J. Quant. Spectrosc. Radiat. Transfer Vol. 48, No. 5/6, pp. 537–566, 1992
Printed in Great Britain

0022-4073/92 $5.00 + 0.00
Pergamon Press Ltd

ENERGY LEVELS, INTENSITIES, AND LINEWIDTHS OF ATMOSPHERIC CARBON DIOXIDE BANDS

L. S. ROTHMAN,†‡ R. L. HAWKINS,† R. B. WATTSON,§ and R. R. GAMACHE¶

†Phillips Laboratory, Geophysics Directorate, Hanscom AFB, MA 01731, §Visidyne, Inc., 10 Corporate Place, Burlington, MA 01803, and ¶University of Massachusetts Lowell, Center for Atmospheric Research, 450 Aiken Street, Lowell, MA 01854, U.S.A.

(Received 9 July 1992)

Abstract—Spectroscopic constants are given for eight isotopic variants of carbon dioxide which provide energy levels for transitions required for terrestrial atmospheric i.r. absorption. A new tabulation is also furnished with bands considered for the latest HITRAN molecular database. This list provides improved band intensities and Herman–Wallis coefficients generated from recent high-resolution measurements and theoretical calculations. Rotationally-dependent air- and self-broadened halfwidths are provided from a survey of recent experiments.

INTRODUCTION

Carbon dioxide is one of the most important components of the HITRAN database. Although it is considered a trace gas in the terrestrial atmosphere, its strong opacity in the infrared (i.r.) has a major impact on the environment. Accurate knowledge of the spectroscopic properties of the carbon dioxide molecule is necessary for understanding the greenhouse effect, industrial combustion processes, space and aircraft vehicle exhausts, and planetary atmospheres. It is a prime factor in atmospheric remote sensing of temperature and constituent profiles. CO_2 is often a contaminant in spectra. For long-path atmospheric transmission problems it has in fact been necessary that eight naturally-occurring isotopes be considered for the HITRAN database, the most of any molecular species contained on the compilation.

Since the last publication of carbon dioxide energy-level and band parameters,[1] significant improvements have been made for the three absorption line parameters: the transition frequency, intensity, and linewidth. The improvements in the line positions or transition frequencies have been brought about primarily through the use of Direct Numerical Diagonalization (DND) calculations[2,3] to extrapolate from observed vibration–rotation transitions to transitions which have not been measured, but are of possible significance in the atmosphere, and a refined, global method of fitting the transitions. In addition, new observations by Benner et al,[4] Esplin et al[5–7] and Blanquet et al[8] have been added to the fit. High-vibrational levels in the 4.3 μm region observed by Bailly,[9] but not immediately relevant to the atmospheric transmission requirement of HITRAN, have also been added to the fit. As before, the goal of this effort has been to generate a self-consistent set of spectroscopic constants from which to calculate the many line transitions on the database.

The greatest amelioration to the database has been in the intensities. This improvement has been made possible by the use of new measurements by Johns,[10,11] Dana et al,[12–15] Benner et al[4] as well as calculations[3] made with the DND technique. Herman–Wallis coefficients, where available, are used to describe deviations from rigid-rotor behavior.

Pressure broadening of CO_2, both by air and CO_2, was determined by fitting polynomials to a number of recent measurements[12,15–18] and calculations.[19]

In the discussions that follow, we use the vibrational quantum notation as defined in Ref. 20.

‡To whom all correspondence should be addressed.

LINE POSITIONS

The least-squares fitting procedure

Carbon dioxide line positions ν were calculated from the upper and lower state rovibrational energies:

$$\nu = E'(v', J') - E''(v'', J'') \tag{1}$$

where a single prime denotes the upper state, double primes the lower, E is the energy of the state, v its vibrational mode, and J the rotational quantum number.

The energies, in turn, have been calculated using effective spectroscopic constants:

$$E(v, J) = G_v + B_v J(J+1) - D_v[J(J+1)]^2 + H_v[(J(J+1)]^3. \tag{2}$$

Wherever possible, the spectroscopic constants G, B, D, and H for a given vibrational state were determined by weighted linear least-squares fitting of observed line positions involving that state. This section describes the fitting procedure used.

For each isotopic species of carbon dioxide, for example $^{12}C^{16}O_2$ (626 in the HITRAN short-hand notation), spectroscopic constants for all vibrational levels were fit simultaneously. Conceptually, this is a straightforward application of linear least-squares. However, the large amount of data involved (almost 20,000 experimentally observed line positions for 626) and the large number of free parameters (almost 500, again for 626) make the practical application less straightforward.

Least-squares fitting was performed using the Givens rotation algorithm.[21] The implementation was based on a modification of the algorithm described by Gentleman.[22] The Givens algorithm is about 40% slower and proportionately more subject to accumulated roundoff error than more common algorithms, but is particularly suited to large, sparse problems such as this one. It processes the data one observation at a time, so that computer memory requirements are independent of the number of observations. Also, the fact that only a small number of the spectroscopic constants are involved in any one observation can be used to reduce the amount of computation required, by properly ordering the observations and the constants. Thus the sparseness of this particular problem can be used to improve the speed and roundoff characteristics of the Givens algorithm.

The presence of roundoff error was examined by fitting the 626 data twice. In one fit, the bands were ordered for maximum efficiency, in the other fit the data were only partially ordered, such that twice as much computation was required. The resulting spectroscopic constants were printed out to 10 significant digits and compared. Not a single digit differed between the two fits. This result indicates that roundoff error was negligible, and that the implementation is more than adequate for problems of this size.

Corrections to the data

Comparison to DND calculated line positions indicated that a number of lines in the 30001 ← 01101 and 11112 ← 01101 bands of the 636 isotope had been incorrectly assigned,[23] due to an avoided crossing between the 30001 level and 11112e sublevel. The lines originally assigned to P27 and higher, and R25 and higher, of the 30001 ← 01101 band were reassigned to the 11112e ← 01101 subband, and vice-versa.

The Q-branch lines of the 22202 ← 01101 band of the 626 isotope[4] gave extremely large residuals in the initial fit. It was found that reducing the J values assigned to these lines by 2 quanta (e.g. Q15 was reassigned to Q13, etc.) gave residuals commensurate with those in the P- and R-branches.

There appears to be a typographical error in the position of the $P14f$ line of the 12202 ← 01101 band of the 628 isotope in the paper by Rinsland and Benner.[24] The value published there, 2055.60013 cm^{-1}, was replaced by the value published in Rinsland et al,[25] 2055.62648 cm^{-1}.

The line positions measured by Guelachvili et al,[26–28] and measurements by Esplin et al[5–7] which were calibrated against Guelachvili's, were recalibrated against the rest of the observational database. A calibration factor was applied to the affected measurements and varied to give the best global fit. A value not significantly different from that suggested by Brown and Toth[29] was obtained in this way.

Levels without connection to the ground state

The observation-by-observation nature of the Givens algorithm permits the fit to be easily updated by adding new observations. This ability was used to address several problems in the data used. In some of the isotopic species, there were bands in the database which had no connection to the ground state. Therefore, only the band center, the difference between term values G_v for the upper and lower state, could be determined for these bands; absolute values for G_v could not. Values for the lower state G_v'' were obtained from the literature and added as pseudo-observations, effectively fixing the lower-level G_v'' to its literature value, and obtaining the upper-level G_v' relative to it. Levels treated in this way are denoted by a "*C*" in the comment field in Table 1.

Extrapolation in J and v

For many levels, observations do not extend to high enough rotational quantum number J to determine H_v. Extrapolation to values of J greater than the highest observed is inaccurate when H is not known. The ability to extrapolate was tested by fitting observations of the 10001 ← 00001, 01111 ← 01101, and 00011 ← 00001 bands of 626 over a restricted set of J values, and comparing the fit both to the observed high-J line positions, and to DND calculated line positions up to $J = 180$. (The highest laboratory-observed J values are $J = 108$ for 10001, $J = 140$ for 00001, $J = 116$ for 01111, $J = 122$ for 01101, and $J = 141$ for 00011. The test fits were performed using only lines with J up to 20, or up to 30, 40, 50 etc.)

When the fit was restricted to lines of such low J that H could not be determined, as indicated by the estimated standard deviation of H being larger than the retrieved value of H, the extrapolated line positions were less accurate than DND calculated positions. But when lines of sufficiently high J to determine H were used, the extrapolated line positions were as accurate as, or more accurate than, DND calculated line positions. This typically required measurements to $J = 70$ or larger.

Since it appeared that, for these well-measured levels, DND provides a better extrapolation than the fit itself when H cannot be determined, an attempt was made to determine H for poorly-measured levels by calculating the energy at $J = 180$ using DND constants, and using this DND energy as a pseudo-observation. In most cases, this process caused the fit to the observed line positions to be significantly worse. In these cases the DND energy was not used, and H was not fit (effectively, it was fixed to zero). The levels where the single DND energy was retained to determine H are denoted by a "†" in the comment field (last column) in Table 1. Note that the pseudo-observation is an *energy*, not a line position, so that only the indicated level is directly affected.

In addition to this use of DND energies to extrapolate measured levels with insufficiently high J, DND spectroscopic constants were used for levels which have not been measured at all. These pure DND levels are indicated by the symbol ⊠ in the last column.

BAND INTENSITIES AND HERMAN–WALLIS FACTORS

New measurements

New measurements since the 1986 edition of HITRAN[30] have improved the intensities of several bands. Of particular significance is the band at 720.805 cm^{-1}. This major side band to the ν_2 fundamental has had its total band intensity altered several times throughout the history of HITRAN. Recent measurements by Johns and Auwera,[11] which have been corroborated by others (Dana,[31] Huet et al,[32] and Varanasi and Chudamani[33]), have increased the intensity of this band by 6% from the previous value. The band is one of the key channels for remote sensing experiments proposed for satellite monitoring. The nearby band at 721.584 cm^{-1} for the 636 isotope has changed even more. Previously it was based simply on the isotopic ratio related to the same transition of the principal isotope (the 1973 calculated value).[34] We calculated a 40% reduction via DND, which was later confirmed by the observations of Johns and Auwera.[11] Another band in the long wavelength region used for remote sensing is at 791.447 cm^{-1}. New measurements[11,12] show a 15% decrease from the previous band intensity in HITRAN and also, as with the bands discussed above, yield values for the Herman–Wallis factors.

