text{H}_4$	949.4	NH <sub>3</sub>	10473 -1045.1
$\text{C}_2\text{H}_4$	2987.0 -2985.7	NH <sub>3</sub>	968.7- %1.7
$\text{C}_2\text{H}_4$	2984.7 -2982.7	NH <sub>3</sub>	933.5 -926.3
$\text{C}_2\text{H}_2$	3271.2 -3254.7	HCN	3272.1 -3270.7
$\text{C}_2\text{H}_2$	743.4 -728.8	$\text{SO}_2$	1348.5-1347.7.
Volatiles	2930	OCS	2071 .4-2069.9

; a) Stronger peaks used only to quantify background.

b) Regions used only to spot check the precision.

The remote sensing of planets (other than the Earth) is hindered by the lack of a dedicated database. GEISA continues to accept new lists that are potentially useful, but that service goes not produce the comprehensive collection required for every planet now being studied. Individual users are left to assemble their own database private collections and create customized compilations. The problem is that they must start the process at a more rudimentary level. What they produce is generally invalidated, undocumented and undistributed.

Achieving the ideal database for the “planetary community” is difficult because the atmosphere of each planet is different. The vapor temperatures range from 800 K on Venus to 50 K in the outer planets (Jupiter and beyond). The abundances of the common species like methane and carbon dioxide vary from planet to planet by orders of magnitude, and planets have different molecules dominant species (carbon dioxide for Venus, hydrogen for the outer planets rather than nitrogen, oxygen on Earth). For example, Table 8 (24,25) below gives a tabulation of species and mixing ratios for Jupiter. For the terrestrial molecules like CO<sub>2</sub>, O<sub>2</sub>, O<sub>3</sub> and N<sub>2</sub>O, there has been extensive laboratory efforts to provide an adequate database for terrestrial studies, but these four species are completely missing in Jupiter. Even for a terrestrial species like methane, the standard databases are often insufficient because the abundances and optical densities in the outer planets are several orders of magnitude greater than for the Earth. Planetary investigators need a HITEMP-like collection that does not reject weak features. Unfortunately, long-term funding has never been committed for the creation of a universal planetary database.

**TABLE 8. THE COMPOSITION OF JUPITER: SPECIES, MIXING RATIOS**

<i>Major Species</i>	<i>Mixing Ratios<sup>d</sup></i>	<i>Disequilibrium Species</i>	<i>Mixing Ratios</i>
H <sub>2</sub>	0.865	PH <sub>3</sub>	(1-2)X10 <sup>-7</sup>
He	<b>0.156±0.006</b>		6x10 <sup>-7</sup> (>1bar)
		CO	2X10 <sup>-9</sup>
<i>Principal Minor Constituents</i>		GeH <sub>4</sub>	<b>7±2x10<sup>-10</sup></b>
H <sub>2</sub> O	-2.6x10 <sup>-3</sup> <10 <sup>-6</sup> (<4 bar) 3.7x10 <sup>-4</sup> (10 bar) ? (20 bar)	ASH <sub>3</sub>	2.2* 1.1X10 <sup>-10</sup>
CH <sub>4</sub>	<b>2.0±0.15x10<sup>-3</sup></b> <b>2.5(+3/-2)x10<sup>-5</sup></b>	<i>Other Minor Constituents</i>	
c2H <sub>6</sub>	1.5 X10 <sup>-6</sup>	H	Variable
C <sub>2</sub> H <sub>2</sub>	2-8x10 <sup>-8</sup> <2.5x10 <sup>-6</sup>	(H <sub>2</sub> ) <sub>2</sub>	Variable
C <sub>2</sub> H <sub>4</sub>	7*3 X10 <sup>-9</sup>	<i>Noble Gases, and Isotopic Ratios</i>	
C <sub>3</sub> H <sub>4</sub>	<b>2.5(+2/-1)x10<sup>-9</sup></b>	l-k	<b>0.156±0.006</b>
C <sub>6</sub> H <sub>6</sub>	<b>2(+2/-1)x10<sup>-9</sup></b>	<sup>20</sup> Ne	2.3 M.25x10 <sup>-5</sup>
NH <sub>3</sub>	2.3-2.9 x10 <sup>-4</sup> -0.2-1X10 <sup>-5</sup>	<sup>36</sup> Ar	1* 0.4X10 <sup>-5</sup>
H <sub>2</sub> S	(1-9)X10 <sup>-5</sup> <1 X10 <sup>-6</sup> <3.3 X10 <sup>-6</sup>	<sup>84</sup> Kr	<b>≤8.5±4x10<sup>-9</sup></b>
		<sup>13</sup> Xe	<5*2.5 x10 <sup>-9</sup>
		<sup>3</sup> He/ <sup>4</sup> He	1.1*0. IX10 <sup>-4</sup>
		D/H	2.2 M.5X10 <sup>-5</sup>
		<sup>12</sup> C/ <sup>13</sup> C	3.5*1.5 X10 <sup>-5</sup>
			91

The lack of a complete database was dealt with temporarily last year for NIMS (Near Infrared Mapping Spectrometer) experiment (26) on the Galileo spacecraft by the creation of an interim collection. Existing calculations and predictions from work in progress were assembled together for the six species in Table 9 below (the number of transitions, wavenumber range, bands, summation of the strengths and data source are shown as well). Air-broadened linewidths were overwritten with linewidths corresponding to an atmosphere composed of 90% hydrogen and 10% helium, For methane, some new predictions were made with a much lower intensity limit (10-27).

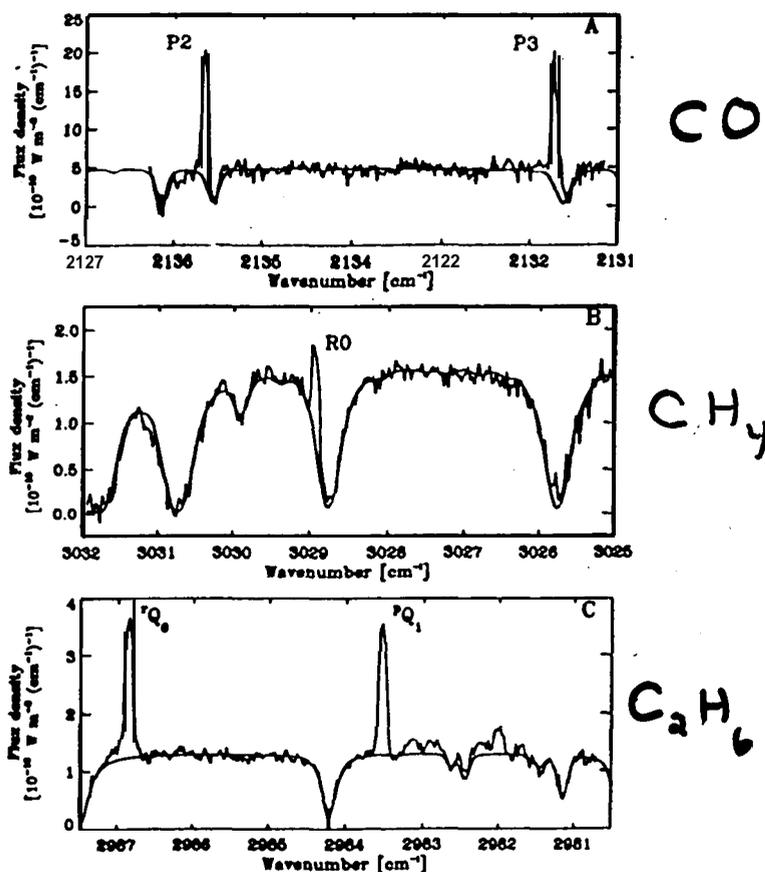
Now, don't expect to see this collection advertised on a Web site! It has been useful for this one application involving low resolution spectra, but it is not yet of good enough quality for general usage. Parts of this NIMS database will give poorer results if used by high resolution experiments in place of HITRAN. I feel that we must be the "gate-keeper" and keep our poorer quality data from being widely distributed. In terms of the methane and ammonia studies indicated in Table 9, when the laboratory studies are finally concluded, new calculations will be generated, validated, documented and then submitted to the standards databases for inclusion. The point is that the individual producers have the responsibility to "do no harm".

