HIGH-RESOLUTION SPECTROSCOPIC DATABASE FOR THE NASA EARTH OBSERVING SYSTEM PROGRAM

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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 is to develop and enhance the HITRAN molecular spectroscopic database and associated software to support the observational programs of the Earth Observing System (EOS). In particular, the focus is on the EOS projects: the Atmospheric Infrared Sounder (AIRS), the High-Resolution Dynamics Limb Sounder (HIRDLS), Measurements of Pollution in the Troposphere (MOPITT), the Tropospheric Emission Spectrometer (TES), and the Stratospheric Aerosol and Gas Experiment (SAGE III). The 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

A focus of this period has been to prepare for a new edition of the HITRAN database. It is anticipated that this edition will be released prior to the next HITRAN meeting in June 2004. This edition 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 halfwidth, temperature-dependence of air-broadened halfwidth, 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 will be 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 cm^{-1}/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 cm^{-1}/(molecule x 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 cm^{-1}/atm @ 296K	iref	6I2	Indices for table of references corresponding to wavenumber, intensity, air- and self-broadened halfwidths, temeperature-dependence, and pressure shift
γ_{self}	F5.4	Self-broadened halfwidth (HWHM) in cm^{-1}/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/HITRAN/). 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 HITRAN molecules	Upper- and Lower-State"global" Quanta
Class 1: Diatomic molecules CO, HF, HCl, HBr, HI, N_2, NO^+	__ v_1 13x I2
Class 2: Diatomic molecules with different electronic levels O_2	__ X v_1 12x A1 I2
Class 3: Diatomic molecules with doublet- Π electronic state NO, OH, ClO	__ X i __ v_1 7x A1 A3 2x I2
Class 4: Linear triatomic N_2O, OCS, HCN	__ v_1 v_2 l_2 v_3 7x I2 I2 I2 I2
Class 5: Linear triatomic with large Fermi resonance CO_2	__ v_1 v_2 l_2 v_3 r 6x I2 I2 I2 I2 I1
Class 6: Non-linear triatomic H_2O, O_3, SO_2, NO_2, HOCl, H_2S, HO_2, HOBr	__ v_1 v_2 v_3 9x I2 I2 I2
Class 7: Linear tetratomic C_2H_2	v_1 v_2 v_3 v_4 v_5 l ± r S I2 I2 I2 I2 I2 I2 A1 I1 A1
Class 8: Pyramidal tetratomic NH_3, PH_3	__ v_1 v_2 v_3 v_4 S 5x I2 I2 I2 I2 I2
Class 9: Non-linear tetratomic H_2CO, H_2O_2, COF_2	__ v_1 v_2 v_3 v_4 v_5 v_6 3x I2 I2 I2 I2 I2 I2
Class 10: Pentatomic or greater polyatomic CH_4	__ v_1 v_2 v_3 v_4 n C 3x I2 I2 I2 I2 A2 A2
CH_3D, CH_3Cl, C_2H_6, HNO_3, SF_6, HCOOH, $ClONO_2$, C_2H_4	**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 $^{12}C_2H_2$. For class 8, S is the symmetry of the level (only for NH_3: for PH_3 S is blank). For H_2O_2 in class 9, v_4 has been replaced by the torsional quanta n and τ described in Refs. [4,5]. For CH_4, 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 HITRAN 2004 edition

Group classification and HITRAN molecules	Upper-State local Quanta	Lower-State local Quanta
Group 1: Asymmetric Rotors†	J' K_a' K_c' F' Sym'	J'' K_a'' K_c'' F'' Sym''
H_2O, O_3, SO_2, NO_2, HNO_3, H_2CO, HOCl, H_2O_2, COF_2, H_2S, HO_2, HCOOH, $ClONO_2$, HOBr, C_2H_4	I3 I3 I3 A5 A1	I3 I3 I3 A5 A1
Group 2: Diatomic and Linear Molecules	F'	*Br* J'' Sym'' F''
CO_2, N_2O, CO, HF, HCl, HBr, HI, OCS, N_2, HCN, C_2H_2, NO^+	10X A5	5X A1 I3 A1 A5
Group 3: Spherical Rotors	J' C' α' F'	J'' C'' α'' F''
SF_6, CH_4	2X I3 A2 I3 A5	2X I3 A2 I3 A5
Group 4: Symmetric Rotors	J' K' l' C' Sym' F'	J'' K'' l'' C'' Sym'' F''
CH_3D, CH_3Cl, C_2H_6, NH_3, PH_3	I3 I3 I2 A2 A1 A4	I3 I3 I2 A2 A1 A4
Group 5: Triplet-Σ Ground Electronic States	F'	*Br* N'' *Br* J'' F'' Sym
O_2	10X A5	1X A1 I3 A1 I3 A5 A1
Group 6: Doublet-Π Ground Electronic States‡	F'	*Br* J'' Sym'' F''
NO, OH, ClO	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 O_2. 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 O_2 and N_2).

