1995 Atmospheric Trace Molecule Spectroscopy (ATMOS) linelist

L. R. Brown, M. R. Gunson, R. A. Toth, F. W. Irion, C. P. Rinsland, and A. Goldman

The Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment uses a Fourier-transform spectrometer on board the Space Shuttle to record infrared solar occultation spectra of the atmosphere at 0.01-cm^{-1} resolution. The current version of the molecular spectroscopic database used for the analysis of the data obtained during three Space Shuttle missions between 1992 and 1994 is described. It is an extension of the effort first described by Brown *et al.* [Appl. Opt. **26,** 5154 (1987)] to maintain an up-to-date database for the ATMOS experiment. The three-part ATMOS compilation contains line parameters of 49 molecular species between 0 and 10000 cm^{-1}. The main list, with nearly 700,000 entries, is an updated version of the HITRAN 1992 database. The second compilation contains supplemental line parameters, and the third set consists of absorption cross sections to represent the unresolvable features of heavy molecules. The differences between the ATMOS database and other public compilations are discussed.

1. Introduction

The Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment records infrared solar occultation spectra of the atmosphere between 580 and 4800 cm^{-1} at 0.01-cm^{-1} resolution by the use of a Fourier-transform spectrometer on board the Space Shuttle.[1] This instrument was first flown in 1985 on Spacelab 3. In 1992, 1993, and 1994, as part of the ATLAS 1, 2, and 3 payloads, it obtained a more extensive set of spectral data for the 69° N to 72° S latitudes with tangent heights between 5 and 150 km, including observations inside the remanent Arctic and Antarctic vortices.[2] These measurements were analyzed to obtain atmospheric pressure, temperature, and volume mixing ratios as a function of the terrestrial coordinates. This article describes the comprehensive, customized catalog of molecular line parameters used for the version 2 analysis of the ATLAS series data and for reprocessing of the Spacelab 3 spectra.

An earlier version of the ATMOS molecular database was compiled in 1987[3] and used for the initial analysis of ATMOS data obtained during the 1985 Spacelab 3 mission. The bulk of the parameters was placed in the main linelist and consisted of major modifications to the 1982 U.S. Air Force Geophysics Laboratory (AFGL) compilation.[4,5] A secondary list, called the Supplemental Linelist, was formed to include preliminary and lower-quality data including parameters for the difficult-to-characterize species like the chlorofluorocarbons. In 1992, the ATMOS investigators set aside its 1987 main list and adopted the 1992 HITRAN database[6] because the public compilation contained most of the revisions needed by ATMOS. As with the 1987 linelists, the improvements in the main 1995 ATMOS database were made in the 580- to 4800-cm^{-1} region using recent laboratory data as well as parameters from the 1991 GEISA compilation.[7] The ATMOS supplemental list was also changed by the removal of artificial line parameters created previously[3] from room-temperature cross sections so that new experimental temperature- and (sometimes) pressure-dependent absorption coefficients could be used for some heavy species. For the 1995 update, a third list was initiated with available experimental absorption cross-section files.[8–19] The philosophy of having three separate lists is so that the one (main) list consists of generally valid parameters based on

L. R. Brown, M. R. Gunson, and R. A. Toth are with the Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109. F. W. Irion is with the Department of Chemical Engineering, California Institute of Technology, Pasadena, California 91125. C. P. Rinsland is with the Chemistry and Dynamics Branch, NASA Langley Research Center, Hampton, Virginia. A. Goldman is with the Department of Physics, University of Denver, Denver, Colorado 80208.

Received 28 September 1995; revised manuscript received 26 January 1996.

0003-6935/96/162828-21$10.00/0

published studies, another (supplemental) is the depository of approximate predictions, and the third list contains empirical absorption coefficients. In contrast to the first ATMOS compilations,[3] few unpublished studies have been included in the 1995 version. An overview of the linelists is given in Table 1, which shows the ATMOS molecule number, species (Molecule), total number of transitions (#Lines), the minimum and maximum ranges (FMIN, FMAX) in wave number (cm^{-1}), followed by the number of isotopes (#ISO), vibrational states (#VIB) and bands (#BANDS), and the total integrated absorption in $cm^{-1}/(molecule \cdot cm^{-2})$ at 296 K. Those parameters marked by s to the left of the molecule number appear in the supplemental list, whereas those marked by c are available in cross-section files. Some species appear in more than one linelist, but, with the exception of the overlapping lists of $CHClF_2$ (CFC-22) cross sections, no spectral band of any species is duplicated in order that all three lists can be used simultaneously.

2. General Description of the ATMOS Linelists

The main and supplemental ATMOS lists contain the same type of molecular parameters as the 1992 HITRAN database, but the format is slightly different. A sample section of the 1995 ATMOS main and supplemental linelists is shown in Table 2 with the name of the molecule given in the first column. The parameters include molecule and isotope code numbers, positions in cm^{-1}, intensities in $cm^{-1}/(molecule \cdot cm^{-2})$ at 296 K, lower state energies in cm^{-1}, air-broadening and self-broadening coefficients in cm^{-1}/atm at 296 K, the transition matrix element ($r2$), the temperature-dependence exponent of the air-broadening coefficients n, and the air-broadened pressure shifts in cm^{-1}/atm at 296 K. These are followed by the upper and the lower vibrational-state index codes (V_{UP} and V_{LO}, respectively), rotational quantum numbers, and the accuracy and the reference-code integers. To summarize the isotopic nomenclature, Table 3 gives the molecule number, species, isotope numbers, the old isotopic codes used before 1986 in the AFGL compilations,[4,5] the chemical formula, and the assumed isotopic abundances.

The upper and the lower state vibration index codes in Table 2 can be translated into corresponding standard vibrational nomenclature by software like those in the FORTRAN program SELECT given with the 1992 HITRAN compilation. Table 4 displays the integer codes for V_{UP} and V_{LO} in Table 2 with their corresponding vibrational quantum numbers. The index is usually incremented in order of increasing energy so that 1 is the ground state (i.e., 000 for H_2O or 00001 for CO_2 or $X0$ for O_2), 2 is the lowest fundamental, and 3 is the next higher state (an overtone or fundamental). The molecules all fall into one of 10 groups. Diatomics are in groups 4, 6, and 7. Species with three atoms are contained in group 1 (asymmetric rotors), group 8 (symmetric rotors), and groups 2 and 3 (linear molecules). Molecules with four atoms are in groups 9 and 10. Group 5 was originally set up for the spherical rotors like CH_4, but it has become the catch-all group for species with five or more atoms, regardless of molecule symmetry. For group 5, the ground state of the nonspherical species has an index of 14. Thus in Table 2 the vibrational indices of 27 14 for the CH_3Br line at 971.2295 cm^{-1} should be interpreted as transitions of the ν_3 band from the ground state.

The accuracy and the reference codes (acc and ref in Table 2) are two sets of three integers each that respectively indicate the estimated uncertainties and the data sources for the positions, intensities, and air-broadening coefficients. The error codes defined by Rothman *et al.*[6] and used by ATMOS are given in Table 5. For example, a code of 564 means that the accuracies are between 0.00001 and 0.0001 cm^{-1} for positions, between 2% and 5% for intensities and from 10% to 20% for air-broadening coefficients. Reference-number fields defined for the 1992 HITRAN linelist give the index of references that correspond to a list distributed electronically with the 1992 HITRAN edition. The publications are grouped by molecule and separated into three subgroups that are numbered individually for positions, intensities, and linewidths. The code 0 0 0 means that the entry was the same in 1986[8] while a code 2 3 4 means that the positions are based on reference 2 of the first subset, intensities on number 3 of the second subset, and widths on number 4 of the third group listed for H_2O. In changing the ATMOS linelist, an attempt has been made to be consistent with the 1992 numbering scheme by incrementing the counter for each new study. However, the reference codes for the new bands in the 1995 ATMOS list will not be consistent with the codes expected on the 1996 HITRAN database because the two databases will be different. In addition, these fields are usually not defined in the supplemental list, as seen in Table 2 for the CH_3I and CH_3Br transitions.

One difference between ATMOS and the two public databases (HITRAN and GEISA) is the molecule code number. The ATMOS number codes for 46 molecules were specified in 1982 to match evolving software at a time when the public databases contained 21 species. As a result, although molecules 1–20 have the same codes on both the ATMOS and the HITRAN databases, all the molecules codes are different between 21 and 50. The correspondence of the numbering schemes between the three compilations is shown in Table 6. The isotope codes are generally the same as the other two databases. One exception is HDO, which is labeled in the ATMOS database as a separate molecule (49) rather than as the minor isotope of molecule 1 (H_2O). In addition, parameters of PH_3 are omitted entirely from the ATMOS linelist, and no parameters are currently included for C_2H_4 (molecule 39).

Table 1. Summary of the ATMOS Main and Supplemental Molecular Parameters

Mol#	Molecule	#Lines	FMIN cm^{-1}	FMAX cm^{-1}	#ISO	#VIB	#Bands	Total Intensity Sum $cm^{-1}/molec \cdot cm^{-2}$ 296 K
1	H_2O	31016	0.40	9999.49	3	45	73	7.279×10^{-17}
2	CO_2	60790	442.00	9648.00	8	319	589	1.126×10^{-16}
3	O_3	196415	0.02	4060.78	5	92	104	1.836×10^{-17}
4	N_2O	26249	0.83	5131.24	5	113	162	7.196×10^{-17}
5	CO	3600	3.46	8464.88	5	9	41	1.059×10^{-17}
6	CH_4	45456	0.01	6184.49	3	40	51	1.772×10^{-17}
7	O_2	1619	0.00	9468.43	3	6	9	9.107×10^{-24}
s 7	O_2	162	1432.50	1676.96	1	1	1	1.470×10^{-27}
8	NO	7385	0.00	3966.00	3	42	50	4.730×10^{-18}
9	SO_2	26225	0.01	2526.03	2	6	7	4.122×10^{-17}
10	NO_2	44975	0.49	2938.37	1	9	9	6.241×10^{-17}
11	NH_3	5817	0.21	2153.76	2	14	16	4.457×10^{-17}
12	HNO_3	129741	0.03	1769.98	1	11	11	1.204×10^{-16}
s 12	HNO_3	8751	845.11	908.83	1	2	2	3.246×10^{-18}
13	OH	3168	0.00	9997.35	3	39	43	4.554×10^{-17}
14	HF	84	41.11	7994.58	1	5	5	7.326×10^{-17}
15	HCl	324	20.24	8454.45	2	7	14	1.709×10^{-17}
16	HBr	398	16.23	9758.56	2	8	16	6.187×10^{-18}
17	HI	237	12.50	8487.30	1	9	9	1.096×10^{-18}
18	ClO	6038	0.01	886.21	2	4	8	1.160×10^{-18}
19	OCS	4096	493.26	4117.99	3	19	21	1.068×10^{-16}
20	H_2CO	2702	0.00	2998.52	3	8	10	2.326×10^{-17}
s 20	H_2CO	587	1707.09	1781.38	1	1	1	7.195×10^{-18}
21	HOCl	15371	0.02	3799.68	2	4	8	3.235×10^{-17}
s 22	HO_2	6820	1032.06	3675.81	1	4	4	1.795×10^{-17}
23	H_2O_2	5444	0.15	1499.48	1	2	2	1.872×10^{-17}
s 24	HONO	2348	779.12	1711.70	1	1	1	2.059×10^{-17}
c 25	HO_2NO_2		802.	804. (at 220K)				1.66×10^{-17}
c 26	N_2O_5		1210.	1275.				4.21×10^{-17}
s 27	$ClONO_2$	23264	763.64	1309.99	2	3	4	3.113×10^{-17}
28	HCN	772	2.87	3421.96	3	6	8	3.086×10^{-17}
s 29	CH_3F	739	987.91	1089.13	1	1	1	1.806×10^{-17}
30	CH_3Cl	10432	661.79	3172.92	2	4	8	5.783×10^{-18}
s 30	CH_3Cl	621	1324.69	1460.14	2	2	3	1.163×10^{-18}
c 31	CF_4		1255.0	1289.				1.61×10^{-16}
c 32	CCl_2F_2		810.	965.				5.95×10^{-17}
c 33	CCl_3F		810.	880.				6.95×10^{-17}
s 34	CH_3CCl_3	251	1382.50	1385.00	1	1	1	1.25×10^{-19}
c 35	CCl_4		770.00	809.99				5.14×10^{-17}
36	COF_2	33932	725.00	1981.27	1	7	7	1.195×10^{-16}
s 37	CFClO	2449	764.11	1907.92	1	2	2	3.957×10^{-17}
38	C_2H_6	10000	745.22	951.65	1	1	1	6.967×10^{-19}
s 38	C_2H_6	115	2976.63	2996.98	1	1	1	2.875×10^{-18}
40	C_2H_2	1267	638.25	3374.22	2	8	9	4.103×10^{-17}
41	N_2	120	1992.62	2625.40	1	1	1	6.719×10^{-27}
c 42	CHF_2Cl (FTS)		780.	839.				2.05×10^{-17}
c 42	CHF_2Cl (TDL)		828.95	829.16				3.11×10^{-19}
s 43	$COCl_2$	32871	828.54	1862.45	1	2	2	3.35×10^{-17}
s 44	CH_3Br	3421	871.32	1038.06	1	1	1	6.427×10^{-19}
s 45	CH_3I	2528	793.46	971.65	1	1	1	1.207×10^{-18}
s 46	HCOOH	3388	1060.96	1161.25	1	1	1	1.757×10^{-17}
47	H_2S	661	994.12	1573.81	1	1	1	7.959×10^{-20}
s 48	$CHFCl_2$	9583	785.00	1099.99	1	1	1	5.284×10^{-17}
49	HDO	8505	0.01	5507.54	2	9	10	7.694×10^{-21}
c 50	SF_6		940.42	952.23				5.243×10^{-17}

The ATMOS Main list: 694359 lines from 0 to 9999 cm^{-1}.
The ATMOS Supplemental list s: 116016 lines from 725 to 3675 cm^{-1}.
The ATMOS Cross Section list c: 8 species from 770 to 1289 cm^{-1}.

Table 2. Sample of the 1995 ATMOS Main and Supplemental Linelists[a]

Molecule	#	Iso	Position	Intensity	E	Air-γ	Self-γ	$r2$	n	Shift	V_{UP}	V_{LO}	Rotational	acc	refs
O_3	3	1	971.210600	5.010E−25	2497.4550	0.0691	0.0849	1.678E−02	0.76	0.000000	19	8	231311 241312	005	1 1 1
CO_2	2	4	971.214903	7.000E−27	1410.1167	0.0790	0.1091	7.013E−04	0.70	0.000000	9	5	R 9 425		1 1 1
O_3	3	2	971.221900	1.000E−24	1216.2510	0.0650	0.0890	1.612E−02	0.76	0.000000	5	1	52 548 53 549	002	1 1 2
COF_2	36	1	971.229400	1.361E−21	50.1023	0.0845	0.1750	0.000E+00	0.94	0.000000	10	1	12 9 4 11 9 3	000	0 111
CH_3Br	44	1	971.229500	2.040E−22	377.1063	0.1000	0.0000	0.000E+00	0.75	0.000000	27	14	33 3 33 2		
COF_2	36	1	971.229600	1.360E−21	50.1021	0.0845	0.1750	0.000E+00	0.94	0.000000	10	1	12 8 4 11 8 3	000	0 111
O_3	3	2	971.230400	8.240E−25	1245.7990	0.0651	0.0890	1.562E−02	0.76	0.000000	5	1	51 744 52 745	002	1 1 2
O_3	3	1	971.231000	4.470E−25	472.7870	0.0708	0.0914	7.651E−07	0.76	0.000000	5	1	26 621 25 818	005	1 1 1
CH_3I	45	1	971.235400	6.000E−23	854.2444	0.1000	0.0000	0.00E+00	0.75	0.000000	27	14	47 9 46 8		
O_3	3	3	971.235500	1.010E−23	667.9365	0.0692	0.0905	1.669E−02	0.76	0.000000	5	1	34 728 35 729	005	1 1 1
CH_3Br	44	1	971.239900	9.350E−23	404.9513	0.1000	0.0000	0.000E+00	0.75	0.000000	27	14	36 0 35 1		

3. Absorption Coefficients

Line parameters are difficult to obtain for some important atmospheric species such as the chlorofluorocarbons and N_2O_5. As an alternative, the remote sensing community has often relied on absorption-coefficient (or cross-section) parameters. In the mid-1980's, the work of Massie *et al.*[9] provided cross sections from pure-gas laboratory spectra at room temperature. By scaling these coefficients by the grid spacing (cm^{-1}/point value), ATMOS transformed some of these into pseudo-line parameters for the supplemental list[3] that could be used in the line-by-line calculations of the forward models within the ATMOS software. This type of transformation also permitted pressure-broadening coefficients to be applied. Later, new pure-gas spectra were obtained for a range of atmospheric temperatures by McDaniel *et al.*[10] and Cantrell *et al.*[11] so that a total of 14 heavy species could be included in the 1992 HITRAN compilation.[6,12] Although these older results can be employed for ATMOS calculations, only the N_2O_5 parameters from Cantrell *et al.*[11] and part of the CFC-22 parameters from McDaniel *et al.*[10] are being used because newer studies[13–19] are available. The current parameters that dominate ATMOS retrievals of eight heavy species are summarized in Table 7, which shows the reference, spectral range, experimental temperatures and total gas pressures, the integrated intensities, and data grid spacing (in inverse centimeters/point). For CCl_4, the new temperature-dependent parameters of Orlando *et al.*[13] are utilized. For CFC-11, CFC-12, SF_6, and the dominant part of a CFC-22 feature, more recent cross sections were obtained[14–17] from laboratory spectra of the gases broadened by N_2 at gas pressures and temperatures that correspond to those of the terrestrial atmosphere.[20] For CCl_3F (CFC-11), cross sections for the 850-cm^{-1} band reported by Li and Varanasi[14] are used. For the 922-cm^{-1} band of CCl_2F_2 (CFC-12), the work of Varanasi and Nemtchinov[15,16] is included. In the case of $CHCl_2F$ (CFC-22), the very high-resolution laser data from Varanasi[17] and Varanasi *et al.*[18] is utilized for the peak of the $2\nu_2$ Q branch at 829 cm^{-1} while the lower-resolution data from McDaniel *et al.*[10] and Massie and Goldman[12] are added to characterize the other portions of the band. Finally, the absorption coefficients at 200 K reported by May and Friedl[19] are used for the HO_2NO_2 band at 803 cm^{-1}. Several decisions were required in order to use these cross sections with the ATMOS analysis software. For example, interpolations to specific atmospheric pressures and temperatures are usually done as functions of temperature for most of the species, except for the peak absorption of $CHClF_2$, for which interpolation is done by log (pressure). If several pressures are available at a single temperature, then the data for the lowest pressure are selected. For temperatures beyond the range of the laboratory data, no extrapolations are done, and laboratory cross-section data nearest the desired temperature are used. Fits to ATMOS ATLAS 3 spectra are illustrated in Fig. 1. The top panel shows the CFC-12 (CCl_2F_2) band at 924 cm^{-1}. The P-branch region is too overlapped by HNO_3 transitions to be included in the retrieval interval. In addition, the wave-number calibration of the CFC-12 absorption coefficients was increased by 0.002 cm^{-1} to align the Q-branch features with the stronger CO_2 transitions appearing in the R branch. The bottom panel shows the CFC-11 (CCl_3F) band at 849 cm^{-1}. The sharp peaks between 856 and 870 cm^{-1} arise from HNO_3, whereas the structures between 830 and 850 cm^{-1} are due to CO_2 and O_3. For CFC-11, no wave-number adjustment has been applied. It is emphasized that the content of the absorption-coefficient database is continually changing. For example, the new data of Newnham *et al.*[21] for the room-temperature data for N_2O_5, the Menoux *et al.* study[22] for collision-induced N_2–N_2 and N_2–O_2, and the temperature-dependent and pressure-broadened cross sections of CF_4 from Varanasi[23] and $CHCl_2F$ from Varanasi *et al.*[18] are being considered for future revisions.