Other regions of the spectrum have also had new measurements: the laser bands,[15] the 2.7 μm doublets,[10] the $3\nu_3$ overtone band,[35] and two bands in the Fermi tetrad[36,37] around 2.2 μm. The observations of Refs. 35–37 have had a major impact on the dipole-moment determination used in DND, and hence on many of the band intensities in Table 2.

Table 1. Spectroscopic constants for CO_2 levels considered for the HITRAN database.

v	G_v	B_v	D_v	H_v	J_{max}	©	‡
$^{12}C^{16}O_2$ (626)							
00001	0.00000	0.39021889	1.33338	0.077	140	18	
01101*e*	667.37996	0.39063900	1.35295	0.099	119	22	
01101*f*	"	0.39125465	1.36088	0.149	122	"	
10002	1285.40834	0.39048223	1.57098	2.173	106	12	ℜ
02201*e*	1335.13161	0.39166676	1.37452	-3.605	110	12	
02201*f*	"	0.39166676	1.38022	0.148	111	"	
10001	1388.18432	0.39018888	1.14919	1.848	108	9	
11102*e*	1932.47013	0.39074498	1.49447	1.005	103	12	
11102*f*	"	0.39169032	1.56357	1.163	104	"	
03301*e*	2003.24615	0.39237834	1.40009	-1.562	101	7	
03301*f*	"	0.39237834	1.40009	-1.179	100	"	
11101*e*	2076.85588	0.39040962	1.25853	0.906	109	13	
11101*f*	"	0.39133390	1.21099	0.451	104	"	
00011	2349.14291	0.38714135	1.32998	0.096	141	5	
20003	2548.36707	0.39110912	1.81217	5.043	92	6	
12202*e*	2585.02213	0.39194333	1.39954	-6.789	98	4	
12202*f*	"	0.39194333	1.53364	1.302	97	"	
20002	2671.14315	0.38956202	1.34939	5.394	90	7	
04401*e*	2671.71459	0.39308193	1.42346	-1.195	98	4	
04401*f*	"	0.39308193	1.42346	-1.195	98	"	
12201*e*	2760.72473	0.39154768	1.41703	-5.991	98	6	
12201*f*	"	0.39154768	1.28224	1.013	95	"	
20001	2797.13591	0.39060563	0.97398	4.277	92	6	
01111*e*	3004.01227	0.38759250	1.34768	0.149	116	6	
01111*f*	"	0.38819027	1.35761	0.172	113	"	
21103*e*	3181.46399	0.39102314	1.63934	2.216	93	3	
21103*f*	"	0.39235111	1.75898	1.633	88	"	
13302*e*	3240.62276	0.39265824	1.50008	-1.665	89	4	
13302*f*	"	0.39265824	1.50008	-0.727	82	"	
21102*e*	3339.35602	0.39003583	1.37969	2.000	79	6	
21102*f*	"	0.39117476	1.38938	2.792	84	"	
05501*e*	3340.52782	0.39377734	1.44701	-1.062	85	2	
05501*f*	"	0.39377734	1.44701	-1.062	85	"	
13301*e*	3442.21534	0.39221531	1.36530	-2.730	91	5	
13301*f*	"	0.39221531	1.36530	-1.065	92	"	
21101*e*	3500.67217	0.39038703	1.17485	2.841	83	5	
21101*f*	"	0.39171524	1.08365	-0.001	82	"	
10012	3612.84080	0.38750292	1.57387	1.981	105	5	
02211*e*	3659.27229	0.38863604	1.36021	-3.407	105	3	
02211*f*	"	0.38863604	1.37396	0.173	106	"	
10011	3714.78193	0.38706302	1.14183	1.830	107	5	ℜ
30004	3792.68438	0.39176146	2.06599	0.	48	1	
22203*e*	3822.01177	0.39235009	1.36150	0.	46	1	
22203*f*	"	0.39235009	1.70097	0.	47	"	
14402*e*	3898.31386	0.39336242	1.52154	-0.986	80	2	ℜ
14402*f*	"	0.39336242	1.52154	-0.986	80	"	
30003	3942.54327	0.38958904	1.67149	0.	54	1	
22202*e*	4007.91450	0.39143698	1.43977	-8.919	62	2	
22202*f*	"	0.39143698	1.41453	1.901	71	"	
06601*e*	4009.67654	0.39446573	1.47806	0.	77	2	
06601*f*	"	0.39446573	1.47806	0.	77	"	
30002	4064.27484	0.38959417	0.99911	2.327	32	1	†

[*continued . . .*]

Table 1—*continued*

v	G_v	B_v	D_v	H_v	J_{max}	©	‡
14401e	4122.26665	0.39287278	1.38161	-3.239	78	3	
14401f	"	0.39287278	1.38161	-3.239	78	"	
22201e	4197.36118	0.39159424	1.62725	0.	60	3	
22201f	"	0.39159424	1.18580	0.	65	"	
30001	4225.09661	0.39098326	0.67819	-5.057	52	1	†
11112e	4247.70486	0.38778212	1.48514	4.360	66	4	
11112f	"	0.38870505	1.56314	1.266	97	"	
03311e	4314.91373	0.38937642	1.38853	-1.349	86	2	
03311f	"	0.38937642	1.38853	-1.005	89	"	
11111e	4390.62856	0.38736478	1.24083	0.849	94	4	
11111f	"	0.38823509	1.20080	0.362	91	"	
31104e	4416.149	0.39136003	1.772	0.	0	1	♀
31104f	"	0.39310013	1.96104	3.149	0	0	■
23303e	4467.1164	0.39303155	1.59639	-2.004	0	0	■
23303f	"	0.39302753	1.57380	-1.749	"	"	■
15502e	4557.59538	0.39405725	1.54626	-0.947	60	1	†
15502f	"	0.39405725	1.54626	-0.947	60	"	†
31103e	4591.11673	0.38992691	1.55056	4.011	51	1	†
31103f	"	0.39121157	1.42980	0.	24	"	†
00021	4673.32546	0.38406605	1.32645	0.066	98	4	
23302e	4676.79054	0.39219216	1.45716	-3.684	45	1	†
23302f	"	0.39219216	1.45716	-0.096	46	"	†
07701e	4679.15606	0.39513421	1.45354	0.	62	1	
07701f	"	0.39513421	1.45354	0.	62	"	
31102e	4753.45338	0.38971170	1.22212	4.413	43	1	†
31102f	"	0.39119264	1.12864	-0.202	0	0	■
15501e	4801.36463	0.39352184	1.39491	-9.509	59	1	
15501f	"	0.39352184	1.39491	-9.509	59	"	
20013	4853.62341	0.38819761	1.81675	5.612	85	4	
12212e	4887.98501	0.38894150	1.31111	0.	51	1	★
12212f	"	0.38894150	1.42134	0.	44	"	
23301e	4890.096	0.39218200	1.61000	0.	0	0	★■
23301f	"	0.39218200	1.61000	0.	"	"	★𝔑
31101e	4938.3535	0.39012318	0.26294	-34.432	0	0	■
31101f	"	0.39217818	0.94746	-2.130	"	"	■
04411e	4970.92829	0.39011400	1.40629	-0.875	88	1	
04411f	"	0.39011400	1.40629	-0.875	88	"	
20012	4977.83500	0.38653399	1.36836	9.598	75	6	
12211e	5061.77818	0.38852520	1.37447	-4.585	87	2	
12211f	"	0.38852520	1.26483	1.179	88	"	
20011	5099.66050	0.38749949	0.96452	3.901	79	4	
40004	5197.1473	0.39014077	2.01648	10.152	0	0	■
32203e	5245.2805	0.39157517	1.59578	-2.747	0	0	■
32203f	"	0.39152343	1.57437	3.022	"	"	■
01121e	5315.71327	0.38454736	1.34194	0.	85	3	
01121f	"	0.38512822	1.35306	0.	92	"	
21113e	5475.07444	0.38815515	1.61	0.	0	1	★
21113f	"	0.38943597	1.75365	1.223	57	"	†
40002	5475.56500	0.39009300	0.89500	0.	0	0	★■
13312e	5531.30325	0.38971557	1.48991	-1.531	72	1	†
13312f	"	0.38971557	1.48991	-0.653	79	"	†
05511e	5627.3314	0.39085398	1.42634	0.103	0	0	■
05511f	"	0.39084848	1.40809	-0.759	"	"	■
21112e	5632.76490	0.38701311	1.31657	0.	58	1	

[*continued*...]

