

HIGH RESOLUTION SPECTROSCOPIC DATABASE FOR THE NASA
EARTH OBSERVING SYSTEM PROGRAM

NASA Grant NAG5-8420

Final Report
For the period 1 May 1999 through 30 April 2004

Principal Investigator
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October 2004

Prepared for

National Aeronautics and Space Administration
Washington, DC 20546

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

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1. Introduction

The purpose of this project has been to develop and enhance the *HITRAN* molecular spectroscopic database [1] and associated software to support the observational programs of the Earth Observing System (EOS). Emphasis has been on the EOS projects: the Atmospheric Infrared Sounder (AIRS), the High-Resolution Dynamics Limb Sounder (HIRDLS), Measurements of Pollution in the Troposphere (MOPITT), the Tropospheric Emission Spectrometer (TES), and the Stratospheric Aerosol and Gas Experiment (SAGE III). The *HITRAN* program is also involved in the Ozone Monitoring Experiment (OMI). The data requirements of these programs in terms of spectroscopy are varied with respect to constituents being observed, required remote-sensing parameters, and spectral coverage. A general requisite is for additional spectral parameters and improvements to existing molecular bands sufficient for the simulation of the observations leading to retrieval of the atmospheric state. In addition, cross-section data for heavier molecular species must be expanded and made amenable to modeling in remote sensing. The effort in the project also includes developing software and distribution to make access, manipulation, and use of *HITRAN* functional to the EOS program.

2. Data Acquisition and Data Improvement

One focus of this project has been to prepare for a new edition of the *HITRAN* database and compilation. A beta-test copy was prepared for the *HITRAN* international advisory committee that was scheduled to meet at the *HITRAN* conference in June 2004. The committee is composed of twelve members, evenly divided between North America and Europe. The members, and their alternates, have been chosen for their experience and contributions in high-resolution molecular spectroscopy, as well as their experience in atmospheric remote-sensing experiments. The mandate of the committee is to validate *HITRAN* data before public release and make recommendations for updates. The committee attempts to convene twice a year, and makes use of attendance at conferences such as the biennial *HITRAN* meeting.

The most recent edition of *HITRAN* will have an expanded format, shown in Table 1. The format replaces the transition probability squared parameter with the Einstein A -coefficient, allows for more explicit and uniform quantum identification of lines, adds uncertainty and reference indices for three more parameters (self-broadened half-width, temperature-dependence of air-broadened half-width, and the pressure shift of the line), adds the option for a procedure to account for line coupling, and adds the upper and lower statistical weights of each transition. The careful development of the Einstein A -coefficient for the transitions, as well as a rigorous standardization of the quantum-assignment notation, has led us to a more thorough understanding of developmental and maintenance issues of the database for the future. Table 2 illustrates the notation that has been implemented for the so-called global quanta. These quanta include mostly the vibrational band designations. Table 3 illustrates the "local quanta"

designations. These quanta are primarily rotational in nature, and in a sense are the unique tags of each *HITRAN* line transition.

Table 1. Line-transition format for new *HITRAN* database.

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

The reasons for replacing the weighted square of the transition moment by the Einstein *A*-coefficient in the *HITRAN* database are numerous. The Einstein *A*-coefficient is desirable for applications in atmospheric non-local thermodynamic equilibrium (non-LTE) problems, astrophysics, and fundamental physics, for example. The coefficient provides a parameter that is independent of the isotopic abundances and temperature. There were also inconsistencies discovered in previous *HITRAN* editions in the implementation of the transition probability squared. A detailed description of the formulation of the Einstein *A*-coefficient for the *HITRAN* molecular species as well as the statistical weights can be found in Ref. [10].

Coincident with the development of the statistical weights of the transitions is a full tabulation of the partition sums for each of the almost 200 isotopologues present in *HITRAN*. The tables have been provided in the *HITRAN* ftp-site (<ftp://cfa-ftp.harvard.edu/pub/hitran04/>). They are given at one-degree intervals covering 70K to 3000K.

The adoption of three more indices for the self-broadening coefficient, temperature dependent coefficient of air width, and the pressure-shift parameter allows for a much more maintainable database for the future. These parameters are now being provided much more thoroughly, as will be seen in the subsequent section.

Finally, the flag for line coupling is a response to earlier discussions and panel sessions at *HITRAN* meetings. This feature will allow the implementation of physically meaningful algorithms to account for line mixing. The algorithms will initially be provided for certain Q-branches of carbon dioxide, and later for affected lines of N_2O , CH_4 , and O_2 . The ground work has been laid to finally treat this phenomenon in a universal way. Retrievals involving limb sensing and tropospheric observations will be greatly improved in specific regions.

Table 2. Notation and format for the ten classes of global quanta identification in the *HITRAN* 2004 edition.

Class definition for <i>HITRAN</i> molecules	Upper- and Lower-State "global" Quanta
Class 1: Diatomic molecules CO, HF, HCl, HBr, HI, N ₂ , NO ⁺	$\overline{13x} \ v_1 \ I2$
Class 2: Diatomic molecules with different electronic levels O ₂	$\overline{12x} \ X \ v_1 \ I2$
Class 3: Diatomic molecules with doublet- Π electronic state NO, OH, ClO	$\overline{7x} \ X \ i \ \overline{2x} \ v_1 \ I2$
Class 4: Linear triatomic N ₂ O, OCS, HCN	$\overline{7x} \ v_1 \ v_2 \ l_2 \ v_3 \ I2$
Class 5: Linear triatomic with large Fermi resonance CO ₂	$\overline{6x} \ v_1 \ v_2 \ l_2 \ v_3 \ r \ I2 \ I1$
Class 6: Non-linear triatomic H ₂ O, O ₃ , SO ₂ , NO ₂ , HOCl, H ₂ S, HO ₂ , HOBr	$\overline{9x} \ v_1 \ v_2 \ v_3 \ I2 \ I2 \ I2$
Class 7: Linear tetratomic C ₂ H ₂	$v_1 \ v_2 \ v_3 \ v_4 \ v_5 \ l \ \pm \ r \ S \ I2 \ I2 \ I2 \ I2 \ I2 \ I2 \ A1 \ I1 \ A1$
Class 8: Pyramidal tetratomic NH ₃ , PH ₃	$\overline{5x} \ v_1 \ v_2 \ v_3 \ v_4 \ S \ I2 \ I2 \ I2 \ I2 \ I2$
Class 9: Non-linear tetratomic H ₂ CO, H ₂ O ₂ , COF ₂	$\overline{3x} \ v_1 \ v_2 \ v_3 \ v_4 \ v_5 \ v_6 \ I2 \ I2 \ I2 \ I2 \ I2 \ I2$
Class 10: Pentatomic or greater polyatomic CH ₄ CH ₃ D, CH ₃ Cl, C ₂ H ₆ , HNO ₃ , SF ₆ , HCOOH, ClONO ₂ , C ₂ H ₄	$\overline{3x} \ v_1 \ v_2 \ v_3 \ v_4 \ n \ C \ I2 \ I2 \ I2 \ I2 \ A2 \ A2$ Explicit mode notation

Notes: In the previous *HITRAN* edition [1], the global quanta were represented by an index (format I3) which was a code corresponding to the vibrational quantum numbers. In the *HITRAN* 2004 edition, the vibrational quantum numbers are directly incorporated as a 15-character field. v_j is the quantum number associated with the normal mode of vibration j , l_j is the vibrational angular momentum quantum number associated with the degenerate bending mode j , and l is defined as the absolute value of the sum of the vibrational angular momentum quantum number l_j . For class 2 and 3, X designates the electronic state of the molecule, and for class 3, i corresponds to either 1/2 (which means $N = J + 1/2$) or 3/2 (which means $N = J - 1/2$). For details of the notation of class 5, see Ref. [2]. For the notation of class 7, see Ref. [3]. Moreover, we added for class 7 the parity u or g of the vibrational level in the S -field for the symmetric isotopologue ¹²C₂H₂. For class 8, S is the symmetry of the level (only for NH₃; for PH₃ S is blank). For H₂O₂ in class 9, v_4 has been replaced by the torsional quanta n and τ described in Refs. [4, 5]. For CH₄, n is a multiplicity index, and C is the symmetry.

Table 3. Notation and format for the six groups of local quanta identification in the *HITRAN2004* edition

Group classification and <i>HITRAN</i> molecules	Upper-State local Quanta					Lower-State local Quanta						
Group 1: Asymmetric Rotors [†] H ₂ O, O ₃ , SO ₂ , NO ₂ , HNO ₃ , H ₂ CO, HOCl, H ₂ O ₂ , COF ₂ , H ₂ S, HO ₂ , HCOOH, ClONO ₂ , HOBr, C ₂ H ₄	<i>J'</i>	<i>K_a'</i>	<i>K_c'</i>	<i>F'</i>	Sym'	<i>J''</i>	<i>K_a''</i>	<i>K_c''</i>	<i>F''</i>	Sym''		
	I3	I3	I3	A5	A1	I3	I3	I3	A5	A1		
Group 2: Diatomic and Linear Molecules CO ₂ , N ₂ O, CO, HF, HCl, HBr, HI, OCS, N ₂ , HCN, C ₂ H ₂ , NO ⁺					<i>F'</i>		<i>Br</i>	<i>J''</i>	Sym''	<i>F''</i>		
				10X	A5	5X	A1	I3	A1	A5		
Group 3: Spherical Rotors SF ₆ , CH ₄	<i>J'</i>	<i>C'</i>	<i>α'</i>	<i>F'</i>		<i>J''</i>	<i>C''</i>	<i>α''</i>	<i>F''</i>			
	2X	I3	A2	I3	A5	2X	I3	A2	I3	A5		
Group 4: Symmetric Rotors CH ₃ D, CH ₃ Cl, C ₂ H ₆ , NH ₃ , PH ₃	<i>J'</i>	<i>K'</i>	<i>l'</i>	<i>C'</i>	Sym'	<i>F'</i>	<i>J''</i>	<i>K''</i>	<i>l''</i>	<i>C''</i>	Sym''	<i>F''</i>
	I3	I3	I2	A2	A1	A4	I3	I3	I2	A2	A1	A4
Group 5: Triplet-Σ Ground Electronic States O ₂					<i>F'</i>	<i>Br</i>	<i>N''</i>	<i>Br</i>	<i>J''</i>	<i>F''</i>	Sym	
				10X	A5	1X	A1	I3	A1	I3	A5	A1
Group 6: Doublet-Π Ground Electronic States [‡] NO, OH, ClO					<i>F'</i>		<i>Br</i>	<i>J''</i>	Sym''	<i>F''</i>		
				10X	A5	3X	A1	F5.1	A1	A5		

Notes: Prime and double primes refer respectively to upper and lower states, respectively; *Br* is the *O*-, *P*-, *Q*-, *R*-, or *S*-branch symbol; *J* is the quantum number associated with the total angular momentum excluding nuclear spin; *F* is the quantum number associated with the total angular momentum including nuclear spin. *F* is shown in A5 FORTRAN format in order to accommodate integer (I5) or half-integer values (F5.1). For group 3, the notations *C* and *α* are described in Ref. [6]. For group 4, the symmetry *C* (which is equal to A+, A- or E) is described in Ref. [7, 8]. *N* is the total angular momentum including spin and rotation for O₂. Sym is either the symmetry *e* or *f* for *l*-type doubling [9], + or - for required symmetry symbols, or *d* or *q* for magnetic-dipole or electric-quadrupole transitions (only for O₂ and N₂).