4. Alterations to Molecular Line Parameters

The following sections discuss the modifications made to the 1992 HITRAN database and the 1987 ATMOS supplemental linelist to create the 1995 ATMOS compilations. Table 8 gives an overview of the available studies[24–114] that were incorporated by showing the species, the region, or band that was modified according to positions ν, intensities I, or air-broadened widths γ. More detailed summaries of the resulting parameters in Tables 9 and 10 list

Table 3. Summary of Isotopes Codes and Abundances

Mol Num	Species	ISO Num	Old Code	Formula	Abundance	Mol Num	Species	ISO Num	Old Code	Formula	Abundance
1	H_2O	1	161	$H2^{16}O$	0.9973	18	ClO	1	56	$^{35}Cl^{16}O$	0.7559
		2	181	$H_2{}^{18}O$	0.002000			2	76	$^{37}Cl^{16}O$	0.2417
		3	171	$H_2{}^{17}O$	0.000372	19	OCS	1	622	$^{16}O^{12}C^{32}S$	0.9374
2	CO_2	1	626	$^{12}C^{16}O^{16}O$	0.9842			2	624	$^{16}O^{12}C^{34}S$	0.04158
		2	636	$^{13}C^{16}O^{16}O$	0.01106			3	632	$^{16}O^{13}C^{32}S$	0.01053
		3	628	$^{12}C^{16}O^{18}O$	0.003947			4	822	$^{18}O^{12}C^{32}S$	0.001880
		4	627	$^{12}C^{16}O^{17}O$	0.000734	20	H_2CO	1	126	$H_2{}^{12}C^{16}O$	0.9862
		5	638	$^{13}C^{16}O^{18}O$	0.00004434			2	136	$H_2{}^{13}C^{13}O$	0.01108
		6	637	$^{13}C^{16}O^{17}O$	0.00000825			3	128	$H_2{}^{12}C^{18}O$	0.00
		7	828	$^{12}C^{18}O^{18}O$	0.000003957	21	HOCl	1	165	$H^{16}O^{35}Cl$	0.7558
		8	728	$^{12}C^{17}O^{18}O$	0.00000147			2	167	$H^{16}O^{37}Cl$	0.2417
3	O_3	1	666	$^{16}O^{16}O^{16}O$	0.9929	22	HO_2	1		HO_2	1.0
		2	668	$^{16}O^{16}O^{18}O$	0.003982	23	H_2O_2	1	1661	H_2O_2	0.9950
		3	686	$^{16}O^{18}O^{16}O$	0.001991	24	HNO_2	1		HNO_2	1.0
		4	667	$^{16}O^{16}O^{17}O$	0.000744	25	HNO_4	1		HNO_4	1.0
		5	676	$^{16}O^{17}O^{16}O$	0.000372	26	N_2O_5	1		N_2O_5	1.0
4	N_2O	1	446	$^{14}N^{14}N^{16}O$	0.9903	27	$ClONO_2$			$ClONO_2$	1.0
		2	456	$^{14}N^{15}N^{16}O$	0.003641	28	HCN	1	124	$H^{12}C^{14}N$	0.9851
		3	546	$^{15}N^{14}N^{16}O$	0.003641			2	134	$H^{13}C^{14}N$	0.01107
		4	448	$^{14}N^{14}N^{18}O$	0.001986			3	125	$H^{12}C^{15}N$	0.003622
		5	447	$^{14}N^{14}N^{17}O$	0.000369	29	CH_3F	1		CH_3F	1.0
5	CO	1	26	$^{12}C^{16}O$	0.9865	30	CH_3Cl	1	215	$^{12}CH_3{}^{35}Cl$	0.7489
		2	36	$^{13}C^{16}O$	0.01108			2	217	$^{12}CH_3{}^{37}Cl$	0.2395
		3	28	$^{12}C^{18}O$	0.001978	31	CF4	1		CF_4	1.0
		4	27	$^{12}C^{17}O$	0.000368	32	CCl_2F_2	1		CCl_2F_2	1.0
		5	38	$^{13}C^{18}O$	0.00002222	33	CCl_3F	1		CCl_3F	1.0
6	CH_4	1	211	$^{12}CH_4$	0.9883	34	CH_3CCl_3	1		CH_3CCl_3	1.0
		2	311	$^{13}CH_4$	0.01110	35	CCl_4	1		CCl_4	1.0
		3	212	$^{12}CH_3D$	0.0006158	36	COF_2	1		COF_2	0.9865
7	O_2	1	66	$^{16}O^{16}O$	0.9953	37	COClF	1		COClF	1.0
		2	68	$^{16}O^{18}O$	0.003991	38	C_2H_6	1	1221	C_2H_6	0.9770
		3	67	$^{16}O^{17}O$	0.000742	39	C_2H_4	1		C_2H_4	1.0
8	NO	1	46	$^{14}N^{16}O$	0.9949	40	C_2H_2	1	1221	$^{12}C^{12}CH_2$	0.9776
		2	56	$^{15}N^{16}O$	0.003654			2	1231	$^{12}C^{13}CH_2$	0.02197
		3	48	$^{14}N^{18}O$	0.001993	41	N_2	1	44	N_2	0.9927
9	SO_2	1	626	$^{32}SO_2$	0.9457	42	CHF_2Cl	1		CHF_2Cl	1.0
		2	646	$^{34}SO_2$	0.04195	43	$COCl_2$	1		$COCl_2$	1.0
10	NO_2	1	646	NO_2	0.9916	44	CH_3Br	1		CH_3Br	1.0
11	NH_3	1	4111	$^{14}NH_3$	0.9959	45	CH_3I	1		CH_3I	1.0
		2	5111	$^{15}NH_3$	0.003661	46	HCOOH	1		HCOOH	1.0
12	HNO_3	1	146	HNO_3	0.9891	47	H_2S	1		$H_2{}^{32}S$	0.9499
13	OH	1	61	^{16}OH	0.9975			2		$H_2{}^{34}S$	0.049
		2	81	^{18}OH	0.002000			3		$H_2{}^{33}S$	0.001
		3	62	^{16}OD	0.0001554	48	$CHFCl_2$	1		$CHFCl_2$	1.0
14	HF	1	19	HF	0.9998						
15	HCl	1	15	$H^{35}Cl$	0.7576						
		2	17	$H^{37}Cl$	0.2423	49	HDO	1	162	$HD^{16}O$	0.0003107
16	HBr	1	19	$H^{79}Br$	0.5068			2	182	$HD^{18}O$	0.0000006
		2	11	$H^{81}Br$	0.4931						
17	HI	1	17	HI	0.9998	50	SF6	1		$^{32}SF_6$	0.9502

the molecule numbers in parentheses, vibrational bands, isotope number, the number of lines (#Lines), the minimum and the maximum wave-number ranges covered (*F*MIN, *F*MAX), the minimum and the maximum intensity ranges (*I*MIN, *I*MAX), the sum of the intensities (*S*-SUM) in $cm^{-1}/(molecule \cdot cm^{-2})$ at 296 K, and the accuracy and references codes. The tables also show the minimum and the maximum values of the air-broadened half-widths (*P*BHW, *P* MAX), self-broadened half-widths (SELF, *S*MAX), and the temperature-dependence coefficient of the air-broadened widths *n* (*N*TDP, *N*MAX). Because most of the pressure shifts are set to zero, these are not included in Table 9 and 10. The temperature-dependence coefficient is used to compute the expected linewidth by the use of

$$\gamma(P, T) = \gamma_0(P_0, T_0 = 296\ \mathrm{K})\left(\frac{296}{T}\right)^n P, \qquad (1)$$

where γ_0 is the half-width in cm^{-1}/atm at $T = 296$ K and P is pressure in atmospheres. Table 9 gives data for only the modified species in the main ATMOS linelist, whereas Table 10 summarizes all the species presently on the supplemental list. Complete summaries of the database can be ob-

Table 4. Vibrational Quantum Numbers Corresponding to Linelist Index Code V_{UP} and V_{LO}

Group 1: H_2O, O_3, SO_2, NO_2, HOCl, HDO, HO_2, H_2S (v_1, v_2, v_3)

1)	000	2)	010	3)	020	4)	100	5)	001	6)	030	7)	110	8)	011
9)	040	10)	120	11)	021	12)	200	13)	101	14)	002	15)	130	16)	031
17)	210	18)	111	19)	012	20)	041	21)	220	22)	121	23)	022	24)	300
25)	201	26)	102	27)	003	28)	131	29)	310	30)	211	31)	112	32)	013
33)	141	34)	042	35)	320	36)	221	37)	301	38)	202	39)	122	40)	023
41)	400	42)	103	43)	004	44)	151	45)	330	46)	231	47)	212	48)	311
49)	410	50)	113	51)	321	52)	222	53)	302	54)	401	55)	420	56)	123
57)	500	58)	203	59)	104	60)		61)	331	62)	213	63)	312	64)	411
65)	303	66)	402	67)	403	68)	421	69)	501	70)	313	71)	412	72)	232
73)	050	74)	060												

Group 2: CO_2 (v_1, v_2, l_2, v_3, index)

1)	00001	2)	01101	3)	10002	4)	02201	5)	10001	6)	11102	7)	03301	8)	11101
9)	00011	10)	20003	11)	12202	12)	20002	13)	04401	14)	12201	15)	20001	16)	01111
17)	21103	18)	13302	19)	21102	20)	05501	21)	13301	22)	21101	23)	10012	24)	02211
25)	10011	26)	30004	27)	22203	28)	14402	29)	30003	30)	22202	31)	06601	32)	30002
33)	14401	34)	22201	35)	30001	36)	11112	37)	03311	38)	11111	39)	00021	40)	31104
41)	31103	42)	31102	43)	20013	44)	12212	45)	23301	46)	31101	47)	04411	48)	20012
49)	12211	50)	20011	51)	01121	52)	40004	53)	32203	54)	21113	55)	40002	56)	13312
57)	05511	58)	21112	59)	13311	60)	21111	61)	10022	62)	02221	63)	10021	64)	30014
65)	22213	66)	14412	67)	41102	68)	30013	69)	06611	70)	22212	71)	30012	72)	41101
73)	14411	74)	22211	75)	30011	76)	11122	77)	03321	78)	11121	79)	00031	80)	31114
81)	23313	82)	31113	83)	23312	84)	31112	85)	15511	86)	20023	87)	23311	88)	12222
89)	31111	90)	20022	91)	12221	92)	20021	93)	01131	94)	40015	95)	32214	96)	40014
97)	32213	98)	40013	99)	51102	100)	32212	101)	40012	102)	21123	103)	32211	104)	21122
105)	40011	106)	21121	107)	10032	108)	02231	109)	10031	110)	41114	111)	41113	112)	41112
113)	11132	114)	03331	115)	11131	116)	20033	117)	12232	118)	20032	119)	12231	120)	20031
121)	21133	122)	21132	123)	21131	124)	23303	125)	15502	126)	23302	127)	07701		

Group 3: N_2O, OCS, HCN (v_1, v_2, l_2, v_3)

1)	0000	2)	0110	3)	0200	4)	0220	5)	1000	6)	0310	7)	0330	8)	1110
9)	0400	10)	0420	11)	1200	12)	1220	13)	2000	14)	0001	15)	0510	16)	1310
17)	1330	18)	2110	19)	0111	20)	1400	21)	1420	22)	2200	23)	2220	24)	3000
25)	0201	26)	0221	27)	1001	28)	2310	29)	3110	30)	0311	31)	0331	32)	1111
33)	4000	34)	3200	35)	2001	36)	1201	37)	1221	38)	0002	39)	2111	40)	0112
41)		42)	0600	43)	0620										

Group 4: CO, HF, HCl, HBr, HI, N_2

1)	0	2)	1	3)	2	4)	3	5)	4	6)	5

Group 5: CH_4, CF_4, CCl_4, SF_6, CH_3D, CH_3Cl, CH_3Br, CH_3I, CH_3F, C_2H_6, HNO_3, HONO, HCOOH, N_2O_5, $ClONO_2$, CCl_2F_2, CCl_3F, CHF_2Cl, $CHFCl_2$

1)	00000000	2)	00000111	3)	01100001	4)	00000202	5)	00000222	6)	01100112
7)	10000000	8)	00011001	9)	02200002	10)	10000111	11)	00011112	12)	01111002
13)	00022002	14)	GROUND	15)	V1	16)	V2	17)	V4	18)	V5
19)	V9	20)	2V5	21)	2V9	22)	3V6	23)	3V9	24)	V5+V9
25)		26)	V6	27)	V3	28)	2V6	29)	00000333	30)	00011223
31)	V7	32)	V8	33)	V8+V9						

Group 6: O_2

1)	X0	2)	X1	3)	A0	4)	A1	5)	B0	6)	B1	7)	B2

Group 7: NO, OH, ClO

1)	X3/2 0	2)	X3/2 1	3)	X3/2 2	4)	X3/2 3	5)	X3/2 4	6)	X3/2 5	7)	X3/2 6	8)	X3/2 7
9)	X3/2 8	10)	X3/2 9	11)	X1/2 0	12)	X1/2 1	13)	X1/2 2	14)	X1/2 3	15)	X1/2 4	16)	X1/2 5
17)	X1/2 6	18)	X1/2 7	19)	X1/2 8	20)	X1/2 9								

Group 8: NH_3 (v_1, v_2, v_3, v_4, inversion)

1)	0000	2)	0100	3)	0200	4)	0001	5)	0000A	6)	0100A	7)	0200A
8)	0001A	9)	0000S	10)	0100S	11)	0200S	12)	0001S				

Group 9: H_2CO, H_2O_2, COF_2, $COCl_2$, COClF (v_1, v_2, v_3, v_4, v_5, v_6)

1)	000000	2)	000002	3)	001100	4)	001001	5)	100000	6)	000010	7)	010100	8)	010001
9)	000001	10)	010000	11)	000100	12)	020000	13)		14)	002001	15)	000020		

Group 10: C_2H_2 (v_1, v_2, v_3, l_3, v_4, l_4, v_5, l_5)

1)	00000000	2)	00000111	3)	00100000	4)	01011110	5)	00011001	6)	
7)	00011110	8)	00011112	9)	00000200	10)	00000222				

Table 5. Definition of the Accuracy Codes

Wave Number		Intensity and Half-Width	
ACC	Error Range	ACC	Error Range
0	≥1. or undefined	0	Undefined
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%

tained from L. Brown. The individual modifications are described below in order of molecular number. Entries for H_2CO, HONO, CH_3F, CH_3CCl_3, CH_3Br, CH_3I, and $CHFCl_2$ in the supplemental list have not changed and are described in the 1987 article.[3]

H_2O (1)

Two changes were made to the H_2O parameters. In the 10-μm region, 39 experimental intensities and 81 air-broadened linewidths from Rinsland *et al.*[24] replaced some of the calculated values for the stronger rotational and ν_2 transitions from 800 to 1100 cm^{-1}. At 3 μm, measured intensities of Toth[25] from 3003 to 4260 cm^{-1} were used for 542 transitions of the $2\nu_2$ band of the main isotope. Because only some of the transitions were replaced, the reference codes shown in Table 9 correspond to the unchanged lines. The reference codes for the altered features are 011111 and 7 7 0, respectively. Other recent measurements of Toth[26,27] have not yet been included.