**TABLE 9. NIMS CUSTOMIZED DATABASE WITH 90% H<sub>2</sub> + 10% He LINE WIDTHS**

MOL.	#LINES	FMIN - FMAX cm <sup>-1</sup>	NUMBER ISO BANDS	STRENGTH x 10 <sup>-17</sup>	SOURCE (et al.)
CH <sub>4</sub>	219208	0.0 -6203.6	3 117	1.77	HILICO / BROWN
NH <sub>3</sub>	18075	0.2 -7037.3	2 45	4.78	KLEINER / BROWN / URBAN
PH <sub>3</sub>	9491	708.1 -2478.8	1 8	2.82	GEISA / TARRAGO
AsH <sub>3</sub>	4445	1923.S -2289.9	1 2	4.04	GEISA / TARRAGO
GeH <sub>4</sub>	824	1937.4 -2221.6	1 1	4.10	GEISA
H <sub>2</sub> O	49444	0.0 -22656.5	4 137	7.28	96 HITRAN/BROWN/GAMACHE

• **STRENGTH** is the summation of all line intensities in units of cm<sup>2</sup>/ (cm<sup>2</sup> molecule) at 296 K.  
 • The database consists of separate files for each molecule covering the range shown above.  
 • Calculations from different sources (and in different formats) were merged together and converted to HITRAN format.  
 • The air-broadened line widths in the database were replaced with widths appropriate for an atmosphere composed of 90% hydrogen and 10% helium.  
 • Results that became available after the release of the 1996 HITRAN compilation were obtained for methane and ammonia.  
 • The number of the methane transitions increased from some 47,000 on HITRAN to over 200,000 because new predictions of bands from the ground state and difference bands of both isotopes were done with a lower state intensity limit of 10<sup>-27</sup>.  
 Note that above 3400 cm<sup>-1</sup>, the NIMS database contains only <sup>13</sup>CH<sub>4</sub> transitions arising from the ground state.

In terms of new remote sensing activities (that were rather unexpected), the people who study comets are having the most fun. First there was the spectacular crash of Shoemaker-Levi-9 comet fragments into Jupiter in 1994. Then there was the surprise appearance of two comets, Hyakutake and Hale-Bopp, which were bright enough to permit good spectra to be recorded at many wavelengths. Even the infrared proved useful as seen by the detection of CO, CH<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> in Hyakutake (27) shown in fig. 7 below.



Flux calibrated spectra of comet C/1996 B2 Hyakutake (solid lines) as observed through the terrestrial atmosphere. Synthesized spectra of atmospheric transmittance for conditions appropriate to Mauna Kea are also shown (dashed lines). The telluric lines are seen in absorption against the cometary continuum, and their cometary counterparts are Doppler shifted to higher frequencies by the comet's motion relative to the observer (-15 km/sec). A. The P2 and P3 lines of the carbon monoxide 1-0 vibrational band. B. The R0 line of the methane  $\nu_3$  band. C. The  ${}^rQ_0$  and  ${}^rQ_1$  branches of the ethane  $\nu_7$  band Mumma et al. 1996.

FIGURE 7. The infrared spectrum of comet Hyakutake (see Ref. 27).

There now have been over two dozen molecular and atomic species detected in cometary vapors using wavelengths from the UV to the microwave. For example, a compilation of observed abundances for some organic species from M. Mumma (28) is shown in Table 10 below. Surprisingly, comets *even* have the “forest fire” species of methanol, formaldehyde and formic acid, as well as many sulfur-bearing species,

For unexpected events like these, the standard databases are lacking, and users have had to survey the literature, dig out information from 30 year-old dissertations, find unpublished collections of low resolution absorption coefficients, and really scramble before they can begin to interpret really some interesting physical processes within the cometary “atmospheres.”

**TABLE 10. ABUNDANCES OF ORGANIC VOLATILES IN COMETS (26)**

Species	Halley	Hyakutake	Hale-Bopp <sup>1,2</sup>
H <sub>2</sub> O	100	100	100
CH <sub>4</sub>	0.2-1.2	0.7	0.7
C <sub>2</sub> H <sub>2</sub>		0.3-0.9	<b>TBD</b>
C <sub>2</sub> H <sub>4</sub>		0.4-1.2	0.2-0.6
CH <sub>3</sub> OH	1.7	<b>0.4-2</b>	2 - 5
H <sub>2</sub> CO	0-5	<b>TBD</b>	1.5
HCOOH			<b>0.13</b>
CO <sub>2</sub>	3		<b>20-30</b>
CO	6	6-10	6-10
HCN	<b>0.50</b>	0.3	<b>0.12</b> - 0.2s
H <sub>2</sub> S			<b>13</b>
OCS			0.07- <b>0.16<sup>3</sup></b>
H <sub>2</sub> CS			0.01s <sup>4</sup>
SO <sub>2</sub>			<b>0.16<sup>5</sup></b>
CS <sub>2</sub>			0.13 <sup>6</sup>

M. Mumma, private communication, Sept., 1997 with:

1. Mumma et al. 1993 and refs therein, Mumma et al. 196, Brooke et al. 1996.
2. Many IAU Circulars; Biver et al. Science 212:1915-1918 (1997).
3. DeLo Russo et al. LAUC 6682, Woodney et al. LAUC 6607
4. Woodney et al. LAUC 6607
5. Wink et al. LAUC 6591
6. If Q(CS) - Q(CS<sub>2</sub>). Biver et al. Science 275, 1915-1918 (1997).

## CONCLUSION

In summary, progress made in the remote sensing applications is tied directly to quality of the database that is available. The standard databases in the infrared and microwave are very good for terrestrial applications, but not for planetary studies in general. To support just the planetary atmospheres community we should:

### Organize:

- Define the needs in terms of species, wavelengths, lower intensity limits, line shape parameters requirements
- Assign tasks to avoid duplication of effort

### Centralize:

- Collect and distribute from a central point with a dedicated staff

### Generalize:

- Anticipate future needs
- Collect more than just what has already been seen in someone's data

### Standardize:

- Define selection of parameters, their units, the computer formats

### Criticize:

- Do critical evaluations to assess data quality and detail inadequacies

### Document:

- Provide thorough and detailed description of the database at the same time it is released.

## ACKNOWLEDGEMENTS

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## REFERENCES

1. Peixoto, J. P., and Oort, A. H., *The Physics of Climate*, New York, AIP, 1992, ch. 1, pg. 3.
2. Grant, W. B., Optical remote measurement of toxic gases, *J. Air Waste Mung. Ass.* 42, 18 (1992).
3. Brown, L. R., Farmer, C. B., **Rinsland, C. P.**, and Zander, R., pp. 97-152, in *Spectroscopy of the Earth's Atmosphere and Interstellar Medium*, Eds. K. Narahari Rao and A. Weber, Academic Press, Inc Boston, USA.
4. Gunson, M. R. (private communication).
5. Goody, R. M. and Yung, Y. L., *Atmospheric Radiation Theoretical Basis*, 2nd Edition, 1989, Oxford University Press, New York, Oxford.
6. Allen, M. (private communication).
7. DeMore, W. B., Sander, S. P., Howard, C. J., Ravishankara, A. R., Golden, D. M., Kolb, C. E., Hampson, R. F., Kurylo, M. J., Molina, M. J., *Chemical kinetics and photochemical data for use in stratospheric modeling*, JPL publication 97-4 (1997). Pasadena, Ca 91009.
8. Demore, W. B. (private communication).
9. Farmer, C. B., and Norton, R. H., A high resolution infrared spectroscopy atlas of the infrared spectrum of the Sun and the Earth from space, *NASA Reference Publication 1224*, vols 1 and 2 (1989).
10. Zander, R., Gunson, M. R., Farmer, C. B., **Rinsland, C. P.**, *J. Atm. Chem.* 15, 171-186 (1992).
11. Rothman, L. S., Gamache, R. R., Tipping, R. H., **Rinsland, C. P.**, Smith, M. A. H., **Benner, D. C.**, DeVi, V. **Malathy, Flaud, J. -M., Camy-Peyret, C., Perrin, A., Goldman, A., Massie, S. T., Brown, L. R., and Toth, R. A., J. Quant. Spectrosc. Rad. Transfer** 48, 1-780 (1992).
12. Selby, J. E. A. et al. **Reims, ASA and L. S. Rothman, et al., JQSRT** (submitted).
13. **Husson, N., Bonnet, B., Scott, N. A., and Chedin, A., J. Quant. Spectrosc. Radiat. Transfer** 48, 509-518 (1992) and **Jacquinet-Husson, N. et al., in preparation.**
14. Pickett, H. M., **Poynter, R. L., Cohen, E. A., Delitsky, M. L., Pearson, J. C., and Muller, H. S. P., Submillimeter, millimeter and microwave spectral line catalog, JPL Publication** 80-23, Rev.4 (1996). Pasadena, CA,
15. Brown, L. R. et al., *Appl. Opt.* 26, 5154-5182 (1987) and *Appl. Opt.* 35, 2828 (1996).
16. Chance, K. V., **Jucks, K. W., Johnson, D. G., and Traub, W. A., J. Quant. Spectrosc. Radiat. Transfer** 52, 447-457 (1994).
17. **Hanst and Hanst**, Digitized Reference Spectra (Infrared), copyright 1993, Infrared Analysis, Inc., Anaheim, CA 92801
18. **Jacquinet-Husson, N.** (private communication).
19. Cohen, E. and **Pickett, H. M.,** (private communication).
20. Chance, K. V., and **Jucks, K. W.** (private communication).
21. Worden, H., Beer, R. and **Rinsland, C. P., J. Geophys. Res.** 102, 1287-1299 (1997).
22. **Griffith, D. W. T., Mankin, W. G., Coffey, M. T., Ward, D. E. and Riebau, A., J. S. Levine Ed., Global Biomass Burning: Atmospheric, climatic and Biospheric Implications, Cambridge, MA, MIT Press, 1991.**
23. Yokelson, R. J., Griffith, D. W. T., Ward, D. E., Open-path FTIR studies of large-scale laboratory biomass fires, *J. Geophys. Res.* 101, 21067-21080 (1997).
24. Or(on, G. S. (private communication).
25. **Atreya, S. K., Wong, M. H., Owen, T., Niemann, H., and Mahaffey, P., The three Galileos: The Man, The Spacecraft, The Telescope, Rahe, J., Barbieri, C., Johnson, T., Sohus, A., Eds., Dordrecht, Kluwer Academic Publishers, 1997.**
26. **Carlson, R. W, Baines, K. H., Encrenaz, T., Taylor, F. W., Drossart, P., Kampl, L. W., Science** 253, 1541-1548 (1991).
27. Mumma, M. J., **Disanti, M. A, Russo, N., D., Fomenkova, M., Magee-Sauer, K., Kaminski C. D., and Xie, D. X., Science** 272, 1310-1314 (1996), and Mumma, M. J. (private communication).