†For NO_2 and HO_2, *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 $J = N + ½$ and – means $J = N - ½$.

‡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 1 of the previous annual report summarizes the molecules and their isotopologues currently in the line-transition portion of HITRAN.

2.1. Recent Improvements to HITRAN Line Parameters

The following sub-sections cover all 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

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

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 H_2O 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 $HD^{16}O$ and $HD^{18}O$ we also used the values from Ref. [17] of the ν_1, ν_2 and ν_3 bands of $HD^{16}O$ 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 $H_2{}^{16}O$, $H_2{}^{18}O$ and $H_2{}^{17}O$ 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 $H_2{}^{16}O$ again assuming negligible vibrational dependence. For the pure rotation region of $HD^{16}O$ and $HD^{18}O$ we similarly adopted the values from Ref. [17] of the ν_1, ν_2 and ν_3 bands of $HD^{16}O$.

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 $H_2{}^{16}O$, $H_2{}^{18}O$ and $H_2{}^{17}O$ isotopologues. For the $HD^{16}O$, $HD^{18}O$ and $HD^{17}O$ isotopologues, values from the SISAM.H_2O 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-μm 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 4 summarizes these values.

Table 4. 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. CO_2 (molecule 2)

Among the several recent studies on CO_2, we have to highlight the global calculation both on positions and intensities for $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{12}C^{16}O^{18}O$ and $^{12}C^{16}O^{17}O$ of Taskun 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 $^{16}O^{12}C^{18}O$ and $^{16}O^{12}C^{17}O$ 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 $^{16}O^{12}C^{17}O$ isotopologue, the hyperfine structure is resolved.

Concerning line positions, several updates have been accomplished. For the main isotopologue $^{12}C^{16}O_2$, 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 $^{12}C^{16}O_2$, 8 bands of $^{13}C^{16}O_2$, 4 bands of $^{12}C^{16}O^{18}O$, and 12 bands of $^{12}C^{16}O^{17}O$. 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 $2\nu_1 + 3\nu_3$ $^{12}C^{16}O_2$ 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 $2\nu_1 + 3\nu_3$ 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 $^{12}C^{16}O^{17}O$ have also been updated from Ref. [41]. A summary of the improvements concerning the line positions is given in Table 5.

Table 5: Bands of CO_2 for which the line positions have been updated.