O_3 (3)

The ozone parameters were updated significantly for the 1992 HITRAN list.[28] For the updated ATMOS main list, some bands were revised, and new entries were added for 36 bands to extend the ozone catalog to 4060 cm^{-1}. The (004) and (310) bands at 2.5 μm and the (103) band at 2.7 μm were included.[29,30] At 3.4 μm, eight hot bands were added between 2841 and 3102 cm^{-1}.[31] At 5.5 μm, the $3\nu_3–\nu_1$ hot band was revised, and at 10 μm, several hot bands were merged.[32] At 17 μm, calculated ν_2 parameters for $^{16}O^{16}O^{17}O$ and $^{16}O^{17}O^{16}O$ were incorporated.[33] However, the scaling of all ozone intensities by some 5% as inferred from the measurements of Pickett *et al.*[34] has been deferred until after confirmation by other investigators. The reference and accuracy codes of the altered transitions are indicated in Table 9. Some more recent studies[35–38] have not been included.

N_2O (4)

The previous N_2O on all the databases were either old predictions from the 1982 AFGL tape[5] for the 500–727- and the 3293–5131-cm^{-1} regions or a composite list prepared by Toth[39] in 1985 for the 894–2839-cm^{-1} interval. For the 1995 ATMOS linelist, transitions between 3046 and 3493 cm^{-1} were revised by replacing six existing bands and adding 26 missing bands by the use of the work of Toth.[40] Modified entries are listed with reference codes of 1 1 1.

CH_3D (6)

The intensities of the CH_3D triad of ν_6, ν_3, and ν_5 between 970 and 1693 cm^{-1} were recalculated to include the intensities results of Tarrago *et al.*[41] The air-broadened widths were set to 0.08 cm^{-1}/atm and the self-broadened to 0.09 cm^{-1}/atm. The CH_3D parameters in the 3.3-μm region that are used for ATMOS retrievals have not been revised since 1982, however. The intensity measurements of five ν_4 lines reported by Rinsland *et al.*[42] have not been included in the expectation that an ongoing study[43] will provide a global revision of the 3.3-μm CH_3D.

Table 6. Molecule Numbers on the ATMOS (A), HITRAN (H), and GEISA[a] (G) Databases

Species	A	H	G	Species	A	H	G	Species	A	H	G
H_2O	1	1	1	ClO	18	18	19	CCl_4	35	0	0
CO_2	2	2	2	OCS	19	19	20	COF_2	36	29	38
O_3	3	3	3	H_2CO	20	20	21	CFClO	37	0	0
N_2O	4	4	4	HOCl	21	21	32	C_2H_6	38	27	22
CO	5	5	5	HO_2	22	0	0	C_2H_4	39	0	25
CH_4	6	6	6	H_2O_2	23	25	35	C_2H_2	40	26	24
O_2	7	7	7	HONO	24	0	0	N_2	41	22	33
NO	8	8	8	HO_2NO_2	25	0	0	CHF_2Cl	42	0	0
SO_2	9	9	9	N_2O_5	26	0	0	$COCl_2$	43	0	0
NO_2	10	10	10	$ClONO_2$	27	0	0	CH_3Br	44	0	0
NH_3	11	11	11	HCN	28	23	27	CH_3I	45	0	0
HNO_3	12	12	13	CH_3F	29	0	0	HCOOH	46	32	37
OH	13	13	14	CH_3Cl	30	24	34	H_2S	47	31	36
HF	14	14	15	CF_4	31	0	0	$CHFCl_2$	48	0	0
HCl	15	15	16	CCl_2F_2	32	0	0	HDO	49	1	1
HBr	16	16	17	CCl_3F	33	0	0	SF_6	50	30	39
HI	17	17	18	CH_3CCl_3	34	0	0	CH_3D	6	6	23

[a]GEISA species Ge_4, C_3H_8, C_2N_2, C_4H_2, HC_3N, C_3H_4, and PH_3 are excluded from the ATMOS lists.

Table 7. Summary of Absorption Cross Sections used for ATMOS Retrievals

Molecule	Ref.	Spectral Range	Temp.	Press.	Integrated Strength	Grid
CCl_2F_2	15,16	810.04 - 964.98	216	0.2236	5.9510^{-17}	0.010
		810.04 - 964.93	233	0.2595	5.9410^{-17}	
		810.06 - 964.93	245	0.4675	5.9310^{-17}	
		810.05 - 964.96	260	0.8612	5.9410^{-17}	
		810.02 - 964.98	273	0.6509	5.9010^{-17}	
		810.08 - 964.97	284	0.6845	5.8910^{-17}	
		810.01 - 964.96	296	0.9214	5.9510^{-17}	
CCl_3F	14	810.01 - 879.98	215	0.2242	6.8810^{-17}	0.012
			225	0.2278	6.8910^{-17}	
			233	0.3299	6.8510^{-17}	
			246	0.3800	6.8610^{-17}	
			272	0.7242	6.9210^{-17}	
			284	0.6857	6.9510^{-17}	
			296	0.9991	6.9510^{-17}	
CHF_2Cl	10	780.01 - 840.00	203	N/A	1.8810^{-17}	0.015
			213		1.9010^{-17}	
(FTS)			233		1.9410^{-17}	
			253		1.9910^{-17}	
			273		2.0110^{-17}	
			293		2.0510^{-17}	
	17	828.95 - 829.16	216	0.0527	4.4710^{-19}	0.00026
		828.95 - 829.16	216	0.1017	4.4910^{-19}	
(TDL)		828.95 - 829.16	216	0.1480	4.4010^{-19}	
		828.95 - 829.16	216	0.2369	4.2710^{-19}	
		828.94 - 829.19	236	0.3548	4.2510^{-19}	
		828.94 - 829.19	252	0.5288	3.7910^{-19}	
		828.94 - 829.18	292	0.9983	3.1110^{-19}	
HO_2NO_2	19	769.99 - 834.99	220	N/A	1.7210^{-17}	0.00247
N_2O_5	11	1210.15 - 1275.76	233	N/A	3.8910^{-17}	0.482
			253		4.0610^{-17}	
			273		4.0910^{-17}	
			293		4.2110^{-17}	
CCl_4	13	770.01 - 809.99	170	N/A	4.9010^{-17}	0.0048
			223		4.9510^{-17}	
			248		5.0710^{-17}	
			273		5.0610^{-17}	
			298		5.1010^{-17}	
			310		5.1410^{-17}	
CF_4	10	1255.01 - 1289.99	203	N/A	1.5210^{-16}	0.015
			213		1.6510^{-16}	
			233		1.5910^{-16}	
			253		1.6510^{-16}	
			273		1.6210^{-16}	
			293		1.6110^{-16}	
SF_6	18	925.00 - 955.00	295	1.00	2.0710^{-16}	0.010
			273	0.723	2.0510^{-16}	
			246	0.468	2.0910^{-16}	
			216	0.0329	2.5510^{-16}	

O_2 (7)

Predictions of the 6-μm transitions arising from the electric quadrupole and magnetic dipole were added, respectively, to the main[44] and the supplemental[45] lists with air- and self-broadened coefficients set to 0.042 and 0.065 cm^{-1}/atm, respectively. A constant value of 0.75 is used for the air-broadened widths' temperature coefficient.

NO (8)

The positions and the intensities of the 1–0 band and the widths of infrared transitions were modified by

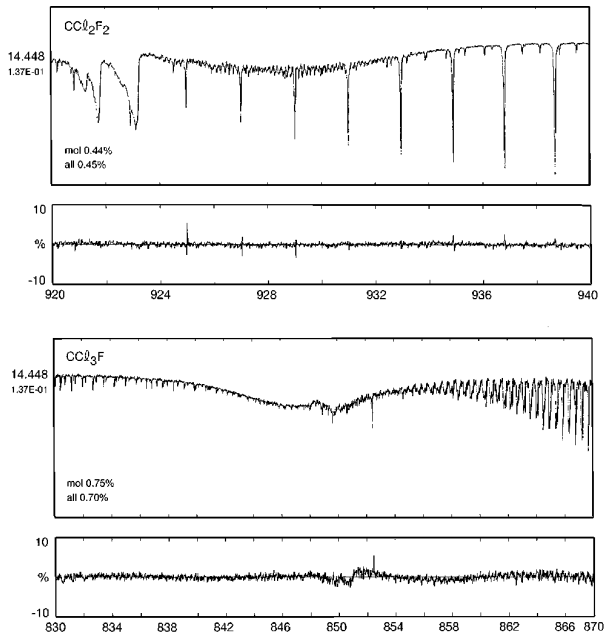

Fig. 1. Modeling of the atmospheric absorption of CFC-12 (top) and CFC-11 (bottom) in ATMOS data by the use of laboratory cross sections.[14–16] The tangent altitude is 14.4 km. The Q and R branches of the CCl_2F_2 band at 924 cm^{-1} are overlapped by the strong CO_2 transitions. The R branch of the CCl_3F band near 850 cm^{-1} is overlapped by manifolds of HNO_3 between 856 and 870 cm^{-1}, and the Q branch is overlapped by weak CO_2 and O_3 transitions.

the use of the work of Spencer *et al.*[46] The new line positions are systematically lower compared with those of the 1992 values: from 0.0003 cm^{-1} at low J and to 0.001 cm^{-1} at $J = 22$. The new intensities of the P and the R branches are 3.6% higher between P 13.5 and R 19.5, but the Q-branch transitions and the higher m P and R branch lines are 8% lower compared with those of the 1992 HITRAN values.[6] Because air and O_2 measurements are not generally available, the linewidths are N_2-broadening coefficient values from Spencer *et al.*[46] The temperature dependences of the widths are set to a constant 0.71. The new measurements are only 1% to 4% different from the prior Ballard *et al.* results[47] that were used in the 1992 HITRAN update.

NO_2 (10)

The 6-μm region was revised for the 1538–1640-cm^{-1} interval by the replacement of an older prediction in the 1992 HITRAN with an experimental linelist from Toth[48] that included transitions of ν_3, $2\nu_2$, and ν_3–ν_2. Linewidths were set to the default values on HITRAN of $\gamma_{air} = 0.067\ cm^{-1}/atm$, $\gamma_{self} = 0.0$, and the temperature coefficient = 0.75, based on the work of Devi *et al.*[49] and May and Webster.[50] The reference codes for these changes are 4 4 1. The more recent work of Perrin *et al.*[51,52] has not yet been incorporated.

HNO_3 (12)

The bands near 11 and 7.5 μm were revised substantially. In the first region, the prediction of the ν_5, $2\nu_9$ parameters of Perrin *et al.*[53,54] replaced the line positions and the relative intensities by Maki and Wells.[55] Approximate parameters for the 11-μm hot bands[56] were moved to the supplemental linelist.

Table 8. Differences between the 1995 ATMOS and 1992 HITRAN Databases

Species	Region	ν	I	γ	References
H_2O	Replace some $2\nu_2$ lines at 3 μm		*		25
	Replace some rotational lines 12–8.7 μm		*	*	24
O_3	10-, 3.3-, 2.7-, 2.5-, and 14-μm isotopes	*	*		29–33
N_2O	3.3- to 3.0-μm bands	*	*	*	39, 40
CH_3D	ν_3, ν_5, ν_6, triad at 7–9 μm		*		41
O_2	6 μm	*	*		44, 45
NO	1–0 (all) and all widths above 1600 cm^{-1}	*	*	*	46
NO_2	6 μm (ν_3, $2\nu_2$, $\nu_2 + \nu_3 - \nu_2$) bands	*	*	*	48–50
HNO_3	ν_5, $2\nu_9$ (11 μm)	*	*		53, 54
	ν_2, ν_3, ν_4 regions intensities scaled		*		56–59
HF	1–0 positions * 0.9999998936 (±13)	*			61, 63
HCl	All bands	*			64–66
ClO	1–0 near 12 μm	*	*		69–73
OCS	500–4100 cm^{-1} for 21 bands	*	*	*	74–78
HOCl	ν_2, ν_3 near 14 μm, 8.1-μm region	*			80
HO_2	fundamentals 3–9 μm	*	*		81–84
$ClONO_2$	ν_4 near 13 μm	*	*	*	85–89
CH_3Cl	ν_3 near 15 μm	*	*		92, 93
	ν_5 RQ_0 branch only	*	*		94, 95
COClF	Approximate parameters for ν_1 at 5.5 μm	*			Present
C_2H_6	ν_9 near 12 μm		*		102–103
	1987 3-μm Q branches + PQ_3	*	*		104–107
C_2H_2	3 μm	*	*		110
$COCl_2$	ν_1, ν_5 bands near 5.5 and 11 μm	*	*		114
$HD^{18}O$	ν_2 near 7.2 μm	*	*		3