## APPENDIX

Note that some of the tables in this appendix have been provided as preliminary drafts for manuscripts currently in preparation by the database organizers. The versions presented here may be somewhat different from the final tables that are published later.

### Summary tables for molecular databases

a. **JPL BIBLIOGRAPHY:** DeMore, W. B., Sander, S. P., Howard, C. J., Ravishankara, A. R., Golden, D. M., Kolb, C. E., Hampson, R. F., Kurylo, M. J., Molina, M. J., *Chemical kinetics and photochemical data for use in stratospheric modeling*, JPL publication 97-4 (1997). Pasadena, Ca 91009.

b. **1996 HITRAN** Rothman, L. S., Gamache, R. R., Tipping, R. H., Rinsland, C. P., Smith, M. A. H., Benner, D. C., Devi, V. Malathy, Flaud, J. -M., Camy-Peyret, C., Perrin, A., Goldman, A., Massie, S. T., Brown, L. R., and Toth, R. A., *J. Quant. Spectrosc. Radiat. Transfer* **48**, 1-780 (1992).

**1996 HITEMP:** Selby, J. E. A. et al. Reims, ASA and L. S. Rothman, et al., *JQSRT* (submitted).

c. **1997 GEISA:** Husson, N., Bonnet, B., Scott, N. A., and Chedin, A., *J. Quant. Spectrosc. Radiat. Transfer* **48**, 509-518 (1992) and Jacquinet-Husson, N. et al., in preparation.

d. **JPL SMM CATALOG:** Pickett, H. M., Poynter, R. L., Cohen, E. A., Delitsky, M. L., Pearson, J. C., and Muller, H. S. P., *Submillimeter, millimeter and microwave spectral line catalog*, JPL Publication 80-23, Rev.4 (1996). Pasadena, CA.

e. **1995 A'PMOS:** Brown, L. R. et al., *Appl. Opt.* **26**, 5154-5182 (1987) and *Appl. Opt.* **35**, 2828 (1996).

f. **1997 SAO:** Chance, K. V., Jucks, K. W., Johnson, D. G., and Traub, W. A., *J. Quant. Spectrosc. Radiat. Transfer* **52**, 447-457 (1994).

g. **LAB SPECTRA CATALOG:** Hanst and Hanst, Digitized Reference Spectra (Infrared), copyright 1993, Infrared Analysis, Inc., Anaheim, CA 92801

a. JPL BIBLIOGRAPHY: DeMore, W. B., Sander, S. P., Howard, C. J., Ravishankara, A. R., Golden, D. M., Kolb, C. E., Hampson, R. F., Kurylo, M. J., Molina, M. J., *Chemical kinetics and photochemical data for use in stratospheric modeling*, JPL publication 97-4 (1997). Pasadena, Ca 91009.

JPL CHEMICAL KINETICS AND PHOTOCHEMICAL DATA 1997

Species and wavelength range (nanometers)

&O <sub>2</sub>	205-240	CCl <sub>4</sub>	174-275
&O <sub>3</sub>	175-362	CCl <sub>3</sub> F	170-260
•O <sub>3</sub>		CCl <sub>2</sub> F <sub>2</sub>	170-240
H <sub>2</sub> O	190-250	CF <sub>2</sub> ClCFCl <sub>2</sub>	184-230
H <sub>2</sub> O	175-189	CF <sub>2</sub> ClCF <sub>2</sub> Cl	172-220
H <sub>2</sub> O <sub>2</sub>	190-350	CF <sub>3</sub> CF <sub>2</sub> Cl	172-204
NO		CF <sub>4</sub>	
& N O <sub>2</sub>	202-422	c <sub>2</sub> F <sub>6</sub>	
• N O <sub>3</sub>	600-670	CCl <sub>2</sub> O	184-229
N <sub>2</sub> O	173-240	CClFO	154-229
N <sub>2</sub> O <sub>5</sub>	200-280	CF <sub>2</sub> O	184-229
NH <sub>3</sub>		# CF <sub>3</sub> OH	
HONO	310-396	CH <sub>3</sub> Cl	186-216
• H N O <sub>3</sub>	190-350	CH <sub>3</sub> CCl <sub>3</sub>	185-240
HO <sub>2</sub> NO <sub>2</sub>	190-325	CHClF <sub>2</sub>	174-204
c o		CH <sub>3</sub> CF <sub>2</sub> Cl	
CO <sub>2</sub>		CF <sub>3</sub> CHCl <sub>2</sub>	
CH <sub>4</sub>		CF <sub>3</sub> CHFCl	
CH <sub>2</sub> O	301-356	CH <sub>3</sub> CFCl <sub>2</sub>	190-220
& CH <sub>3</sub> O <sub>2</sub>	210-290	CF <sub>3</sub> CF <sub>2</sub> CHCl <sub>2</sub>	190-220
& C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	2 15-29S	CF <sub>2</sub> ClCF <sub>2</sub> CHFCl	190-220
CH <sub>3</sub> OOH	210-280	# CH <sub>3</sub> OCl	230-394
# CH <sub>3</sub> C(O)O <sub>2</sub> NO <sub>2</sub>	190-350	BrO	313-374
HCN		# HOBr	300-37s
CH <sub>3</sub> CN		* BrONO <sub>2</sub> +	200-300
Cl <sub>2</sub>	260-360	# BrCl	200-380
& OClO	272-475	CH <sub>3</sub> Br	200-380
& ClO <sub>3</sub>		& CF <sub>3</sub> Br	190-272
& Cl <sub>2</sub> O	200-320	& CF <sub>2</sub> Br <sub>2</sub>	190-272
& Cl <sub>2</sub> O <sub>2</sub>	190-386	& CF <sub>2</sub> BrCF <sub>2</sub> Br	190-272
• Cl <sub>2</sub> O <sub>3</sub>	220-320	& CF <sub>2</sub> ClBr	190-272
Cl <sub>2</sub> O <sub>4</sub>	200-310	CF <sub>3</sub> I	240-344
Cl <sub>2</sub> O <sub>6</sub>	200-380	SO <sub>2</sub>	
HCl	140-220	H <sub>2</sub> S	
HF		CS <sub>2</sub>	
& HOCl	200-380	Ocs	186-226
ClNO	190-500	SF <sub>6</sub>	
# FNO	180-350	NaOH	
ClNO <sub>2</sub>	190-370	NaCl	189-292
ClOO	220-280		
ClONO	235-400		
• ClONO <sub>2</sub>	196-414		

(1) Hudson • nd Kleffer [132]. (2) Turco [305]. # New Entry.

• Indicates a change in the recommendation from the previous evaluation.