Band Center (cm^{-1})	Upper Vib $v_1 v_2 l_2 v_3 r$	Lower Vib $v_1 v_2 l_2 v_3 r$	ν_{min} (cm^{-1})	ν_{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	0 0 0 1 1	1 0 0 0 1	886	1002	75	0	74	32
1063.735	0 0 0 1 1	1 0 0 0 2	986	1105	77	0	76	32
2076.856	1 1 1 0 1	0 0 0 0 1	2010	2145	127	0	88	32
2224.656	1 0 0 1 2	1 0 0 0 1	2158	2264	68	0	68	32
2274.422	0 6 6 1 1	0 6 6 0 1	2244	2299	62	6	34	29
2275.842	1 4 4 1 1	1 4 4 0 1	2251	2297	42	4	28	29
2277.173	2 2 2 1 1	2 2 2 0 1	2259	2294	23	10	22	29
2278.387	1 4 4 1 2	1 4 4 0 2	2243	2306	77	4	39	29
2280.618	2 2 2 1 2	2 2 2 0 2	2250	2305	61	4	34	29
2281.674	2 2 2 1 3	2 2 2 0 3	2243	2310	85	2	42	29
2286.804	0 5 5 1 1	0 5 5 0 1	2234	2322	133	5	56	29
2311.701	0 1 1 2 1	0 1 1 1 1	2246	2350	162	1	67	32
2324.141	0 2 2 1 1	0 2 2 0 1	2227	2371	250	2	92	32
2324.183	0 0 0 2 1	0 0 0 1 1	2244	2366	80	1	79	32
2326.598	1 0 0 1 1	1 0 0 0 1	2231	2372	91	0	90	32
2327.433	1 0 0 1 2	1 0 0 0 2	2231	2374	93	0	92	32
2336.632	0 1 1 1 1	0 1 1 0 1	2227	2384	278	1	101	32
2349.143	0 0 0 1 1	0 0 0 0 1	2230	2397	109	0	108	32
2429.374	1 0 0 1 1	1 0 0 0 2	2364	2467	66	0	66	32
3365.269	3 1 1 0 2	1 0 0 0 1	3331	3403	33	8	48	29
3398.219	2 1 1 1 3	1 1 1 0 1	3374	3420	46	6	28	38
3465.439	2 0 0 1 3	1 0 0 0 1	3410	3505	61	0	60	32
3496.141	2 3 3 1 3	1 3 3 0 2	3464	3522	68	3	36	29
3504.987	1 4 4 1 2	0 4 4 0 1	3461	3537	108	4	48	29
3506.713	3 1 1 1 4	2 1 1 0 3	3473	3534	73	2	38	29
3518.664	2 2 2 1 3	1 2 2 0 2	3468	3554	124	2	54	29
3527.808	2 2 2 1 2	1 2 2 0 1	3484	3559	100	2	47	29
3542.604	2 1 1 1 3	1 1 1 0 2	3476	3586	171	1	70	38
3543.095	4 0 0 0 2	1 1 1 0 2	3502	3592	82	1	63	38
3552.854	1 2 2 1 2	0 2 2 0 1	3476	3598	203	2	78	38
3554.964	2 3 3 0 1	0 2 2 0 1	3504	3611	188	2	68	38
3555.909	2 1 1 1 2	1 1 1 0 1	3492	3593	152	1	64	32
3568.215	2 0 0 1 3	1 0 0 0 2	3490	3615	81	0	80	32
3589.651	2 0 0 1 2	1 0 0 0 1	3506	3628	79	0	78	32
3612.841	1 0 0 1 2	0 0 0 0 1	3509	3661	99	0	98	32
3659.272	0 2 2 1 1	0 0 0 0 1	3582	3715	82	4	86	32
3692.427	2 0 0 1 2	1 0 0 0 2	3606	3731	81	0	80	32
3703.157	3 1 1 1 1	2 1 1 0 1	3680	3723	43	6	27	29
3703.510	2 2 2 1 2	1 2 2 0 2	3651	3736	124	2	54	29
3704.112	2 3 3 1 2	1 3 3 0 2	3675	3727	56	3	32	29
3711.476	2 0 0 1 1	1 0 0 0 1	3635	3757	79	0	78	32
3712.412	2 3 3 1 1	1 3 3 0 1	3689	3733	42	7	28	29

3713.720	2 1 1 1 1	1 1 1 0 1	3648	3755	166	1	68	32
3713.809	2 2 2 1 1	1 2 2 0 1	3665	3747	118	2	52	29
3714.782	1 0 0 1 1	0 0 0 0 1	3610	3763	99	0	98	32
3724.133	1 5 5 1 1	0 5 5 0 1	3702	3743	33	5	25	29
3726.396	1 4 4 1 1	0 4 4 0 1	3678	3759	119	4	51	29
3814.252	2 0 0 1 1	1 0 0 0 2	3753	3854	65	0	64	32
3980.582	0 1 1 2 1	0 2 2 0 1	3975	4003	59	8	47	32
4005.946	0 0 0 2 1	0 1 1 0 1	3934	4029	78	2	63	32
4416.149	3 1 1 0 4	0 0 0 0 1	4426	4452	16	12	42	29
4687.796	3 0 0 1 4	1 0 0 0 1	4652	4719	42	2	42	32
4722.649	3 2 2 1 4	1 2 2 0 2	4705	4740	23	10	22	29
4733.518	2 3 3 1 3	0 3 3 0 1	4696	4763	87	3	42	29
4735.611	4 0 0 1 5	2 0 0 0 3	4712	4757	24	6	28	29
4753.454	3 1 1 0 2	0 0 0 0 1	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

$^{16}O^{13}C^{16}O$, 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
$^{16}O^{12}C^{18}O$, 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
$^{16}O^{12}C^{17}O$, 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.