Table 9. Summary of Alterations to the Main ATMOS Linelist

Species		#ISO	#Lines	FMIN cm^{-1}	FMAX cm^{-1}	IMIN cm^{-1}	IMAX /(molecule × cm^{-2})	S-SUM	ACC	REF	PBHW (cm^{-1}/atm)	PMAX (cm^{-1}/atm)	SELF	SMAX	NTDP	NMAX
H_2O	(1)															
000	000	1	1731	0.401	1647.767	1.01E-32	2.67E-18	5.268E-17	000	0 0 0	0.008	0.105	0.000	0.000	0.64	0.64
020	000	1	1132	2565.280	4338.475	1.00E-26	2.98E-21	8.161E-20	000	0 0 0	0.009	0.105	0.000	0.000	0.64	0.64
O_3	(3)															
010	000	4	5641	584.251	820.380	3.51E-27	5.57E-25	3.804E-22	450	5 5 0	0.065	0.087	0.079	0.112	0.76	0.76
010	000	5	2846	591.161	822.795	3.52E-27	6.06E-25	2.075E-22	450	5 5 0	0.065	0.087	0.079	0.112	0.76	0.76
102	101	1	1130	922.344	1002.238	9.94E-26	2.69E-24	8.293E-22	450	4 4 0	0.065	0.087	0.083	0.111	0.76	0.76
003	101	1	192	931.056	1004.900	9.93E-26	6.38E-25	4.092E-23	450	4 4 0	0.067	0.082	0.088	0.101	0.76	0.76
201	200	1	791	931.896	1008.602	9.92E-26	9.81E-25	2.941E-22	450	4 4 0	0.067	0.087	0.088	0.112	0.76	0.76
003	002	1	1364	935.836	1020.250	9.90E-26	5.16E-24	1.666E-21	450	4 4 0	0.065	0.087	0.081	0.112	0.76	0.76
102	002	1	206	940.504	1014.917	9.95E-26	6.37E-25	4.723E-23	450	4 4 0	0.067	0.082	0.087	0.099	0.76	0.76
300	101	1	196	1159.487	1208.161	9.98E-26	1.83E-25	2.671E-23	450	4 4 0	0.071	0.084	0.097	0.109	0.76	0.76
003	100	1	1270	1863.333	2093.154	1.00E-25	3.90E-24	1.234E-21	450	4 4 0	0.065	0.087	0.083	0.112	0.76	0.76
102	100	1	1132	1885.468	2064.958	1.00E-25	2.31E-24	3.704E-22	450	4 4 0	0.065	0.086	0.081	0.111	0.76	0.76
003	001	1	1861	1894.594	2088.217	1.00E-25	1.22E-23	1.507E-21	450	4 4 0	0.065	0.087	0.082	0.111	0.76	0.76
102	001	1	2159	1966.935	2066.712	1.02E-25	4.32E-23	1.469E-20	450	4 4 0	0.064	0.087	0.076	0.111	0.76	0.76
201	100	1	1968	1999.192	2132.692	1.00E-25	3.00E-23	1.041E-20	450	4 4 0	0.064	0.087	0.078	0.112	0.76	0.76
201	001	1	948	2014.848	2204.232	1.00E-25	1.91E-24	2.468E-22	450	4 4 0	0.066	0.086	0.080	0.110	0.76	0.76
300	100	1	849	2101.905	2251.240	1.00E-25	1.72E-24	2.174E-22	450	4 4 0	0.065	0.084	0.086	0.110	0.76	0.76
300	001	1	1075	2210.164	2302.772	1.01E-25	2.73E-24	8.457E-22	450	4 4 0	0.066	0.087	0.083	0.111	0.76	0.76
103	100	1	970	2841.156	2930.506	1.00E-25	1.83E-24	5.530E-22	450	2 2 0	0.065	0.087	0.085	0.112	0.76	0.76
103	001	1	200	2873.465	3019.922	1.00E-25	2.54E-24	1.040E-22	450	2 2 0	0.066	0.084	0.086	0.108	0.76	0.76
310	100	1	15	2877.462	2927.423	1.01E-25	3.26E-25	2.731E-24	450	2 2 0	0.071	0.078	0.093	0.104	0.76	0.76
004	100	1	125	2877.632	2972.559	1.01E-25	7.59E-25	2.611E-23	450	2 2 0	0.069	0.084	0.086	0.106	0.76	0.76
004	001	1	1452	2878.938	2992.258	1.00E-25	9.18E-24	2.941E-21	450	2 2 0	0.065	0.087	0.081	0.111	0.76	0.76
310	001	1	142	2882.411	2974.307	1.01E-25	7.88E-25	2.670E-23	450	2 2 0	0.065	0.077	0.086	0.104	0.76	0.76
013	010	1	1639	2902.203	3049.761	1.00E-25	1.22E-23	4.026E-21	450	2 2 0	0.065	0.087	0.080	0.112	0.76	0.76
112	010	1	636	2923.918	3102.695	1.00E-25	1.76E-24	1.707E-22	450	2 2 0	0.065	0.084	0.088	0.109	0.76	0.76
003	000	1	3394	2926.875	3192.978	1.00E-25	4.05E-22	1.306E-19	450	4 4 0	0.064	0.087	0.072	0.112	0.76	0.76
102	000	1	3103	2938.639	3175.149	1.00E-25	6.65E-23	1.231E-20	450	4 4 0	0.064	0.087	0.076	0.112	0.76	0.76
201	000	1	2094	2967.273	3204.319	1.00E-25	2.81E-23	9.702E-21	450	4 4 0	0.064	0.087	0.078	0.112	0.76	0.76
300	000	1	1155	3190.171	3357.246	1.00E-25	2.55E-24	3.902E-22	450	4 4 0	0.065	0.086	0.084	0.111	0.76	0.76
103	010	1	461	3273.600	3332.613	1.01E-25	4.13E-25	9.687E-23	450	4 4 0	0.068	0.086	0.092	0.111	0.76	0.76
004	010	1	14	3294.749	3331.276	1.03E-25	1.20E-25	1.535E-24	450	4 4 0	0.072	0.082	0.098	0.105	0.76	0.76
310	010	1	1	3327.465	3327.465	1.06E-25	1.06E-25	1.060E-25	450	4 4 0	0.072	0.072	0.094	0.094	0.76	0.76
013	000	1	1736	3595.887	3748.539	1.01E-25	1.96E-23	6.146E-21	450	3 3 0	0.065	0.087	0.079	0.112	0.76	0.76
112	000	1	485	3624.469	3762.052	1.00E-25	2.83E-24	1.383E-22	450	3 3 0	0.065	0.081	0.081	0.106	0.76	0.76
004	000	1	681	3892.776	4060.783	1.00E-25	1.29E-23	5.741E-22	450	2 2 0	0.065	0.085	0.088	0.109	0.76	0.76
310	000	1	1219	3894.373	4049.936	1.00E-25	7.90E-24	4.463E-22	450	2 2 0	0.065	0.087	0.088	0.112	0.76	0.76
103	000	1	2150	3912.153	4032.648	1.00E-25	4.33E-23	1.378E-20	450	2 2 0	0.064	0.087	0.077	0.112	0.76	0.76
N_2O	(4)															
1310	0000	1	60	3046.220	3074.625	1.09E-24	2.73E-24	1.221E-22	466	1 1 1	0.070	0.089	0.085	0.116	0.75	0.82
0002	1000	1	58	3101.829	3154.201	1.03E-24	2.71E-24	1.144E-22	466	1 1 1	0.071	0.089	0.086	0.116	0.75	0.82
2110	0000	1	81	3162.794	3197.532	1.05E-24	7.12E-24	3.262E-22	466	1 1 1	0.069	0.093	0.080	0.121	0.73	0.82
0201	0000	2	59	3266.276	3320.368	1.05E-24	2.73E-24	1.183E-22	466	1 1 1	0.071	0.089	0.086	0.116	0.75	0.82
1111	0200	1	91	3280.070	3355.758	1.01E-24	1.52E-23	7.431E-22	466	1 1 1	0.069	0.097	0.080	0.127	0.73	0.82
1111	0220	1	172	3280.981	3353.934	1.01E-24	1.06E-23	1.016E-21	466	1 1 1	0.070	0.093	0.081	0.121	0.75	0.82
2111	0330	1	121	3281.457	3482.857	1.01E-24	1.10E-23	5.725E-22	466	1 1 1	0.070	0.090	0.081	0.119	0.75	0.82
0311	0110	1	260	3285.230	3383.462	1.02E-24	1.51E-22	1.506E-20	466	1 1 1	0.069	0.097	0.077	0.127	0.73	0.82
2111	0310	1	34	3288.513	3321.113	1.01E-24	1.14E-24	3.649E-23	466	1 1 1	0.074	0.080	0.097	0.105	0.75	0.77
0201	0000	1	136	3295.982	3408.309	1.08E-24	1.65E-21	8.290E-20	466	1 1 1	0.069	0.097	0.076	0.127	0.73	0.82
0201	0000	3	81	3296.447	3363.125	1.03E-24	7.52E-24	3.686E-22	466	1 1 1	0.070	0.093	0.082	0.121	0.75	0.82
0201	0000	4	82	3307.838	3373.540	1.02E-24	6.72E-24	3.332E-22	466	1 1 1	0.070	0.093	0.082	0.121	0.75	0.82
1201	1000	1	71	3310.979	3373.094	1.06E-24	4.51E-24	2.136E-22	466	1 1 1	0.070	0.090	0.083	0.119	0.75	0.82
0221	0000	1	82	3319.826	3414.419	1.04E-24	7.16E-24	3.204E-22	466	1 1 1	0.069	0.077	0.077	0.101	0.73	0.82
1001	0000	2	112	3370.824	3462.689	1.02E-24	1.15E-22	5.722E-21	466	1 1 1	0.069	0.097	0.078	0.127	0.73	0.82
1001	0000	4	109	3378.948	3463.967	1.02E-24	5.82E-23	2.981E-21	466	1 1 1	0.069	0.097	0.078	0.127	0.73	0.82
1001	0000	3	115	3381.794	3473.528	1.04E-24	1.23E-22	6.218E-21	466	1 1 1	0.069	0.097	0.077	0.127	0.73	0.82
1111	0110	2	158	3382.909	3448.822	1.02E-24	6.92E-24	6.575E-22	466	1 1 1	0.070	0.097	0.082	0.127	0.75	0.82
2001	1000	1	112	3384.988	3476.512	1.02E-24	1.13E-22	5.624E-21	466	1 1 1	0.069	0.097	0.078	0.127	0.73	0.82
1001	0000	1	156	3386.212	3513.862	1.03E-24	3.31E-20	1.650E-18	466	1 1 1	0.069	0.097	0.070	0.127	0.73	0.82
1111	0110	1	338	3394.709	3506.679	1.03E-24	1.86E-21	1.854E-19	466	1 1 1	0.069	0.097	0.076	0.127	0.73	0.82
1111	0110	4	130	3396.960	3452.701	1.02E-24	3.42E-24	3.098E-22	466	1 1 1	0.070	0.089	0.085	0.116	0.75	0.82

The intensities of the ν_5 and $2\nu_9$ near 900 cm^{-1} and ν_4 and ν_3 near 1300 cm^{-1} were renormalized by the use of Goldman *et al.*[57] and Giver *et al.*,[58] unpublished laboratory data and ATMOS atmospheric data. There are considerable differences in absolute intensity studies; for the interim, it is thought that the normalization selected here sets the relative band intensities to within ±10%, but the absolute uncertainties for the integrated band intensities may be 10% to 15%. The relative intensities within bands

Table 9. (**continued**)

Species		#ISO	#Lines	FMIN cm^{-1}	FMAX cm^{-1}	IMIN cm^{-1}	IMAX /(molecule × cm^{-2})	S-SUM	ACC	REF	PBHW (cm^{-1}/atm)	PMAX (cm^{-1}/atm)	SELF (cm^{-1}/atm)	SMAX	NTDP	NMAX
H_2O	(1)															
000	000	1	1731	0.401	1647.767	1.01E-32	2.67E-18	5.268E-17	000	0 0 0	0.008	0.105	0.000	0.000	0.64	0.64
020	000	1	1132	2565.280	4338.475	1.00E-26	2.98E-21	8.161E-20	000	0 0 0	0.009	0.105	0.000	0.000	0.64	0.64
O_3	(3)															
010	000	4	5641	584.251	820.380	3.51E-27	5.57E-25	3.804E-22	450	5 5 0	0.065	0.087	0.079	0.112	0.76	0.76
010	000	5	2846	591.161	822.795	3.52E-27	6.06E-25	2.075E-22	450	5 5 0	0.065	0.087	0.079	0.112	0.76	0.76
102	101	1	1130	922.344	1002.238	9.94E-26	2.69E-24	8.293E-22	450	4 4 0	0.065	0.087	0.083	0.111	0.76	0.76
003	101	1	192	931.056	1004.900	9.93E-26	6.38E-25	4.092E-23	450	4 4 0	0.067	0.082	0.088	0.101	0.76	0.76
201	200	1	791	931.896	1008.602	9.92E-26	9.81E-25	2.941E-22	450	4 4 0	0.067	0.087	0.088	0.112	0.76	0.76
003	002	1	1364	935.836	1020.250	9.90E-26	5.16E-24	1.666E-21	450	4 4 0	0.065	0.087	0.081	0.112	0.76	0.76
102	002	1	206	940.504	1014.917	9.95E-26	6.37E-25	4.723E-23	450	4 4 0	0.067	0.082	0.087	0.099	0.76	0.76
300	101	1	196	1159.487	1208.161	9.98E-26	1.83E-25	2.671E-23	450	4 4 0	0.071	0.084	0.097	0.109	0.76	0.76
003	100	1	1270	1863.333	2093.154	1.00E-25	3.90E-24	1.234E-21	450	4 4 0	0.065	0.087	0.083	0.112	0.76	0.76
102	100	1	1132	1885.468	2064.958	1.00E-25	2.31E-24	3.704E-22	450	4 4 0	0.065	0.086	0.081	0.111	0.76	0.76
003	001	1	1861	1894.594	2088.217	1.00E-25	1.22E-23	1.507E-21	450	4 4 0	0.065	0.087	0.082	0.111	0.76	0.76
102	001	1	2159	1966.935	2066.712	1.02E-25	4.32E-23	1.469E-20	450	4 4 0	0.064	0.087	0.076	0.111	0.76	0.76
201	100	1	1968	1999.192	2132.692	1.00E-25	3.00E-23	1.041E-20	450	4 4 0	0.064	0.087	0.078	0.112	0.76	0.76
201	001	1	948	2014.848	2204.232	1.00E-25	1.91E-24	2.468E-22	450	4 4 0	0.066	0.086	0.080	0.110	0.76	0.76
300	100	1	849	2101.905	2251.240	1.00E-25	1.72E-24	2.174E-22	450	4 4 0	0.065	0.084	0.086	0.110	0.76	0.76
300	001	1	1075	2210.164	2302.772	1.01E-25	2.73E-24	8.457E-22	450	4 4 0	0.066	0.087	0.083	0.111	0.76	0.76
103	100	1	970	2841.156	2930.506	1.00E-25	1.83E-24	5.530E-22	450	2 2 0	0.065	0.087	0.085	0.112	0.76	0.76
103	001	1	200	2873.465	3019.922	1.00E-25	2.54E-24	1.040E-22	450	2 2 0	0.066	0.084	0.086	0.108	0.76	0.76
310	100	1	15	2877.462	2927.423	1.01E-25	3.26E-25	2.731E-24	450	2 2 0	0.071	0.078	0.093	0.104	0.76	0.76
004	100	1	125	2877.632	2972.559	1.01E-25	7.59E-25	2.611E-23	450	2 2 0	0.069	0.084	0.086	0.106	0.76	0.76
004	001	1	1452	2878.938	2992.258	1.00E-25	9.18E-24	2.941E-21	450	2 2 0	0.065	0.087	0.081	0.111	0.76	0.76
310	001	1	142	2882.411	2974.307	1.01E-25	7.88E-25	2.670E-23	450	2 2 0	0.065	0.077	0.086	0.104	0.76	0.76
013	010	1	1639	2902.203	3049.761	1.00E-25	1.22E-23	4.026E-21	450	2 2 0	0.065	0.087	0.080	0.112	0.76	0.76
112	010	1	636	2923.918	3102.695	1.00E-25	1.76E-24	1.707E-22	450	2 2 0	0.065	0.084	0.088	0.109	0.76	0.76
003	000	1	3394	2926.875	3192.978	1.00E-25	4.05E-22	1.306E-19	450	4 4 0	0.064	0.087	0.072	0.112	0.76	0.76
102	000	1	3103	2938.639	3175.149	1.00E-25	6.65E-23	1.231E-20	450	4 4 0	0.064	0.087	0.076	0.112	0.76	0.76
201	000	1	2094	2967.273	3204.319	1.00E-25	2.81E-23	9.702E-21	450	4 4 0	0.064	0.087	0.078	0.112	0.76	0.76
300	000	1	1155	3190.171	3357.246	1.00E-25	2.55E-24	3.902E-22	450	4 4 0	0.065	0.086	0.084	0.111	0.76	0.76
103	010	1	461	3273.600	3332.613	1.01E-25	4.13E-25	9.687E-23	450	4 4 0	0.068	0.086	0.092	0.111	0.76	0.76
004	010	1	14	3294.749	3331.276	1.03E-25	1.20E-25	1.535E-24	450	4 4 0	0.072	0.082	0.098	0.105	0.76	0.76
310	010	1	1	3327.465	3327.465	1.06E-25	1.06E-25	1.060E-25	450	4 4 0	0.072	0.072	0.094	0.094	0.76	0.76
013	000	1	1736	3595.887	3748.539	1.01E-25	1.96E-23	6.146E-21	450	3 3 0	0.065	0.087	0.079	0.112	0.76	0.76
112	000	1	485	3624.469	3762.052	1.00E-25	2.83E-24	1.383E-22	450	3 3 0	0.065	0.081	0.081	0.106	0.76	0.76
004	000	1	681	3892.776	4060.783	1.00E-25	1.29E-23	5.741E-22	450	2 2 0	0.065	0.085	0.088	0.109	0.76	0.76
310	000	1	1219	3894.373	4049.936	1.00E-25	7.90E-24	4.463E-22	450	2 2 0	0.065	0.087	0.088	0.112	0.76	0.76
103	000	1	2150	3912.153	4032.648	1.00E-25	4.33E-23	1.378E-20	450	2 2 0	0.064	0.087	0.077	0.112	0.76	0.76
N_2O	(4)															
1310	0000	1	60	3046.220	3074.625	1.09E-24	2.73E-24	1.221E-22	466	1 1 1	0.070	0.089	0.085	0.116	0.75	0.82
0002	1000	1	58	3101.829	3154.201	1.03E-24	2.71E-24	1.144E-22	466	1 1 1	0.071	0.089	0.086	0.116	0.75	0.82
2110	0000	1	81	3162.794	3197.532	1.05E-24	7.12E-24	3.262E-22	466	1 1 1	0.069	0.093	0.080	0.121	0.73	0.82
0201	0000	2	59	3266.276	3320.368	1.05E-24	2.73E-24	1.183E-22	466	1 1 1	0.071	0.089	0.086	0.116	0.75	0.82
1111	0200	1	91	3280.070	3355.758	1.01E-24	1.52E-23	7.431E-22	466	1 1 1	0.069	0.097	0.080	0.127	0.73	0.82
1111	0220	1	172	3280.981	3353.934	1.01E-24	1.06E-23	1.016E-21	466	1 1 1	0.070	0.093	0.081	0.121	0.75	0.82
2111	0330	1	121	3281.457	3482.857	1.01E-24	1.10E-23	5.725E-22	466	1 1 1	0.070	0.090	0.081	0.119	0.75	0.82
0311	0110	1	260	3285.230	3383.462	1.02E-24	1.51E-22	1.506E-20	466	1 1 1	0.069	0.097	0.077	0.127	0.73	0.82
2111	0310	1	34	3288.513	3321.113	1.01E-24	1.14E-24	3.649E-23	466	1 1 1	0.074	0.080	0.097	0.105	0.75	0.77
0201	0000	1	136	3295.982	3408.309	1.08E-24	1.65E-21	8.290E-20	466	1 1 1	0.069	0.097	0.076	0.127	0.73	0.82
0201	0000	3	81	3296.447	3363.125	1.03E-24	7.52E-24	3.686E-22	466	1 1 1	0.070	0.093	0.082	0.121	0.75	0.82
0201	0000	4	82	3307.838	3373.540	1.02E-24	6.72E-24	3.332E-22	466	1 1 1	0.070	0.093	0.082	0.121	0.75	0.82
1201	1000	1	71	3310.979	3373.094	1.06E-24	4.51E-24	2.136E-22	466	1 1 1	0.070	0.090	0.083	0.119	0.75	0.82
0221	0000	1	82	3319.826	3414.419	1.04E-24	7.16E-24	3.204E-22	466	1 1 1	0.069	0.077	0.077	0.101	0.73	0.82
1001	0000	2	112	3370.824	3462.689	1.02E-24	1.15E-22	5.722E-21	466	1 1 1	0.069	0.097	0.078	0.127	0.73	0.82
1001	0000	4	109	3378.948	3463.967	1.02E-24	5.82E-23	2.981E-21	466	1 1 1	0.069	0.097	0.078	0.127	0.73	0.82
1001	0000	3	115	3381.794	3473.528	1.04E-24	1.23E-22	6.218E-21	466	1 1 1	0.069	0.097	0.077	0.127	0.73	0.82
1111	0110	2	158	3382.909	3448.822	1.02E-24	6.92E-24	6.575E-22	466	1 1 1	0.070	0.097	0.082	0.127	0.75	0.82
2001	1000	1	112	3384.988	3476.512	1.02E-24	1.13E-22	5.624E-21	466	1 1 1	0.069	0.097	0.078	0.127	0.73	0.82
1001	0000	1	156	3386.212	3513.862	1.03E-24	3.31E-20	1.650E-18	466	1 1 1	0.069	0.097	0.070	0.127	0.73	0.82
1111	0110	1	338	3394.709	3506.679	1.03E-24	1.86E-21	1.854E-19	466	1 1 1	0.069	0.097	0.076	0.127	0.73	0.82
1111	0110	4	130	3396.960	3452.701	1.02E-24	3.42E-24	3.098E-22	466	1 1 1	0.070	0.089	0.085	0.116	0.75	0.82

may also vary by more than 20% in many cases. The air-broadened widths of 0.11 cm^{-1}/atm and a temperature coefficient of $n = 0.75$ have been taken from May and Webster.[59] The recent results for the hot bands have not been included.[60]

Analysis of the ATMOS atmospheric spectral data encompassing both the ν_2 and the ν_5 bands revealed a systematic bias between the profiles retrieved from individual HNO_3 bands. In order that a consistent set of profiles of HNO_3 could be derived, the ν_2 band

Table 9. (**continued**)