& Indicates a change in the note.

b. 1996 HITRAN Rothman, L. S., Gamache, R. R., Tipping, R. H., Rinsland, C. P., Smith, M. A. H., Benner, D. C., Devi, V. Malathy, Flaud, J. -M., Camy-Peyret, C., Perrin, A., Goldman, A., Massie, S. T., Brown, L R., and Toth, R. A., *J. Quant. Spectrosc. Rad. Transfer* 48, 1-780 ( 1992).

- 1996 HITEMP: Selby, J. E. A. et al. Reims, ASA and L. S. Rothman, et al., *JQSRT* (submitted).

Table 2 Summary of species represented in HITRAN

Mol No	Species	Number of Isotopes	Number of Bands	Number of Lines	Spectral Cover. (cm <sup>-1</sup> )
1	HO	4	137	49444	0-22657
2	CO <sub>2</sub>	8	589	60802	442 - 9649
3	O <sub>3</sub>	3	106	275 133	0-4033
4	N <sub>2</sub> O	5	164	26174	0-5132
5	CO	5	47	4477	3 - 6418
6	CH <sub>4</sub>	3	51	48032	0 - 6185
7	O <sub>2</sub>	3	19	6292	0-15928
8	NO	3	50	15331	0- 3%7
9	SO <sub>2</sub>	2	9	38853	0-4093
10	NO <sub>2</sub>	1	12	103680	0-2939
11	NH <sub>3</sub>	2	40	11 152	0-5295
12	HNO <sub>3</sub>	1	13	165426	0-1770
13	OH	3	103	8676	0 - 9997
14	HF	1	6	107	41-11536
15	HCl	2	17	533	20-13458
16	HBr	2	16	576	16-9759
17	HI	1	9	237	12-8488
18	ClO	2	12	7230	0-1208
19	Ocs	4	7	858	0-2089
20	H <sub>2</sub> CO	3	10	2702	0-2999
21	HOCl	2	6	15 565	0-3800
22	N <sub>2</sub>	1	1	120	1922-2626
23	HCN	3	8	772	2-3422
24	CH <sub>3</sub> Cl	2	8	9355	679.3173
25	H <sub>2</sub> O <sub>2</sub>	1	2	5 444	0-1502
26	C <sub>2</sub> H <sub>2</sub>	2	11	1 668	604 - 3375
27	C <sub>2</sub> H <sub>6</sub>	1	2	4749	720 - 3001
28	PH <sub>3</sub>	1	2	2886	708-1411
29	COF <sub>2</sub>	1	7	54866	725-1982
30	SF <sub>6</sub>	1	1	11 520	940-953
31	H <sub>2</sub> S		15	7 151	2-2892
32	HCOOH	1	1	3388	1060-1162
33	HOI	1	4	26%3	0-3676
34	O	1	1	2	68-159
35	ClONO <sub>2</sub>	1	3	32199	763-798
36	NO <sup>+</sup>	1	6	1 206	1634-2531
37	HOBr	2	2	4358	0-316

Band Stats for Supplemental files	
3 High-vib O <sub>3</sub>	184724
36 NO <sup>+</sup>	1206
37 HOBr	4358
Band Stats for HITEMP	
1 H <sub>2</sub> O	1174009
2 CO <sub>2</sub>	1032269
5 CO	113022
Band Stats for UV	
702	110201
Cross-section Sizes	
N <sub>2</sub> O - W	143308 Bytes
SO <sub>2</sub> - UV	2377758 Bytes
IR	17963586 Bytes
Aerosols	
	229014 Bytes

Detailed Content of GEISA97 Edition

Mol.	ID	# Lines	Intensity average	Alpha average	Iso. ID	# Lines	F. Min (cm <sup>-1</sup> )	F. Max (cm <sup>-1</sup> )	Int. Min (cm.mol <sup>-1</sup> )	Int. Max (cm.mol <sup>-1</sup> )
I2O	1	50217	1.450E-21	0.069	161	30117	0.401	22656.465	1.010E-32	2.670E-18
					162	9799	0.007	5507.548	1.240E-32	2.700E-22
					171	3744	6.471	11150.790	1.490E-27	7.830E-22
					181	6357	6.785	13900.421	1.000E-27	5.390E-21
					182	200	1231.680	1607.611	1.000E-26	7.940E-26
					626	27896	442006	9648.007	0.000E+00	3.520E-18
CO2	2	62816	1.793E-21	0.071	636	9154	497.201	8104.666	0.000E+00	3.570E-20
					628	13554	507.860	8132.017	1.390E-36	6.850E-21
					627	6625	554.909	6961.226	1.000E-27	1.280E-21
					638	2312	567.596	4946.384	3.700E-27	7.230E-23
					637	1584	584.754	3641.072	3.710E-27	1.360E-23
					828	1107	615.974	3669.609	1.760E-40	1.310E-23
					728	288	626.438	2358.226	3.870E-27	2.500E-24
					838	296	2115.685	2276.481	4.870E-42	1.760E-25
					666	167755	0.026	4060.783	4.060E-29	4.200E-20
					668	19147	0.921	1177.493	4.880E-28	7.760E-23
					686	7513	1.177	1145.690	7.500E-28	7.560E-23
667	58254	0.289	820.380	5.340E-31	5.570E-25					
676	28938	0.213	822.795	1.490E-31	6.060E-25					
N2O	4	26771	2.688E-21	0.075	446	19423	0.838	5131.249	4.000E-27	1.000E-18
					447	1004	542.242	3482917	3.430E-26	4.150E-22
					448	2034	545.179	3463.967	1.230E-25	2.050E-21
					456	2128	5.028	3462689	5.220E-26	3.670E-21
					546	2182	4.858	3473.528	4.720E-26	3.600E-21
					26	5908	3.530	8464.883	7.880E-78	4.460E-19
CO	5	13515	7.545E-22	0.047	27	74a	3.714	6338.061	8.190E-40	1.600E-22
					28	77C	3.629	6266.578	7.610E-39	8.320E-22
					36	4768	3.414	8180.219	3.610E-73	4.680E-21
					38	741	3.462	6123.294	2.580E-40	8.700E-24
					37	58f	1807.871	6196.551	1.030E-36	1.680E-24
					211	56985	0.010	6184.492	4.000E-34	2.062E-19
					311	9894	0.032	6069.086	4.100E-34	2.329E-21
					66	1435	0.000	15927.806	0.000E+00	8.833E-24
67	418f	0.000	14536.515	1.147E-47	5.337E-26					
68	671	1.572	15851.213	1.186E-35	1.710E-26					
NO	8	94738	9.89E-23	0.053	46	9336f	0.000	9273.214	1.401E-85	6.211E-20
					48	675	1601.905	2038.846	4.190E-28	1.390E-22
					56	695	1649.585	2060.462	4.430E-28	2.550E-22
SO2	9	38853	1.065E-21	0.114	626	3856f	0.017	4092.948	1.020E-28	6.090E-20
					646	287	2463.47C	2496.088	9.740E-24	3.430E-23
N2O2	10	10368f	6.194E-22	0.067	646	10068f	0.498	2938.381	4.240E-28	1.300E-19
NH3	11	11152	4.275E-21	0.077	411	1006f	0.215	5294.501	2.970E-29	5.450E-19
					511	109f	0.375	5179.786	5.460E-29	1.990E-21
PH3	12	4635	6.457E-21	0.075	131	463f	17.805	2445.553	3.690E-28	2.930E-19
HN03	13	171504	6.879E-22	0.105	146	171504	0.035	1769.982	3.490E-27	3.020E-20
OH	14	41786	1.048E-21	0.044	61	4163	0.005	19267.869	1.401E-85	3.458E-18
					62	9f	0.01f	11824	2090E-30	5.780E-29
					81	6f	0.05f	6325	1.200E-30	1.200E-26
HF	15	107	6.772E-19	0.044	19	10f	41.111	11635.570	1.100E-26	1.440E-17
HCl	16	533	1.89E-20	0.040	15	28f	20.27f	13457.841	1.090E-26	5.030E-19
					17	24f	20.24f	10994.721	1.010E-26	1.610E-19
					19	28f	16.23f	9758.564	1.000E-26	1.210E-19
HBr	17	576	1.072E-20	0.051	11	28	16.23f	9757.189	1.010E-26	1.180E-19
					17	23	12.50f	8487.305	1.020E-26	1.540E-19
HI	18	237	4.623E-21	0.05f	56	359f	0.02f	1207.639	1.520E-29	3.240E-21
					76	363	0.01f	1199.840	5.090E-30	1.030E-21

Detailed Content of **GEISA97** Edition

(continued)