[†]For NO₂ and HO₂, *N* (the quantum number associated with the rotational angular momentum) is used instead of *J*, and the Sym field +/- (which is not a symmetry) is the *J*-coding defined as follows: + means $J = N + \frac{1}{2}$ and - means $J = N - \frac{1}{2}$.

[‡]For OH, the format of branch (*Br*) in the lower-state quanta field is 2A1 to accommodate the total orbital angular momentum *N* as well as *J*.

Highlighted in the next sections are some salient features of the most recent improvements. Table 4 summarizes the molecules and their isotopologues currently in the line-transition portion of *HITRAN*.

Table 4. Summary of isotopologues represented in *HITRAN*

No.	Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral coverage (cm ⁻¹)	Number of lines
1	H ₂ O	161	0.997317	0-25233	36114
		181	0.00199983	0-14519	9548
		171	0.000372	10-11335	6120
		162	0.00031069	0-7514	9628
		182	0.000000623	0-3825	1611
		172	0.000000116	1234-1599	175
		626	0.98420	442-9649	27979
		636	0.01106	497-8105	8836
		628	0.0039471	0-8133	13445
2	CO ₂	627	0.000734	0-6962	7739
		638	0.00004434	567-4947	2312
		637	0.00000825	584-3642	1593
		828	0.0000039573	615-3670	721
		728	0.00000147	626-2359	288
		666	0.992901	0-4061	183785
		668	0.00398194	0-2114	21718
3	O ₃	686	0.00199097	1-2075	8937
		667	0.000740	0-2122	65106
		676	0.000370	0-2101	31935
		446	0.990333	0-5135	33066
		456	0.0036409	5-5086	4222
4	N ₂ O	546	0.0036409	4-4704	4592
		448	0.00198582	542-4672	4250
		447	0.000369	550-4430	1705
		26	0.98654	3-8465	917
5	CO	36	0.01108	3-6279	780
		28	0.0019782	3-6267	760
		27	0.000368	3-6339	728
		38	0.00002222	3-6124	712
		37	0.00000413	1807-6197	580
6	CH ₄	211	0.98827	0-9200	187128
		311	0.01110	0-6070	28793
		212	0.00061575	7-3307	35519
7	O ₂	66	0.995262	0-15927	1430
		68	0.00399141	1-15852	671
		67	0.000742	0-14537	4326
8	NO	46	0.993974	0-9274	100902
		56	0.0036543	1609-2061	699
		48	0.00199312	1601-2039	679
9	SO ₂	626	0.94568	0-4093	38566
		646	0.04195	2463-2497	287
10	NO ₂	646	0.991616	0-3075	104223
11	NH ₃	4111	0.9958715	0-5295	27994
		5111	0.0036613	0-5180	1090
12	HNO ₃	146	0.989110	0-1770	271166

Table 4 (continued)

		61	0.997473	0-19268	41166
13	OH	81	0.00200014	0-329	295
		62	0.00015537	0-332	912
14	HF	19	0.99984425	41-11536	107
15	HCl	15	0.757587	20-13458	324
		17	0.242257	20-10995	289
		19	0.50678	16-9759	651
16	HBr	11	0.49306	16-9758	642
17	HI	17	0.99984425	12-8488	806
18	ClO	56	0.75591	0-1208	3599
		76	0.24172	0-1200	3631
		622	0.93739	0-4119	10553
		624	0.04158	0-4116	4186
19	OCS	632	0.01053	0-4013	2283
		623	0.007399	509-4116	1802
		822	0.001880	0-4042	1096
		126	0.98624	0-2999	1772
20	H ₂ CO	136	0.01108	0-73	563
		128	0.0019776	0-48	367
		165	0.75579	1-3800	8877
21	HOCl	167	0.24168	1-3800	7399
22	N ₂	44	0.9926874	1922-2626	120
		124	0.98511	0-3424	2955
23	HCN	134	0.01107	2-3405	652
		125	0.0036217	2-3420	646
		215	0.74894	0-3173	16411
24	CH ₃ Cl	217	0.23949	0-3162	14708
25	H ₂ O ₂	1661	0.994952	0-1500	100781
26	C ₂ H ₂	1221	0.97760	604-6686	3232
		1231	0.02197	613-6589	285
27	C ₂ H ₆	1221	0.97699	720-2978	4749
28	PH ₃	1111	0.99953283	770-2472	11790
29	COF ₂	269	0.98654	725-2002	70601
30	SF ₆	29	0.95018	929-964	22901
		121	0.94988	2-4257	12330
31	H ₂ S	141	0.04214	5-4172	4894
		131	0.007498	5-4099	3564
32	HCOOH	126	0.983898	10-1235	24808
33	HO ₂	166	0.995107	0-3676	38804
34	O	6	0.997628	68-159	2
		5646	0.74957	763-798	21988
35	ClONO ₂	7646	0.23970	765-791	10211
36	NO ⁺	46	0.993974	1634-2531	1206
		169	0.5056	0-316	2177
37	HOBr	161	0.4919	0-316	2181
		221	0.9773	701-3243	12697
38	C ₂ H ₄	231	0.02196	2947-3181	281
39	CH ₃ OH	2161	0.98593	0-1408	19899

Note: SF₆ and ClONO₂ are relegated to a supplemental directory.

2.1. Recent Improvements to *HITRAN* Line Parameters

The following sub-sections cover molecules whose parameters have been updated since the last edition of *HITRAN* [1]. The descriptions are generally by band regions. Future improvements are also mentioned where necessary.

2.1.1. H_2O (molecule 1)

For water vapor, a major improvement has been done especially for the main isotopologue $H_2^{16}O$.

In the pure-rotation region, 952 lines of HDO^{18} have been added to *HITRAN*. Line positions and intensities come from the JPL catalog [11]. Note that this isotopologue was not previously present in *HITRAN* in this region.

Updates of line positions have been done for 1396 lines of $H_2^{17}O$ and $H_2^{18}O$ between 0-500 cm^{-1} based on the work of Toth [12], and of line intensities for 2523 lines of $H_2^{17}O$, $H_2^{18}O$, and $HD^{16}O$ between 0-500 cm^{-1} based on the work of Pearson [13].

Between 0 and 800 cm^{-1} , the calculations of Coudert et al. [14, 15, 16] have been used to update line positions and line intensities of the 000-000, 010-010, 020-020, 100-100, and 001-001 bands, and to add six new bands into *HITRAN* (100-001, 100-020, 020-100, 020-001, 001-100, 001-020). These updates and improvements are for positions and intensities of 2852 lines involving the first eight vibrational states. To account for the fact that at small wavenumbers, that is for the microwave region, a higher sensitivity is experimentally achieved as well as for theoretical reasons, the intensity cutoff, S_{cut} , was taken here as

$$S_{cut} = S_{min} \times [1 - e^{-hc\nu/kT}] \quad (1)$$

where $S_{min} = 10^{-27}$ cm/molecule, h is Planck's constant, c is the speed of light, ν is the wavenumber of the transition, k is Boltzmann's constant, and T is the temperature.

Moreover, a complete update for positions and line intensities has been done for all isotopologues between 500-8000 cm^{-1} based on the work of Toth [17]. This update does not concern lines previously discussed which come from the work of Coudert.

Between 9600 to 11400 cm^{-1} , the line positions and intensities of the isotopologue $H_2^{17}O$, which comes from a preliminary study of Camy-Peyret et al [18], have been updated. The number of lines has been increased to 1063 from 370.

Another significant improvement concerns the 11400-12895 cm^{-1} and 13184-25000 cm^{-1} regions for which the lines lists generated from the work of Mérienne et al [19] and from the work of Coheur et al. [20] have been used to replace *HITRAN* lines of $H_2^{16}O$ in these two regions. Only assignments, line positions and line intensities have been taken from Refs. [19, 20].

Concerning the air-broadening coefficients, a complete update has been done based on the work of Jacquemart [21] for the $H_2^{16}O$, $H_2^{18}O$ and $H_2^{17}O$ isotopologues and on the work of Toth [17] for the $HD^{16}O$, $HD^{18}O$ and $HD^{17}O$ isotopologues. For the air-broadening coefficients of the H_2O isotopologues, semi-empirical calculations have been used [21]. For each rotational transition, a fit of recent experimental data [17, 19, 20, 22, 23] and recent theoretical data [24, 25, 26] has been done using Eq. (15) of Ref. [27]. The coefficients deduced from the fit allow us to obtain any air-broadening coefficient of transitions having same rotational quantum numbers

but different vibrational quantum numbers. The coefficients from Ref. [21] have been used to calculate the air-broadening coefficients of transitions for all H₂O isotopologues present in this *HITRAN* 2004 edition. For the air-broadening coefficients of the HDO isotopologues, we used directly the values of Toth [17] between 500-8000 cm⁻¹, and for the pure rotation region of HD¹⁶O and HD¹⁸O we also used the values from Ref. [17] of the ν_1 , ν_2 and ν_3 bands of HD¹⁶O making the assumption that the vibrational dependence is negligible.

For the self-broadening coefficients, values from Toth [17] have been used between 500-8000 cm⁻¹. For the 0-800 cm⁻¹ region of the H₂¹⁶O, H₂¹⁸O and H₂¹⁷O isotopologues (except for lines from Toth [17] between 500-800 cm⁻¹), we used the values from Ref. [17] of the ν_1 , ν_2 and ν_3 bands H₂¹⁶O again assuming negligible vibrational dependence. For the pure rotation region of HD¹⁶O and HD¹⁸O we similarly adopted the values from Ref. [17] of the ν_1 , ν_2 and ν_3 bands of HD¹⁶O.