Species			#ISO	#Lines	FMIN cm^{-1}	FMAX cm^{-1}	IMIN cm^{-1}	IMAX /(molecule × cm^{-2})	S-SUM	ACC	REF	PBHW (cm^{-1}/atm)	PMAX (cm^{-1}/atm)	SELF (cm^{-1}/atm)	SMAX	NTDP	NMAX
	1111	0110	3	160	3397.027	3462.016	1.02E-24	6.90E-24	6.681E-22	466	1 1 1	0.070	0.097	0.082	0.127	0.75	0.82
	2111	1110	1	150	3398.949	3464.340	1.01E-24	6.15E-24	5.793E-22	466	1 1 1	0.070	0.090	0.083	0.119	0.75	0.82
	1201	0200	1	111	3400.729	3492.494	1.11E-24	1.07E-22	5.346E-21	466	1 1 1	0.069	0.097	0.078	0.127	0.73	0.82
	2111	0001	1	31	3403.331	3440.339	1.01E-24	1.42E-24	3.752E-23	466	1 1 1	0.073	0.083	0.094	0.110	0.75	0.79
	1221	0220	1	260	3403.821	3495.847	1.02E-24	1.03E-22	1.027E-20	466	1 1 1	0.069	0.093	0.078	0.121	0.73	0.82
	1001	0000	5	89	3411.522	3482.917	1.06E-24	1.22E-23	6.060E-22	466	1 1 1	0.069	0.097	0.081	0.127	0.73	0.82
	0221	0310	1	148	3412.643	3477.046	1.03E-24	6.08E-24	5.703E-22	466	1 1 1	0.070	0.090	0.083	0.119	0.75	0.82
	0600	0000	3	5	3419.532	3461.685	1.12E-24	9.39E-24	2.805E-23	466	1 1 1	0.072	0.073	0.094	0.094	0.79	0.80
	0600	0000	1	17	3428.066	3511.764	1.07E-24	4.10E-22	8.154E-22	466	1 1 1	0.069	0.070	0.079	0.082	0.73	0.78
	0620	0000	1	13	3450.219	3503.988	1.28E-24	4.72E-22	9.133E-22	466	1 1 1	0.071	0.072	0.087	0.094	0.80	0.82
CH_4	(6)																
	V6	GROUND	3	1406	970.390	1427.138	1.00E-26	1.75E-23	1.342E-21	3321516	0	0.080	0.080	0.090	0.090	0.75	0.75
	V3	GROUND	3	561	1060.783	1438.420	1.03E-26	1.97E-23	9.498E-22	3321516	0	0.080	0.080	0.090	0.090	0.75	0.75
	V5	GROUND	3	1031	1262.749	1693.489	1.00E-26	3.83E-24	3.205E-22	3321516	0	0.080	0.080	0.090	0.090	0.75	0.75
O_2	(7)																
	X1	X0	1	146	1407.321	1705.649	3.68E-30	1.49E-28	6.159E-27	354	1 1 0	0.042	0.062	0.000	0.000	0.75	0.75
NO	(8)																
X3/2	1 X3/2	0	1	205	1733.303	1973.284	1.72E-26	3.34E-20	1.585E-18	305	0 1 1	0.041	0.067	0.054	0.077	0.71	0.71
X1/2	1 X1/2	0	1	212	1736.671	1971.989	4.45E-27	6.25E-20	2.997E-18	305	0 1 1	0.041	0.069	0.054	0.076	0.71	0.71
NO_2	(10)																
	001	000	1	3222	1538.182	1662.424	1.22E-23	2.56E-19	5.728E-17	454	4 4 1	0.067	0.067	0.000	0.000	0.75	0.75
	020	000	1	155	1554.220	1653.517	2.97E-23	1.36E-21	6.825E-20	454	4 4 1	0.067	0.067	0.000	0.000	0.75	0.75
	011	010	1	802	1556.174	1639.205	1.05E-22	6.33E-21	1.198E-18	454	4 4 1	0.067	0.067	0.000	0.000	0.75	0.75
HNO_3	(12)																
	V5	00000000	1	19302	816.189	946.493	7.15E-24	1.29E-20	1.144E-17	444	9 9 9	0.110	0.110	0.300	0.300	0.75	0.75
	2V9	00000000	1	18666	826.268	959.186	7.15E-24	8.69E-21	8.292E-18	444	9 9 9	0.110	0.110	0.300	0.300	0.75	0.75
	V3	GROUND	1	20747	1098.376	1387.849	1.00E-23	3.35E-20	2.712E-17	000	7 7 1	0.110	0.110	0.000	0.000	0.75	0.75
	V8+V9	GROUND	1	6214	1165.014	1232.483	1.61E-23	1.58E-21	1.199E-18	000	6 6 1	0.110	0.110	0.000	0.000	0.75	0.75
	V4	GROUND	1	19082	1229.867	1387.561	1.11E-23	2.00E-20	1.366E-17	000	7 8 1	0.110	0.110	0.000	0.000	0.75	0.75
	V2	GROUND	1	21946	1650.014	1769.982	2.12E-24	4.24E-20	4.381E-17	000	1 1 1	0.110	0.110	0.000	0.000	0.75	0.75
HF	(14)																
	1	0	1	29	3269.779	4368.140	1.15E-26	2.37E-18	1.572E-17	462	2 1 2	0.010	0.105	0.075	0.729	0.22	1.00
HCl	(15)																
	1	1	2	12	20.240	239.339	1.01E-26	3.95E-25	2.220E-24	482	1 1 1	0.009	0.089	0.080	0.245	0.29	0.76
	1	1	1	13	20.270	258.994	1.98E-26	1.23E-24	6.902E-24	482	1 1 1	0.010	0.097	0.075	0.264	0.29	0.76
	0	0	2	21	20.847	418.738	4.42E-26	4.63E-19	2.585E-18	582	1 1 1	0.005	0.089	0.050	0.245	0.29	0.76
	0	0	1	22	20.878	437.392	1.95E-26	1.45E-18	8.096E-18	582	1 1 1	0.010	0.097	0.050	0.264	0.29	0.76
	1	0	2	38	2398.957	3151.461	1.22E-26	1.61E-19	1.518E-18	472	2 1 1	0.005	0.089	0.050	0.253	0.13	0.76
	1	0	1	39	2400.278	3160.444	1.81E-26	5.03E-19	4.749E-18	472	2 1 1	0.005	0.089	0.050	0.253	0.13	0.76
	2	1	1	21	2554.264	2962.536	1.43E-26	7.71E-25	7.419E-24	472	1 1 1	0.013	0.089	0.085	0.253	0.13	0.76
	2	1	2	19	2577.751	2947.382	1.15E-26	2.49E-25	2.382E-24	472	1 1 1	0.016	0.089	0.022	0.253	0.13	0.76
	2	0	1	35	5159.439	5829.709	2.29E-26	1.18E-20	1.077E-19	462	1 1 1	0.005	0.098	0.055	0.253	0.13	0.76
	2	0	2	33	5194.557	5825.543	3.71E-26	3.76E-21	3.434E-20	462	1 1 1	0.005	0.089	0.055	0.253	0.13	0.76
	3	1	1	13	5321.585	5568.350	1.13E-26	3.22E-26	2.738E-25	462	1 1 1	0.033	0.089	0.154	0.253	0.35	0.76
	3	1	2	2	5510.529	5525.897	1.03E-26	1.04E-26	2.068E-26	462	1 1 1	0.062	0.072	0.237	0.245	0.71	0.72
	3	0	1	29	7895.987	8454.457	1.12E-26	8.09E-23	7.180E-22	352	1 1 1	0.006	0.089	0.065	0.253	0.13	0.76
	3	0	2	27	7933.979	8448.539	1.36E-26	2.58E-23	2.288E-22	352	1 1 1	0.007	0.089	0.070	0.253	0.05	0.76
ClO	(18)																
X1/2	1 X1/2	0	2	190	770.401	875.322	1.06E-24	2.17E-22	1.641E-20	442	1 1 1	0.093	0.093	0.000	0.000	0.75	0.75
X3/2	1 X3/2	0	2	226	773.840	878.516	1.21E-24	1.03E-21	7.841E-20	442	1 1 1	0.093	0.093	0.000	0.000	0.75	0.75
X1/2	1 X1/2	0	1	204	776.285	882.995	1.11E-24	6.83E-22	5.117E-20	442	1 1 1	0.093	0.093	0.000	0.000	0.75	0.75
X3/2	1 X3/2	0	1	236	779.760	886.215	1.18E-24	3.24E-21	2.444E-19	442	1 1 1	0.093	0.093	0.000	0.000	0.75	0.75

Table 9. (**continued**)

Species		#ISO	#Lines	FMIN cm^{-1}	FMAX cm^{-1}	IMIN cm^{-1}	IMAX /(molecule × cm^{-2})	S-SUM	ACC	REF	PBHW (cm^{-1}/atm)	PMAX (cm^{-1}/atm)	SELF (cm^{-1}/atm)	SMAX	NTDP	NMAX
OCS (19)																
0110	0000	1	209	493.260	549.975	3.76E-23	4.53E-21	3.421E-19	521	1 1 1	0.082	0.109	0.116	0.169	0.30	0.90
1000	0000	1	160	822.740	887.377	1.42E-22	1.55E-20	1.109E-18	531	1 3 1	0.082	0.109	0.113	0.169	0.30	0.90
0200	0000	1	160	1018.894	1083.744	4.88E-23	5.22E-21	3.757E-19	531	1 4 1	0.082	0.109	0.113	0.169	0.30	0.90
2000	0000	1	140	1676.692	1733.200	1.07E-22	2.92E-21	2.097E-19	521	1 1 1	0.082	0.109	0.116	0.169	0.30	0.90
1200	0000	1	160	1860.771	1925.538	4.38E-23	3.67E-21	2.697E-19	521	2 5 1	0.082	0.109	0.113	0.169	0.30	0.90
1310	0110	1	276	1863.083	1920.944	2.75E-23	6.21E-22	8.977E-20	521	2 5 1	0.082	0.106	0.116	0.169	0.30	0.90
0001	0000	3	159	1970.284	2034.044	1.30E-22	1.16E-20	8.421E-19	991	9 9 1	0.082	0.109	0.113	0.169	0.30	0.90
0001	0000	1	220	2003.194	2091.720	5.51E-23	1.19E-18	8.579E-17	521	2 5 1	0.000	0.109	0.000	0.169	0.00	0.90
0111	0110	1	356	2008.832	2081.552	1.67E-22	8.56E-20	1.230E-17	521	2 5 1	0.082	0.106	0.113	0.169	0.30	0.90
0001	0000	2	159	2022.958	2085.346	5.55E-22	4.40E-20	3.216E-18	991	9 9 1	0.082	0.109	0.113	0.169	0.30	0.90
0400	0000	1	140	2082.385	2139.251	1.45E-22	5.68E-21	3.927E-19	521	2 5 1	0.082	0.109	0.116	0.169	0.30	0.90
0510	0110	1	236	2093.757	2143.976	7.00E-23	7.31E-22	9.976E-20	521	2 5 1	0.082	0.106	0.120	0.169	0.30	0.90
3000	0000	1	140	2518.644	2575.061	6.79E-24	1.56E-22	1.140E-20	521	2 5 1	0.082	0.109	0.116	0.169	0.30	0.90
0111	0000	1	209	2542.361	2598.907	7.83E-25	7.83E-23	5.691E-21	531	2 2 1	0.082	0.109	0.116	0.169	0.30	0.90
2200	0000	1	140	2701.118	2757.748	6.60E-24	1.59E-22	1.160E-20	521	2 5 1	0.082	0.109	0.116	0.169	0.30	0.90
1111	0110	1	316	2860.425	2925.128	1.20E-23	1.02E-21	1.497E-19	521	2 5 1	0.082	0.106	0.113	0.169	0.30	0.90
1001	0000	1	180	2867.400	2939.850	3.43E-23	1.26E-20	9.255E-19	521	2 5 1	0.082	0.109	0.113	0.169	0.30	0.90
1400	0000	1	140	2912.288	2969.087	1.49E-24	1.62E-22	1.044E-20	521	2 5 1	0.082	0.109	0.116	0.169	0.30	0.90
0201	0000	1	160	3059.953	3124.613	1.04E-23	9.41E-22	6.868E-20	521	2 5 1	0.082	0.109	0.113	0.169	0.30	0.90
0311	0110	1	276	3063.233	3120.931	6.00E-24	1.41E-22	2.029E-20	521	2 5 1	0.082	0.106	0.116	0.169	0.30	0.90
0002	0000	1	160	4053.648	4117.994	7.56E-23	7.90E-21	5.718E-19	521	1 1 1	0.082	0.109	0.113	0.169	0.30	0.90
HOCl (21)																
001	000	1	845	679.018	757.953	5.38E-23	4.95E-21	1.273E-18	331	1 1 0	0.060	0.060	0.000	0.000	0.75	0.75
001	000	2	530	679.476	755.946	4.63E-23	4.82E-21	6.904E-19	331	1 1 0	0.060	0.060	0.000	0.000	0.75	0.75
010	000	1	611	1180.966	1249.953	1.47E-22	3.17E-20	4.901E-18	331	1 1 0	0.060	0.060	0.000	0.000	0.75	0.75
010	000	2	523	1185.936	1249.946	1.55E-22	1.03E-20	1.644E-18	331	1 1 0	0.060	0.060	0.000	0.000	0.75	0.75
CH_3Cl (30)																
V3	GROUND	2	1752	661.793	765.094	1.01E-23	3.67E-21	9.715E-19	351	1 1 0	0.080	0.080	0.000	0.000	0.75	0.75
V3	GROUND	1	1993	666.344	771.445	1.00E-23	1.13E-20	2.960E-18	351	1 1 0	0.080	0.080	0.000	0.000	0.75	0.75
C_2H_6 (38)																
V9	GROUND	1	10000	745.225	951.650	6.88E-27	1.03E-21	6.967E-19	331	1 1 1	0.100	0.100	0.000	0.000	0.75	0.75
C_2H_4 (40)																
00011110	00000000	1	119	1192.333	1469.865	1.37E-27	1.38E-19	2.664E-18	000	1 1 1	0.040	0.116	0.110	0.162	0.75	0.75
01011110	00000000	1	63	3204.731	3351.912	2.22E-21	2.46E-19	4.961E-18	460	2 2 1	0.045	0.116	0.110	0.162	0.75	0.75
00100000	00000000	1	62	3211.602	3358.285	8.93E-22	2.22E-19	4.355E-18	460	2 2 1	0.043	0.116	0.110	0.162	0.75	0.75
HDO (49)																
000	000	1	461	0.007	100.490	1.24E-32	1.27E-22	2.585E-21	000	0 0 0	0.008	0.103	0.000	0.000	0.64	0.64
010	000	1	1653	1104.970	1894.299	1.00E-27	2.67E-23	2.816E-21	000	0 0 0	0.008	0.103	0.000	0.000	0.64	0.64
010	000	2	200	1231.680	1607.611	1.00E-26	7.94E-26	5.832E-24	443	7 7 0	0.031	0.105	0.000	0.000	0.75	0.75
100	000	1	1333	2332.099	3132.932	1.01E-27	9.75E-24	6.337E-22	000	0 0 0	0.008	0.103	0.000	0.000	0.64	0.64
020	000	1	953	2486.140	3361.318	1.00E-27	1.23E-24	8.468E-23	000	0 0 0	0.008	0.103	0.000	0.000	0.64	0.64
001	000	1	1651	3236.354	4121.496	1.01E-27	1.75E-23	1.416E-21	000	0 0 0	0.008	0.103	0.000	0.000	0.64	0.64
110	000	1	860	3843.445	4496.503	1.00E-27	9.36E-25	6.426E-23	000	0 0 0	0.019	0.103	0.000	0.000	0.64	0.64
030	000	1	602	3879.178	4639.031	1.01E-27	8.76E-25	3.504E-23	000	0 0 0	0.024	0.103	0.000	0.000	0.64	0.64
011	000	1	576	4850.495	5384.821	3.01E-27	5.53E-25	3.671E-23	000	0 0 0	0.019	0.103	0.000	0.000	0.64	0.64
200	000	1	216	5154.643	5507.548	3.07E-27	2.94E-25	1.589E-23	000	0 0 0	0.029	0.103	0.000	0.000	0.64	0.64

strength was scaled by 1.1. This awaits confirmation by experimental measurements, but it is still within the estimated absolute uncertainty of the band strengths and hence remains a valid choice.

HF (14)

The line positions of the 1–0 fundamental band were multiplied by a scaling factor of 0.99999989 to normalize the original frequency calibration[61] to the current calibration standards for CO.[62] The resulting positions agree to better than 0.00001 cm^{-1} with the five heterodyne HF frequencies given by Goddon *et al.*[63]

HCl (15)

The computation errors in the positions of all HCl lines on the 1992 HITRAN[6,64] were corrected by the work of Rinsland *et al.*[65] for the 1–0 band and for all other bands by Tipping.[66] The intensities and the widths were not changed and remain consistent with the measurements of Pine *et al.*[67,68] The reference codes are 2 1 1 for the 1–0 band and 1 1 1 for the remainder.