Table 1—*continued*

v	G_v	B_v	D_v	H_v	J_{max}	©	‡
21112*f*	"	0.38811592	1.34365	0.	59	"	
13311*e*	5730.60511	0.38924791	1.32457	0.	66	1	†
13311*f*	"	0.38924791	1.32457	0.	67	"	†
21111*e*	5790.57598	0.38740648	1.13096	2.383	58	2	
21111*f*	"	0.38862059	1.06749	0.819	59	"	
10022	5915.21219	0.38452898	1.57606	1.810	76	3	†
02221*e*	5958.51212	0.38560687	1.34912	-2.429	78	2	
02221*f*	"	0.38560687	1.36906	0.288	77	"	
10021	6016.69005	0.38393530	1.13905	2.312	70	3	
30014	6075.98035	0.38890584	2.12621	15.255	59	2	
22213*e*	6103.686	0.38948235	2.98	0.	0	1	♀
22213*f*	"	0.38939756	1.58	0.	"	"	♀
14412*e*	6176.7013	0.39046900	1.54147	0.232	0	0	■
14412*f*	"	0.39044868	1.49278	-1.553	"	"	■
41102*e*	6178.6922	0.38928314	0.04590	-41.247	0	0	■
41102*f*	"	0.39156514	0.96661	-1.508	"	"	■
30013	6227.91706	0.38671097	1.71434	9.966	63	1	
06611*e*	6284.0982	0.39179878	1.83005	11.037	0	0	■
06611*f*	"	0.39179862	1.82960	11.037	"	"	■
22212*e*	6288.5325	0.38851273	1.56510	2.030	0	0	■
22212*f*	"	0.38846264	1.38597	1.637	"	"	■
30012	6347.85146	0.38645486	0.98129	5.609	63	1	
41101*e*	6387.8675	0.39004831	0.15622	-23.424	0	0	■
41101*f*	"	0.39270574	0.94095	-0.746	"	"	■
14411*e*	6398.1110	0.39002331	1.44739	2.971	0	0	■
14411*f*	"	0.39027095	2.47711	66.381	"	"	■
22211*e*	6474.534	0.38864364	1.498	0.	0	1	♀
22211*f*	"	0.38864364	1.25	0.	"	"	♀
30011	6503.08090	0.38797369	0.71684	0.	57	1	
11122*e*	6537.95879	0.38481636	1.47088	0.	63	1	
11122*f*	"	0.38572340	1.55681	0.	62	"	
03321*e*	6601.71318	0.38637502	1.38391	0.	69	2	
03321*f*	"	0.38637502	1.38391	0.	60	"	
11121*e*	6679.70568	0.38431555	1.23015	0.	53	1	
11121*f*	"	0.38513542	1.19188	0.	58	"	
31114*e*	6688.177	0.38854452	1.75	0.	0	1	♀
31114*f*	"	0.39025487	1.91	0.	"	"	♀
23313*e*	6736.7641	0.39014120	1.57645	-1.988	0	0	■
23313*f*	"	0.39014728	1.58667	-0.534	"	"	■
31113*e*	6863.55646	0.38692624	1.41194	0.	44	1	
31113*f*	"	0.38833672	1.51749	0.	41	"	
23312*e*	6944.7345	0.38923044	1.24637	-6.244	0	0	■
23312*f*	"	0.38928796	1.42639	0.776	"	"	■
00031	6972.57734	0.38099334	1.32399	0.128	91	5	
31112*e*	7023.67530	0.38674989	1.20482	5.539	46	1	†
31112*f*	"	0.38811818	1.15475	1.717	39	"	†
15511*e*	7064.6605	0.39101706	1.72862	-6.288	0	0	■
15511*f*	"	0.39100320	1.69113	-6.088	"	"	■
20023	7133.824	0.38528576	1.72	0.	0	1	♀
23311*e*	7154.6273	0.38972910	1.76931	12.418	0	0	■
23311*f*	"	0.38941145	0.79298	-25.940	"	"	■
12222*e*	7166.0220	0.38570429	1.11545	-10.056	0	0	■
12222*f*	"	0.38571109	1.23533	-4.972	"	"	■
31111*e*	7203.829	0.38759651	0.99	0.	0	1	♀

[*continued . . .*]

Table 1—*continued*

v	G_v	B_v	D_v	H_v	J_{max}	©	‡
31111f	"	0.38915188	0.94	0.	"	"	♀
20022	7259.7483	0.38357496	1.56688	10.090	0	0	■
40015	7283.978	0.38958480	2.51	0.	0	1	♀
32214e	7307.6717	0.39002494	1.37512	-10.224	0	0	■
32214f	"	0.38993691	1.79515	0.740	"	"	■
12221e	7338.1573	0.38553755	1.49566	5.769	0	0	■
12221f	"	0.38548534	1.23075	0.512	"	"	■
20021	7377.6240	0.38435399	0.86925	-1.851	0	0	■
40014	7460.527	0.38734776	1.99	0.	0	1	♀
32213e	7505.2335	0.38866573	1.58933	-0.746	0	0	■
32213f	"	0.38860454	1.54600	2.740	"	"	■
40013	7593.695	0.38558301	1.176	0.	0	1	♀
01131e	7602.51399	0.38150413	1.33736	0.	68	3	
01131f	"	0.38206918	1.35007	0.	59	"	
51102e	7615.5901	0.38939488	0.31976	-19.669	0	0	■
51102f	"	0.39204422	0.92733	-0.309	"	"	■
32212e	7694.3884	0.38867442	2.76983	58.658	0	0	■
32212f	"	0.38826130	1.19679	2.613	"	"	■
40012	7734.448	0.38699702	1.151	0.	0	1	♀
21123e	7743.6727	0.38550802	1.64452	-1.003	0	0	■
21123f	"	0.38649732	1.67100	-1.201	"	"	■
32211e	7897.57300	0.38896500	1.33000	0.	0	0	■
32211f	"	0.38896500	0.93900	0.	"	"	■
21122e	7901.47900	0.38400800	1.31000	0.	0	0	■
21122f	"	0.38512800	1.38000	0.	"	"	■
40011	7920.838	0.38854999	0.55	0.	0	1	♀
21121e	8055.9391	0.38486062	2.66924	90.587	0	0	■
21121f	"	0.38552049	1.06522	1.473	"	"	■
41114e	8081.8348	0.38714174	1.69618	4.381	0	0	■
41114f	"	0.38888587	1.83021	4.973	"	"	■
10032	8192.55067	0.38155873	1.56724	0.	63	2	
02231e	8232.88409	0.38257946	1.34291	0.	55	2	
02231f	"	0.38257946	1.36419	0.	56	"	
41113e	8250.632	0.38625109	1.387	0.	0	1	♀
41113f	"	0.38782425	1.348	0.	"	"	♀
10031	8293.95124	0.38080572	1.12750	0.	65	2	
41112e	8425.005	0.38682258	0.999	0.	0	1	♀
41112f	"	0.38851738	0.94	0.	"	"	♀
50015	8676.716	0.38818320	2.30	0.	0	1	♀
11132e	8803.270	0.38185849	1.47	0.	0	1	♀
11132f	"	0.38274510	1.55	0.	"	"	♀
50014	8831.482	0.38514658	0.954	0.	0	1	♀
03331e	8863.67909	0.38337322	1.37287	0.	68	2	
03331f	"	0.38337322	1.37287	0.	69	"	
11131e	8944.140	0.38126452	1.219	0.	0	1	♀
11131f	"	0.38203190	1.17	0.	"	"	♀
50013	8965.225	0.38592420	0.746	0.	0	1	♀
50012	9137.799	0.38778745	0.66	0.	0	1	♀
00041	9246.93393	0.37792307	1.32018	0.	78	2	
20033	9388.994	0.38238062	1.85	0.	0	1	♀
12232e	9419.1180	0.38318877	1.57657	0.414	0	0	■
12232f	"	0.38315988	1.64309	3.887	"	"	■
20032	9516.969	0.38049550	1.389	0.	0	1	♀
12231e	9589.8190	0.38250452	1.43905	5.351	0	0	■

[continued . . .]

Table 1—*continued*

v	G_v	B_v	D_v	H_v	J_{max}	⊕	‡
12231*f*	"	0.38248205	1.29888	5.076	"	"	■
20031	9631.353	0.38124472	1.007	0.	0	1	♀
01141*e*	9864.45178	0.37846333	1.33393	0.	69	2	
01141*f*	"	0.37901329	1.34681	0.	58	"	
21133*e*	9987.2099	0.38247990	1.56291	-0.734	0	0	■
21133*f*	"	0.38361013	1.70432	-0.310	"	"	■
21132*e*	10145.509	0.38085571	-0.286	0.	0	1	♀
21132*f*	"	0.38216714	1.087	0.	"	"	♀
21131*e*	10297.083	0.38185513	1.012	0.	0	1	♀
21131*f*	"	0.38241578	1.259	0.	"	"	♀
10042	10444.89201	0.37859441	1.56824	0.	62	1	
02241*e*	10482.42758	0.37955413	1.33148	0.	58	2	
02241*f*	"	0.37955413	1.35930	0.	67	"	
10041	10546.61303	0.37767751	1.12694	0.	64	1	
03341*e*	11100.85249	0.38037288	1.36122	0.	51	2	
03341*f*	"	0.38037288	1.36122	0.	66	"	
00051	11496.43720	0.37485584	1.31742	0.	77	2	
01151*e*	12101.57111	0.37542458	1.32895	0.	68	2	
01151*f*	"	0.37596060	1.34414	0.	57	"	
02251*e*	12707.18932	0.37653146	1.32105	0.	57	2	
02251*f*	"	0.37653146	1.35395	0.	68	"	
03351*e*	13313.28168	0.37737617	1.35858	0.	48	1	
03351*f*	"	0.37737617	1.35858	0.	45	"	
00061	13721.13625	0.37179189	1.31530	0.	80	2	
01161*e*	14313.92343	0.37238910	1.32523	0.	57	2	
01161*f*	"	0.37291165	1.34178	0.	54	"	
02261*e*	14907.22350	0.37351166	1.31002	0.	52	2	
02261*f*	"	0.37351166	1.34958	0.	55	"	
00071	15921.08782	0.36873129	1.31300	0.	79	2	
01171*e*	16501.56838	0.36935885	1.32074	0.	54	2	
01171*f*	"	0.36988656	1.33874	0.	55	"	
02271*e*	17082.59233	0.37049609	1.29869	0.	51	1	
02271*f*	"	0.37049609	1.34464	0.	46	"	
00081	18096.35669	0.36567447	1.31083	0.	66	2	
01181*e*	18664.57385	0.36632863	1.31705	0.	51	2	
01181*f*	"	0.36682577	1.33536	0.	54	"	
00091	20247.01630	0.36262179	1.30678	0.	61	2	
01191*e*	20803.01674	0.36330405	1.30812	0.	50	1	
01191*f*	"	0.36378941	1.33039	0.	53	"	
000X1	22373.14890	0.35957366	1.30654	0.	60	2	
000Y1	24474.84685	0.35652993	1.30196	0.	55	2	
000Z1	26552.21158	0.35349217	1.29624	0.	34	1	
		$^{13}C^{16}O_2$ (636)					
00001	0.00000	0.39023754	1.33346	0.151	122	7	
01101*e*	648.47803	0.39061133	1.35489	0.497	113	12	
01101*f*	"	0.39124542	1.36377	0.305	116	"	
10002	1265.82778	0.39091592	1.58290	2.406	104	7	
02201*e*	1297.26326	0.39161360	1.32714	-0.634	106	7	
02201*f*	"	0.39161360	1.38798	-0.256	103	"	
10001	1370.06211	0.38971769	1.20251	2.207	104	7	
11102*e*	1896.53799	0.39096282	1.49053	0.	49	4	
11102*f*	"	0.39202155	1.56117	0.	98	"	
03301*e*	1946.34998	0.39228792	1.38603	-1.128	95	4	
03301*f*	"	0.39228792	1.38603	-0.039	98	"	

[*continued*...]