Mol	ID	# Lines	Intensity average	Alpha average	1s0 ID	# Lines	F-M in (cm <sup>-1</sup> )	F-Max (cm <sup>-1</sup> )	Int-Min (cm molec <sup>-1</sup> )	Int-Max (cm mol <sup>-1</sup> )
OCS	20	24922	4.251 E-21	0.090	622	14500	0.406	4118.004	1.560E-25	8.550E-20
					624	4764	0.396	4115.931	6.400 [1.27	4.720E-20
					632	2403	0.404	4012.468	1.720E-27	1.200E-20
					623	1802	509.007	4115.588	1.010E-23	8.430E-21
					822	1096	0.381	4041.565	2.620E-28	2.090E-21
					634	357	1972.188	2910.543	1.010E-23	5.240E-22
H2CO	21	2702	8.610E-21	0.120	126	1772	0.000	2998.527	1.020E-38	7.500E-20
					128	367	0.035	47.486	1.160E-30	1.110E-22
					136	563	0.037	75.745	2.020E-30	6.29[353.22
C2H6	22	1498	2.686E-22	0.101	226	8944	765.027	3000.486	5.800E-27	3.210E-20
					236	6037	725.603	918.717	1.320E-28	1.770E-23
CH3D	23	11524	9.333E-25	0.060	212	11524	7.760	3146.460	5.570E-30	4.030E-22
C2H2	24	1668	2.340E-20	0.061	211	1432	604.774	3358.285	1.370E-27	1.080E-18
					231	236	613.536	3374.226	3.820E-26	1.580E-20
C2H4	25	12978	1.411E-21	0.087	211	12967	701.203	3242.172	6.940E-26	8.410E-20
					311	281	2947.832	3180.288	5.060E-24	1.620S3-21
GeH4	26	824	4.978E-20	0.100	824	804	1937.371	2224.570	1.960E-22	3.680E-19
HCN	27	2575	1.205E-20	0.132	124	2275	2.956	18407.973	1.780E-28	7.100E-19
					125	115	2.870	9671.953	5.110E-26	2730E-21
					134	185	2.880	9627.961	4.150E-26	8.290E-21
C3H8	28	9019	4.168E-23	0.080	221	9019	700.015	799.930	3.770E-24	4.310E-22
C2N2	29	2571	2.668E-21	0.080	224	2577	203.955	2181.690	6.590E-24	2.580E-20
C4H2	30	1405	3.445 E-21	0.100	211	1405	190.588	654.425	2.650E-24	6.930E-20
HC3N	31	2027	2.693 E-21	0.100	124	2027	474.293	690.860	6.360E-24	4.420E-20
HOCl	32	15565	2.295E-21	0.060	165	8057	0.024	3799.249	1.650E-27	3.590E-20
					167	7508	0.349	3799.682	7.220E-28	1.140E-20
					44	117	2001.711	2619.230	2.330E-34	3.410E-28
N2	33	117	5.729E-29	0.047	44	117	2001.711	2619.230	2.330E-34	3.410E-28
CH3Cl	34	9355	5.584E-22	0.08s	215	5311	679.050	3172.927	1.250E-25	1.130E-20
					217	4044	674.143	3161.830	4.190E-26	3.540E-21
					166	100781	0.043	1499.487	5.090E-29	5.610E-20
H2O2	35	100781	5.090E-22	0.107	166	100781	0.043	1499.487	5.090E-29	5.610E-20
H2S	36	20788	2.992E-22	0.136	121	12330	2.985	4256.547	1.450E-26	1.360E-19
					131	3564	5.601	4098.234	2.020E-26	5.990E-21
					141	4894	5.615	4171.176	2.020E-26	1.080E-21
HCOOF	37	3388	5.186E-21	0.400	261	3388	1060.962	1161.251	2.140E-22	2.840s3-20
COF2	38	54866	2.178E-21	0.084	269	54866	725.005	1981.273	4.740E-24	3.830E-20
SF6	39	11520	4.551E-21	0.050	236	11520	940.425	952.238	2.160E-22	1.500E-20
C3H4	40	3390	4.277E-22	(*)	341	3390	290.274	359.995	2.020E-23	3.180E-21
HO2	41	26963	9.907 E-21	0.088	166	26963	0.055	3675.819	3.550E-27	2.900E-20
ClONO	42	32199	1.093E-22	0.140	564	21988	763.641	797.741	1.250E-24	3.850S7-22
					764	10211	765.212	790.805	6.340E-25	1.260E-22

TOTAL LINES IN GEISA1997:1,346,266

(\*) missing value; set to 0.000

d. JPL SMM CATALOG: Pickett, H. M., Poynter, R. L., Cohen, E. A., Delitsky, M. L., Pearson, J. C., and Muller, H. S. P., *Submillimeter, millimeter and microwave spectral line catalog*, JPL Publication 80-23, Rev.4 (1996). Pasadena, CA.

SPECTRA OF THE 1000 JPL SUBMILLIMETER, MILLIMETER AND MICROWAVE SPECTRAL LINE CATALOGS FIDELITY, POWER, COMB, MULTIPLY, POLARITY, WAVELEN, WAVELEN

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
10001	10002	10003	10004	10005	10006	10007	10008	10009	10010	10011	10012	10013	10014	10015	10016	10017	10018	10019	10020	10021	10022	10023	10024	10025	10026	10027	10028	10029	10030	10031	10032	10033	10034	10035	10036	10037	10038	10039	10040	10041	10042	10043	10044	10045	10046	10047	10048	10049	10050	10051	10052	10053	10054	10055	10056	10057	10058	10059	10060	10061	10062	10063	10064	10065	10066	10067	10068	10069	10070	10071	10072	10073	10074	10075	10076	10077	10078	10079	10080	10081	10082	10083	10084	10085	10086	10087	10088	10089	10090	10091	10092	10093	10094	10095	10096	10097	10098	10099	10100