ClO (18)

The updated parameters of the ClO fundamental near 840 cm^{-1} were taken from the work of Goldman

Table 10. Summary of the 1995 Supplemental Linelist

Species		ISO	#Lines	FMIN cm^{-1}	FMAX cm^{-1}	IMIN (cm^{-1}/molecule × cm^{-2})	IMAX S-SUM	ACC	REF	PBHW (cm^{-1}/atm)	PMAX SELF (cm^{-1}/atm)	SMAX	NTDP	NMAX
O_2	(7)													
X1	X0	1	162	1432.508	1676.962	5.14E-33	4.41E-29 1.470E-27	344	2 2 0	0.042	0.062	0.000	0.000	0.75 0.75
HNO_3	(12)													
3V9	V9	1	4780	845.111	908.834	8.14E-23	2.78E-21 2.030E-18	000	0 0 0	0.110	0.110	0.000	0.000	0.75 0.75
V5+V9	V9	1	3971	847.611	904.221	8.13E-23	1.70E-21 1.216E-18	000	0 0 0	0.110	0.110	0.000	0.000	0.75 0.75
H_2CO	(20)													
010001	000000	1	587	1707.093	1781.387	3.00E-22	5.98E-20 7.195E-18	000	0 0 0	0.100	0.100	0.000	0.000	0.75 0.75
HO_2	(22)													
001	000	1	1146	1032.068	1144.963	1.00E-23	6.80E-21 1.247E-18	000	0 0 0	0.080	0.080	0.100	0.100	0.75 0.75
000	000	1	2372	1055.186	1454.546	4.41E-23	2.89E-20 1.394E-17	000	0 0 0	0.100	0.100	0.000	0.000	0.75 0.75
010	000	1	1229	1145.513	1459.718	1.01E-23	1.11E-20 2.077E-18	000	0 0 0	0.080	0.080	0.100	0.100	0.75 0.75
100	000	1	2073	3202.033	3675.819	1.00E-23	3.08E-21 6.847E-19	000	0 0 0	0.080	0.080	0.100	0.100	0.75 0.75
HONO	(24)													
	000000	1	2348	779.126	1711.707	1.39E-22	2.76E-20 2.059E-17	000	0 0 0	0.100	0.100	0.000	0.000	0.75 0.75
HO_2NO_2	(25)													
V4	00000000	1	341	802.478	803.654	6.75E-24	5.98E-21 9.140E-19	000	0 0 0	0.100	0.100	0.000	0.000	0.75 0.75
N_2O_5	(26)													
V3	GROUND	1	401	725.000	765.000	1.18E-20	2.03E-19 3.674E-17	000	0 0 0	0.800	0.800	0.000	0.000	0.75 0.75
	GROUND	1	360	1221.886	1269.014	7.57E-22	3.79E-19 4.677E-17	000	0 0 0	7.500	25.000	0.000	0.000	0.75 0.75
V1	GROUND	1	2739	1671.050	1807.950	3.56E-22	1.42E-19 1.639E-16	000	0 0 0	20.000	20.000	0.000	0.000	0.75 0.75
$ClONO_2$	(27)													
	V9	1	6411	763.641	797.741	1.25E-24	4.98E-22 9.191E-19	000	0 492	0.140	0.140	0.800	0.800	0.75 0.75
V4	GROUND	2	6208	765.212	790.805	6.41E-25	2.52E-22 4.656E-19	000	0 492	0.140	0.140	0.800	0.800	0.75 0.75
V4	GROUND	1	6970	766.150	792.488	3.87E-24	7.70E-22 1.439E-18	000	0 492	0.140	0.140	0.800	0.800	0.75 0.75
V2	GROUND	1	3675	1270.007	1309.991	2.00E-24	2.03E-20 2.831E-17	000	0 0 0	0.030	0.100	0.000	0.000	0.75 0.75
CH_3F	(29)													
V1	GROUND	1	739	987.918	1089.135	5.41E-23	1.16E-19 1.806E-17	000	0 0 0	0.100	0.100	0.000	0.000	0.75 0.75
CH_3Cl	(30)													
V2	GROUND	1	513	1324.697	1377.725	5.06E-23	6.16E-21 1.057E-18	000	0 0 0	0.100	0.100	0.000	0.000	0.75 0.75
V5	GROUND	2	61	1458.986	1459.770	5.43E-24	1.05E-21 2.714E-20	000	0 0 0	0.080	0.080	0.300	0.300	0.75 0.75
V5	GROUND	1	47	1459.218	1460.144	1.78E-22	3.12E-21 7.940E-20	000	0 0 0	0.080	0.080	0.300	0.300	0.75 0.75
CCl_2F_2	(32)													
REGION		1	381	920.038	924.202	5.22E-21	5.98E-20 8.285E-18	000	0 0 0	0.055	0.055	0.000	0.000	0.75 0.75
V1	REGION	1	5179	1070.038	1129.996	3.52E-25	2.55E-20 4.580E-17	000	0 0 0	0.030	0.030	0.000	0.000	0.75 0.75
V8	REGION	1	593	1147.277	1161.279	4.23E-23	1.04E-19 5.851E-18	000	0 0 0	0.030	0.030	0.000	0.000	0.75 0.75
CCl_3F	(33)													
V4	REGION	1	842	833.500	860.500	4.55E-22	1.52E-18 6.119E-17	000	0 0 0	0.100	5.000	0.000	0.000	0.75 0.75
V1	REGION	1	3651	1060.004	1099.998	6.56E-22	1.55E-20 2.421E-17	000	0 0 0	0.030	0.030	0.000	0.000	0.75 0.75
CH_3CCl_3	(34)													
V2	Q BRANCH	1	251	1382.500	1385.000	6.97E-24	2.07E-21 1.250E-19	000	0 0 0	0.100	0.100	0.000	0.000	0.75 0.75

et al.[69] For these, the line positions were calculated with the rotational constants of Burkholder *et al.*[70] with corrections of the presented Hamiltonian. Line intensities were computed according to the method outlined by Gillis and Goldman[71] by the use of the dipole moment and Herman–Wallis terms reported by Burkholder *et al.*[72] The averaged value of the N_2-broadening coefficient of 0.093 cm^{-1}/atm at[72,73] 296 K was used for the air-broadened widths and the temperature-dependence coefficient was set

Table 10. (continued)

Species		ISO	#Lines	FMIN cm^{-1}	FMAX cm^{-1}	IMIN (cm^{-1}/molecule × cm^{-2})	IMAX S-SUM	ACC	REF (cm^{-1}/atm)	PBHW (cm^{-1}/atm)	PMAX SELF SMAX	NTDP	NMAX
$CFClO$	(37)												
010001	000000	1	413	764.111	764.720	1.58E-22	6.89E-21 1.114E-18	000	0 0 0	0.100 0.100	0.000 0.000	0.75	0.75
100000	000000	1	2036	1850.078	1907.929	4.29E-21	1.96E-19 3.845E-17	222	1 1 1	0.100 0.100	0.000 0.000	0.75	0.75
C_2H_6	(38)												
V7	Q BRANCHES	1	115	2976.635	2996.980	3.85E-23	2.32E-19 2.875E-18	331	1 1 1	0.090 0.090	0.150 0.150	0.75	0.75
$COCl_2$	(43)												
000010	000000	1	12456	828.549	875.502	3.83E-23	7.60E-21 1.976E-17	222	1 1 1	0.100 0.100	0.000 0.000	0.75	0.75
100000	000000	1	20415	1780.214	1862.452	2.66E-23	3.91E-21 1.374E-17	222	1 1 1	0.100 0.100	0.000 0.000	0.75	0.75
CH_3Br	(44)												
V3	GROUND	1	3421	871.326	1038.060	5.01E-23	8.22E-22 6.427E-19	000	0 0 0	0.100 0.100	0.000 0.000	0.75	0.75
CH_3I	(45)												
V3	GROUND	1	2528	793.467	971.654	5.01E-23	2.61E-21 1.207E-18	000	0 0 0	0.100 0.100	0.000 0.000	0.75	0.75
$HCOOH$	(46)												
V6	GROUND	1	3388	1060.962	1161.251	2.14E-22	2.84E-20 1.757E-17	000	0 0 0	0.100 0.100	0.000 0.000	0.75	0.75
$CHFCl_2$	(48)												
V3	GROUND	1	9583	785.000	1099.992	4.84E-23	2.16E-20 5.284E-17	000	0 0 0	0.030 0.030	0.000 0.000	0.75	0.75

to 0.75.[73] Additional details are given by Goldman *et al.*[69]

OCS (19)

The carbonyl sulfide parameters were modified completely with newer results. The 1987 ATMOS linelists contained four infrared bands on the main list (from the 1982 AFGL tape) and two bands based on unpublished data in the supplemental linelist. The 1991 GEISA provided[7] a complete calculation of 19 infrared bands of the main isotope with positions obtained by Fayt *et al.*[74] and band strengths based unpublished data and reported band strengths of Kagann (Ref. 75 and the references therein). Later it was noted that a computational error had occurred for the intensities, and a corrected prediction was kindly supplied by Fayt.[76] In addition, two isotopic bands of ν_3 based on the work of Blanquet *et al.*[77] were taken from the 1987 ATMOS linelist. The old microwave prediction was removed. For air-broadened widths, the values on the 1992 HITRAN were assumed. For the self-broadened linewidths, the measurements of Bouanich *et al.*[78] were merged. The temperature-dependence coefficient measured for self-broadening[78] was employed for the air broadening.

The update of the OCS parameters was much needed. There were sufficient experimental intensities that demonstrated that the ν_3 band strength needed to be increased on the compilations by almost 9%. Atmospheric investigators should note this difference when comparing present and prior OCS field measurements. However, the OCS linelist is incomplete because many isotopic and hot bands[62,79] have not been included.

HOCl (21)

The HOCl parameters appearing in the 1992 HITRAN had not been updated since 1982, so the predictions of the ν_2 and ν_3 bands provided by Lafferty and Olson[80] for the 1987 ATMOS list were used. The ν_1 band has not been revised.

HO_2 (22)

The approximate predictions of HO_2 in the 1987 supplemental list were replaced by predictions provided by Nelson, Zahniser, and co-workers[81–84] for all three fundamentals.

HO_2NO_2 (25)

The pseudo-lines from the supplemental linelist were removed so that the cross sections of May and Friedl[19] could be used instead.

$ClONO_2$ (27)

The $ClONO_2$ parameters in the supplemental list have been described previously by Rinsland *et al.*[85] and are summarized here as a convenience to the reader. Near 780 cm^{-1}, the experimental cross sections of Ballard *et al.*[86] have been set aside in favor of a line-by-line prediction based on the study by Bell *et al.*[87] of ν_4 of both isotopes of Cl and one hot band $\nu_4 + \nu_9 - \nu_4$. The relative intensities have been normalized to the values of Ballard *et al.*,[86] Davidson *et al.*,[88] Tuazon *et al.*,[89] and results from other laboratory data.[90] The air-broadened coefficient was

set to the averaged N_2 width reported by Bell *et al.*[87] with the temperature coefficient of 0.75 assumed. Parameters of the 1292-cm^{-1} band published by Orphal *et al.*[90] are being sought along with revised values for the 780-cm^{-1} band from McPheat and Duxbury.[91]

CH_3Cl (30)

A prediction of the ν_3 region at 732 cm^{-1} based on the positions of Ref. 92 and the intensities of Dang-Nhu *et al.*[93] has been added to the existing HITRAN parameters in the main list. In addition, a preliminary calculation of RQ_0 at 1459 cm^{-1} appears in the supplemental linelist. This has been obtained from a refinement of the Henfrey and Thrush study[94] by Tarrago *et al.*[95] The linewidths of Blanquet and co-workers[96–98] have not been included, however, and no changes have been made to revise the incomplete prediction available for the 3.3-μm region.

CF_4 (31)

The 1987 parameters[3] for this species were a combination of a modified calculation of the Q branch of the ν_3 fundamental based on the work of Takami *et al.*[99] with measured P- and R-branch manifolds using the Fourier-transform spectrometer at Kitt Peak. Because this list is incomplete, it is thought that it will soon be replaced by either cross sections[10,23] or results of new analyses.[100,101] The information given in Table 7 corresponds to the data of McDaniel *et al.*[10]

CCl_2F_2 (32)

The 922-cm^{-1} band is represented by the cross sections of Varanasi and Nemtchinov.[15,16] All older pseudo-parameters (which contained only default values for the lower state energies) have been removed from the supplemental list. Figure 1 shows observed and synthetic spectra based on the new parameters.

CCl_3F (33)

The cross sections of Li and Varanasi[14] are being used for the CFC-11 bands, and so all data for this species has been removed from the supplemental list.

CCl_4 (35)

The pseudo-lines in the 1987 supplemental list for this species have been removed from the supplemental list, and the cross sections of Orlando *et al.*[13] are being used. It should be noted that the new integrated intensity is 33% different from the value used for the 1987 linelist.[3,9]

COClF (37)

An experimental list of line positions in the ν_1 region near 1800 cm^{-1} was obtained for the supplemental linelist by the use of laboratory spectra recorded at Kitt Peak by L. Brown. The relative intensities are very crude line intensities (within a factor of 3). If this species were detected, much additional work would be needed to obtain adequate line parameters.

C_2H_6 (38)

In the 1987 ATMOS paper, we noted that there was a difference in reported intensity measurements for the ν_9 band near 820 cm^{-1}. Daunt *et al.*[102] had produced a prediction whose integrated strength differed by 25% from that reported by Henry *et al.*[103] and an integrated RQ_0 strength of Goldman *et al.*[104] The 1992 HITRAN contained the Daunt *et al.* prediction, but for the ATMOS linelist, we have normalized the intensities to match the other two studies.

The 1992 HITRAN included a representation of the Q branches of ν_7 near 3000 cm^{-1} produced by Dang-Nhu and Goldman.[105] The 1987 ATMOS linelist contained a set of pseudo-lines obtained from unpublished Kitt Peak spectra and normalized to the intensities of Rinsland *et al.*[106] Because the newer prediction was in poor agreement with the lab data, these parameters were removed from the main list. In the supplemental list, newer PQ_3 branch parameters from Rinsland *et al.*[107] were merged with approximate values from the 1987 supplemental list. The 3.3-μm region of ethane is difficult to model[108] and thus still remains incompletely catalogued in all the databases. The only anticipated revisions for this region are the new intensity and air-broadening measurements of Pine and Stone[109] for RQ_0 and PQ_3.

C_2H_2 (40)

Two bands of C_2H_2 at 3 μm were replaced with the positions and the intensities of Auwera *et al.*[110] and the line widths of Devi *et al.*[111] The other recent studies[112,113] have not yet been incorporated.

CHF_2Cl (42)

The cross sections[10,17] are being used for the CFC-22 band, and so all older values for this species have been removed from the supplemental list. Newer cross sections[18] will eventually be used in place of the older values.[10]

$COCl_2$ (43)

Predictions of the ν_1 and the ν_5 bands of phosgene based on the work of Yamamato *et al.*[114] replaced the approximate 1987 supplemental linelist parameters for this species. Default linewidths of 0.1 cm^{-1}/atm were selected. If this species is ever detected, the assumed intensities will need to be validated.

HDO (49)

In the main list, nine bands of HDO parameters were labeled as molecule number 49 and isotope 1. In addition, a linelist of the ν_2 band of $HD^{18}O$ from Toth via the 1987 ATMOS linelist[3] was added.

SF_6 (50)

The partial prediction of the ν_3 region that appeared in the 1992 HITRAN database was removed so that the cross-section data of Varanasi *et al.*[18] could be

used. This change represents a significant improvement for the tropospheric retrievals.

5. Database Improvements Needed

Any atmospheric remote sensing investigation depends on the molecular database's being complete and accurate. However, the databases generally have numerous faults and limitations either because existing laboratory data have not been included or sufficient laboratory studies have not been performed. At present, the molecular databases contain fairly reliable rotation–vibration line parameters or laboratory cross sections for many of the species for the far- to mid-infrared spectral regions below 2800 cm^{-1}. However, there are gaps for the near-infrared parameters, and no readily available and well-documented public database exists for the visible and ultraviolet wavelengths. For example, some important deficiencies above 2800 cm^{-1} include the omission of weak transitions of CH_4, O_3, H_2O, and N_2O and a number of trace species. In addition, spectral effects occur in tropospheric data that are generally avoided in the lower-pressure stratospheric regimes. The databases do not contain parameters to describe all the (high) pressure-induced phenomena that are required for computing tropospheric spectra. Some of these involving collision-induced continua can be obtained from individual sources, but insufficient studies have been done for the effects of line mixing in species like H_2O and CH_4.

The 1995 ATMOS and the 1996 HITRAN databases will not be exactly the same because the ATMOS catalog is tailored to met the goals of a specific experiment operating in a designated spectral interval. The compilations will also differ because modification of the main ATMOS linelist was suspended in mid-1994 to facilitate a consistent basis for analysis of all ATMOS Shuttle data sets with the same molecular parameters. It is anticipated[115] that the 1996 HITRAN database will contain additional improvements. Table 11 shows some of the changes that will be considered for revision of the ATMOS linelists.