Table 1—*continued*

v	G_v	B_v	D_v	H_v	J_{max}	©	‡
11101*e*	2037.09334	0.39005116	1.27429	0.318	97	5	
11101*f*	"	0.39091846	1.23846	1.829	100	"	
00011	2283.48711	0.38727344	1.32916	0.143	123	6	
20003	2507.52954	0.39166590	1.84886	4.501	90	1	
12202*e*	2531.67814	0.39211394	1.15471	0.	30	1	
12202*f*	"	0.39211394	1.48752	0.	37	"	
04401*e*	2595.759	0.39295427	1.41097	0.	95	1	C
04401*f*	"	0.39295427	1.41097	0.	95	"	C
20002	2645.06786	0.38968668	1.39851	0.	82	2	
12201*e*	2700.26444	0.39118149	1.32898	-1.207	88	2	
12201*f*	"	0.39118149	1.28874	-0.174	89	"	
20001	2750.59644	0.38972586	0.99291	0.	54	1	
01111*e*	2920.23792	0.38768022	1.34923	0.585	112	3	
01111*f*	"	0.38829411	1.35938	0.280	115	"	
21103*e*	3127.3533	0.39137580	1.62320	1.517	0	0	■
21103*f*	"	0.39289978	1.77443	2.154	"	"	■
13302*e*	3169.4416	0.39276884	1.46614	-2.030	0	0	■
13302*f*	"	0.39276269	1.43718	-2.089	"	"	■
05501*e*	3245.4464	0.39362204	1.42960	-1.089	0	0	■
05501*f*	"	0.39362236	1.43069	-1.028	"	"	■
21102*e*	3289.70119	0.38999405	1.44486	2.679	53	2	†
21102*f*	"	0.39113417	1.32892	-0.992	42	"	†
13301*e*	3361.39969	0.39185731	1.37856	0.	45	1	
13301*f*	"	0.39185731	1.37856	0.	34	"	
21101*e*	3433.77073	0.38973276	1.20684	0.	41	3	
21101*f*	"	0.39094098	1.09206	0.	32	"	
10012	3527.73747	0.38803647	1.57716	2.349	105	3	
02211*e*	3557.31234	0.38869955	1.32077	0.	105	2	
02211*f*	"	0.38869955	1.38420	0.	104	"	
10011	3632.91026	0.38672378	1.19863	2.111	103	3	
30001	4145.76667	0.39050355	2.41245	0.	50	1	★
11112*e*	4147.23205	0.38801702	1.30863	0.	72	2	★
11112*f*	"	0.38914170	1.54833	0.	97	"	
03311*e*	4194.70585	0.38940346	1.37467	-0.864	94	1	
03311*f*	"	0.38940346	1.37467	0.221	97	"	
11111*e*	4287.69801	0.38713084	1.26068	0.641	96	2	
11111*f*	"	0.38794439	1.23446	2.096	99	"	
00021	4543.54803	0.38431127	1.32467	0.081	104	3	
20013	4748.06569	0.38884257	1.83742	4.324	91	2	
12212*e*	4770.97523	0.38925882	1.23021	-7.835	59	1	†
12212*f*	"	0.38925882	1.53244	1.401	56	"	†
04411*e*	4832.437	0.39010992	1.39303	0.	96	1	C
04411*f*	"	0.39010992	1.39303	0.	96	"	C
20012	4887.39069	0.38683530	1.39009	0.	81	3	
12211*e*	4938.83470	0.38828219	1.29088	0.	87	2	
12211*f*	"	0.38828219	1.26742	0.	88	"	
20011	4991.35306	0.38670813	0.95417	0.	67	1	
01121*e*	5168.59893	0.38474991	1.34385	0.609	99	2	
01121*f*	"	0.38534498	1.35457	0.073	86	"	
21113*e*	5357.00437	0.38862235	1.54217	0.	44	1	
21113*f*	"	0.39009954	1.70134	0.	47	"	
13312*e*	5397.25181	0.38991611	1.31004	0.	42	1	
13312*f*	"	0.38991611	1.31004	0.	43	"	
05511*e*	5470.4704	0.39073350	1.06007	-10.054	0	0	■

[*continued*...]

Table 1—*continued*

v	G_v	B_v	D_v	H_v	J_{max}	©	‡
05511*f*	"	0.39101557	1.91781	13.734	"	"	■
21112*e*	5519.92411	0.38706726	1.29464	0.	50	2	
21112*f*	"	0.38821573	1.33087	0.	47	"	
13311*e*	5588.02625	0.38902176	1.32031	0.	52	1	
13311*f*	"	0.38902176	1.32031	0.	53	"	
21111*e*	5662.25817	0.38686742	1.16396	0.	52	1	
21111*f*	"	0.38796327	1.12598	0.	47	"	
10022	5766.18045	0.38515797	1.58121	0.	36	1	
02221*e*	5793.99179	0.38578539	1.31992	0.	46	2	
02221*f*	"	0.38578539	1.38238	0.	49	"	
10021	5872.55125	0.38372777	1.16667	0.	42	1	
30014	5951.604	0.38963872	2.349	0.	0	1	♀
22213*e*	5970.9998	0.38997049	1.24177	-9.500	0	0	■
22213*f*	"	0.38988827	1.65403	0.552	"	"	■
30013	6119.623	0.38759258	1.839	0.	0	1	♀
22212*e*	6155.5078	0.38854751	1.39602	-2.620	0	0	■
22212*f*	"	0.38850487	1.41634	1.578	"	"	■
30012	6241.972	0.38585543	1.102	0.	0	1	♀
22211*e*	6326.0756	0.38840094	2.31481	46.501	0	0	■
22211*f*	"	0.38807583	1.04196	-0.337	"	"	■
30011	6363.624	0.38702900	0.888	0.	0	1	♀
11122*e*	6374.5313	0.38533315	1.41979	-2.108	0	0	■
11122*f*	"	0.38625970	1.52616	0.422	"	"	■
31114*e*	6552.925	0.38904363	1.522	0.	0	1	♀
31114*f*	"	0.39095379	2.035	0.	"	"	♀
31113*e*	6736.696	0.38734810	1.52	0.	0	1	♀
31113*f*	"	0.38887533	1.368	0.	"	"	♀
00031	6780.21036	0.38135150	1.32256	0.292	73	2	†
31112*e*	6892.1160	0.38704604	3.43070	123.463	0	0	■
31112*f*	"	0.38773648	1.25359	3.495	"	"	■
31111*e*	7046.031	0.38683504	0.992	0.	0	1	♀
31111*f*	"	0.38823442	0.893	0.	"	"	♀
01131*e*	7393.58992	0.38182094	1.34166	0.630	48	2	†
01131*f*	"	0.38239697	1.35603	0.586	53	"	†
40013	7481.570	0.38538693	1.445	0.	0	1	★♀
40012	7600.127	0.38587749	0.833	0.	0	1	♀
10032	7981.186	0.38227783	1.566	0.	0	1	♀
02231*e*	8007.33146	0.38287278	1.31655	0.	37	1	
02231*f*	"	0.38287278	1.37511	0.	44	"	
10031	8089.028	0.38073941	1.229	0.	0	1	♀
00041	8993.50726	0.37639388	1.32032	0.485	58	2	†
01141*e*	9595.24601	0.37889274	1.33727	0.922	55	2	†
01141*f*	"	0.37945451	1.35369	0.763	54	"	†
00051	11183.47756	0.37543875	1.31858	0.820	57	2	†
01151*e*	11773.60748	0.37596632	1.32879	0.	54	2	
01151*f*	"	0.37651304	1.34949	0.	63	"	
00061	13350.16635	0.37248573	1.31145	0.	56	2	
01161*e*	13928.72148	0.37304288	1.32516	0.	63	2	
01161*f*	"	0.37357533	1.34956	0.	62	"	
00071	15493.62510	0.36953621	1.30864	0.	59	2	
01171*e*	16060.64231	0.37012259	1.32507	0.	64	2	
01171*f*	"	0.37064065	1.34755	0.	53	"	
00081	17613.91274	0.36659002	1.30579	0.	58	2	
01181*e*	18169.43152	0.36720407	1.31692	0.	47	2	

[*continued*...]