A major update has been performed for the air-pressure shift coefficients in this 2004 *HITRAN* edition; most of water-vapor transitions in *HITRAN* have a non-zero value now. As has been done for the air-broadening coefficients, semi-empirical calculations [21] have been used for the air-pressure shift coefficients for all lines of H₂¹⁶O, H₂¹⁸O and H₂¹⁷O isotopologues. For the HD¹⁶O, HD¹⁸O and HD¹⁷O isotopologues, values from the SISAM.H₂O line list from Toth [17] have been used when available.

For the temperature dependence of the air-broadening coefficients, values from Ref. [28] covering transitions in the 6- μ m region have been used. Note that these values are only m -dependent, where $m = -J''$ for $\Delta J = -1$, $m = J''$ for $\Delta J = 0$, and $m = J'' + 1$ for $\Delta J = +1$, and these coefficients have now been used for all transitions of all isotopologues of water vapor throughout the database. Table 5 summarizes these values.

Table 5. Summary of the coefficients of temperature dependence of the air-broadening coefficients n_{air} from Ref. [28].

$ m $	n_{air}
0	0.78
1	0.78
2	0.78
3	0.77
4	0.73
5	0.69
6	0.64
7	0.59
8	0.53
9	0.49
10	0.45
11	0.41
12	0.39
13	0.37
14	0.36
15	0.36
16	0.38
≥ 17	0.41

2.1.2. CO₂ (molecule 2)

Among the several recent studies on CO₂, we have to highlight the global calculation both on positions and intensities for ¹²C¹⁶O₂, ¹³C¹⁶O₂, ¹²C¹⁶O¹⁸O and ¹²C¹⁶O¹⁷O of Tashkun et al. [29]. This calculation has led to a Carbon Dioxide Spectroscopic Database at 296K (CDSD-296). This work has been compared with the earlier calculations using the Direct Numerical Diagonalization (DND) technique [30] and has been found to be an improvement. Following what has been done previously [31], high-quality experimental data are preferred when available compared to calculated data. For this reason, the data of CDSD-296 have been used to update *HITRAN* only when no laboratory observed data are available.

Two line lists in the pure rotation region have been added in this edition for the isotopologues ¹⁶O¹²C¹⁸O and ¹⁶O¹²C¹⁷O since a small observable permanent dipole moment exists for these asymmetric species. The positions, the energies of the lower state of the transitions, and the line intensities come from the JPL catalog [11]. Note that for the ¹⁶O¹²C¹⁷O isotopologue, the hyperfine structure is resolved.

Concerning line positions, several updates have been accomplished. For the main isotopologue ¹²C¹⁶O₂, the recent work of Miller and Brown [32] has been used to update line positions of 83 bands in a large range of the infrared. Moreover, the calculation of Taskun et al. [29] has been used to improve the line positions that had been calculated in *HITRAN92* [33] using spectroscopic constants [31] coming either from DND calculation [30], from Venus observations [34], or from the calculation of Rothman and Benedict [35] for the other isotopologues. The work of Taskun et al. [29] has led to the update of line positions of 51 bands of ¹²C¹⁶O₂, 8 bands of ¹³C¹⁶O₂, 4 bands of ¹²C¹⁶O¹⁸O, and 12 bands of ¹²C¹⁶O¹⁷O. As was stressed in the work of Goldman et al [36], the work of Ding et al. [37] has been used to update the line positions for the 2ν₁ + 3ν₃ ¹²C¹⁶O₂ triad. The spectroscopic constants of Ref. [37] have also been used to update the line positions of two hot bands involving the levels of the 2ν₁ + 3ν₃ triad. For the 21113-11102, 21113-11101, 12212-02201, 40002-11102, and 23301-02201 interacting bands (for notations, see Table 3), the line positions have been taken from the work of Benner [38]. The positions of the two laser bands of ¹²C¹⁶O¹⁷O have also been updated from Ref. [41]. A summary of the improvements concerning the line positions is given in Table 6.

Table 6. Bands of CO₂ for which the line positions have been updated.

Band Center (cm ⁻¹)	Upper Vib ν ₁ ν ₂ l ₂ ν ₃ r	Lower Vib ν ₁ ν ₂ l ₂ ν ₃ r	v _{min} (cm ⁻¹)	v _{max} (cm ⁻¹)	No. of Lines	J _{min}	J _{max}	Ref.
¹⁶ O ¹² C ¹⁶ O, first most abundant isotopologue (626 in AFGL notation)								
608.828	1 0 0 1 2	0 1 1 1 1	576	644	67	1	47	32
618.028	1 0 0 0 2	0 1 1 0 1	546	687	136	1	91	32
645.105	2 3 3 0 3	2 2 2 0 3	645	646	15	10	24	29
654.869	0 1 1 1 1	0 0 0 1 1	607	708	98	1	67	32
655.260	0 2 2 1 1	0 1 1 1 1	621	696	144	1	52	32
667.380	0 1 1 0 1	0 0 0 0 1	593	752	153	0	102	32
667.752	0 2 2 0 1	0 1 1 0 1	600	750	275	1	94	32
688.672	1 1 1 0 1	1 0 0 0 1	625	756	126	0	84	32
710.770	1 0 0 1 1	0 1 1 1 1	677	745	67	1	47	32
720.804	1 0 0 0 1	0 1 1 0 1	649	791	137	1	92	32
741.724	1 1 1 0 1	0 2 2 0 1	675	802	233	2	81	32
791.448	1 1 1 0 1	1 0 0 0 2	737	849	109	0	74	32
927.156	0 1 1 1 1	1 1 1 0 1	868	964	138	1	60	32

960.959	00011	10001	886	1002	75	0	74	32
1063.735	00011	10002	986	1105	77	0	76	32
2076.856	11101	00001	2010	2145	127	0	88	32
2224.656	10012	10001	2158	2264	68	0	68	32
2274.422	06611	06601	2244	2299	62	6	34	29
2275.842	14411	14401	2251	2297	42	4	28	29
2277.173	22211	22201	2259	2294	23	10	22	29
2278.387	14412	14402	2243	2306	77	4	39	29
2280.618	22212	22202	2250	2305	61	4	34	29
2281.674	22213	22203	2243	2310	85	2	42	29
2286.804	05511	05501	2234	2322	133	5	56	29
2311.701	01121	01111	2246	2350	162	1	67	32
2324.141	02211	02201	2227	2371	250	2	92	32
2324.183	00021	00011	2244	2366	80	1	79	32
2326.598	10011	10001	2231	2372	91	0	90	32
2327.433	10012	10002	2231	2374	93	0	92	32
2336.632	01111	01101	2227	2384	278	1	101	32
2349.143	00011	00001	2230	2397	109	0	108	32
2429.374	10011	10002	2364	2467	66	0	66	32
3365.269	31102	10001	3331	3403	33	8	48	29
3398.219	21113	11101	3374	3420	46	6	28	38
3465.439	20013	10001	3410	3505	61	0	60	32
3496.141	23313	13302	3464	3522	68	3	36	29
3504.987	14412	04401	3461	3537	108	4	48	29
3506.713	31114	21103	3473	3534	73	2	38	29
3518.664	22213	12202	3468	3554	124	2	54	29
3527.808	22212	12201	3484	3559	100	2	47	29
3542.604	21113	11102	3476	3586	171	1	70	38
3543.095	40002	11102	3502	3592	82	1	63	38
3552.854	12212	02201	3476	3598	203	2	78	38
3554.964	23301	02201	3504	3611	188	2	68	38
3555.909	21112	11101	3492	3593	152	1	64	32
3568.215	20013	10002	3490	3615	81	0	80	32
3589.651	20012	10001	3506	3628	79	0	78	32
3612.841	10012	00001	3509	3661	99	0	98	32
3659.272	02211	00001	3582	3715	82	4	86	32
3692.427	20012	10002	3606	3731	81	0	80	32
3703.157	31111	21101	3680	3723	43	6	27	29
3703.510	22212	12202	3651	3736	124	2	54	29
3704.112	23312	13302	3675	3727	56	3	32	29
3711.476	20011	10001	3635	3757	79	0	78	32
3712.412	23311	13301	3689	3733	42	7	28	29
3713.720	21111	11101	3648	3755	166	1	68	32
3713.809	22211	12201	3665	3747	118	2	52	29
3714.782	10011	00001	3610	3763	99	0	98	32
3724.133	15511	05501	3702	3743	33	5	25	29
3726.396	14411	04401	3678	3759	119	4	51	29
3814.252	20011	10002	3753	3854	65	0	64	32
3980.582	01121	02201	3975	4003	59	8	47	32
4005.946	00021	01101	3934	4029	78	2	63	32
4416.149	31104	00001	4426	4452	16	12	42	29
4687.796	30014	10001	4652	4719	42	2	42	32
4722.649	32214	12202	4705	4740	23	10	22	29
4733.518	23313	03301	4696	4763	87	3	42	29
4735.611	40015	20003	4712	4757	24	6	28	29
4753.454	31102	00001	4706	4800	72	2	60	29