TABLE 1 SUMMARY OF THE ATMOS MAIN AND SUPPLEMENTAL MOLECULAR PARAMETERS

mol#	MOLECULE	#LINES	FMIN cm <sup>-1</sup>	FMAX cm <sup>-1</sup>	#ISO	#VIB	#BANDS	Total Intensity Sum cm <sup>-1</sup> /molec·cm <sup>-2</sup> 296K
1	H <sub>2</sub> O	31016	0.40	9999.49	3	45	11	7.279 x10 <sup>-17</sup>
2	C	60790	442.00	9648.00	8	319	589	1.126 x10 <sup>-16</sup>
3	CO <sub>2</sub>	196415	0.02	4060.78	5	92	104	1.636 x10 <sup>-17</sup>
4	N <sub>2</sub> O	26249	0.23	5131.24	s	113	162	7.196 x10 <sup>-17</sup>
5	CO	3600	3.46	8464.55	5	9	41	1.059 x10 <sup>-17</sup>
6	CH <sub>4</sub>	45456	0.01	61 84.49	3	40	51	1.772 x10 <sup>-17</sup>
7	O <sub>2</sub>	1619	0.00	9468.43	3	6	9	9.107 x10 <sup>-18</sup>
8	SO <sub>2</sub>	7385	0.00	3963.00	3	42	50	4.730 x10 <sup>-16</sup>
9	SO <sub>2</sub>	2622s	0.01	2526.03	2	6	7	4.122 x10 <sup>-17</sup>
10	NO <sub>2</sub>	44973	0.49	2935.37	1	9	9	6.241 x10 <sup>-17</sup>
11	NH <sub>3</sub>	3217	0.21	2153.76	2	14	16	4.457 x10 <sup>-17</sup>
12	HNO <sub>3</sub>	129741	0.03	1769.98	1	11	11	1.204 x10 <sup>-16</sup>
12	HNO <sub>3</sub>	8751	(345.11	904.63	1	2	2	3.246 x10 <sup>-16</sup>
13	OH	3168	0.00	9997.35	3	39	43	4.554 x10 <sup>-17</sup>
14	NF	84	41.11	7994.3s	1	5	5	7.326 x10 <sup>-17</sup>
15	HC1	324	20.24	8454.45	2	7	14	1.709 x10 <sup>-16</sup>
16	HBr	398	16.23	9758.56	2	8	16	6.137 x10 <sup>-16</sup>
17	HI	237	12.50	2427.30	1	9	9	1.096 x10 <sup>-16</sup>
18	ClO	6038	0.01	886.21	2	4	8	1.160 x10 <sup>-16</sup>
19	Ocs	4096	493.26	4117.99	3	19	21	1.0643 X1 O <sup>-16</sup>
20	H <sub>2</sub> CO	2702	0.00	2998.52	3	8	10	2.326 x10 <sup>-17</sup>
020	H <sub>2</sub> CO	5s7	1707.09	1781.38	1	1	1	7.195 x10 <sup>-16</sup>
21	HOCl	15371	0.02	3799.6s	2	4	8	3.23s x10 <sup>-17</sup>
22	NO <sub>2</sub>	6220	1032.06	3673.81	1	4	4	1.795 x10 <sup>-17</sup>
23	N <sub>2</sub> O <sub>2</sub>	3444	0.15	1499.48	1	2	2	1.872 x10 <sup>-17</sup>
24	HONO	2348	779.12	1711.70	1	1	1	2.059 x10 <sup>-17</sup>
c 25	NO <sub>2</sub> NO <sub>2</sub>		502.	604. (at 220K)				1.66 x10 <sup>-17</sup>
c 26	H <sub>2</sub> O		1210.	1275.				4.21 x10 <sup>-17</sup>
27	ClONO <sub>2</sub>	23264	763.64	1309.99	2	3	4	3.113 x10 <sup>-17</sup>
28	HCH	772	2.87	3421.96	3	6	8	3.086 x10 <sup>-17</sup>
12 9	CH <sub>3</sub> F	739	987.91	10s9.13	1	1	1	1.806 x10 <sup>-17</sup>
30	CH <sub>3</sub> Cl	10432	661.79	3172.92	2	4	8	5.763 x10 <sup>-16</sup>
s 30	CH <sub>3</sub> Cl	621	1324.69	1460.14	2	2	3	1.163 x10 <sup>-16</sup>
c 31	CF <sub>4</sub>		1255.0	12s9.				1.61 x10 <sup>-16</sup>
c 32	CCl <sub>2</sub> F <sub>2</sub>		810.	96s.				5.55 x10 <sup>-17</sup>
c 33	CCl <sub>3</sub> F		810.	MO.				6.95 x10 <sup>-17</sup>
s 34	CH <sub>2</sub> CCl <sub>2</sub>	231	1362.50	136s.00	1	1	1	1.25 x10 <sup>-16</sup>
c 35	CCl <sub>4</sub>		770.00	809.99				5.14 x10 <sup>-17</sup>
36	COF <sub>2</sub>	33932	725.00	1931.27	1	7	7	1.193 x10 <sup>-16</sup>
s 37	CFClO	2U9	764.11	1907.92	1	2	2	3.937 x10 <sup>-17</sup>
38	C <sub>2</sub> H <sub>6</sub>	10000	745.22	951.65	1	1	1	6.967 x10 <sup>-16</sup>
s 38	C <sub>2</sub> H <sub>6</sub>	115	2976.63	2996. -	1	1	1	2.875 x10 <sup>-16</sup>
40	C <sub>2</sub> H <sub>2</sub>	1267	638.25	5376.22	2	8	9	4.103 x1 O <sup>-17</sup>
41	N <sub>2</sub>	120	1992.62	2625.40	1	1	1	6.719 x10 <sup>-17</sup>
c 42	CHF <sub>2</sub> Cl (FTS)		7s0.	239.				2.05 X10 <sup>-17</sup>
c 42	CHF <sub>2</sub> Cl (TOL)		628.93	829.16				3.11 x10 <sup>-16</sup>
s 43	COCl <sub>2</sub>	32871	828.54	1862.45	1	2	2	3.35 x10 <sup>-17</sup>
s 44	CH <sub>2</sub> Br	3421	871.32	1038.06	1	1	1	6.427 x10 <sup>-16</sup>
s 45	CH <sub>3</sub> I	2528	793.46	971.65	1	1	1	1.207 x10 <sup>-16</sup>
s 46	HCOOH	3388	1060.96	1161.25	1	1	1	1.757 x10 <sup>-17</sup>
47	H <sub>2</sub> S	661	994.12	1573.81	1	1	1	7.959 x10 <sup>-16</sup>
s 48	CHCl <sub>3</sub>	9523	785.00	10W.W	1	1	1	5.224 x10 <sup>-17</sup>
49	HDO	8505	0.01	5507.54	2	9	10	7.694 x1 O <sup>-17</sup>
c 50	SF <sub>6</sub>		940.42	952.23				5.243 x10 <sup>-17</sup>

The ATMOS Main list : 694359 lines from 0 to 9999 cm<sup>-1</sup>  
 The ATMOS Supplemental list s : 116016 lines from 725 to 3673 cm<sup>-1</sup>  
 The ATMOS Cross Section list c : 8 species from 770 to 12s9 cm<sup>-1</sup>

Table 7 Summary Of Absorption Cross Sections used for ATMOS Retrievals

Molecule	Ref	Spectral Range cm <sup>-1</sup>	Temp. K	Press. atm.	Integrated Strength cm <sup>2</sup> /(molecule cm <sup>-2</sup> )	Grid cm <sup>-1</sup> /pt
CO <sub>2</sub> F <sub>2</sub>	15,16	81001- 964.98	216	0.2236	5.9510 <sup>-17</sup>	0010
		810.04 - 964.92	233	0.2595	5.9410 <sup>-17</sup>	
		810M - 964.92	245	0.4673	5.9310 <sup>-17</sup>	
		810.05- 964.96	260	0.8612	5.9410 <sup>-17</sup>	
		810.02 - 964.98	273	0.6509	5.9010 <sup>-17</sup>	
		81008- 964.97	284	0.6845	5.8910 <sup>-17</sup>	
61001- 964.96	296	0.9214	5.9510 <sup>-17</sup>			
CO <sub>2</sub> F	14	81001- 879.98	215	0.2242	6.8810 <sup>-17</sup>	0.012
			225	0.2276	6.8910 <sup>-17</sup>	
			233	0.3299	6.8510 <sup>-17</sup>	
			246	0.3800	6.8610 <sup>-17</sup>	
			272	0.7242	6.9210 <sup>-17</sup>	
			284	0.6857	6.9510 <sup>-17</sup>	
	296	0.9991	6.93 10 <sup>-17</sup>			
CHF <sub>2</sub> Cl (FIS)	10	780.01 - 840.00	203	N/A	1.8810 <sup>-17</sup>	0.015
			213		1.9010 <sup>-17</sup>	
			233		1.9410 <sup>-17</sup>	
			253		1.9910 <sup>-17</sup>	
			272		2.0110 <sup>-17</sup>	
			293		2.0510 <sup>-17</sup>	
(IDL)	17	828.95 - 829.16	216	0.0527	4.4710 <sup>-19</sup>	0.00026
		828.95 - 829.16	216	CL1017	4.4910 <sup>-19</sup>	
		828.95 - 829.16	216	0.1480	4.4010 <sup>-19</sup>	
		828.95 - 829.16	216	0.2369	4.2710 <sup>-19</sup>	
		828.94 - 829.19	236	0.3548	4.2510 <sup>-19</sup>	
		828.94 - 62719	252	0.5288	3.7910 <sup>-19</sup>	
828.94 - 829.18	29a	0.9983	3.1110 <sup>-19</sup>			
HO <sub>2</sub> NO <sub>2</sub>	19	769.99- 834.99	220	N/A	1.7210 <sup>-17</sup>	0.00247
N <sub>2</sub> O <sub>3</sub>	11	121035- 1275.76	233	N/A	3.8910 <sup>-17</sup>	0482
			283		4.0610 <sup>-17</sup>	
			273		4.0921P	
			292		4.2110 <sup>-17</sup>	
CCl <sub>4</sub>	23	770.01 - 809.99	170	N/A	4.9010 <sup>-17</sup>	om42
			171		4.9510 <sup>-17</sup>	
			240		5.0710 <sup>-17</sup>	
			273		5.0610 <sup>-17</sup>	
			296		5.1010 <sup>-17</sup>	
			310		5.1410 <sup>-17</sup>	
CF <sub>4</sub>	10	1235.01- 1289.99	203	N/A	1.5210 <sup>-16</sup>	0.015
			213		1.6510 <sup>-16</sup>	
			233		1.5910 <sup>-16</sup>	
			253		1.6510 <sup>-16</sup>	
			m		1.6210 <sup>-16</sup>	
	292		1.6110 <sup>-16</sup>			
SF <sub>6</sub>	18	925.00 - 955.00	295	1.00	2.0710 <sup>-16</sup>	0010
			m	0rc.?	2.0510 <sup>-16</sup>	
			246	0.468	2.0910 <sup>-16</sup>	
			216	0.0329	2.5510 <sup>-16</sup>	