Table 1—*continued*

v	G_v	B_v	D_v	H_v	J_{max}	⊕	‡
01181*f*	"	0.36770944	1.34183	0.	40	"	
00091	19711.09554	0.36364750	1.30325	0.	55	2	
01191*e*	20255.15756	0.36429083	1.31469	0.	44	1	
01191*f*	"	0.36478554	1.36062	0.	39	"	
000X1	21785.24776	0.36070904	1.30067	0.	48	2	
000Y1	23836.45190	0.35777449	1.29563	0.	57	2	
000Z1	25864.79849	0.35484531	1.29223	0.	56	1	
$^{16}O^{12}C^{18}O$ (628)							
00001	0.00000	0.36818450	1.18701	-0.015	119	11	
01101*e*	662.37335	0.36860192	1.20678	0.186	113	10	
01101*f*	"	0.36915324	1.20692	-0.285	111	"	
10002	1259.42520	0.36812143	1.36612	1.819	103	6	
02201*e*	1325.141	0.36956416	1.24872	-3.814	100	3	C
02201*f*	"	0.36956416	1.23158	0.603	98	"	C
10001	1365.84343	0.36851237	1.02206	0.963	100	5	
11102*e*	1901.73695	0.36852010	1.32316	1.576	75	3	
11102*f*	"	0.36931323	1.36848	0.443	92	"	
03301*e*	1988.328	0.37026432	1.29798	-0.519	97	1	C†
03301*f*	"	0.37026432	1.29798	0.517	0	"	C†
11101*e*	2049.33885	0.36862827	1.11901	0.388	92	3	
11101*f*	"	0.36950956	1.08162	0.427	99	"	
00011	2332.11231	0.36528675	1.18424	0.014	118	4	
20003	2500.75995	0.36849295	1.58393	3.438	63	1	
12202*e*	2549.449	0.369659	1.30	0.	0	0	
12202*f*	"	0.369659	1.34	0.	"	"	
20002	2614.24775	0.36774362	1.09684	3.563	64	1	
04401*e*	2651.931	0.37091415	1.29016	-0.576	96	1	C†
04401*f*	"	0.37091415	1.29016	-0.576	96	"	C†
12201*e*	2728.24134	0.36966999	1.32197	0.	49	1	
12201*f*	"	0.36966999	1.13708	0.	44	"	
20001	2757.17770	0.36904215	0.88719	0.	35	1	
01111*e*	2982.11105	0.36573112	1.20268	0.217	114	2	
01111*f*	"	0.36626757	1.20380	-0.296	110	"	
21103*e*	3127.35412	0.36863303	1.45042	1.566	45	1	†
21103*f*	"	0.36972232	1.54854	1.893	43	"	†
13302*e*	3200.192	0.370371	1.34	0.	0	0	
13302*f*	"	0.370371	1.34	0.	"	"	
21102*e*	3281.01692	0.36814783	1.19318	0.	46	2	
21102*f*	"	0.36917925	1.18942	0.	46	"	
13301*e*	3405.062	0.370274	1.24	0.	0	0	
13301*f*	"	0.370274	1.24	0.	"	"	
21101*e*	3454.011	0.368759	1.06	0.	0	0	
21101*f*	"	0.369167	1.12	0.	"	"	
10012	3571.14016	0.36530734	1.37493	1.813	102	2	
02211*e*	3632.524	0.36670707	1.23511	-3.705	99	1	C
02211*f*	"	0.36670707	1.22499	0.444	99	"	C
10011	3675.13269	0.36557351	1.01195	0.808	99	3	
30003	3856.658	0.367404	1.25	0.	0	0	
30002	3987.595	0.36823159	0.964	0.	0	0	
11112*e*	4201.15072	0.36571694	1.32213	2.243	74	2	
11112*f*	"	0.36649734	1.37302	0.553	91	"	
03311*e*	4283.373	0.36743345	1.29394	0.	96	1	C
03311*f*	"	0.36743345	1.29394	0.	0	"	C
11111*e*	4346.18586	0.36575789	1.11060	1.003	91	2	

[*continued*. . .]

Table 1—*continued*

v	G_v	B_v	D_v	H_v	J_{max}	Φ	‡
11111*f*	"	0.36656255	1.07470	0.704	98	"	
00021	4639.50157	0.36239125	1.18191	0.080	93	2	
20013	4791.25976	0.36575852	1.57728	0.	60	1	
12212*e*	4836.559	0.36680918	-0.14472	0.	32	1	⋆C
12212*f*	"	0.36680918	-0.16675	0.	32	"	C
20012	4904.86008	0.36484197	1.07386	0.	54	2	
04411*e*	4934.660	0.36811032	1.28109	0.	95	1	C
04411*f*	"	0.36811032	1.28109	0.	95	"	C
12211*e*	5012.615	0.36681630	1.22498	-20.242	53	1	C
12211*f*	"	0.36681630	1.13612	6.971	54	"	C
20011	5042.58248	0.36613133	0.85461	-1.027	51	1	†
01121*e*	5277.15210	0.36286199	1.19923	0.	51	2	♀
01121*f*	"	0.36338427	1.20185	0.	60	"	
21113*e*	5406.070	0.36589919	1.347	0.	0	1	♀
21113*f*	"	0.36699169	1.592	0.	"	"	♀
21112*e*	5558.566	0.36521505	1.236	0.	0	1	♀
21112*f*	"	0.36631024	1.233	0.	"	"	♀
21111*e*	5727.047	0.365954	0.99	0.	0	0	
21111*f*	"	0.367160	1.03	0.	"	"	
10022	5858.028	0.36250096	1.385	0.	0	1	♀
02221*e*	5915.234	0.363842	1.23	0.	0	0	
02221*f*	"	0.363842	1.22	0.	"	"	
10021	5959.956	0.36262984	1.018	0.	0	1	♀
30014	5993.586	0.36635464	1.817	0.	0	1	♀
30013	6127.783	0.36451882	1.407	0.	0	1	♀
30012	6254.594	0.36528569	0.8646	0.	0	1	♀
30011	6429.176	0.36663261	0.6227	0.	0	1	♀
00031	6922.19672	0.35949797	1.17897	0.	66	2	♀
31113*e*	6762.656	0.365047	1.20	0.	0	0	
31113*f*	"	0.366263	1.27	0.	"	"	
31112*e*	6927.645	0.365297	1.07	0.	0	0	
31112*f*	"	0.366614	1.02	0.	"	"	
01131*e*	7547.52735	0.35999435	1.19595	0.	50	1	
01131*f*	"	0.36050264	1.19191	0.	39	"	
10032	8120.109	0.35970368	1.398	0.	0	1	♀
10031	8220.364	0.35968221	1.004	0.	0	1	♀
00041	9180.23221	0.35660734	1.17712	0.	58	2	
00051	11413.64929	0.35371888	1.17250	0.	49	2	
00061	13622.49542	0.35083374	1.17063	0.	52	2	
00071	15806.82594	0.34795170	1.16843	0.	53	2	
00081	17966.70358	0.34507337	1.16689	0.	52	2	
00091	20102.19914	0.34219890	1.16180	0.	37	2	
000X1	22213.38382	0.33933560	1.17709	0.	36	1	
		$^{16}O^{12}C^{17}O$ (627)					
00001	0.00000	0.37861462	1.26428	0.	51	8	
01101*e*	664.72914	0.37902973	1.26216	0.	41	3	
01101*f*	"	0.37961283	1.27387	0.	41	3	
10002	1272.28663	0.37870010	1.46815	0.	39	1	
02201*e*	1329.843	0.380030	1.31	0.	0		
02201*f*	"	0.380030	1.30	0.	"		
10001	1376.02747	0.37877938	1.08312	0.	43	2	
11102*e*	1916.69308	0.37903763	1.40981	0.	39	1	
11102*f*	"	0.37989164	1.28444	0.	24	1	
03301*e*	1995.352	0.380725	1.32	0.	0		

[*continued*...]

Table 1—*Continued*

v	G_v	B_v	D_v	H_v	J_{max}	©	‡
03301*f*	"	0.380725	1.32	0.	"		
11101*e*	2062.09865	0.37894151	1.18811	0.	50	1	
11101*f*	"	0.37984267	1.13166	0.	31	1	
00011	2340.01370	0.37563150	1.26053	0.	41	1	
20003	2524.24812	0.37920541	1.68286	0.	39	1	
12202*e*	2566.648	0.380210	1.35	0.	0		
12202*f*	"	0.380210	1.43	0.	"		
20002	2641.24038	0.37804734	1.20449	0.	45	1	
12201*e*	2743.485	0.380019	1.37	0.	0		
12201*f*	"	0.380019	1.21	0.	"		
20001	2775.55765	0.37935305	1.48387	0.	31	1	
01111*e*	2992.310	0.376102	1.23	0.	0		
01111*f*	"	0.376664	1.23	0.	"		
10012	3591.251	0.375812	1.46	0.	0		
02211*e*	3644.990	0.377079	1.30	0.	0		
02211*f*	"	0.377079	1.29	0.	"		
10011	3693.346	0.375745	1.07	0.	0		
11112*e*	4223.434	0.376157	1.39	0.	0		
11112*f*	"	0.377014	1.45	0.	"		
11111*e*	4366.812	0.375973	1.18	0.	0		
11111*f*	"	0.376829	1.14	0.	"		
00021	4655.204	0.37265080	1.25	0.	0	1	♀
20013	4821.515	0.37639562	1.716	0.	0	1	♀
20012	4939.351	0.375118	1.21	0.	0		
20011	5068.930	0.376263	0.91	0.	0		
21112*e*	5593.645	0.375625	1.23	0.	0		
21112*f*	"	0.376758	1.22	0.	"		
30013	6175.954	0.37498224	1.512	0.	0	1	♀
30012	6298.116	0.37531350	0.888	0.	0	1	♀
00031	6945.608	0.369671	1.24	0.	0		
		$^{16}O^{13}C^{18}O$ (638)					
00001	0.00000	0.36818116	1.18498	0.	102	7	
01101*e*	643.329	0.36856153	1.20496	0.	94	1	C
01101*f*	"	0.36911244	1.20134	0.	101	1	
10002	1244.90023	0.36853201	1.38123	0.	84	2	
02201*e*	1286.982	0.36949264	1.22940	0.	86	1	C
02201*f*	"	0.36949264	1.22900	0.	77	1	
10001	1342.27778	0.36802125	1.01052	0.	83	2	
11101*e*	2005.44617	0.36825410	1.07427	0.	33	1	
11101*f*	"	0.36908204	1.00379	0.	36	1	
00011	2265.97128	0.36539121	1.18187	0.	101	1	
20002	2588.18210	0.36757742	1.31998	0.	37	1	
01111*e*	2897.709	0.36580015	1.20125	0.	95	1	C
01111*f*	"	0.36633437	1.19855	0.	102	1	
10012	3490.39555	0.36582920	1.38376	0.	83	2	
02211*e*	3529.789	0.36674444	1.22423	0.	85	1	C
02211*f*	"	0.36674444	1.21844	0.	76	1	
10011	3587.54964	0.36518960	1.00668	0.	82	2	
00021	4508.748	0.36260820	1.205	0.	0	1	♀
20013	4692.179	0.36651099	1.643	0.	0	1	♀
20012	4814.570	0.364815	1.12	0.	0		
20011	4925.013	0.365556	0.88	0.	0		

[*continued*...]