4755.707	3 1 1 1 4	1 1 1 0 2	4712	4792	102	1	50	29
4768.554	2 2 2 1 3	0 2 2 0 1	4711	4807	144	2	60	32
4784.681	2 0 0 2 3	0 0 0 1 1	4762	4805	21	7	27	29
4786.701	3 1 1 1 3	1 1 1 0 1	4750	4814	78	2	41	32
4790.572	3 0 0 1 4	1 0 0 0 2	4733	4834	65	0	64	32
4807.694	2 1 1 1 3	0 1 1 0 1	4741	4854	91	1	72	32
4808.185	4 0 0 0 2	0 1 1 0 1	4758	4857	80	1	55	29
4839.733	3 0 0 1 3	1 0 0 0 1	4780	4874	61	0	60	32
4853.624	2 0 0 1 3	0 0 0 0 1	4772	4903	85	0	84	32
4910.605	2 0 0 2 2	0 0 0 1 1	4872	4937	41	1	41	29
4912.160	4 0 0 1 4	2 0 0 0 3	4879	4936	35	2	36	29
4920.211	3 2 2 1 3	1 2 2 0 2	4893	4942	49	6	30	29
4922.552	4 0 0 1 3	2 0 0 0 2	4889	4946	35	2	36	29
4937.312	4 0 0 1 2	2 0 0 0 1	4922	4953	8	12	20	29
4941.488	2 3 3 1 2	0 3 3 0 1	4897	4972	103	3	47	29
4942.509	3 0 0 1 3	1 0 0 0 2	4872	4978	69	0	68	32
4946.819	3 1 1 1 2	1 1 1 0 1	4900	4979	102	1	50	32
4953.401	2 2 2 1 2	0 2 2 0 1	4890	4991	158	2	64	32
4959.667	3 0 0 1 2	1 0 0 0 1	4892	4996	67	0	66	32
4965.385	2 1 1 1 2	0 1 1 0 1	4884	5007	198	1	77	32
4977.835	2 0 0 1 2	0 0 0 0 1	4881	5018	89	0	88	32
5028.481	2 0 0 2 1	0 0 0 1 1	5000	5052	31	3	33	29
5062.443	3 0 0 1 2	1 0 0 0 2	5002	5096	61	0	60	32
5099.661	2 0 0 1 1	0 0 0 0 1	5017	5148	85	0	84	32
5114.896	3 0 0 1 1	1 0 0 0 1	5060	5155	61	0	60	32
5123.196	2 1 1 1 1	0 1 1 0 1	5050	5167	185	1	73	32
5126.973	3 1 1 1 1	1 1 1 0 1	5086	5158	91	1	45	32
5139.402	2 2 2 1 1	0 2 2 0 1	5081	5176	145	2	60	32
5151.381	2 3 3 1 1	0 3 3 0 1	5112	5181	90	3	43	29
5217.672	3 0 0 1 1	1 0 0 0 2	5176	5251	48	0	46	32
5315.713	0 1 1 2 1	0 0 0 0 1	5251	5342	93	0	64	32
5584.393	0 0 0 3 1	1 0 0 0 1	5541	5601	39	2	40	32
5687.169	0 0 0 3 1	1 0 0 0 2	5638	5703	42	2	42	32
5972.540	3 2 2 1 4	0 2 2 0 1	5949	5995	46	6	29	29
5998.570	4 0 0 1 5	1 0 0 0 2	5967	6028	37	2	38	29
6020.797	3 1 1 1 4	0 1 1 0 1	5975	6059	108	1	52	32
6075.980	3 0 0 1 4	0 0 0 0 1	6019	6121	66	0	66	32
6149.365	4 1 1 1 4	1 1 1 0 2	6160	6164	5	14	18	29
6170.102	3 2 2 1 3	0 2 2 0 1	6132	6198	82	2	41	32
6175.119	4 0 0 1 4	1 0 0 0 2	6130	6207	50	0	50	32
6196.176	3 1 1 1 3	0 1 1 0 1	6137	6233	136	1	60	32
6205.511	4 0 0 1 3	1 0 0 0 1	6160	6232	47	0	46	32
6227.917	3 0 0 1 3	0 0 0 0 1	6150	6266	75	0	74	32
6308.287	4 0 0 1 3	1 0 0 0 2	6260	6335	49	0	48	32
6346.264	4 0 0 1 2	1 0 0 0 1	6303	6376	47	0	46	32
6347.852	3 0 0 1 2	0 0 0 0 1	6271	6385	73	0	74	32
6356.295	3 1 1 1 2	0 1 1 0 1	6297	6392	134	1	59	32
6359.257	3 2 2 1 2	0 2 2 0 1	6322	6386	80	2	40	29
6387.868	4 1 1 0 1	0 0 0 0 1	6348	6430	45	8	52	29
6503.081	3 0 0 1 1	0 0 0 0 1	6447	6545	63	0	62	32
6532.654	4 0 0 1 1	1 0 0 0 1	6506	6557	29	4	32	29
6536.449	3 1 1 1 1	0 1 1 0 1	6489	6572	107	1	51	32
6562.441	3 2 2 1 1	0 2 2 0 1	6547	6577	15	11	19	29
6870.800	1 1 1 3 2	1 1 1 0 2	6848	6885	30	9	24	29
6905.767	1 0 0 3 1	1 0 0 0 1	6850	6922	47	0	46	32
6907.143	1 0 0 3 2	1 0 0 0 2	6846	6924	51	0	50	32

6935.134	0 1 1 3 1	0 1 1 0 1	6846	6952	156	1	65	32
6972.577	0 0 0 3 1	0 0 0 0 1	6856	6989	79	0	78	32
7283.978	4 0 0 1 5	0 0 0 0 1	7253	7314	37	2	38	29
7414.455	4 1 1 1 4	0 1 1 0 1	7386	7438	57	4	32	29
7460.527	4 0 0 1 4	0 0 0 0 1	7411	7494	54	0	54	32
7583.252	4 1 1 1 3	0 1 1 0 1	7550	7608	70	2	37	29
7593.695	4 0 0 1 3	0 0 0 0 1	7535	7623	57	0	56	32
7734.448	4 0 0 1 2	0 0 0 0 1	7687	7766	51	0	50	32
7757.625	4 1 1 1 2	0 1 1 0 1	7741	7773	18	11	21	32
7920.838	4 0 0 1 1	0 0 0 0 1	7897	7944	25	6	30	29
8103.586	2 0 0 3 3	1 0 0 0 2	8080	8119	18	8	26	29
8135.890	1 1 1 3 2	0 1 1 0 1	8079	8154	98	1	48	29
8192.551	1 0 0 3 2	0 0 0 0 1	8099	8210	70	0	70	32
8231.561	2 0 0 3 2	1 0 0 0 2	8207	8246	18	8	26	37
8243.169	2 0 0 3 1	1 0 0 0 1	8224	8256	11	10	20	37
8276.760	1 1 1 3 1	0 1 1 0 1	8216	8293	101	1	49	29
8293.951	1 0 0 3 1	0 0 0 0 1	8206	8310	65	0	64	32
9516.969	2 0 0 3 2	0 0 0 0 1	9454	9533	51	0	50	37
9631.353	2 0 0 3 1	0 0 0 0 1	9583	9649	42	2	42	37

¹⁶O¹³C¹⁶O, second most abundant isotopologue (636 in AFGL notation)

573.683	1 3 3 0 2	0 4 4 0 1	573	574	25	7	31	29
595.675	2 1 1 0 3	1 2 2 0 2	579	597	40	5	31	29
619.824	2 1 1 0 3	2 0 0 0 3	591	650	57	2	42	29
637.764	1 3 3 0 2	1 2 2 0 2	613	669	100	2	41	29
649.687	0 5 5 0 1	0 4 4 0 1	625	682	92	4	41	29
2225.024	0 5 5 1 1	0 5 5 0 1	2206	2243	24	5	23	29
2227.810	1 3 3 1 2	1 3 3 0 2	2202	2249	44	7	29	29
2229.651	2 1 1 1 3	2 1 1 0 3	2202	2253	56	4	32	29

¹⁶O¹²C¹⁸O, third most abundant isotopologue (628 in AFGL notation)

561.121	1 2 2 0 2	0 3 3 0 1	547	562	68	7	29	29
647.712	1 2 2 0 2	1 1 1 0 2	617	685	266	1	49	29
2287.110	1 2 2 1 2	1 2 2 0 2	2251	2315	170	2	43	29
2295.045	0 3 3 1 1	0 3 3 0 1	2241	2330	284	3	59	29

¹⁶O¹²C¹⁷O, fourth most abundant isotopologue (627 in AFGL notation)

586.850	1 1 1 0 2	0 2 2 0 1	548	626	294	2	53	29
649.955	1 2 2 0 2	1 1 1 0 2	620	685	244	1	46	29
665.114	0 2 2 0 1	0 1 1 0 1	614	726	427	1	74	29
665.509	0 3 3 0 1	0 2 2 0 1	623	715	348	2	62	29
681.386	1 2 2 0 1	1 1 1 0 1	656	712	208	1	41	29
732.256	1 1 1 0 1	0 2 2 0 1	691	771	302	2	54	29
748.133	1 2 2 0 1	0 3 3 0 1	733	749	72	7	29	29
963.986	0 0 0 1 1	1 0 0 0 1	925	991	85	1	43	41
1067.727	0 0 0 1 1	1 0 0 0 2	1024	1098	97	0	48	41
2306.741	1 1 1 1 2	1 1 1 0 2	2253	2342	258	1	58	29
2315.147	0 2 2 1 1	0 2 2 0 1	2246	2355	362	2	71	29
2317.319	1 0 0 1 1	1 0 0 0 1	2249	2356	141	0	70	29
2318.964	1 0 0 1 2	1 0 0 0 2	2249	2359	145	0	72	29
2327.581	0 1 1 1 1	0 1 1 0 1	2248	2370	416	1	80	29

Note: The second and third columns, Upper Vib and Lower Vib, use the AFGL vibrational notation for carbon dioxide [4]. The sixth column indicates the number of lines that have been replaced in *HITRAN*.

For the line intensities, numerous experimental studies have been performed since the last *HITRAN* updates [1]. Several works have been taken into account to improve the current edition: the work of Mandin et al. [39] for the 10012-10001 band of $^{12}\text{C}^{16}\text{O}_2$ centered at 2225 cm^{-1} the work of Claveau et al. [40] for three hot bands of $^{16}\text{O}^{12}\text{C}^{17}\text{O}$ between 550 and 765 cm^{-1} , for the $\nu_2 + \nu_3 - \nu_2$ band of $^{16}\text{O}^{12}\text{C}^{17}\text{O}$, and for the laser bands of $^{16}\text{O}^{12}\text{C}^{17}\text{O}$ and $^{16}\text{O}^{12}\text{C}^{18}\text{O}$ [41]; the work of Teffo et al. for the 10031-00001 and 10032-00001 bands of the main isotopologue centered at 8294 cm^{-1} and at 8192 cm^{-1} [42] and for the fundamental ν_3 of $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ [43]; the work of Henningsen and Simonsen [44] for the $2\nu_1 + 2\nu_2 + \nu_3$ band of $^{12}\text{C}^{16}\text{O}_2$ at 6348 cm^{-1} ; the work of Kshirsagar et al. for the $2\nu_3$ of $^{16}\text{O}^{12}\text{C}^{18}\text{O}$ at 4639 cm^{-1} [45] and for the 00031-10001 and 00031-10002 bands of $^{12}\text{C}^{16}\text{O}_2$ at 5584 cm^{-1} and 5687 cm^{-1} [46]; the work of Giver et al. [47] for five bands of $^{12}\text{C}^{16}\text{O}_2$ between 5218 cm^{-1} and 5349 cm^{-1} ; the work of Malathy Devi et al. [48] for 33 bands of $^{12}\text{C}^{16}\text{O}_2$ between 3090 - 3850 cm^{-1} ; and the work of Benner [38] for five interacting bands around 3400 cm^{-1} . We also used the calculation of Tashkun et al. from CDSD-296 [29] in order to replace line intensities that came into *HITRAN* from the early calculation of Rothman and Benedict [35]: line intensities for 4 bands of $^{12}\text{C}^{16}\text{O}_2$ and for 15 bands of $^{12}\text{C}^{16}\text{O}^{17}\text{O}$ have thus been updated. A summary of the bands for which the line intensities have been updated can be found in Table 7. One should note that the 23301-02201 band, which was not present in the 2000 *HITRAN* edition [1], has been added from the work of Benner [38].