Table 1. SAO database Statistic

Mol	Num lines	Low Freq	High Freq.	Strongest	Weakest	Comment
H <sub>2</sub> O	3896	10	1600	267x 10 <sup>-7</sup>	1.31x10 <sup>-30</sup>	161 Iso
CO <sub>2</sub>	16792	449	1415	2.98x10 <sup>-19</sup>	1.00x10 <sup>-26</sup>	
O <sub>3</sub>	21351	10	1495	4.20x10 <sup>-20</sup>	5.02x10 <sup>-26</sup>	666 Iso., v''=0
N <sub>2</sub> O	8554	10	1600	1.66x10 <sup>-19</sup>	1.82x10 <sup>-30</sup>	
c o	480	10	190	1.45x10 <sup>-21</sup>	8.11 x10 <sup>-6</sup>	
CH <sub>4</sub>	12056	73	1600	9.68x10 <sup>-20</sup>	1.00x10 <sup>-25</sup>	
O <sub>2</sub>	910	10	1600	5.21x10 <sup>-a</sup>	1.10x10 <sup>-35</sup>	
NO	422	11	99	2.95x10 <sup>-22</sup>	7.20x10 <sup>-25</sup>	
s o	571	11	1397	6.09x10 <sup>-27</sup>	1.00x10 <sup>-21</sup>	
NO <sub>2</sub>	33339	10	1600	1.13X10 <sup>-1*</sup>	3.00x10 <sup>-24</sup>	
NH <sub>3</sub>	445	19	1600	5.50x10 <sup>-19</sup>	1.00x10 <sup>-20</sup>	
HNO <sub>3</sub>	78371	10	1371	302x10-M	1.00x10 <sup>-22</sup>	
OH	1395	31	990	1.90x10 <sup>-18</sup>	2.80x10 <sup>-12</sup>	
HF	22	41	615	1.44x10 <sup>-17</sup>	1.56x10 <sup>-26</sup>	
HCl	230	20	438	4.60x10 <sup>-19</sup>	1.00x10 <sup>-26</sup>	
HBr	256	16	383	1.21x10 <sup>-19</sup>	1.39x10 <sup>-26</sup>	
HI	44	12	320	1.54x10 <sup>-19</sup>	1.32x10 <sup>-26</sup>	
ClO	3672	10	887	3.24x 10-21	1.00x10 <sup>-25</sup>	
Ocs	6173	10	1090	1.55x10 <sup>-20</sup>	2.72x10 <sup>-21</sup>	
H <sub>2</sub> CO	492	10	100	6.12x 10-W	1.00x10 <sup>-22</sup>	
HOCl	6525	10	1307	3.59x10 <sup>-20</sup>	1.00x10 <sup>-22</sup>	
HCN	671	11	1537	7.1 OX10-1*	2.40x10 <sup>-25</sup>	
CH <sub>3</sub> Cl	2668	674	768	1.23x10 <sup>-20</sup>	4.19x10 <sup>-26</sup>	
H <sub>2</sub> O <sub>2</sub>	9083	12	1330	561 x10-M	4.00x10 <sup>-22</sup>	
C <sub>2</sub> H <sub>2</sub>	732	646	1441	1.08x10 <sup>-1*</sup>	1.00x10 <sup>-21</sup>	
c. H <sub>6</sub>	2019	748	903	3.42x10 <sup>-3*</sup>	1.00x10 <sup>-22</sup>	
COF <sub>2</sub>	20991	745	1283	3.64x10 <sup>-20</sup>	5.00x10 <sup>-22</sup>	
SF <sub>6</sub>	3001	925	955	6.30x 10-1*	4.34 X10-3*	Pseudo lines
H <sub>2</sub> S	1264	10	1444	1.36x 10 <sup>-7</sup>	1.00x10 <sup>-22</sup>	
HCOOH	2205	1063	1139	2.84x 10-M	1.00x10 <sup>-21</sup>	
H <sub>2</sub> O	14131	10	1458	2.74x10 <sup>-20</sup>	1.00x10 <sup>-23</sup>	
O <sup>3</sup> P	2	68	158	1.13x10 <sup>-21</sup>	9.63x 10-2]	
ClNO	33889	403	831	1.25x10 <sup>-20</sup>	8.30x10 <sup>-31</sup>	Pseudo, real
HOBr	4358	10	316	1.73x10 <sup>-20</sup>	s 26x10 <sup>-21</sup>	
H <sub>2</sub> OIS	2864	10	1600	5.39x10 <sup>-21</sup>	1.49x10 <sup>-27</sup>	171 and 181
H <sub>2</sub> O	2668	10	1600	2.76x10 <sup>-22</sup>	7.61 x10-22	
O <sub>3</sub> ISO	30393	10	1178	7.76x10 <sup>-27</sup>	SOOX10-2'	668, 686, 667, 676
HotO <sub>3</sub>	53687	10	1434	1.38x10 <sup>-21</sup>	1.00x10 <sup>-25</sup>	666 Iso., v'' >0
O <sub>2</sub> <sup>1</sup> D	66	11	189	2.80x10 <sup>-23</sup>	1.24x10 <sup>-34</sup>	
N <sub>2</sub> O <sub>5</sub>	13347	257	1286	9.02x10 <sup>-18</sup>	8.67x10 <sup>-21</sup>	Pseudo lines
HNO <sub>2</sub>	341	802	804	5.98x10 <sup>-22</sup>	6.7sx10 <sup>-24</sup>	Pseudo lines
CFC12	25001	850	1200	1.40X10-9	1.20x10 <sup>-38</sup>	Pseudo lines
CFC11	14001	810	1120	5.00x10 <sup>-20</sup>	1.87x10 <sup>-30</sup>	Pseudo lines
CC14	4001	770	810	4.44x10 <sup>-20</sup>	6.36x10 <sup>-22</sup>	Pseudo lines
CF <sub>4</sub>	9001	1250	129S	5.88x10 <sup>-19</sup>	1.00x10 <sup>-36</sup>	Pseudo lines
CFC113	408	786	990	6.17x 10 <sup>-27</sup>	6.89x10 <sup>-21</sup>	Pseudo lines
HCFC22	21479	776	1335	9.80x 10-M	1.41X10-3*	Pseudo lines
HCFC23	9583	785	1100	2.16x10 <sup>-20</sup>	4.84x10 <sup>-22</sup>	Pseudo lines
HCFC140	2s1	1382	1385	2.07x10 <sup>-21</sup>	6.97x10 <sup>-24</sup>	Pseudo lines

# Hanst and Hanst

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## ALPHABETICAL INDEX Compounds, Common File Names\*, and Classes

\* Compound file names are given here without prefix. Each digitized file has a prefix Z, H, O or T indicating the resolution of the file.

Acetaldehyde 314AA H  
Acetic acid 35AAC G  
Acetic acid, monomer and dimer 110AAC G  
Acetone 23ACT I  
Acetonitrile (dissolved in water) 456AN N  
Acetyl chloride ACCL350 T  
Acrylonitrile 18AC A  
Acrylonitrile ACRO140 H  
Acrylic acid monomer and dimer 240ACYA G  
Acrylic acid, methyl methacrylate 180ACYA G  
Acrylonitrile ACN1632 N  
Allyl alcohol 200AA J  
Alpha Pinene 100APIN C  
Ammonia 85NH3 E  
Aruene A53-700 E  
Benzaldehyde 796BZA N  
Benzene 1082 D  
Beta Pinene 100BPIN C  
Boron trichloride BCL150 T  
Bromochloroethane 200BR2 S  
Bromochloroethane 300BR2M P  
Bromoform 300BRF P  
Bromo methane 930BRM P  
1,3-Butadiene 103BD A  
Butane 151BU A  
2-Butanone MEK762 I  
n-Butyl acetate 600AC K  
n-Butyl alcohol 300BALC J  
n-Butylaldehyde 190BAL H  
Carbon dioxide 100CO2 F  
Carbon disulfide 50CS2 O  
Carbon monoxide 225CO F  
Carbon tetrachloride 27CT P  
Carbonyl fluoride 36COF2 T  
Carbonyl sulfide 36COS O  
Chloroacetylene 114CBZ S  
1-Chloro-1,1-difluoro ethane 60GT Q  
Chlorodifluoroethane 64F22 P  
Chloroethane 55ICE Q  
Chloroform 43CLF P  
Chloroform 652CLM P  
2-Chloroethane 100CLTO S  
4-Chloroethane 100CLTL S  
Chlorotrifluoroethylene 80CTFE R  
Chlorotrifluoroethylene F13-43 P  
C — 114CRA H  
Cyclohexane 48CHX C  
Cyclohexane 114CHX C  
Cyclopentane CYP282 B  
Cyclopropane CYP115 A  
1,2-Difluoro ethane 228ED8 Q  
Difluoroethane 300DFM P  
m-Dichloro benzene 300MDCB S  
o-Dichloro benzene 1000DCB S  
p-Dichloro benzene 300PDCB S  
Dichlorodifluoroethane 20F12 P  
1,1-Dichloroethane 11DC174 Q  
1,2-Dichloroethane 220DCE Q  
cis 1,2-Dichloroethylene 100DCEL R