Table 1—*continued*

v	G_v	B_v	D_v	H_v	J_{max}	©	‡
			$^{16}O^{13}C^{17}O$ (637)				
00001	0.00000	0.37861700	1.24220	0.	80	1	
01101*e*	645.744	0.378961	1.22	0.	0		
01101*f*	"	0.379600	1.23	0.	"		
10002	1255.330	0.379142	1.48	0.	0		
02201*e*	1291.827	0.379969	1.25	0.	0		
02201*f*	"	0.379969	1.30	0.	"		
10001	1355.117	0.378283	1.11	0.	0		
00011	2274.08840	0.37574440	1.23940	0.	81	1	
01111*e*	2908.197	0.376152	1.27	0.	0		
01111*f*	"	0.376734	1.27	0.	"		
10012	3508.376	0.376353	1.48	0.	0		
02211*e*	3542.625	0.377129	1.24	0.	0		
02211*f*	"	0.377129	1.29	0.	"		
10011	3608.559	0.375380	1.11	0.	0		
			$^{12}C^{18}O_2$ (828)				
00001	0.00000	0.34681727	1.05368	0.042	128	3	
01101*e*	657.331	0.34723371	1.07024	0.	111	1	C
01101*f*	"	0.34772525	1.07696	0.	122	1	
10002	1230.32420	0.34652340	1.16834	0.925	98	1	
02201*e*	1315.084	0.34812573	1.15253	0.	94	1	C
02201*f*	"	0.34812573	1.09342	0.	101	1	
10001	1347.09265	0.34740293	0.91732	-0.015	98	1	
00011	2314.04834	0.34409045	1.05115	0.048	127	2	
01111*e*	2959.131	0.34453039	1.06695	0.	110	1	C
01111*f*	"	0.34500966	1.07486	0.	121	1	
10012	3525.20346	0.34385814	1.17867	1.135	97	3	
02211*e*	3604.653	0.34543473	1.14019	0.	93	1	C
02211*f*	"	0.34543473	1.08974	0.	100	1	
10011	3638.06460	0.34465129	0.91058	-0.060	97	3	
00021	4603.69909	0.34136553	1.04775	0.	76	4	
00031	6868.97831	0.33864346	1.04565	0.	65	1	
			$^{17}O^{12}C^{18}O$ (728)				
00001	0.00000	0.356939	1.10	0.	0		
01101*e*	659.7057	0.357360	1.10	0.	0		
01101*f*	"	0.357871	1.14	0.	"		
00011	2322.436	0.354121	1.11	0.	0		

The notation in the first column is described in Ref. 20 with $X = 10$, $Y = 11$, and $Z = 12$ for the very high vibrational levels of Ref. 9. The units are cm^{-1}; D_v should be multiplied by 10^{-7} and H_v by 10^{-13}. The sixth column, J_{max}, is the highest observed J for the level, or sublevel in the case of ℓ-doubled bands. The seventh column, ©, indicates the number of different bands in which this level was observed. The characters in the comments column, ‡, are interpreted as folows: $\mathcal{R}$ = level observed in Raman spectroscopy (Refs. 86,89); † = a single DND energy at $J = 180$ was used to help determine H_v; ♀ = observed in Venus spectra (Ref. 39); ⊠ = DND constants are given, no observations were available; ★ = a perturbed level; C = constraint applied to force lower level of G_v'' in fit to a literature value.[85]

Models used

We assume that the transition moment squared $|R|^2$ can be separated into a rotationless dipole moment squared, $|R_v|^2$, a rotational line strength or Hönl–London factor $L(J, \ell)$, where ℓ is the angular momentum associated with the bending mode, and a Herman–Wallis factor $F(J)$, i.e.

$$|R|^2 = |R_v|^2 L(J, \ell) F(J). \tag{3}$$

The total internal partition sum $Q(T)$ can be approximated by the product of a vibrational part $Q_v(T)$ and a rotational part $Q_R(T)$,

$$Q(T) = g_j\, Q_v(T) Q_R(T), \tag{4}$$

where g_j is the state-independent nuclear spin factor, and depends on the isotopic species.

Table 2. Intensity parameters for CO_2 bands on the HITRAN database.

ν_0	v'	v''	ISO	S_v^0	a_1	a_2	a_3	b_2	Ref-S	Ref-ν
471.5112	20003	11101	626	0.0115	0.00049	0.898	0.	0.	3	
479.8980	13302	12201	626	0.00145	0.00098	0.57	0.	0.	3 ⊥	
508.1663	12202	11101	626	0.0609	0.00107	0.547	0.	0.	3	
510.3208	21103	20002	626	0.00470	0.00083	1.54	0.	0.	3	
526.4759	11102	10001	636	0.0139	0.00084	1.83	0.	0.	3	
535.8935	11102	10001	628	0.0207	0.00077	-1.09	0.	0.	3	
542.2202	21102	20001	626	0.00810	0.00096	-2.37	0.	0.	3	
544.2858	11102	10001	626	3.279	0.0008	0.	0.	5.7	11	
557.7860	14402	05501	626	0.00302	0.00087	-0.632	0.	0.	3	
561.1210	12202	03301	628	0.00765	0.00085	-0.468	0.	0.	3	
564.9089	20002	11101	628	0.00326	0.0009	-0.827	0.	0.	3	
568.9082	13302	04401	626	0.0807	0.00091	-0.598	0.	0.	3	
573.6826	13302	04401	636	0.00147	0.00094	-0.551	0.	0.	3 ⊥	
576.5960	11102	02201	628	0.193	0.00093	-0.46	0.	0.	3	
578.6313	21102	12201	626	0.0415	0.00111	0.379	0.	0.	3	
579.1417	20002	11101	627	0.00072	0.	0.	0.	0.	⊥	
581.3891	22203	13302	626	0.0109	0.00101	-0.602	0.	0.	3	
581.7760	12202	03301	626	2.16	0.00096	-0.554	0.	0.	3	
585.3282	12202	03301	636	0.0365	0.0010	-0.483	0.	0.	3	
586.8501	11102	02201	627	0.0439	0.	0.	0.	0.		
594.2873	20002	11101	626	0.994	0.00104	-0.874	0.	0.	3	
595.6752	21103	12202	636	0.00457	0.00123	-3.77	0.	0.	3	
596.4419	21103	12202	626	0.280	0.00117	-2.14	0.	0.	3	
597.0518	10002	01101	628	4.66	0.00085	-0.69	0.	0.	3	
597.3385	11102	02201	626	56.18	0.00095	0.	0.	-0.86	11	40
599.0230	20003	11102	628	0.0270	0.00082	-0.094	0.	0.	3	
599.2747	11102	02201	636	0.920	0.00113	-1.93	0.	0.	3	
601.5712	10002	01101	638	0.055	0.	0.	0.	0.		
603.1872	30003	21102	626	0.00544	0.00103	-0.612	0.	0.	3	
607.5550	20003	11102	627	0.0052	0.	0.	0.	0.	⊥	
607.5575	10002	01101	627	1.17	0.	0.	0.	0.		
607.9745	20002	11101	636	0.0204	0.00102	-0.466	0.	0.	3	
608.8285	10012	01111	626	0.0190	0.00083	-0.368	0.	0.	3	
609.5860	10002	01101	637	0.0106	0.	0.	0.	0.		
610.9915	20003	11102	636	0.111	0.00078	1.66	0.	0.	3	
611.2204	30004	21103	626	0.0259	0.0008	1.36	0.	0.	3	
615.8969	20003	11102	626	7.36	0.00087	0.468	0.	0.	3	
617.3497	10002	01101	636	24.04	0.00114	0.	0.	0.	11	41
618.0283	10002	01101	626	1567.5	0.000959	0.	0.	-3.13	11	40,60
619.8238	21103	20003	636	0.00932	0.00087	0.864	0.	0.	3	
630.7103	11102	10002	636	2.84	0.00099	0.166	0.	0.	3	
633.0969	21103	20003	626	0.665	0.00097	0.196	0.	0.	3	
634.8641	11112	10012	626	0.00278	0.00089	-0.25	0.	0.	3	
635.1401	12202	11102	636	0.211	0.00144	-2.57	0.	0.	3	
636.7508	01111	00011	636	0.0127	0.00094	-0.073	0.	0.	3	
637.7635	13302	12202	636	0.0132	0.0013	-0.41	0.	0.	3	
640.5478	22203	21103	626	0.0451	0.00148	-2.51	0.	0.	3	
642.3118	11102	10002	628	0.950	0.00091	-0.22	0.	0.	3	
643.3290	01101	00001	638	3.57	0.	0.	0.	0.		
643.6530	02201	01101	638	0.3	0.	0.	0.	0.		
644.4065	11102	10002	627	0.15	0.	0.	0.	0.		
644.6333	21102	20002	636	0.00353	0.00113	-0.078	0.	0.	3	
645.1047	23303	22203	626	0.00265	0.00131	-0.378	0.	0.	3	
645.7440	01101	00001	637	0.642	0.	0.	0.	0.		
646.0830	02201	01101	637	0.055	0.	0.	0.	0.		
647.0618	11102	10002	626	230.	0.001127	0.	0.	-3.58	11	40,60
647.7121	12202	11102	628	0.0737	0.00111	-0.259	0.	0.	3	
648.4780	01101	00001	636	878.3	0.00077	0.	0.	0.	11	40,60,68
648.7852	02201	01101	636	72.2	0.00126	-0.707	0.	0.	3	41,68
649.0867	03301	02201	636	4.58	0.00122	-0.111	0.	0.	3	68
649.4090	04401	03301	636	0.258	0.00128	-0.005	0.	0.	3	
649.6874	05501	04401	636	0.0136	0.00135	0.093	0.	0.	3	

[continued...]