Table 7. Bands of CO_2 for which the line intensities have been updated.

Band Center (cm^{-1})	Upper Vib $\nu_1 \nu_2 l_2 \nu_3 r$	Lower Vib $\nu_1 \nu_2 l_2 \nu_3 r$	ν_{\min} (cm^{-1})	ν_{\max} (cm^{-1})	No. of Lines	Sum of Line Intensities	Ref.
$^{16}\text{O}^{12}\text{C}^{16}\text{O}$, first most abundant isotopologue (626 in AFGL notation)							
2224.656	1 0 0 1 2	1 0 0 0 1	2158	2264	68	1.12E-22	39
3181.464	2 1 1 0 3	0 0 0 0 1	3131	3239	78	1.19E-23	48
3275.163	3 0 0 0 3	0 1 1 0 1	3232	3317	65	1.91E-24	48
3305.708	3 1 1 0 3	1 0 0 0 2	3270	3344	36	4.42E-25	48
3339.356	2 1 1 0 2	0 0 0 0 1	3279	3398	105	1.02E-22	48
3340.534	2 2 2 0 2	0 1 1 0 1	3294	3394	145	8.19E-24	48
3341.659	2 3 3 0 2	0 2 2 0 1	3311	3379	55	4.04E-25	48
3365.269	3 1 1 0 2	1 0 0 0 1	3331	3403	33	3.27E-25	48
3396.895	3 0 0 0 2	0 1 1 0 1	3349	3441	52	1.92E-24	48
3398.219	2 1 1 1 3	1 1 1 0 1	3374	3420	46	2.52E-25	38
3465.439	2 0 0 1 3	1 0 0 0 1	3410	3505	61	1.49E-23	48
3496.141	2 3 3 1 3	1 3 3 0 2	3464	3522	68	6.37E-25	48
3500.672	2 1 1 0 1	0 0 0 0 1	3445	3561	100	6.18E-23	48
3504.987	1 4 4 1 2	0 4 4 0 1	3461	3537	108	3.67E-24	48
3518.664	2 2 2 1 3	1 2 2 0 2	3468	3554	124	1.14E-23	48
3527.613	3 0 0 1 4	2 0 0 0 3	3476	3565	57	8.61E-24	48
3528.057	1 3 3 1 2	0 3 3 0 1	3467	3568	162	1.01E-22	48
3529.981	2 2 2 0 1	0 1 1 0 1	3488	3580	131	4.15E-24	48
3542.604	2 1 1 1 3	1 1 1 0 2	3476	3586	171	2.81E-22	38
3543.095	4 0 0 0 2	1 1 1 0 2	3502	3592	82	1.09E-23	38
3552.854	1 2 2 1 2	0 2 2 0 1	3476	3598	203	2.80E-21	38
3554.964	2 3 3 0 1	0 2 2 0 1	3504	3611	188	2.78E-23	38
3555.909	2 1 1 1 2	1 1 1 0 1	3492	3593	152	9.39E-23	48
3556.774	3 0 0 1 3	2 0 0 0 2	3506	3591	55	5.69E-24	48
3566.069	1 0 0 2 2	0 0 0 1 1	3509	3604	62	2.05E-23	48
3568.215	2 0 0 1 3	1 0 0 0 2	3490	3615	81	3.09E-21	48
3589.651	2 0 0 1 2	1 0 0 0 1	3506	3628	79	1.60E-21	48
3659.272	0 2 2 1 1	0 0 0 0 1	3582	3715	82	1.93E-22	38

3667.547	10021	00011	3606	3704	64	3.47E-23	48
3676.708	30012	20002	3626	3711	55	7.09E-24	48
3679.550	30013	20003	3622	3710	57	8.07E-24	48
3692.427	20012	10002	3606	3731	81	3.64E-21	48
3700.295	21112	11102	3629	3738	170	2.87E-22	48
3711.476	20011	10001	3635	3757	79	2.93E-21	48
3713.720	21111	11101	3648	3755	166	2.22E-22	48
3726.646	12211	02201	3646	3770	208	4.68E-21	48
3727.359	13311	03301	3662	3766	168	1.76E-22	48
3799.484	30012	20003	3774	3819	24	1.35E-25	48
3814.252	20011	10002	3753	3854	65	5.90E-23	48
3858.106	21111	11102	3818	3888	87	1.84E-24	48
4808.185	40002	01101	4758	4857	80	2.44E-23	29
5061.778	12211	00001	4992	5112	69	4.47E-24	29
5217.672	30011	10002	5176	5251	48	2.13E-24	47
5247.833	10022	01101	5217	5271	61	1.37E-24	47
5291.132	02221	01101	5248	5316	130	3.52E-24	47
5315.713	01121	00001	5251	5342	93	4.72E-23	47
5349.310	10021	01101	5301	5357	43	5.77E-25	47
5584.393	00031	10001	5541	5601	39	5.58E-25	46
5687.169	00031	10002	5641	5703	40	6.31E-25	46
6347.852	30012	00001	6271	6385	73	4.42E-22	44
6387.868	41101	00001	6348	6430	45	2.45E-25	29
8192.551	10032	00001	8099	8210	70	4.15E-23	42
8293.951	10031	00001	8194	8310	71	6.18E-23	42
<hr/>							
¹⁶ O ¹² C ¹⁸ O, third most abundant isotopologue (628 in AFGL notation)							
966.269	00011	10001	918	997	108	2.01E-24	41
1072.687	00011	10002	1020	1107	118	5.19E-24	41
4639.501	00021	00001	4579	4663	115	1.44E-23	45
<hr/>							
¹⁶ O ¹² C ¹⁷ O, fourth most abundant isotopologue (627 in AFGL notation)							
586.850	11102	02201	548	626	294	4.23E-24	29
607.555	20003	11102	578	640	123	5.41E-25	29
607.558	10002	01101	554	659	208	1.05E-22	40
644.407	11102	10002	601	693	183	1.74E-23	29
649.955	12202	11102	620	685	244	1.27E-24	29
665.114	02201	01101	614	726	427	9.55E-22	29
681.386	12201	11101	656	712	208	6.17E-25	29
686.071	11101	10001	643	732	178	1.12E-23	29
711.298	10001	01101	659	765	210	1.30E-22	40
713.459	20001	11101	688	742	105	3.07E-25	29
724.547	20002	11102	700	749	89	1.90E-25	29
732.256	11101	02201	691	771	302	4.94E-24	29
748.133	12201	03301	733	749	72	9.72E-26	29
789.812	11101	10002	762	821	114	4.08E-25	29
963.986	00011	10001	925	991	85	4.00E-25	41
1067.727	00011	10002	1024	1098	97	8.34E-25	41
2306.741	11112	11102	2253	2342	258	1.17E-23	29
2315.147	02211	02201	2246	2355	362	2.03E-22	29
2317.319	10011	10001	2249	2356	141	8.20E-23	29
2318.964	10012	10002	2249	2359	145	1.36E-22	29
2327.581	01111	01101	2244	2370	434	5.20E-21	29
<hr/>							
¹⁶ O ¹³ C ¹⁷ O, sixth most abundant isotopologue (637 in AFGL notation)							
2274.088	00011	00001	2198	2316	157	7.33E-22	48

Note: The second and third columns, Upper Vib and Lower Vib, use the AFGL vibrational notation for carbon dioxide [4]. The sixth column indicates the number of lines that have been replaced in *HITRAN*.

Air pressure-induced shifts have been added for the two laser bands of $^{16}\text{CO}_2$ based on the work of Devi et al. [49]. These data have also been used for the two laser bands of the other isotopologues assuming that the dependence with the type of isotopologue is negligible. Concerning the air- and self-broadening coefficients, and the temperature dependence of the air-broadened width, the values recommended in Ref. [33] for the *HITRAN92* edition as well the subsequent editions, have been used for all CO_2 transitions.

2.1.3. N_2O (molecule 4)

For nitrous oxide, the line list is almost completely new. For positions and intensities we have used the line list of Toth [50] that covers the 5 isotopologues present in *HITRAN* between 500 and 7500 cm^{-1} . However, we substituted the positions and intensities of Daumont et al. [51] for those of Ref. [50] for the (00^01-10^00) and (02^20-00^00) bands in the 10- μm region, and by those of Johns et al [52] for the ν_2 band in the 17- μm region. Moreover, we kept the *HITRAN* positions and intensities [1] between 0 to 50 cm^{-1} . We are carrying out a major effort making intercomparisons of theoretical calculations [51, 53] and the experimental results [50, 51, 54] to determine the best line list throughout for $^{14}\text{N}_2^{16}\text{O}$.

For the air-broadening coefficients, a polynomial fit based on experimental results from Toth [55], Lacombe et al. [56], and Nemtchinov et al [57] has been used for all lines and for all isotopologues in *HITRAN*. The expression used for the air-broadening coefficients (in $\text{cm}^{-1}/\text{atm}$ at 296K) is

$$\gamma_{\text{air}} = 0.0964 \quad 0 \leq |m| \leq 1 \quad (2a)$$

$$\gamma_{\text{air}} = 0.0964 - 1.72 \times 10^{-3} |m| + 3.81 \times 10^{-5} |m|^2 - 2.96 \times 10^{-7} |m|^3 \quad 2 \leq |m| \leq 67 \quad (2b)$$

$$\gamma_{\text{air}} = 0.0632 \quad |m| > 67, \quad (2c)$$

where the running index $m = -J''$ for the P branch, $m = J''$ for the Q branch, and $m = J'' + 1$ for the R branch.

Concerning the self-broadening coefficients, a polynomial fit based on experimental results from Toth [58] has been used for all lines and for all isotopologues in *HITRAN*. The expression used for the self-broadening coefficients (in $\text{cm}^{-1}/\text{atm}$ at 296K) is

$$\gamma_{\text{self}} = 0.127 \quad 0 \leq |m| \leq 1 \quad (3a)$$

$$\gamma_{\text{self}} = 0.1238 - 1.803 \times 10^{-3} |m| + 2.54 \times 10^{-5} |m|^2 - 1.4 \times 10^{-7} |m|^3 \quad 2 \leq |m| \leq 86 \quad (3b)$$

$$\gamma_{\text{self}} = 0.0676 \quad |m| > 86. \quad (3c)$$

For the temperature dependence of the air-broadened width, a mean value of 0.75 has been used for every line based on the work of Lacombe et al. [56], and Nemtchinov et al [57].

Concerning the air pressure shift coefficients, the expression of Toth [50], as a function of the wavenumber and $|m|$, has been used for all lines except those of between 0 to 45 cm^{-1} for which a zero default value has been used (a reasonable assumption consistent with the usual vibrational dependence expected for pressure shifts).