At present, parameters in some form exist for all the detectable species that are being monitored by the ATMOS experiment. The database inaccuracies that affect retrievals the most are those associated with intensities because these propagate into the error budget of a retrieval on a 1:1 basis. To provide an overview of the impact spectroscopic uncertainties have on the retrievals, estimates of intensity uncertainties are given in Table 12 by species. The spectral regions used for ATMOS retrievals are shown to emphasize that these estimates pertain to only the parameters within the specific wave-number intervals used by ATMOS and are not necessarily correct for all the intensities of a species throughout the database. For example, the CH_3D listed in Table 12 with 20% accuracies corresponds only to the current parameters at 3.3 μm (which has not been studied extensively in the laboratory); the CH_3D parameters of the three revised fundamentals near 8 μm (which are not being used

Table 11. Revisions to be taken from HITRAN 1996

Species	Anticipated Update
CO_2	Revised intensities
O_3	Default values for pressure shifts
NO	Hot bands at 5.1 μm
NO_2	Prediction of bands at 6 μm
NH_3	New bands at 4, 3, 2.3, and 2 μm
HNO_3	New hot bands at 11 μm
CH_3Cl	Air-broadened widths
COF_2	Revised prediction of ν_4 region
C_2H_2	ν_5 at 14-μm region
H_2S	ν_1, ν_3, and $2\nu_2$ at 4 μm

Table 12. Estimated Intensity Uncertainties in Regions Used by ATMOS

Species	Region (cm^{-1})	% Acc. (2σ)	Recommendations/ Comments
H_2O	1380–1980	4	
	2960–3300	4	
HDO	1420–1515	5	
$H_2{}^{18}O$	1415–1690	5	
$H_2{}^{17}O$	1455–1776	5	
CO_2	650–960	4	
	1910–2400	3	/may be 2%
	3205–3630	3	/may be 2%
$^{12}C^{18}O^{16}O$	1230–1385	5	
O_3	770–3170	4	higher cm^{-1} should be
O_3-686	980–1000	10	improved and abundance
O_3-668	1090–1091	20	assumptions should be checked for both 668 and 686
N_2O	1150–3460	3	/may be 2%
CO	2070–2200	3	/may be 2%
CH_4	1230–4315	3	
CH_3D	2950–3100	20	complete analysis needed
NO	1840–1920	3	
NO_2	1580–1640	4	
	2915–2925	6	
HNO_3	865–1730	15	hot bands needed
HF	3790–4140	3	
HCl	2730–2980	3	
OCS	2040–2055	8	
HNO_4	801–805	20	need data more/cross sections at 220 K only
N_2O_5	1210–1260	15	
$ClONO_2$	779–781	20	hot bands needed
HCN	3270–3360	4	
CH_3Cl	2966–2968	10	complete prediction needed/only partial list
CF_4	1282–1285	10	
CCl_2F_2	920–940	8	
CCl_3F	830–870	10	
CCl_4	776–783	20	
COF_2	772–774,	10	
	1936–1940		
C_2H_6	2976–2977	10	complete prediction needed/only partial list
C_2H_2	755–776	6	
$CHClF_2$	828–829	10	
SF_6	945–952	10	/linelist on 1992 HITRAN should be removed

for ATMOS retrievals) have accuracies closer to 7%.[41] The best accuracies of 3% are associated with linear species (CO, NO, HF, HCl, CO_2, and N_2O) because the transitions of these fairly stable species are readily measured and modeled by simple expressions. The largest uncertainties of 15% to 20% occur for the heavier or less stable gases (HNO_3, N_2O_5, $ClONO_2$, and CCl_4). The remainder fall in the range 5%–10%, depending on the species. These estimates in Table 12 are thought to be conservative (perhaps 2σ) in that the numbers are generally larger than the values given in the original laboratory studies.

There are a number of laboratory studies that would significantly enhance the accuracy of the ATMOS retrievals. The absolute intensities of normal and ^{18}O-substituted heavy ozone are in need of improvement. As discussed above, the 5% scaling of $^{16}O_3$ intensities at 10 μm based on the work of Pickett *et al.*[34] has not been adopted here because we believe further studies are needed to validate this result. Studies of heavy ozone enrichments require more accurate absolute intensities of $^{16}O^{16}O^{18}O$ and $^{16}O^{18}O^{16}O$ relative to $^{16}O_3$. This is a difficult experimental problem given the fractionation effects known to occur in an electric discharge.[116] The 3000-cm^{-1} region of CH_3D has never been successfully modeled to provide a prediction of relative intensities, and only a few individual line intensities have been measured.[42] Further studies are also needed to provide accurate intensities in nitric acid and carbon tetrachloride bands. Measurements and analyses of the numerous hot bands are needed for several molecules, especially those in the ν_4 region of $ClONO_2$, the ν_3 region of SF_6, and all regions of the infrared bands of HNO_3. Absorption cross sections as functions of temperature and pressure are needed at 802 cm^{-1} to improve retrievals of HO_2NO_2. Complete parameters for the fundamental bands of C_2H_6 near 3000 cm^{-1}, CH_3Cl near 1400 and 3000 cm^{-1}, and the isotopic OCS bands for the 500–4100-cm^{-1} region are also needed, as well as general revision of the positions, intensities, and widths of H_2O in the 600–1100-cm^{-1} region of H_2O. It should be noted that these are the areas of highest priority for ATMOS and that additional problems exist in the databases that will have a serious impact on other remote sensing experiments.

6. Conclusion

This article describes the 1995 ATMOS database of parameters used for the analysis of the atmospheric data recorded during the ATLAS 1, 2, and 3 Shuttle missions between 1992 and 1994. The updates have been done for the mid-infrared parameters of 26 gases. Anyone wishing to obtain these linelists should contact L. Brown.

The authors are indebted to all the individuals who provided linelists in electronic form or evaluations: J. Auwera, C. Camy-Peyret, E. Cohen, A. Fayt, J.-M. Flaud, N. Jacquinet-Husson, W. Lafferty, A. Maki, A. Perrin, L. S. Rothman, G. Tarrago, R. Tipping, P. Varanasi, S. Yamamato, and M. Zahniser. The research described in this paper was carried out by the Jet Propulsion Laboratory, California Institute of Technology, and by Langley Research Center, Hampton, Va., under contract with the National Aeronautics and Space Administration. Reference herein to any specific commercial process, or service by trade name, trademark, manufacturer of otherwise, does not constitute or imply its endorsement by the United States Government or the Jet Propulsion Laboratory, California Institute of Technology.

References

1. C. B. Farmer and R. H. Norton, "A high resolution infrared spectroscopy atlas of the infrared spectrum of the Sun and the Earth from space," NASA Ref. Pub. 1224 (NASA, Washington, D.C., 1989), Vols. 1 and 2; C. B. Farmer, "High resolution infrared spectroscopy of the Sun and the Earth's atmosphere from space," Mikrochem. Acta (Vienna) **3,** 189 (1987).
2. M. R. Gunson, M. M. Abbas, M. C. Abrams, M. Allen, L. R. Brown, T. L. Brown, A. Y. Chang, A. Goldman, F. W. Irion, L. L. Lowes, E. Mahieu, G. L. Manney, H. A. Michelsen, M. J. Newchurch, C. Rinsland, R. J. Salawitch, G. P. Stiller, G. C. Toon, Y. L. Yung, and R. Zander, "The atmospheric trace molecular spectroscopy (ATMOS) experiment: deployment on the ATLAS Space Shuttle Missions," submitted to Geophys. Res. Lett.
3. L. R. Brown, C. B. Farmer, C. P. Rinsland, and R. A. Toth, "Molecular line parameters of the atmospheric trace molecule spectroscopy experiment," Appl. Opt. **26,** 5154–5182 (1987).
4. L. S. Rothman, A. Goldman, J. R. Gillis, R. R. Gamache, H. M. Pickett, R. L. Poynter, N. Husson, and A. Chedin, "AFGL trace gas compilation—1982 version," Appl. Opt. **22,** 1616–1627 (1983).
5. L. S. Rothman, R. R. Gamache, A. Barbe, A. Goldman, J. R. Gillis, L. R. Brown, R. A. Toth, J.-M. Flaud, and C. Camy-Peyret, "AFGL atmospheric absorption-line parameters compilation—1982 edition," Appl. Opt. **22,** 2247–2256 (1983).
6. L. S. Rothman, R. R. Gamache, R. H. Tipping, C. P. Rinsland, M. A. H. Smith, D. Chris Benner, V. Malathy Devi, J.-M. Flaud, C. Camy-Peyret, A. Perrin, A. Goldman, S. T. Massie, L. R. Brown, and R. A. Toth, "The HITRAN molecular database editions of 1991 and 1992," J. Quant. Spectrosc. Radiat. Transfer **48,** 469–507 (1992). Hitran is high-resolution transmission molecular absorption.
7. N. Husson, B. Bonnet, N. A. Scott, and A. Chedin, "Management and study of spectroscopic information: the GEISA program," J. Quant. Spectrosc. Radiat. Transfer **48,** 509–518 (1992). GEISA is Gestion et Etude des Informations Spectroscopiques Atmospheriques.
8. L. S. Rothman, R. R. Gamache, A. Goldman, L. R. Brown, R. A. Toth, H. M. Pickett, R. L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C. P. Rinsland, and M. A. H. Smith, "The HITRAN database: 1986 edition," Appl. Opt. **26,** 4058–4097 (1987).
9. S. T. Massie, A. Goldman, D. G. Murcray, and J. C. Gille, "Approximate absorption cross sections of F12, F11, $ClONO_2$, N_2O_5, HNO_3, CCl_4, CF_4, F21, F113, F114, and HNO_4," Appl. Opt. **24,** 3426–3427 (1985).
10. A. H. McDaniel, C. A. Cantrell, J. A. Davidson, R. E. Shetter, and J. G. Calvert, "The temperature dependent, infrared absorption cross sections for the chlorofluorocarbons: CFC-11, CFC-12, CFC-13, CFC-14, CFC-22, CFC-113, CFC-114, and CFC-115," J. Atmos. Chem. **12,** 211–227 (1991).

11. C. A. Cantrell, J. A. Davidson, A. H. McDaniel, R. E. Shetter, and J. G. Calvert, "Infrared absorption cross-sections for N_2O_5," Chem. Phys. Lett. **148,** 358–362 (1988).
12. S. T. Massie and A. Goldman, "Absorption parameters of very dense molecular spectra for the HITRAN compilation," J. Quant. Spectrosc. Radiat. Transfer **48,** 713–719 (1992).
13. J. J. Orlando, G. S. Tyndall, A. Huang, and J. G. Calvert, "Temperature dependence of the infrared absorption cross sections of carbon tetrachloride," Geophys. Res. Lett. **19,** 1005–1008 (1992).
14. Z. H. Li and P. Varanasi, "Measurement of the absorption cross sections of CFC-11 at conditions representing various model atmospheres," J. Quant. Spectrosc. Radiat. Transfer **52,** 137–144 (1994).
15. P. Varanasi and V. Nemtchinov, "Thermal infrared absorption coefficients of CFC-12 at atmospheric conditions," J. Quant. Spectrosc. Radiat. Transfer **51,** 125–125 (1994).
17. P. Varanasi, "Absorption spectra of HCFC-22 around 829 cm^{-1} at atmospheric conditions," J. Quant. Spectrosc. Radiat. Transfer **47,** 251–255 (1992).
18. P. Varanasi, Z. Li, V. Nemtchinov, and A. Cherukuri, "Spectral absorption-coefficient data on HCFC-22 and SF_6 for remote-sensing applications," J. Quant. Spectrosc. Radiat. Transfer **52,** 323–332 (1994).
19. R. D. May and R. R. Friedl, "Integrated band intensities of HO_2NO_2 at 220K," J. Quant. Spectrosc. Radiat. Transfer **50,** 257–266 (1993).
20. *U.S. Standard Atmosphere,* Pub. NOAA-S/T76-1562 (U.S. Government Printing Office, Washington D.C., 1976).
21. D. Newnham, J. Ballard, and M. Page, "Infrared absorbance cross-sections for dinitrogen pentoxide vapour," J. Quant. Spectrosc. Radiat. Transfer **48,** 571–577 (1993).
22. V. Menoux, R. Le. Doucen, C. Boulet, A. Robin, and A. M. Bouchardy, "Collision-induced absorption in the fundamental band of N_2–N_2 and N_2–O_2 pairs," Appl. Opt. **32,** 263–268 (1993).
23. P. Varanasi, SUNY at Stony Brook, Marine Science Research Center, Institute of Terrestrial and Planetary Atmospheres, Stony Brook, New York 11794 (personal communication, 1995).
24. C. P. Rinsland, A. Goldman, M. A. H. Smith, and V. Malathy Devi, "Measurements of Lorentz air-broadening coefficients and relative intensities in the $H_2{}^{16}O$ pure rotational and ν_2 bands from long horizontal path atmospheric spectra," Appl. Opt. **30,** 1427–1438 (1991).
25. R. A. Toth, "$2\nu_2$–ν_2 and $2\nu_2$ bands of $H_2{}^{16}O$, $H_2{}^{17}O$, and $H_2{}^{18}O$: line positions and strengths," J. Opt. Soc. Am. B **10,** 1526–1544 (1993).
26. R. A. Toth, "ν_1–ν_2, ν_3–ν_2, ν_1, and ν_3 bands of $H_1{}^{16}O$: line positions and strengths," J. Opt. Soc. Am. B **10,** 2006–2029 (1993).
27. R. A. Toth, "The ν_1 and ν_3 bands of $H_2{}^{17}O$ and $H_2{}^{18}O$—line positions and strengths," J. Mol. Spectrosc. **166,** 184–203 (1994).
28. J.-M. Flaud, C. Camy-Peyret, A. Perrin, and C. P. Rinsland, "Improved spectroscopic line parameters for the ozone molecule," J. Quant. Spectrosc. Radiat. Transfer **48,** 611–615 (1992).
29. A. Perrin, A. M. Vesserot, J.-M. Flaud, C. Camy-Peyret, V. Malathy Devi, M. A. H. Smith, C. P. Rinsland, A. Barbe, S. Bouazza, and J. J. Plateaux, "The 2.5-μm bands of ozone: line positions and intensities," J. Mol. Spectrosc. **149,** 519–529 (1991).
30. V. Malathy Devi, A. Perrin, J.-M. Flaud, C. Camy-Peyret, C. P. Rinsland, and M. A. H. Smith, "Line positions and intensities for the $\nu_2 + 3\nu_3$ band of $^{16}O_3$ around 2.7 μm," J. Mol. Spectrosc. **143,** 381–388 (1990).
31. J.-M. Flaud, C. Camy-Peyret, A. Perrin, V. Malathy Devi, A. Barbe, S. Bouazza, J. J. Plateaux, C. P. Rinsland, M. A. H. Smith, and A. Goldman, "Line parameters for ozone hot bands in the 3.3-μm spectral region," J. Mol. Spectrosc. **160,** 378–386 (1993).
32. J.-M. Flaud, C. Camy-Peyret, C. P. Rinsland, V. Malathy Devi, M. A. H. Smith, and A. Goldman, "Improved line parameters for ozone bands in the 10-μm spectral region," Appl. Opt. **29,** 3667–3671 (1990).
33. C. P. Rinsland, M. A. H. Smith, V. Malathy Devi, A. Perrin, J.-M. Flaud, and C. Camy-Peyret, "The ν_2 bands of $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$: line positions and intensities," J. Mol. Spectrosc. **149,** 474–480 (1991).
34. H. M. Pickett, D. B. Peterson, and J. S. Margolis, "Absolute absorption of ozone in the midinfrared," J. Geophys. Res. A **97,** 20787–20793 (1992).
35. A. Barbe, J. J. Plateaux, S. Bouazza, J.-M. Flaud, and C. Camy-Peyret, "Spectral properties of ozone in the 5 μm region," J. Quant. Spectrosc. Radiat. Transfer **48,** 599–610 (1992).
36. S. Bouazza, A. Barbe, S. Mikhailenko, and J. J. Plateaux, "Line positions and intensities of the $\nu_1 + 2\nu_2 + \nu_3$ and $2\nu_2 + 2\nu_3$ bands of $^{16}O_3$," J. Mol. Spectrosc. **166,** 365–371 (1994).
37. A. Barbe, J. J. Plateaux, S. Bouazza, O. Sulakshina, S. Mikhailenko, V. Tyuterev, and S. Tashkun, "Experimental and theoretical study of absolute intensities of ozone spectral lines in the range 1850–2300 cm^{-1}," J. Quant. Spectrosc. Radiat. Transfer **52,** 341–355 (1994).
38. D. Consalvo, A. Perrin, J.-M. Flaud, C. Camy-Peyret, A. Valentin, and Ch. Chardonnet, "The 10-μm bands of the $^{17}O_3$ isotopic species of ozone," J. Mol. Spectrosc. **168,** 92–98 (1994).
39. R. A. Toth, "Line frequency measurements and analysis of N_2O between 900–4700 cm^{-1}," Appl. Opt. **30,** 5289–5315 (1991).
40. R. A. Toth, "Line strengths (900–3600 cm^{-1}), self-broadened linewidths, and frequency shifts (1800–2360 cm^{-1}) of N_2O," Appl. Opt. **30,** 7326–7365 (1993).
41. G. Tarrago, G. Restelli, and F. Cappellani, "Absolute absorption intensities in the triad ν_3, ν_5, and ν_6 of $^{12}CH_3D$ at 6–10 μm," J. Mol. Spectrosc. **129,** 326–332 (1988).
42. C. P. Rinsland, M. R. Gunson, J. C. Foster, R. A. Toth, C. B. Farmer, and R. Zander, "Stratospheric profiles of heavy water vapor isotopes and CH_3D from analysis of the ATMOS Spacelab-3 infrared solar spectra," J. Geophys. Res. **96,** 1057–1068 (1991).
43. J. P. Champion, University of Bourgogne, Centre National de la Recherche Scientifique, Ura 1796, 6 Bd Gabríel, F-21000, Dijon, France (personal communication, 1995).
44. A. Goldman, C. P. Rinsland, B. Canova, R. Zander, and M. Dang-Nhu, "Improved spectral parameters for the $^{16}O_2$ infrared forbidden lines in the $X^3\Sigma_g^-$ (0–1) band of oxygen," J. Quant. Spectrosc. Radiat. Transfer **54,** 757–765 (1995).
45. M. Dang-Nhu, R. Zander, A. Goldman, and C. P. Rinsland, "Identification of magnetic dipole infrared transitions of the fundamental band of oxygen," J. Mol. Spectrosc. **144,** 366–373 (1990).
46. M. N. Spencer, C. Chackerian, Jr., L. Giver, and L. R. Brown, "The nitric oxide fundamental band: frequency and shape parameters for rovibrational lines," J. Mol. Spectrosc. **165,** 506–524 (1994).
47. J. Ballard, W. B. Johnston, B. J. Kerredge, and J. J. Remedios, "Experimental spectral line parameters in the 1–0 band of nitric oxide," J. Mol. Spectrosc. **127,** 70–82 (1988).
48. R. A. Toth, "High resolution measurements and analysis of $^{14}N^{16}O_2$ in the (001)–(000) and (011)–(010) bands," J. Opt. Soc. Am. B **9,** 433–461 (1992).
49. V. M. Devi, B. Fridovich, G. D. Jones, D. G. S. Snyder, and A.