Dichloro-1-fluoro ethane (dissolved in water) 125G5 Q  
Dichloromethane 160DCM P  
1,2-Dichloropropane 300DCP T  
1,3-Dichloropropane 300DCPR T  
1,2-Dichlorotetrafluoroethane 114-318 Q  
Diethyl ether 24DEAM N  
Diethyl ether 144DEE L  
Diethyl ketone 320DEK I  
Diisopropyl ether 114DIE L  
Dimethyl ether 240DME L  
1,1-Dimethyl hydrazine DMH2846 N  
Dimethyl sulfide 363DMS O  
Dinitrogen pentoxide 175N2O5 M  
Ethane 260ET A  
Ethanol 320ETA J  
Ethyl acetate 93EAC K  
Ethyl acetate 93EAC K  
Ethyl acrylate 93EAY K  
Ethyl benzene 300EBZ D  
Ethyl butyrate 91EBU K  
Ethyl formate 103ETF K  
Ethylene 82ETY A  
Ethylene oxide 125EO F  
Ethyl vinyl ether 160EVE L  
Eucal 87 gasoline 250GAS T  
Fluoro benzene 64FBZ S  
Formaldehyde 176FA H  
Formic acid, monomer 140FAC G  
Furan FURAN133 P  
n-Heptane 213HEP C  
n-Hexane 121HX C  
Hydrazine 400H2 E  
Hydrogen bromide 635HBR E  
Hydrogen chloride 285HCL E  
Hydrogen cyanide 36HCN M  
Hydrogen fluoride 30HF E

Hydrogen iodide 100HI E  
Hydrogen peroxide 160H2O2 P  
Hydrogen sulfide 32KH2S O  
Isobutane 148IBU A  
Iodo methane 796IM P  
Isobutanol 190IBA J  
Isobutylene 190IBY A  
Isoprene 147IP B  
Isopropyl acetate 228IPA J  
Isopropyl acetone 300IPB D  
K-1 Kerosene 200KER T  
Mesitylene 285MTY D  
Methane 128ME A  
Methanol 141MA J  
Methyl acetate 100MAC K  
Methyl acrylate 135MACR K  
Methyl amine 400MAM N  
2-Methyl butane 1108UT B  
2-Methyl-2-butene 2M2BU474 B  
3-Methyl-1-butene 3M1BU474 B  
Methyl formate 57MF E  
Methyl isobutyl ketone M2IMBK I  
Methyl mercaptan 1500MHC O  
Methyl methacrylate 114MM K  
Methyl nitrite MN1300 N  
2-Methyl pentane 2MP114 C  
3-Methyl pentane 3MP118 C  
2-Methyl-1-pentene 185MPE C  
2-Methyl-2-pentene 2M2P282 C  
4-Methyl-2-pentene 4M2P290 C  
Methyl vinyl ether MVE1474 L  
Methyl vinyl ketone 356MVK I  
Nitric acid 140HNO3 M  
Nitric oxide 825NO M  
Nitro benzene NB223 M

Dichloro-1-fluoro ethane (dissolved in water) 125G5 Q  
Dichloromethane 160DCM P  
1,2-Dichloropropane 300DCP T  
1,3-Dichloropropane 300DCPR T  
1,2-Dichlorotetrafluoroethane 114-318 Q  
Diethyl ether 24DEAM N  
Diethyl ether 144DEE L  
Diethyl ketone 320DEK I  
Diisopropyl ether 114DIE L  
Dimethyl ether 240DME L  
1,1-Dimethyl hydrazine DMH2846 N  
Dimethyl sulfide 363DMS O  
Dinitrogen pentoxide 175N2O5 M  
Ethane 260ET A  
Ethanol 320ETA J  
Ethyl acetate 93EAC K  
Ethyl acetate 93EAC K  
Ethyl acrylate 93EAY K  
Ethyl benzene 300EBZ D  
Ethyl butyrate 91EBU K  
Ethyl formate 103ETF K  
Ethylene 82ETY A  
Ethylene oxide 125EO F  
Ethyl vinyl ether 160EVE L  
Eucal 87 gasoline 250GAS T  
Fluoro benzene 64FBZ S  
Formaldehyde 176FA H  
Formic acid, monomer 140FAC G  
Furan FURAN133 P  
n-Heptane 213HEP C  
n-Hexane 121HX C  
Hydrazine 400H2 E  
Hydrogen bromide 635HBR E  
Hydrogen chloride 285HCL E  
Hydrogen cyanide 36HCN M  
Hydrogen fluoride 30HF E  
Hydrogen iodide 100HI E  
Hydrogen peroxide 160H2O2 P  
Hydrogen sulfide 32KH2S O  
Isobutane 148IBU A  
Iodo methane 796IM P  
Isobutanol 190IBA J  
Isobutylene 190IBY A  
Isoprene 147IP B  
Isopropyl acetate 228IPA J  
Isopropyl acetone 300IPB D  
K-1 Kerosene 200KER T  
Mesitylene 285MTY D  
Methane 128ME A  
Methanol 141MA J  
Methyl acetate 100MAC K  
Methyl acrylate 135MACR K  
Methyl amine 400MAM N  
2-Methyl butane 1108UT B  
2-Methyl-2-butene 2M2BU474 B  
3-Methyl-1-butene 3M1BU474 B  
Methyl formate 57MF E  
Methyl isobutyl ketone M2IMBK I  
Methyl mercaptan 1500MHC O  
Methyl methacrylate 114MM K  
Methyl nitrite MN1300 N  
2-Methyl pentane 2MP114 C  
3-Methyl pentane 3MP118 C  
2-Methyl-1-pentene 185MPE C  
2-Methyl-2-pentene 2M2P282 C  
4-Methyl-2-pentene 4M2P290 C  
Methyl vinyl ether MVE1474 L  
Methyl vinyl ketone 356MVK I  
Nitric acid 140HNO3 M  
Nitric oxide 825NO M  
Nitro benzene NB223 M

Nitro ethane 114NE N  
Nitro methane 140NM M  
Nitrogen dioxide 125NO2 M  
Nitrogen dioxide (and NO) 100NO2 M  
Nitroso benzene 300NBZ N  
Nitrous acid HNO2-10 U  
Nitrous oxide 80N2O M  
n-Octane 219OCT C  
Oxone 321OZ P  
n-Pentane 152P B  
1-Pentene 1PENT564 B  
2-Pentene 2PENT564 B  
Perfluoro butane 300PFBU T  
Peroxy acetyl nitrate BOPAN N  
Phenylene Carbonyl chloride 60PHG T  
Phenylene PhG-945 E  
Phosphorus trichloride PTC700 T  
Propane 118PP A  
Propionaldehyde 274PA H  
Propionic acid, monomer and dimer 257PAC G  
Propionic acid, methyl methacrylate 170PAC G  
n-Propyl acetate 60PAC K  
n-Propyl acetone 300PBZ D  
Propylene 128PPY A  
Propylene oxide 388PYO P  
Silicon tetrafluoride 1651F4 T  
Styrene 145STY D  
Sulfur dioxide 125SO2 O  
Sulfur hexafluoride 45F6 O  
Tertiary butyl benzene 100TBZ D  
1,1,1,2-Tetrachloroethane TETC36 Q  
1,1,2,2-Tetrachloroethane 400TCE Q  
Tetrafluoroethylene 125TFE R  
Tetrafluoroethane 57TFM P  
Tetrahydrofuran 200THF P

Tetrahydrofuran 200THF O  
Thiophene 200TF O  
Toluene 137TO D  
1,1,1-Trichloroethane 95TC1 Q  
1,1,2-Trichloroethane 125TC2 Q  
Trichloroethylene 160TCE R  
Trichlorofluoroethane 38F11 P  
1,2,3-Trichloropropane 300TCP T  
1,2,4-Trichloroethane 113-141 Q  
1,2,4-Trimethyl benzene 300TMBZ D  
Vinyl acetate VIAC474 E  
Vinyl chloride 200VC R  
Vinylidene chloride VC482 R  
Water 180H2O E  
m-Xylene 200MXL D  
o-Xylene 100OXL D  
p-Xylene 300PXL D