2.1.4. CO (molecule 5)

Several updates have been completed for this edition of *HITRAN3k* for carbon monoxide. For the first overtone of $^{12}\text{C}^{16}\text{O}$ near $2.4\ \mu\text{m}$, line intensities have been updated from the work of Brault et al. [59]. These new results show that the line intensities of the previous *HITRAN* edition [1] were systematically larger by 4.2% than those of Ref. [59]. Note that two recent studies [55, 56] also demonstrate that the former *HITRAN* values were too large for the (2-0) band (1 to 6 % larger than these measured values).

For the second overtone (3-0) of $^{12}\text{C}^{16}\text{O}$ around $1.6\ \mu\text{m}$, different groups [62 - 65] have come to the conclusion that the intensity values in *HITRAN* were overestimated by 5 to 7%. Refs. [64, 65] agree very well with each other, and we chose to use the calculated values of Sung and Varanasi. [65] to update *HITRAN*.

Recent laboratory measurements of air-broadening coefficients [60, 65, 66] in the fundamental and first two overtones agree within $\pm 2\%$ for transitions with $3 < |m| < 19$. Outside this range, the *HITRAN* air-broadening coefficients [1] are 3 to 10% smaller than the measured values. For this reason, we chose to update the air-broadening coefficients using the Eq. (2) of Ref. [65].

Concerning the self-broadening coefficients, the *HITRAN* values and recent measurements [62 - 71] all agree within $\pm 5\%$. However, recent works using a collisional-narrowing profile [65, 67, 68, 70, 71] are in a much better agreement as shown in Ref. [71]. The more important difference between these works and those using a Voigt profile concern the rotational dependence of the self-broadening coefficients. An update of the self-broadening coefficients has been performed in *HITRAN* using experimental values of Ref. [71].

The temperature dependence exponent for air-broadening is now equal to $0.75\ \text{cm}^{-1}/\text{atm}$ for all CO transitions in *HITRAN3k*. This constant value comes from the recent laboratory study in the 1-0 and 2-0 bands [60].

Pressure air shifts have also been added in *HITRAN2004* for the 1-0, 2-0 and 3-0 bands of $^{12}\text{C}^{16}\text{O}$. The experimental values of Zou and Varanasi [60] have been used for the fundamental band and the first overtone for the range $-24 \leq m \leq 25$. Outside this range constant values of $-0.003\ \text{cm}^{-1}/\text{atm}$ and $-0.0055\ \text{cm}^{-1}/\text{atm}$ have been used respectively for the fundamental band and the first overtone. For the second overtone, the experimental values of Sung and Varanasi [65], who report air-shifts between -0.003 and $-0.009\ \text{cm}^{-1}/\text{atm}$, have been used between in the range $-24 \leq m \leq 26$. Outside this range the constant value of $-0.0075\ \text{cm}^{-1}/\text{atm}$ has been used as a default value.

2.1.5. CH₄ (molecule 6)

In the pure rotation region, the quantum number K of the $^{12}\text{CH}_3\text{D}$ isotopologue, which had been omitted in the previous *HITRAN* editions, has been added using the JPL catalog [11]. Moreover, positions and line intensities from the JPL catalog have also been used to update *HITRAN*.

A major improvement has also been accomplished concerning the near infrared region for $^{12}\text{CH}_4$. First, a new line list of 4937 positions and intensities from Brown [72] covering the 4800 to $5500\ \text{cm}^{-1}$ region has replaced the 273 lines between 4800 and $4938\ \text{cm}^{-1}$ of *HITRAN* [1]. In addition, 35320 positions and intensities have been added between 6180 and $9200\ \text{cm}^{-1}$, a spectral region where *HITRAN* [1] did not previously contain information on this molecule.

2.1.6. HNO_3 (molecule 12)

Several updates have been done for nitric acid. The recent work of Zu et al. [73] in the 683 GHz region shows a comparison between an observed spectrum and calculation using either the JPL catalog [11] or the previous *HITRAN* database [1]. This comparison stressed the fact that the calculation from the JPL catalog is more accurate than the calculation from *HITRAN*. Thus the pure rotation nitric acid line list in *HITRAN* [1], which covered 0 to 43 cm^{-1} region, has been replaced by the line list of the JPL catalog [11] which covers the 0 to 84 cm^{-1} region.

The intensities of the ν_3 , ν_4 , ν_5 and $2\nu_9$ cold bands have been normalized based on an accurate analysis of the 11- μm region using new laboratory high-resolution Fourier transform spectra [74]. According to this study, the individual line intensities of the ν_3 , ν_4 , ν_5 and $2\nu_9$ bands have been multiplied by a factor equal to 0.879.

The two hot bands $\nu_5 + \nu_9 - \nu_9$ and $3\nu_9 - \nu_9$ located respectively at 885.424 and 830.6 cm^{-1} have been updated. Let us recall that these two bands had been removed from *HITRAN96* [75] and replaced by the hot band $\nu_5 + \nu_9 - \nu_9$ from Goldman et al [76] in *HITRAN2000* [1]. In the *HITRAN2004* edition, the $3\nu_9 - \nu_9$ band has been added using the line positions and intensities from Ref. [77]. Concerning the $\nu_5 + \nu_9 - \nu_9$ band, which is the most commonly used for the retrieval of HNO_3 in the atmosphere, the positions and the intensities have been updated from Ref. [78].

Prior this edition, the self-broadening coefficients were equal to zero for most of the lines of nitric acid. In the new *HITRAN* edition, this halfwidth has been fixed to the constant value of 0.8 $\text{cm}^{-1}/\text{atm}$ for all lines. This value has been chosen considering Refs. [73, 79].

2.2 Validations

There have been numerous independent validations of the new data that have either been incorporated into the *HITRAN* database, or have replaced older data. The overriding issue is how do these new spectroscopic data, whether line parameters or cross-sections improve our ability at retrieving atmospheric profiles or simulating real atmospheric transmission and radiance.

One aim is to reduce residuals. An example is shown in Fig. 1 for carbon dioxide. This work, by Miller and Brown [32] at the Jet Propulsion Laboratory, is part of an ongoing effort to substantially improve the line parameters of CO_2 for the Orbiting Carbon Observatory project of NASA. These data are being taken with state-of-the art procedures using the Fourier transform spectrometer at Kitt Peak National Solar Observatory, and are improving *HITRAN* substantially.

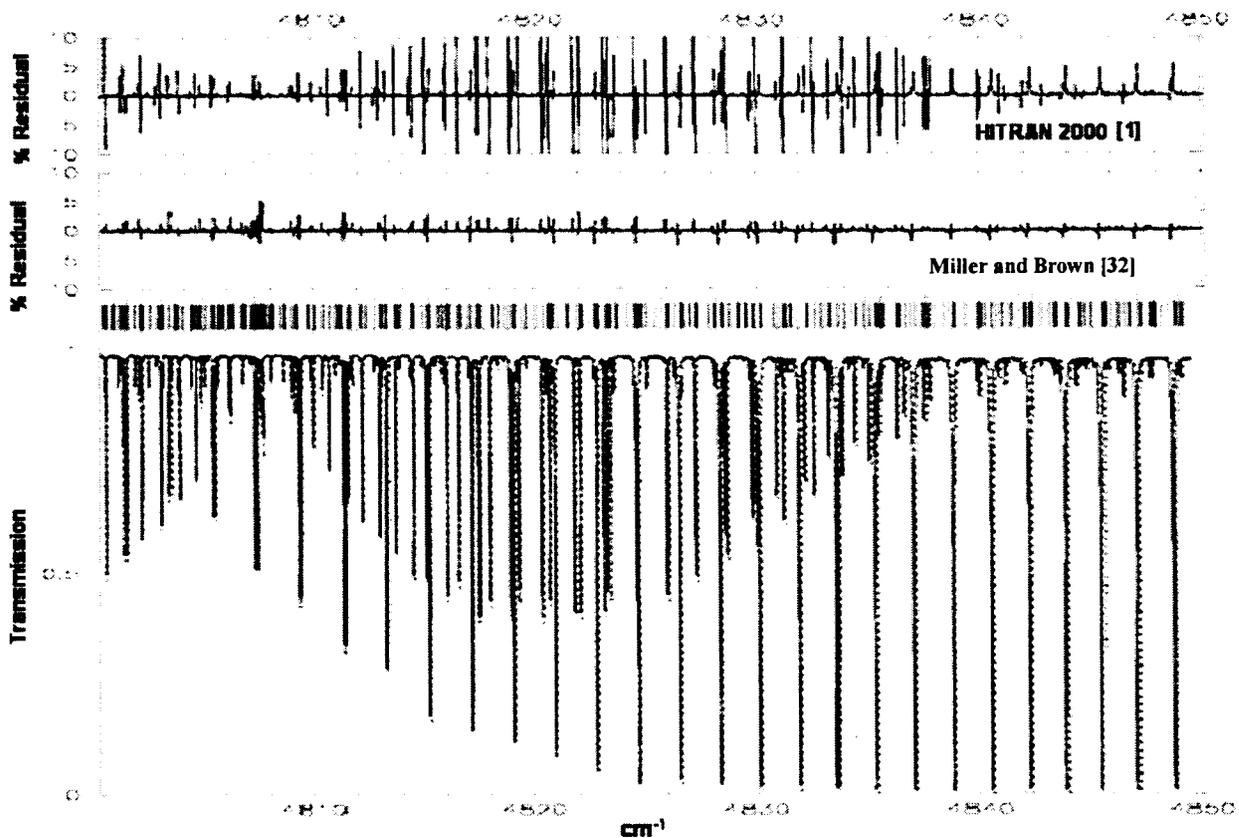


Figure 1. Comparison between experimental (solid line) and simulated (dashed line) CO₂ laboratory spectra in the 2- μ m region. The experimental conditions of the bottom panel are 30 torr CO₂ and 25 m path. Top panel: Residuals from simulating the experimental spectrum using the previous *HITRAN* database [1]. RMS error = 2.75%. Middle panel: Simulation residuals using the line positions reported in Miller and Brown [32] with unpublished intensity data. RMS error = 0.11%.

Another example of improved residuals is shown in Fig. 2 for water vapor. The measurements of Liu et al at Stanford University [80] show a substantial improvement of the line intensities in a region of the spectrum that has long needed attention in *HITRAN*. The measurements of Hanson's group at Stanford were made in the laboratory with an external cavity diode laser. Measurements at elevated temperature also show significant improvement of *HITRAN*2004 from the previous edition of *HITRAN* [1] for the strongest lines.