Neuendorffer, "Temperature-dependence of the widths of N_2-broadened lines of the ν_3 band of $^{14}N^{16}O_2$," Appl. Opt. **21,** 1537–1538 (1982).
50. R. D. May and C. R. Webster, "Laboratory measurements of NO_2 line parameters near 1600 cm^{-1}," Geophys. Res. Lett. **17,** 2157–2160 (1990).
51. A. Perrin, J.-M. Flaud, C. Camy-Peyret, D. Hurtmans, M. Herman, and G. Guelachvili, "The $\nu_2 + \nu_3$ and $\nu_2 + \nu_3 - \nu_2$ bands of $^{14}N^{16}O_2$: line positions and intensities," J. Mol. Spectrosc. **168,** 54–66 (1994).
52. A. Perrin, J.-M. Flaud, C. Camy-Peyret, A. M. Vasserot, G. Guelachvili, A. Goldman, F. J. Murcray, and R. D. Blatherwick, "The ν_1, $2\nu_2$, and ν_3 interacting bands of $^{14}N^{16}O_2$—line positions and intensities," J. Mol. Spectrosc. **154,** 391–406 (1992).
53. A. Perrin, V. Jaouen, A. Valentin, J.-M. Flaud, and C. Camy-Peyret, "The ν_5 and $2\nu_9$ bands of HNO_3," J. Mol. Spectrosc. **157,** 112–121 (1993).
54. A. Perrin, J.-M. Flaud, C. Camy-Peyret, V. Jaouen, R. Farrenq, G. Guelachvili, Q. Kou, F. LeRoy, M. Morillon-Chapey, J. Orphal, M. Badaoui, J.-Y. Mandin, and V. Dana, "Line intensities in the 11 μm band and the 7.6 μm band of HNO_3," J. Mol. Spectrosc. **160,** 524–539 (1993).
55. A. G. Maki and J. S. Wells, "Measurement and analysis of the Fermi resonance between ν_5 and $2\nu_9$ of nitric acid," J. Mol. Spectrosc. **152,** 69–79 (1992).
56. A. Goldman, J. R. Gillis, C. P. Rinsland, F. J. Murcray, and D. G. Murcray, "Stratospheric HNO_3 quantification from line-by-line nonlinear least-squares analysis of high-resolution balloon-bourne solar absorption spectra in the 870 cm^{-1} region," Appl. Opt. **23,** 3252–3255 (1984).
57. A. Goldman, T. G. Kyle, and F. S. Bonomo, "Statistical band model parameters and integrated intensities for the 5.9-μ, 7.5-μ, and 11.3-μ bands of HNO_3 vapor," Appl. Opt. **10,** 65–73 (1971).
58. L. P. Giver, P. J. Valero, and D. Goorvitch, "Nitric-acid band intensities and band-model parameters from 610 to 1760 cm^{-1}," J. Opt. Soc. Am. B **1,** 715–722 (1984).
59. R. D. May and C. R. Webster, "Measurements of line positions, intensities and collisional air-broadening coefficients in the HNO_3 7.5-μm band using a computer-controlled tunable diode laser spectrometer," J. Mol. Spectrosc. **138,** 383–397 (1989).
60. A. Perrin, J.-M. Flaud, C. Camy-Peyret, B. P. Winnewisser, S. Klee, A. Goldman, F. J. Murcray, R. D. Blatherwick, F. S. Bonomo, and D. G. Murcray, "First analysis of the $3\nu_9$–ν_9, $3\nu_9$–ν_5, and $3\nu_9$–$2\nu_9$ bands of HNO_3—torsional splitting in the ν_9 vibrational mode," J. Mol. Spectrosc. **166,** 224–243 (1994).
61. G. Guelachvili, "Absolute wavenumber measurements of the 1–0, 2–0, HF and 2–0, $H^{35}Cl$, $H^{37}Cl$ absorption bands," Opt. Commun. **19,** 150–154 (1976).
62. A. G. Maki and J. S. Wells, "New wavenumber calibration tables from heterodyne frequency measurements," J. Res. Nat. Inst. Stand. Technol. **97,** 409–470 (1992).
63. D. Goddon, A. Groh, H. J. Hanses, M. Schneider, and W. Urban, "Heterodyne frequency measurements of the 1–0 band of HF at 2.7 μm," J. Mol. Spectrosc. **147,** 392–397 (1991).
64. R. H. Tipping, "Calculation of spectroscopic parameters for diatomic molecules of atmospheric interest," GL-TR-90-0127 Rep. (Geophysics Laboratory, Hanscom Air Force Base, Mass., 1990).
65. C. P. Rinsland, M. A. H. Smith, A. Goldman, V. Malathy Devi, and D. C. Benner, "The fundamental bands of $H^{35}Cl$ and $H^{37}Cl$—line positions from high-resolution laboratory data," J. Mol. Spectrosc. **159,** 274–278 (1992).
66. R. H. Tipping, Department of Physics and Astronomy, University of Alabama, Tuscaloosa, Alabama 35487 (personal communication, 1993).
67. A. S. Pine, A. Fried, and J. W. Elkins, "Spectral intensities in the fundamental bands of HF and HCl," J. Mol. Spectrosc. **109,** 30–45 (1985).
68. A. S. Pine and A. Fried, "Self-broadening in the fundamentals of HF and HCl," J. Mol. Spectrosc. **114,** 148–162 (1985).
69. A. Goldman, J. R. Gillis, C. P. Rinsland, and J. B. Burkholder, "Improved line parameters for the $x^2\pi$–$x^2\pi$ (1–0) bands of ^{35}ClO and ^{37}ClO," J. Quant. Spectrosc. Radiat. Transfer **52,** 357–359 (1994).
70. J. B. Burkholder, P. D. Hammer, C. J. Howard, A. G. Maki, G. Thompson, and C. Chackerian Jr., "Infrared measurements of the ClO radical," J. Mol. Spectrosc. **124,** 139–161 (1987).
71. J. R. Gillis and A. Goldman, "Spectral line parameters for the $x^2\pi$–$x^2\pi$ (1, 0) bands of OH and ClO for atmospheric applications," J. Quant. Spectrosc. Radiat. Transfer **26,** 23–31 (1981).
72. J. B. Burkholder, P. D. Hammer, C. J. Howard, and A. Goldman, "Infrared line intensity measurements in the v = 0–1 band of the ClO radical," J. Geophys. Res. A **94,** 2225–2234 (1989).
73. C. P. Rinsland and A. Goldman, "Search for infrared absorption lines of atmospheric chlorine monoxide (ClO)," J. Quant. Spectrosc. Radiat. Transfer **48,** 685–692 (1992).
74. A. Fayt, R. Vanderhaute, and J. G. Lahaye, "Global rovibrational analysis of carbonyl sulfide," J. Mol. Spectrosc. **119,** 233–266 (1986).
75. R. H. Kagann, "Infrared absorption intensities for OCS," J. Mol. Spectrosc. **94,** 192–198 (1982).
76. A. Fayt, Molecular Spectroscopy Laboratory, Catholic University Louvain, Chem Cyclotron 2/B-1348, Louvain La Neuve, Belgium (personal communication, 1992).
77. G. Blanquet, J. Walrand, and C. P. Courtoy, "The ν_3 band of $^{16}O^{12}C^{34}S$ and $^{16}O^{13}C^{34}S$," J. Mol. Spectrosc. **81,** 473–479 (1980).
78. J. P. Bouanich, G. Blanquet, J. Walrand, and C. P. Courtoy, "Diode-laser measurements of line strengths and collisional half-widths in the ν_1 band of OCS 298 K and 200 K," J. Quant. Spectrosc. Radiat. Transfer **36,** 295–306 (1986).
79. N. Hunt, S. C. Foster, J. W. C. Johns, and A. R. W. McKellar, "High resolution spectroscopy of 16 bands of OCS in the region 1975–2140 cm^{-1} for diode laser calibration," J. Mol. Spectrosc. **111,** 42–53 (1985).
80. W. J. Lafferty and W. B. Olson, "The high-resolution infrared spectra of the ν_2 and ν_3 bands of HOCl," J. Mol. Spectrosc. **120,** 111–248 (1986).
81. D. D. Nelson Jr. and M. S. Zahniser, "Diode laser spectroscopy of the ν_3 vibration of HO_2 radical," J. Mol. Spectrosc. **150,** 527–534 (1991).
82. M. S. Zahniser and A. C. Stanton, "A measurement of the vibrational band strength for the ν_3 band of the HO_2 radical," J. Chem. Phys. **80,** 4951–4960 (1984).
83. M. S. Zahniser, K. E. McCurdy and A. C. Stanton, "Quantitative spectroscopic studies of the HO_2 radical: band strength measurements for the ν_1 and ν_2 vibrational bands," J. Phys. Chem. **93,** 1065–1070 (1989).
84. D. D. Nelson Jr. and M. S. Zahniser, "Air-broadened linewidth measurements in the ν_2 vibrational band of the hydroperoxyl radical," J. Mol. Spectrosc. **166,** 273–279 (1994).
85. C. P. Rinsland, M. R. Gunson, M. C. Abrams, R. Zander, E. Mahieu, A. Goldman, M. K. W. Ko, J. M. Rodriguez, and N. D. Sze, "Profiles of stratospheric chlorine nitrate ($ClONO_2$) from atmospheric trace molecule spectroscopy (ATMOS)/ATLAS 1 infrared solar occultation spectra," J. Geophys. Res. **99,** 18895–18900 (1994).
86. J. Ballard, W. B. Johnston, M. R. Gunson, and P. T. Wassell, "Absolute absorption coefficients of $ClONO_2$ infrared bands

at stratospheric temperatures," J. Geophys. Res. **93,** 1659–1665 (1988).
87. W. Bell, G. Duxbury, and D. D. Stuart, "High resolution spectra of the ν_4 band of chlorine nitrate," J. Mol. Spectrosc. **152,** 283–297 (1992).
88. J. A. Davidson, C. A. Cantrell, R. E. Shelter, A. H. McDaniel, and J. G. Calvert, "Absolute infrared absorption cross sections for $ClONO_2$ at 296 and 223 K," J. Geophys. Res. A **92,** 10921–10925 (1987).
89. E. C. Tuazon and T. J. Wallington, "Infrared absorption coefficients of gaseous chlorine nitrate," Geophys. Res. Lett. **16,** 331–334 (1989).
90. J. Orphal, J. Morillon-Chapey, and G. Guelachvili, "High-resolution absorption cross sections of chlorine nitrate in the ν_2 band region around 1292 cm^{-1} at stratospheric temperatures," J. Geophys. Res. A **99,** 14549–14555 (1994).
91. R. McPheat and G. Duxbury, "Absorption coefficients of $ClONO_2$ at 780 cm^{-1}," J. Geophys. Res. **101,** 6803–6810 (1996).
92. M. Betrencourt, M. Morillon-Chapey, G. Blanquet, and J. Walrand, "Diode-laser spectroscopy of methl-chloride near 14 μm toward its detection in the stratosphere," J. Mol. Spectrosc. **128,** 433–433 (1988).
93. M. Dang-Nhu, G. Blanquet, J. Walrand, and F. Derie, "Spectral intensities in the ν_3 band of the $^{12}CH_3{}^{35}Cl$ at 13 μm," Mol. Phys. **65,** 77–83 (1988).
94. N. F. Henfrey and B. A. Thrush, "The analysis of high resolution spectra of the ν_2 and ν_5 bands of $CH_3{}^{35}Cl$ and $CH_3{}^{37}Cl$," J. Mol. Struct. **146,** 71–83 (1986).
95. G. Tarrago, I. Kleiner, and L. R. Brown, Physics, Molecular and Applications Laboratory, Centre National de la Recherche Scientifique, University of Paris, Unite Propre, Lab Associe, Tour 13, 4 Pl. Jussieu, F-75252, Paris 05, France (personal communication, 1992).
96. G. Blanquet, J. Walrand, and J.-P. Bouanich, "Diode-laser measurements of N_2-broadening coefficients in the ν_3 band of $CH_3{}^{35}Cl$," J. Mol. Spectrosc. **160,** 253–257 (1993).
97. G. Blanquet, J. Walrand, and J.-P. Bouanich, "Diode-laser measurements of O_2-broadening coefficients in the ν_3 band of $CH_3{}^{35}Cl$," J. Mol. Spectrosc. **159,** 137–143 (1993).
98. J.-P. Bouanich, G. Blanquet, and J. Walrand, "Theoretical O_2- and N_2-broadening coefficients of CH_3Cl spectral lines," J. Mol. Spectrosc. **161,** 416–426 (1993).
99. M. Takami, "Double resonance and high resolution infrared spectroscopy of the CF_4 fundamental. 1. Infrared radiofrequency double resonance," J. Chem. Phys. **73,** 2665–2672 (1980).
100. T. Gabard, A. Nikitin, J. P. Champion, G. Pierre, and A. S. Pine, "$2\nu_3$ of $^{12}CF_4$ and its simultaneous analysis with ν_3," J. Mol. Spectrosc. **170,** 431–448 (1995).
101. T. Gabard, G. Pierre, and M. Takami, "Study of the ν_3 and $2\nu_4$ interacting states of $^{12}CF_4$," Mol. Phys. **85,** 735–744 (1995).
102. S. J. Daunt, A. K. Atakan, W. E. Blass, G. W. Halsey, D. E. Jennings, D. C. Reuter, J. Susskind, and J. W. Brault, "The 12 micron band of ethane: high resolution laboratory analysis with candidate lines for infrared heterodyne searches," Astrophysics **280,** 921–936 (1984).
103. L. Henry, A. Valentin, W. J. Lafferty, J. T. Hougen, V. Malathy Devi, P. P. Das, and K. Narahari Rao, "Analysis of high resolution Fourier transform and diode laser spectra of the ν_9 band of ethane," J. Mol. Spectrosc. **100,** 260–289 (1983).
104. A. Goldman, C. P. Rinsland, F. J. Murcray, D. G. Murcray, M. T. Coffey, and W. G. Mankin, "Balloon-borne and aircraft infrared measurements of ethane in the upper troposphere and lower stratosphere," J. Atmos. Chem. **2,** 211–221 (1984).
105. M. Dang-Nhu and A. Goldman, "Line parameters for C_2H_6 in the 3000 cm^{-1} region," J. Quant. Spectrosc. Radiat. Transfer **38,** 159–161 (1987).
106. C. P. Rinsland, G. A. Harvey, V. Malathy Devi, K. B. Thakur, J. S. Levine, and M. A. H. Smith, "Q branches of the ν_7 fundamental of ethane (C_2H_6): integrated intensity measurements for atmospheric measurement applications," Appl. Opt. **25,** 2872–2873 (1986).
107. C. P. Rinsland, R. Zander, C. B. Farmer, R. H. Norton, and J. M. Russell III, "Concentration of ethane (C_2H_6) in the lower stratosphere and upper troposphere and acetylene (C_2H_2) in the upper troposphere deduced from atmospheric trace molecule spectroscopy/Spacelab 3 spectra," J. Geophys. Res. **92,** 11951–11964 (1987).
108. A. S. Pine and W. J. Lafferty, "Torsional splittings and assignments of the Doppler-limited spectrum of ethane in the C-H stretching region," J. Res. Nat. Bur. Stand. **87,** 237–255 (1982).
109. A. S. Pine and S. C. Stone, "Torsional tunneling and A_1–A_2 splittings and air-broadening of the $^RQ_0$ and $^PQ_3$ subbranches of the ν_7 band of ethane," J. Mol. Spectrosc. **175,** 21–30 (1996).
110. J. Vander Auwera, D. Hurtmans, M. Carleer, and M. Herman, "The ν_3 fundamental in C_2H_2," J. Mol. Spectrosc. **157,** 337–357 (1993).
111. V. Malathy Devi, D. C. Benner, C. P. Rinsland, M. A. H. Smith, and B. D. Sidney, "Tunable diode laser measurements of N_2- and air-broadened halfwidths: lines in the $(\nu_4 + \nu_5)_0$ band of $^{12}C_2H_2$," J. Mol. Spectrosc. **114,** 49–53 (1985).
112. R. D'Cunha, Y. A. Sarma, G. Guelachvili, R. Farrenq, and K. Narahari Rao, "Analysis of the $^{13}C^{12}CH_2$ bands in the FTIR spectrum of acetylene," J. Mol. Spectrosc. **160,** 181–185 (1993).
113. D. Lambot, J. C. Populaire, D. Walrand, G. Blanquet, and J. P. Bouanich, "Diode laser measurements of self-broadening coefficients in the ν_5 band of C_2H_2 at low temperature," J. Mol. Spectrosc. **165,** 1–11 (1994).
114. S. Yamamoto, T. Nakanaga, H. Takeo, C. Matsumura, M. Nakata, and K. Kuchitsu, "Equilibrium structure and anharmonic potential function of phosgene: diode laser spectra of the ν_1 and ν_5 bands," J. Mol. Spectrosc. **106,** 376–387 (1984).
115. L. S. Rothman, U.S. Air Force, Geophysics Directorate, Phillips Laboratory, Bedford, Mass. 01731 (personal communication, 1994).
116. S. M. Anderson, J. Morton, and K. Mauersburger, "Laboratory measurements of ozone isotopomers by tunable diode laser absorption spectroscopy," Chem. Phys. Lett. **156,** 175–180 (1989).