Table 2—*continued*

ν_0	v'	v''	ISO	S_ν^0	a_1	a_2	a_3	b_2	Ref-S	Ref-ν
649.9549	12202	11102	627	0.0118	0.	0.	0.	0.		
652.5520	12202	11102	626	16.5	0.00132	-1.03	0.	0.	3	
654.8694	01111	00011	626	0.898	0.00092	-0.077	0.	0.	3	
655.2600	02211	01111	626	0.0739	0.00108	0.112	0.	0.	3	
655.6006	13302	12202	626	0.966	0.00124	-0.151	0.	0.	3	
655.6414	03311	02211	626	0.00454	0.00107	0.086	0.	0.	3	
657.3310	01101	00001	828	0.343	0.	0.	0.	0.		
657.6911	14402	13302	626	0.0510	0.00129	-0.018	0.	0.	3	
657.7532	02201	01101	828	0.0277	0.	0.	0.	0.		
659.2815	15502	14402	626	0.00253	0.00136	0.096	0.	0.	3	
659.7057	01101	00001	728	0.0635	0.	0.	0.	0.		
661.1353	13301	12201	636	0.00560	0.00132	0.251	0.	0.	3	
662.3734	01101	00001	628	331.6	0.00106	0.	0.	0.	11	40
662.7676	02201	01101	628	26.3	0.00099	0.731	0.	0.	3	
663.1711	12201	11101	636	0.0987	0.0013	0.801	0.	0.	3	
663.1870	03301	02201	628	1.56	0.00102	0.227	0.	0.	3	
663.6030	04401	03301	628	0.0820	0.00107	0.206	0.	0.	3	
664.7291	01101	00001	627	61.5	0.001198	0.	0.	0.	11	40
665.1139	02201	01101	627	4.88	0.	0.	0.	0.		
665.5090	03301	02201	627	0.285	0.	0.	0.	0.		
667.0312	11101	10001	636	1.40	0.0011	0.025	0.	0.	3	
667.3799	01101	00001	626	83065.	0.000964	0.	0.	0.	11	40,54
667.7516	02201	01101	626	6304.	0.000957	0.	0.	0.	11	40,60
668.1145	03301	02201	626	366.9	0.00106	0.	0.	0.	11	40,60
668.2129	21102	20002	626	0.296	0.00111	-0.123	0.	0.	3	
668.4684	04401	03301	626	19.1	0.00123	0.144	0.	0.	3	40
668.5585	22202	21102	626	0.0195	0.00133	0.768	0.	0.	3	
668.8132	05501	04401	626	0.920	0.0013	0.201	0.	0.	3	
669.1487	06601	05501	626	0.0424	0.00137	0.264	0.	0.	3	
669.4795	07701	06601	626	0.00190	0.00145	0.332	0.	0.	3	
675.8466	11111	10011	626	0.00167	0.00094	-0.084	0.	0.	3	
678.9024	12201	11101	628	0.0394	0.00092	2.36	0.	0.	3	
680.0533	14401	13301	626	0.0195	0.00133	0.378	0.	0.	3	
681.3863	12201	11101	627	0.0082	0.	0.	0.	0.	⊥	
681.4906	13301	12201	626	0.419	0.00125	0.507	0.	0.	3	
683.1743	21101	20001	636	0.00235	0.00116	-0.388	0.	0.	3	
683.4954	11101	10001	628	0.674	0.00091	-0.423	0.	0.	3	
683.8689	12201	11101	626	8.35	0.00115	1.8	0.	0.	3	
686.0712	11101	10001	627	0.13	0.	0.	0.	0.		
688.6716	11101	10001	626	143.89	0.001089	0.	0.	0.83	11	40,60
696.6890	22201	21101	626	0.0101	0.00103	3.22	0.	0.	3	
698.9488	10001	01101	638	0.058	0.	0.	0.	0.		
703.4701	10001	01101	628	8.32	0.00073	-1.08	0.	0.	3	
703.5362	21101	20001	626	0.212	0.0011	-0.995	0.	0.	3	
707.8388	20001	11101	628	0.0210	0.00074	-2.77	0.	0.	3	
709.3730	10001	01101	637	0.0094	0.	0.	0.	0.		
710.7696	10011	01111	626	0.0175	0.00072	-0.076	0.	0.	3	
711.2983	10001	01101	627	1.26	0.	0.	0.	0.		42
712.5108	20002	11102	628	0.0154	0.00074	-0.182	0.	0.	3	
713.4590	20001	11101	627	0.0038	0.	0.	0.	0.		
713.5031	20001	11101	636	0.0363	0.00091	-0.784	0.	0.	3	
720.2800	20001	11101	626	4.15	0.0008	-3.02	0.	1.44	14,3	
720.8043	10001	01101	626	1599.	0.00107	0.	0.	2.19	11,31,32,33	40,60
721.5841	10001	01101	636	11.7	0.001238	0.	0.	0.	11	41
724.1978	11101	02201	628	0.315	0.00081	1.58	0.	0.	3	
724.4244	30001	21101	626	0.00622	0.0009	-3.91	0.	0.	3	
724.5473	20002	11102	627	0.0024	0.	0.	0.	0.	⊥	
724.9188	30002	21102	626	0.00700	0.00088	-0.906	0.	0.	3	
732.2557	11101	02201	627	0.0474	0.	0.	0.	0.		
733.5063	21101	12201	636	0.00147	0.00108	1.64	0.	0.	3 ⊥	
738.6730	20002	11102	626	2.46	0.00034	0.	0.	5.12	13,11	
739.8301	11101	02201	636	0.576	0.00095	0.373	0.	0.	3	
739.9134	12201	03301	628	0.0122	0.00071	0.112	0.	0.	3	

[*continued*...]

Table 2—*continued*

ν_0	v'	v''	ISO	S^0_v	a_1	a_2	a_3	b_2	Ref-*S*	Ref-ν
739.9474	21101	12201	626	0.136	0.00096	2.44	0.	0.	3	
741.7243	11101	02201	626	63.4	0.000758	0.	0.	3.29	14,11	40
748.1330	12201	03301	627	0.0025	0.	0.	0.	0.	⊥	
748.5299	20002	11102	636	0.0194	0.00087	0.662	0.	0.	3	
754.3339	21102	12202	626	0.120	0.00096	0.126	0.	0.	3	
755.1458	22201	13301	626	0.00481	0.00092	0.203	0.	0.	3	
757.4786	12201	03301	626	2.45	0.00107	0.	0.	1.33	13,11	
761.0793	30003	21103	626	0.00435	0.00084	0.629	0.	0.	3	
765.6407	13301	04401	636	0.00115	0.00074	0.025	0.	0.	3 ⊥	
767.2917	22202	13302	626	0.00526	0.00079	0.07	0.	0.	3	
770.5008	13301	04401	626	0.0951	0.00073	0.035	0.	0.	3	
771.2656	11101	10002	636	0.131	0.00058	0.749	0.	0.	3	
781.7408	14401	05501	626	0.00365	0.00068	-0.06	0.	0.	3	
789.8120	11101	10002	627	0.01	0.	0.	0.	0.		
789.9136	11101	10002	628	0.0199	0.00059	-1.69	0.	0.	3	
790.9889	21102	20003	626	0.0357	0.00048	0.709	0.	0.	3	
791.4476	11101	10002	626	7.65	0.001016	-1.6	0.	-3.5	12,11	40
803.7264	12201	11102	636	0.00329	0.00073	-0.052	0.	0.	3	
828.2546	12201	11102	626	0.151	0.	0.	0.	0.	71	
829.5290	21101	20002	626	0.00633	0.00071	-1.9	0.	0.	3	
857.1932	13301	12202	626	0.00527	0.00015	-0.134	0.	0.	3	
864.6658	20001	11102	626	0.042	0.	0.	0.	0.	71	8
883.1446	01111	11101	636	0.00599	-0.00109	-0.461	0.	0.	3	47
898.5476	02211	12201	626	0.0146	-0.00102	-0.459	0.	0.	3	
910.6378	00021	10011	636	0.	0.	0.	0.	0.	@	50
913.4250	00011	10001	636	0.080	0.	0.	0.	0.	71	43
915.6500	21101	12202	626	0.00071	-0.00127	-4.7	0.	0.	3 ⊥	
917.6461	10011	20001	626	0.00990	-0.00089	-0.997	0.	0.	3	
927.1564	01111	11101	626	0.414	-0.00056	0.	0.	0.	15	44,55
941.6976	10012	20002	626	0.0138	-0.0008	-0.47	0.	0.	3	
955.8873	00031	10021	626	0.	0.	0.	0.	0.	@	49
958.5435	00021	10011	626	0.00015	0.	0.	0.	0.	@	49
960.9586	00011	10001	626	6.13	-0.00078	-1.06	0.	0.	15	43
963.9862	00011	10001	627	0.0045	0.	0.	0.	0.		
965.6345	00021	10011	828	0.	0.	0.	0.	0.	@	48
966.2689	00011	10001	628	0.018	0.	0.	0.	0.	71	43
1017.6593	00011	10002	636	0.054	0.	0.	0.	0.	71	43
1023.6999	01111	11102	636	0.00605	-0.00027	1.17	0.	0.	3	
1043.6387	10011	20002	626	0.0158	-0.00049	0.233	0.	0.	3	
1057.3651	00031	10022	626	0.	0.	0.	0.	0.	@	45
1060.4847	00021	10012	626	0.0002	0.	0.	0.	0.	@	45,49
1063.7346	00011	10002	626	9.15	0.	1.33	0.	0.	15	43
1064.4737	10012	20003	626	0.0318	-0.00044	1.33	0.	0.	3	45
1066.2409	11112	21103	626	0.00307	-0.00032	0.835	0.	0.	3	
1067.7271	00011	10002	627	0.0064	0.	0.	0.	0.		
1071.5421	01111	11102	626	0.757	-0.0001	0.	0.	0.	15	45
1072.6871	00011	10002	628	0.036	0.	0.	0.	0.	71	43
1074.2502	02211	12202	626	0.0305	-0.00039	0.925	0.	0.	3	
1078.4956	00021	10012	828	0.	0.	0.	0.	0.	@	48
1080.3741	01111	11102	628	0.00434	-0.00031	0.684	0.	0.	3	
1239.3636	11102	01101	628	0.0223	-0.000135	0.	0.	0.	63	63
1244.9002	10002	00001	638	0.00267	0.00046	-9.73	0.	0.	63	63
1259.4252	10002	00001	628	0.320	-0.00027	1.52	0.	0.	63	63
1272.2866	10002	00001	627	0.0152	-0.000895	4.34	0.	0.	63	63
1342.2778	10001	00001	638	0.00625	0.00035	-2.76	0.	0.	63	63
1365.8434	10001	00001	628	0.359	-0.000293	-0.84	0.	0.	63	63
1376.0275	10001	00001	627	0.0221	-0.00032	-2.09	0.	0.	63	63
1386.9655	11101	01101	628	0.0342	0.	0.	0.	0.	63	63
1846.3324	21103	02201	626	0.00120	-0.15	0.	0.	0.	72	
1880.9871	20003	01101	626	0.01597	-0.1572	17.3	-0.485	0.	64	64
1883.2001	12202	01101	636	0.00160	-0.060	0.	0.	0.	64	64
1896.0557	21103	10002	626	0.00711	-0.0899	5.10	0.	0.	64	64
1896.5380	11102	00001	636	0.0175	-0.0729	6.6	-0.123	6.6	64	64

[*continued*. . .]