Concerning 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 $^{12}C^{16}O_2$ centered at 2225 cm^{-1} the work of Claveau et al. [40] for three hot bands of $^{16}O^{12}C^{17}O$ between 550 and 765 cm^{-1}, for the $\nu_2 + \nu_3 - \nu_2$ band of $^{16}O^{12}C^{17}O$, and for the laser bands of $^{16}O^{12}C^{17}O$ and $^{16}O^{12}C^{18}O$ [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 $^{16}O^{13}C^{17}O$ [43]; the work of Henningsen and Simonsen [44] for the $2\nu_1 + 2\nu_2 + \nu_3$ band of $^{12}C^{16}O_2$ at 6348 cm^{-1}; the work of Kshirsagar et al. for the $2\nu_3$ of $^{16}O^{12}C^{18}O$ at 4639 cm^{-1} [45] and for the 00031-10001 and 00031-10002 bands of $^{12}C^{16}O_2$ at 5584 cm^{-1} and 5687 cm^{-1} [46]; the work of Giver et al. [47] for five bands of $^{12}C^{16}O_2$ between 5218 cm^{-1} and 5349 cm^{-1}; the work of Malathy Devi et al. [48] for 33 bands of $^{12}C^{16}O_2$ 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 Taskun 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 $^{12}C^{16}O_2$ and for 15 bands of $^{12}C^{16}O^{17}O$ have thus been updated. A summary of the bands for which the line intensities have been updated can be found in Table 6. 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 6. Bands of CO_2 for which the line intensities have been updated.

Band Center (cm^{-1})	Upper Vib $v_1 v_2 l_2 v_3 r$	Lower Vib $v_1 v_2 l_2 v_3 r$	ν_{min} (cm^{-1})	ν_{max} (cm^{-1})	No. of Lines	Sum of Line Intensities	Ref.
$^{16}O^{12}C^{16}O$, 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	1 0 0 2 1	0 0 0 1 1	3606	3704	64	3.47E-23	48
3676.708	3 0 0 1 2	2 0 0 0 2	3626	3711	55	7.09E-24	48
3679.550	3 0 0 1 3	2 0 0 0 3	3622	3710	57	8.07E-24	48
3692.427	2 0 0 1 2	1 0 0 0 2	3606	3731	81	3.64E-21	48
3700.295	2 1 1 1 2	1 1 1 0 2	3629	3738	170	2.87E-22	48
3711.476	2 0 0 1 1	1 0 0 0 1	3635	3757	79	2.93E-21	48
3713.720	2 1 1 1 1	1 1 1 0 1	3648	3755	166	2.22E-22	48
3726.646	1 2 2 1 1	0 2 2 0 1	3646	3770	208	4.68E-21	48
3727.359	1 3 3 1 1	0 3 3 0 1	3662	3766	168	1.76E-22	48
3799.484	3 0 0 1 2	2 0 0 0 3	3774	3819	24	1.35E-25	48

3814.252	2 0 0 1 1	1 0 0 0 2	3753	3854	65	5.90E-23	48
3858.106	2 1 1 1 1	1 1 1 0 2	3818	3888	87	1.84E-24	48
4808.185	4 0 0 0 2	0 1 1 0 1	4758	4857	80	2.44E-23	29
5061.778	1 2 2 1 1	0 0 0 0 1	4992	5112	69	4.47E-24	29
5217.672	3 0 0 1 1	1 0 0 0 2	5176	5251	48	2.13E-24	47
5247.833	1 0 0 2 2	0 1 1 0 1	5217	5271	61	1.37E-24	47
5291.132	0 2 2 2 1	0 1 1 0 1	5248	5316	130	3.52E-24	47
5315.713	0 1 1 2 1	0 0 0 0 1	5251	5342	93	4.72E-23	47
5349.310	1 0 0 2 1	0 1 1 0 1	5301	5357	43	5.77E-25	47
5584.393	0 0 0 3 1	1 0 0 0 1	5541	5601	39	5.58E-25	46
5687.169	0 0 0 3 1	1 0 0 0 2	5641	5703	40	6.31E-25	46
6347.852	3 0 0 1 2	0 0 0 0 1	6271	6385	73	4.42E-22	44
6387.868	4 1 1 0 1	0 0 0 0 1	6348	6430	45	2.45E-25	29
8192.551	1 0 0 3 2	0 0 0 0 1	8099	8210	70	4.15E-23	42
8293.951	1 0 0 3 1	0 0 0 0 1	8194	8310	71	6.18E-23	42

$^{16}O^{12}C^{18}O$, third most abundant isotopologue (628 in AFGL notation)

966.269	0 0 0 1 1	1 0 0 0 1	918	997	108	2.01E-24	41
1072.687	0 0 0 1 1	1 0 0 0 2	1020	1107	118	5.19E-24	41
4639.501	0 0 0 2 1	0 0 0 0 1	4579	4663	115	1.44E-23	45

$^{16}O^{12}C^{17}O$, fourth most abundant isotopologue (627 in AFGL notation)