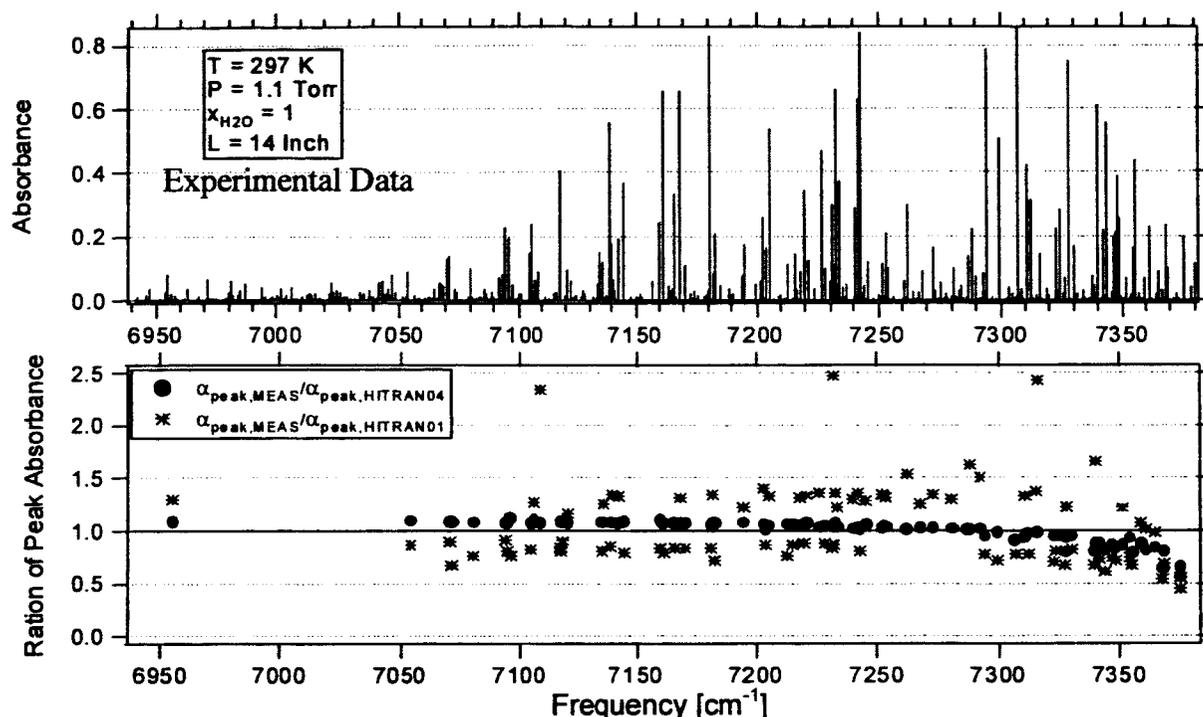


Figure 2. External cavity diode laser absorption measurements in the 1.4- μm region for water vapor. Comparison with new *HITRAN* edition and previous edition [1].

A further avenue of validation is to compare the retrievals using different spectral bands in *HITRAN*. Bernath and Boone at the University of Waterloo in Canada have been testing the new *HITRAN* database against results from the Atmospheric Chemistry Experiment (ACE) [81]. Figure 3 shows retrievals from two different occultations, using both the previous *HITRAN* edition [1] and the new *HITRAN* in the 2.7- μm region. Clearly, the consistency with the 6- μm region is superior.

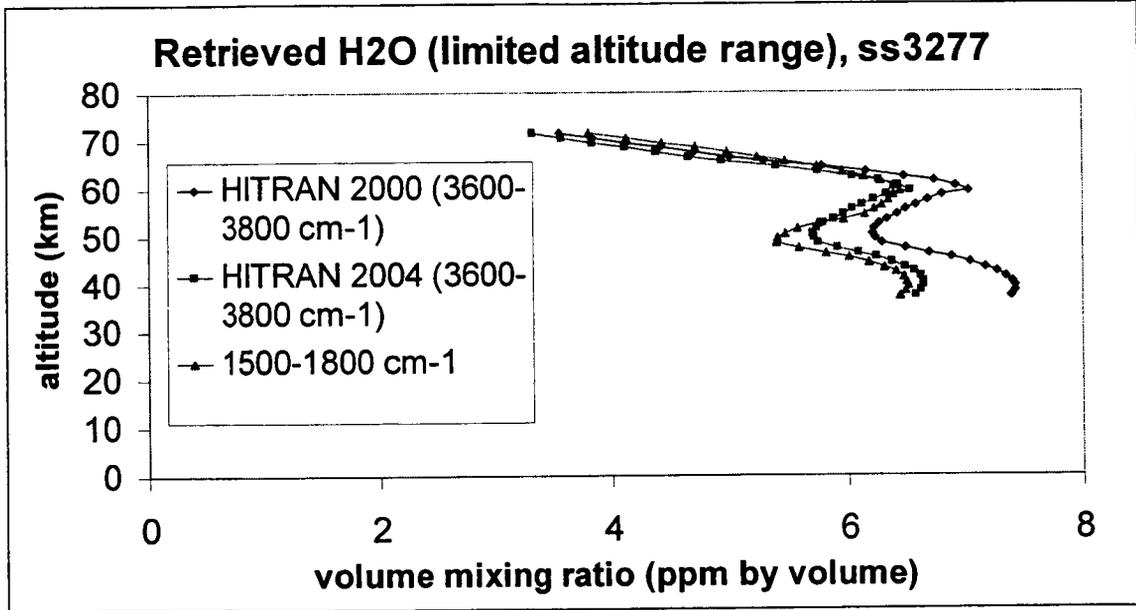
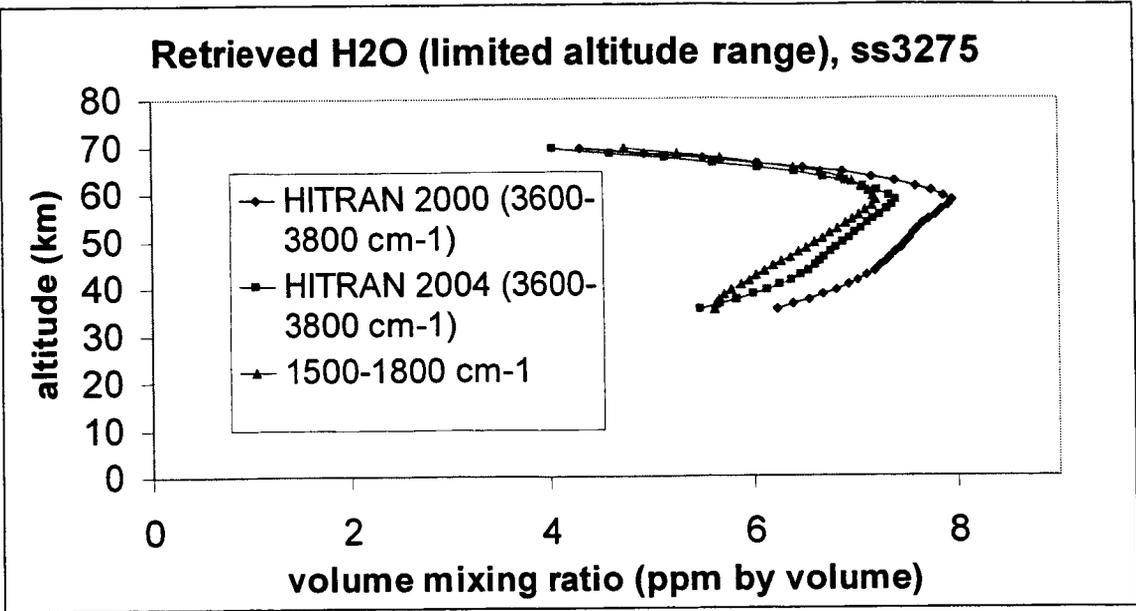


Figure 3. Retrievals of water-vapor profiles from two different occultations made by ACE. Comparison using HITRAN2000[1] and the new HITRAN2004.

Another study by Boone and Bernath [81] made retrievals of nitric acid from the Atmospheric Chemistry Experiment (ACE). The retrievals were of tropical occultation, Arctic occultation, and a northern mid-latitude occultation taken in 2004. In Fig. 4, comparisons are made using both the HITRAN2000 edition [1] and the current edition. Three prominent bands of HNO_3 were used and the consistency using the new edition of *HITRAN* has reduced discrepancies significantly. It should be remarked, that the improvement shown in Fig. 4b, only validates the relative intensities of the three bands in *HITRAN*, not the absolute intensities. In other words, there is still the possibility of a uniform shift in all three bands. Nevertheless, these validations demonstrate a significant improvement in *HITRAN*.

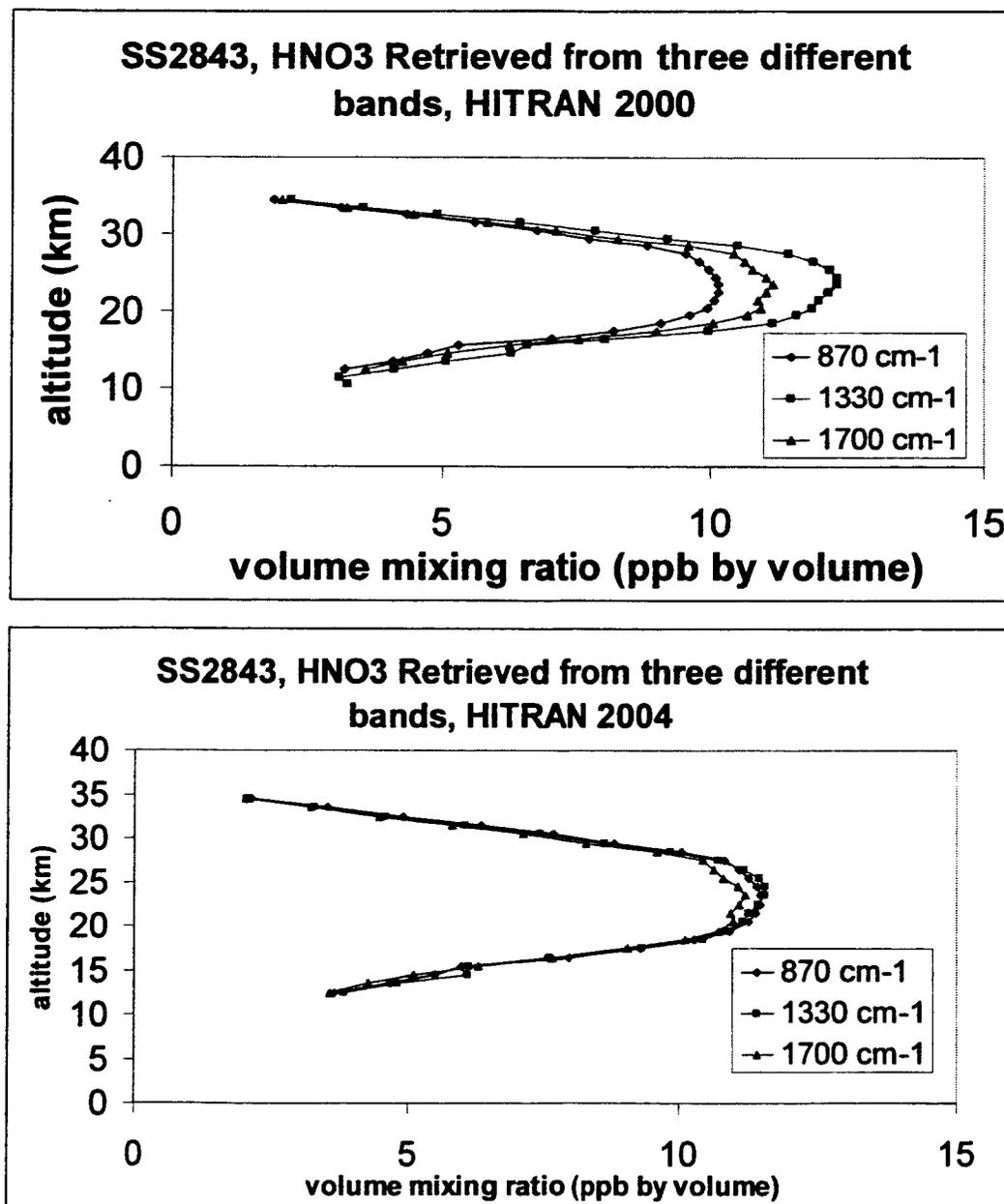


Figure 4. Improvement of consistency using 3 different bands of nitric acid in *HITRAN*. Fig. 4a uses HITRAN2000 [1], and Fig. 4b uses new *HITRAN*.

3. Administration of *HITRAN* project

3.1. Labor effort

A major change in the administration of this grant has been the termination of the sub-contract with the ONTAR Corporation. The work that comprised the main part of their effort, namely developing the software system JavaHAWKS, that is the interface and filtering system for the *HITRAN* compilation, had reached a mature state. There is still work to be done, however, such as developing a server-based interface that will permit users to work mostly on files at the SAO, rather than have to down-load all files and work on their resident computer. To this end, we plan to bring in a post-doctoral candidate who has experience in not only high-resolution spectroscopy, but programming on the level needed for implementation and maintenance of the *HITRAN* project.

During this project period, David Jacquemart, a post-doc from the group of C. Camy-Peyret at the University of Paris, joined the *HITRAN* team here. He has worked primarily on the updating of the line-by-line portion of *HITRAN*. He has also worked on implementing the Einstein *A*-coefficients and the new format for *HITRAN*. His value to the program has been enormous.

3.2. Meetings

Two International *HITRAN* Conferences have been conducted at the Smithsonian Astrophysical Observatory during this grant (June 2000 and June 2002), and a third one is planned for 2004. The Proceedings of these conferences have been published in the web-site.

In November 2003, Jacquemart and Rothman had a working meeting at JPL. The primary purpose was to meet with Linda Brown and Charles Miller. Discussions focused on problems and issues of various molecules that they are working on, or ones that we jointly have good collaborative efforts with other groups. We met with Robert Toth to assess and obtain his work on water vapor and nitrous oxide. Meetings with Reinhard Beer, Goeff Toon, Helen Worsden, and others at JPL were also conducted. Issues involved requirements for NASA satellite remote-sensing experiments.

A lot of effort has been going into the preparation for the upcoming Biennial *HITRAN* Conference. The conference will be held at the Harvard-Smithsonian Center for Astrophysics, 16-18 June 2004. The International *HITRAN* Advisory committee will meet the day before the meeting. Information about the Conference has been placed in the *HITRAN* web-site, and the program was made available in April.

3.3. Documentation

We have been carefully documenting the changes and reasons for changes to *HITRAN*. This will be presented as an article in a Special Issue of *JQSRT*. We encouraged some contributors to *HITRAN* to publish their articles in this issue. Work has also been done to update the JavaHAWKS manual. The manual and articles describing *HITRAN* have been placed in the documentation sub-page of the *HITRAN* web-site.

3.4. Future Plans

More work is going on in validations and comparisons of *HITRAN* data. This has become more and more of an issue, both because more laboratories are doing similar measurements and because of the high emphasis on accuracy.

For the line-by-line portion of *HITRAN*, the effort proceeds on several fronts. We will be adding many bands in the shorter wavelength regions, which are either lacking or severely deficient. Additional molecules will be added to the *HITRAN* list. A major effort is being undertaken to provide line-coupling parameters and algorithms. The latter effect has an impact on many simulations. Collision-induced bands, such as for oxygen and nitrogen, will be parametrized, much in the manner that the absorption cross-section part of *HITRAN* has done. We expect to add to the molecules in the cross-section portion, and also provide more access to UV data sets.

4. Publications and Presentations during this grant

A major accomplishment with respect to documentation of *HITRAN* was the publication in November 2003 of a Special Issue of the Journal of Quantitative Spectroscopy and Radiative Transfer, volume 82. This issue contained 30 refereed articles relevant to the *HITRAN* compilation and topics significant to the EOS program. The Guest Editors were L.S. Rothman, K. Chance, and A. Goldman. It should be noted that the articles describing the *HITRAN* database editions are among the most cited in the geosciences and engineering.

Publications during this grant:

- “Total Internal Partition Sums for Molecules in the Terrestrial Atmosphere,” R.R. Gamache, S. Kennedy, R.L. Hawkins, and L.S. Rothman, *Journal of Molecular Structure* **517/518**, 407-425 (2000).
- “*HITRAN* Partition Functions and Weighted Transition-Moments Squared,” A. Goldman, R.R. Gamache, A. Perrin, J.-M. Flaud, C.P. Rinsland, and L.S. Rothman, *J. Quant. Spectrosc. and Rad. Transfer* **66**, 455-486 (2000).
- “Atmospheric Molecules,” L.S. Rothman and M. Živković-Rothman, Atomic and Molecular Data and their Applications, eds. K.A. Berrington and K.L. Bell, AIP Conference Proceedings 543, 92-103 (2000).
- “Atmospheric Ultraviolet Spectroscopy,” K. Chance and L.S. Rothman, Chapter 13, p. 475-497 in Ultraviolet Spectroscopy and Ultraviolet Lasers, eds. P. Misra and M.A. Dubinskii, Marcel Dekker, New York (2002).
- “The spectrum of acetylene in the 5- μm region from new line parameter measurements,” D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, J.-J. Plateaux, D. Décatoire, and L.S. Rothman, *J. Quant. Spectrosc. and Rad. Transfer* **76**, 237-267 (2003).
- “The *HITRAN* Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001,” L.S. Rothman et al, *J. Quant. Spectrosc. and Rad. Transfer* **82**, 5-44 (2003).
- “The 1- μm CO_2 bands and the O_2 (0-1) $X^3\Sigma_g^- - a^1\Delta_g$ and (1-0) $X^3\Sigma_g^- - b^1\Sigma_g^+$ bands in the Earth atmosphere,” A. Goldman, T.M. Stephen, L.S. Rothman, L.P. Giver, J.-Y. Mandin, R.R. Gamache, C.P. Rinsland, and F.J. Murcray, *J. Quant. Spectrosc. and Rad. Transfer* **82**, 197-205 (2003).
- “The IR acetylene spectrum in *HITRAN*: update and new results,” D. Jacquemart, J.-Y. Mandin, V. Dana, C. Claveau, J. Vander Auwera, L.S. Rothman, L. Régalia-Jarlot, and A. Barbe, *J. Quant. Spectrosc. and Rad. Transfer* **82**, 363-382 (2003).

“Total Internal Partition Sums for Molecular Species in the 2000 edition of the HITRAN database,” J. Fischer, R.R. Gamache, A. Goldman, L.S. Rothman, and A. Perrin, *J. Quant. Spectrosc. and Rad. Transfer* **82**, 401-412 (2003).

Presentations during this grant:

“HITRAN2000,” Fifth Atmospheric Spectroscopy Applications Conference, Reims, France (September 1999). (Invited)

“UV Spectral Data for HITRAN2000,” Paper EP7, Fifth Atmospheric Spectroscopy Applications Conference, Reims, France (September 1999).

“HAWKS (HITRAN Atmospheric Workstation),” Fifth Atmospheric Spectroscopy Applications Conference, Reims, France (September 1999).

“HITRAN and HITEMP,” Atmospheric Transmission Workshop, US Army Night Vision Directorate, Fort Belvoir, Virginia (September 1999).

“HITRAN Database,” Seminar, National Institute of Environmental Studies, Tsukuba, Japan (February 2000). (Invited)

“Atmospheric Molecules,” International Conference on Atomic and Molecular Data (ICAMDATA), Oxford, UK (March 2000). (Invited)

“HITRAN2000,” The Sixth Biennial HITRAN Database Conference, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts (June 2000); XVIth International Conference on High Resolution Infrared Spectroscopy, Prague, Czech Republic (September 2000).

“The Venus 1- μm CO₂ Bands and the O₂ (0-1) $X^3\Sigma_g^- - a^1\Delta_g$ and (1-0) $X^3\Sigma_g^- - b^1\Sigma_g^+$ Bands in the Earth’s Atmosphere,” The Sixth Biennial HITRAN Database Conference, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts (June 2000); XVIth International Conference on High Resolution Infrared Spectroscopy, Prague, Czech Republic (September 2000).

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

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

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“Millenium HITRAN Compilation,” L.S. Rothman, D. Jacquemart, and K. Chance, The 18th Colloquium on High Resolution Molecular Spectroscopy, Dijon, France (September 2003).

“The Next HITRAN Edition: Description of New Parameters,” D. Jacquemart and L.S. Rothman, The 18th Colloquium on High Resolution Molecular Spectroscopy, Dijon, France (September 2003).

“The HITRAN Quest for Accurate Long-path Atmospheric Transmission in Tactical Arenas,” L.S. Rothman, 26th Annual Review of Atmospheric Transmission Models, Lexington, Massachusetts (September 2003). (Invited)

“Recent Advances in the HITRAN Spectroscopic Database for Atmospheric and Environmental Modeling,” L.S. Rothman, Ninth Topical Meeting, Laser Applications to Chemical and Environmental Analysis (LACEA), Annapolis, Maryland (February 2004). (Invited)

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