586.850	1 1 1 0 2	0 2 2 0 1	548	626	294	4.23E-24	29
607.555	2 0 0 0 3	1 1 1 0 2	578	640	123	5.41E-25	29
607.558	1 0 0 0 2	0 1 1 0 1	554	659	208	1.05E-22	40
644.407	1 1 1 0 2	1 0 0 0 2	601	693	183	1.74E-23	29
649.955	1 2 2 0 2	1 1 1 0 2	620	685	244	1.27E-24	29
665.114	0 2 2 0 1	0 1 1 0 1	614	726	427	9.55E-22	29
681.386	1 2 2 0 1	1 1 1 0 1	656	712	208	6.17E-25	29
686.071	1 1 1 0 1	1 0 0 0 1	643	732	178	1.12E-23	29
711.298	1 0 0 0 1	0 1 1 0 1	659	765	210	1.30E-22	40
713.459	2 0 0 0 1	1 1 1 0 1	688	742	105	3.07E-25	29
724.547	2 0 0 0 2	1 1 1 0 2	700	749	89	1.90E-25	29
732.256	1 1 1 0 1	0 2 2 0 1	691	771	302	4.94E-24	29
748.133	1 2 2 0 1	0 3 3 0 1	733	749	72	9.72E-26	29
789.812	1 1 1 0 1	1 0 0 0 2	762	821	114	4.08E-25	29
963.986	0 0 0 1 1	1 0 0 0 1	925	991	85	4.00E-25	41
1067.727	0 0 0 1 1	1 0 0 0 2	1024	1098	97	8.34E-25	41
2306.741	1 1 1 1 2	1 1 1 0 2	2253	2342	258	1.17E-23	29
2315.147	0 2 2 1 1	0 2 2 0 1	2246	2355	362	2.03E-22	29
2317.319	1 0 0 1 1	1 0 0 0 1	2249	2356	141	8.20E-23	29
2318.964	1 0 0 1 2	1 0 0 0 2	2249	2359	145	1.36E-22	29
2327.581	0 1 1 1 1	0 1 1 0 1	2244	2370	434	5.20E-21	29

$^{16}O^{13}C^{17}O$, sixth most abundant isotopologue (637 in AFGL notation)

2274.088	0 0 0 1 1	0 0 0 0 1	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 $^{16}CO_2$ 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 HITRAN 92 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 $(00^01\text{-}10^00)$ and $(02^20\text{-}00^00)$ 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 $^{14}N_2{}^{16}O$.

For the air-broadening coefficients, a polynomial fit based on experimental results from Toth [55], Lacome 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 cm^{-1}/atm at 296K) is

$$\gamma_{air} = 0.0964 \qquad 0 \le |m| \le 1 \qquad (2a)$$

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

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

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 cm^{-1}/atm at 296K) is

$$\gamma_{self} = 0.127 \qquad 0 \le |m| \le 1 \qquad (3a)$$

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

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

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 Lacome 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 $^{12}C^{16}O$ near 2.4 μm, 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 $^{12}C^{16}O$ around 1.6 μm, 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 HITRAN3k.

Recent laboratory measurements of air-broadening coefficients [60, 65, 66] in the fundamental and first two overtones agree within ± 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 ± 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 HITRAN3k using experimental values of Ref. [71].

The temperature dependence exponent for air-broadening is now equal to 0.75 cm^{-1}/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 HITRAN3k for the 1-0, 2-0 and 3-0 bands of $^{12}C^{16}O$. 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 cm^{-1}/atm and –0.0055 cm^{-1}/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 cm^{-1}/atm, have been used between in the range $-24 \leq m \leq 26$. Outside this range the constant value of -0.0075 cm^{-1}/atm has been used as a default value.

2.1.5. CH_4 (molecule 6)

In the pure rotation region, the quantum number K of the $^{12}CH_3D$ 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 $^{12}CH_4$. First, a new line list of 4937 positions and intensities from Brown [72] covering the 4800 to 5500 cm^{-1} region has replaced the 273 lines between 4800 and 4938 cm^{-1} of HITRAN [1]. In addition, 35320 positions and intensities have been added between 6180 and 9200 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 HITRAN 2000 [1]. In the HITRAN 2004 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 cm^{-1}/atm for all lines. This value has been chosen considering Refs. [73,79].

3. Administration of HITRAN project

3.1. Labor effort

A major change in the administration of this grant during this period 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 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

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 will be 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 are encouraging some contributors to HITRAN to publish their articles in this issue. Work has also been done to update the JavaHAWKS manual.

3.3. 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 period

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.

Publications during this period:

"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 period:

"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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