Table 2—*continued*

ν_0	v'	v''	ISO	S_ν^0	a_1	a_2	a_3	b_2	Ref-S	Ref-ν
1901.7370	11102	00001	628	0.01956	-0.0511	0.	0.	0.	64	64
1905.4911	13302	02201	626	0.00990	-0.0711	0.	0.	0.	64	64
1916.6931	11102	00001	627	0.00329	-0.0537	0.	0.	0.	64	64
1917.6422	12202	01101	626	0.1979	-0.067	5.5	0.029	5.5	64	64
1932.4701	11102	00001	626	3.425	-0.06044	5.53	-0.111	4.91	65	51,65
1951.1717	21102	10001	626	0.00768	-0.0469	0.	0.	0.	64	64
1996.5898	20002	01101	636	0.00289	-0.0483	0.	0.	0.	64	64
2003.2462	03301	00001	626	0.	-0.0413	0.	0.	0.	66	66
2003.7632	20002	01101	626	0.01711	-0.05703	13.7	0.	-23.	24	24
2004.2245	21102	02201	626	0.00219	-0.0279	0.	0.	0.	64	64
2005.4462	11101	00001	638	0.00078	-0.0366	0.	0.	0.	64 @	64
2023.8734	21102	10002	636	0.00099	-0.050	0.	0.	0.	24	24
2037.0933	11101	00001	636	0.4584	-0.0417	0.	0.	0.	24	24
2049.3388	11101	00001	628	0.1431	-0.0334	0.	0.	-1.8	24	24
2051.7864	12201	01101	636	0.0481	-0.0436	0.	0.	0.	24	24
2053.9477	21102	10002	626	0.0849	-0.0404	0.	0.	0.	24	24
2062.0987	11101	00001	627	0.0258	-0.0389	0.	0.	0.	24	24
2063.7086	21101	10001	636	0.00297	-0.0273	0.	0.	0.	24	24
2064.1365	13301	02201	636	0.00610	-0.0325	0.	0.	0.	24	24
2065.8680	12201	01101	628	0.0166	-0.0327	0.	0.	0.	24	24
2075.4444	22202	11102	626	0.0103	-0.0377	0.	0.	0.	24	24
2076.8559	11101	00001	626	41.55	-0.03772	0.52	0.	-0.58	67	51,67
2093.3448	12201	01101	626	4.01	-0.03838	3.30	-0.121	0.	67	51,67
2094.8044	20001	01101	628	0.0092	-0.0305	0.	0.	0.	67	67
2102.1184	20001	01101	636	0.0217	-0.0482	0.	0.	0.	67	67
2107.0838	13301	02201	626	0.289	-0.0394	0.80	-0.054	0.	67	67
2110.8285	20001	01101	627	0.0018	-0.04	0.	0.	0.	67	67
2112.4878	21101	10001	626	0.1700	-0.0414	0.	0.	0.	67	51,67
2119.0225	14401	03301	626	0.0183	-0.0414	0.	0.	0.	67	67
2120.5053	22201	11101	626	0.0119	-0.0470	0.	0.	0.	67	67
2129.7559	20001	01101	626	2.132	-0.04202	-1.6	0.053	1.9	67	51,67
2131.8047	30002	11102	626	0.0050	-0.0425	0.	0.	0.	67	67
2136.5075	21101	02201	636	0.0022	-0.03	0.	0.	0.	67	67
2148.2407	30001	11101	626	0.0077	-0.048	0.	0.	0.	67	67
2157.6753	10012	10001	636	0.00788	0.	0.	0.	0.	67	67
2165.5406	21101	02201	626	0.0920	-0.0516	0.	0.	0.	67	67
2167.9430	21101	10002	636	0.0009	-0.045	0.	0.	0.	67	67
2170.8490	11112	11101	626	0.0426	0.	0.	0.	0.	67	67
2180.6991	20012	20001	626	0.0012	0.	0.	0.	0.	67	67
2182.4803	20013	20002	626	0.0028	0.	0.	0.	0.	67	67
2194.1150	22201	03301	626	0.0037	-0.068	0.	0.	0.	67	67
2205.2967	10012	10001	628	0.00517	0.00003	-1.7	0.	0.	3	
2215.2638	21101	10002	626	0.0331	-0.0648	5.55	0.	0.	3	
2224.6565	10012	10001	626	1.19	-0.00002	-0.945	0.	0.	3	
2224.9910	01131	01121	636	0.	0.	0.	0.	0.	@	9
2225.0240	05511	05501	636	0.00254	-0.00014	-0.309	0.	0.	3	
2227.8102	13312	13302	636	0.00366	-0.00080	-2.3	0.	0.	3	
2229.6511	21113	21103	636	0.00447	0.	0.	0.	0.	3	
2230.2229	21112	21102	636	0.00198	-0.00003	0.06	0.	0.	3	
2236.6624	00031	00021	636	0.00001	0.	0.	0.	0.	@	9
2236.6784	04411	04401	636	0.0603	-0.00012	-0.017	0.	0.	3	58
2238.5703	12211	12201	636	0.0354	-0.00013	-0.013	0.	0.	3	58
2239.2971	12212	12202	636	0.0818	-0.00010	0.008	0.	0.	3	
2240.5362	20013	20003	636	0.0459	-0.00013	-0.021	0.	0.	3	58
2240.7566	20011	20001	636	0.0136	-0.00013	0.021	0.	0.	3	
2242.3228	20012	20002	636	0.0229	-0.00014	-0.063	0.	0.	3	58
2242.8071	02211	02201	638	0.149	0.	0.	0.	0.		58
2245.2719	10011	10001	638	0.0555	0.	0.	0.	0.		58
2245.4953	10012	10002	638	0.0816	0.	0.	0.	0.		58
2248.3559	03311	03301	636	1.43	-0.00012	0.009	0.	0.	3	58
2248.3610	01121	01111	636	0.0250	-0.00015	0.	0.	0.	3	9,58
2250.6047	11111	11101	636	0.897	-0.00014	-0.013	0.	0.	3	58
2250.6941	11112	11102	636	1.81	0.	0.	0.	0.	3	58

[*continued*]

Table 2—*continued*

ν_0	v '	v "	ISO	S_v^0	a_1	a_2	a_3	b_2	Ref-*S*	Ref-ν
2250.7980	02211	02201	637	0.0264	0.	0.	0.	0.		
2253.0460	10012	10002	637	0.0146	0.	0.	0.	0.		
2253.4420	10011	10001	637	0.0098	0.	0.	0.	0.		
2254.3798	01111	01101	638	3.48	0.	0.	0.	0.		58
2260.0491	02211	02201	636	33.7	-0.00013	0.012	0.	0.	3	53,9
2260.0609	00021	00011	636	0.279	-0.00015	0.007	0.	0.	3	9,58
2261.9097	10012	10002	636	19.5	-0.00014	-0.005	0.	0.	3	53
2261.9659	03331	03321	626	0.	0.	0.	0.	0.	@	28
2262.4530	01111	01101	637	0.628	0.	0.	0.	0.		
2262.8481	10011	10001	636	11.6	-0.00014	0.017	0.	0.	3	53
2265.2792	00031	00021	828	0.	0.	0.	0.	0.	@	9
2265.9713	00011	00001	638	38.8	0.	0.	0.	0.		53
2271.7599	01111	01101	636	771.6	-0.00015	0.	0.	0.	10	53,9
2274.0884	00011	00001	637	7.15	0.	0.	0.	0.		58
2274.3720	02231	02221	626	0.	0.	0.	0.	0.	@	28
2274.4217	06611	06601	626	0.00599	-0.00024	-0.827	0.	0.	3	
2275.8424	14411	14401	626	0.00339	-0.00011	-0.152	0.	0.	3	
2277.1728	22211	22201	626	0.00231	-0.00012	-0.106	0.	0.	3	
2277.2612	10031	10021	626	0.	0.	0.	0.	0.	@	52
2277.3385	10032	10022	626	0.	0.	0.	0.	0.	@	52
2277.9842	30011	30001	626	0.00100	-0.00009	0.043	0.	0.	3	
2278.3874	14412	14402	626	0.0102	-0.00037	-0.89	0.	0.	3	
2280.6180	22212	22202	626	0.00584	-0.00012	-0.034	0.	0.	3	
2281.6742	22213	22203	626	0.0147	-0.00010	-0.01	0.	0.	3	
2282.7286	04411	04401	628	0.0178	-0.00010	0.017	0.	0.	3	70
2283.2960	30014	30004	626	0.00843	-0.00012	-0.033	0.	0.	3	
2283.4871	00011	00001	636	9286.	-0.00013	0.	0.	0.	10	53,9
2283.5766	30012	30002	626	0.00216	-0.00012	0.031	0.	0.	3	
2284.3739	12211	12201	628	0.0121	-0.00011	0.008	0.	0.	3	
2285.3738	30013	30003	626	0.00394	-0.00013	-0.1	0.	0.	3	
2286.7994	03321	03311	626	0.00273	-0.00012	0.016	0.	0.	3	28
2286.8007	01131	01121	626	0.00002	0.	0.	0.	0.	@	28
2286.8036	05511	05501	626	0.156	-0.00011	-0.032	0.	0.	3	
2287.1097	12212	12202	628	0.0290	0.	0.	0.	0.	3	
2288.3898	13311	13301	626	0.0931	-0.00011	-0.028	0.	0.	3	46
2289.0771	11121	11111	626	0.00185	-0.00014	-0.001	0.	0.	3 @	52
2289.5689	02211	02201	828	0.0127	0.	0.	0.	0.		56
2289.6508	00021	00011	828	0.00009	0.	0.	0.	0.	@	9
2289.9038	21111	21101	626	0.069	-0.00012	-0.05	0.	0.	3	
2290.2539	11122	11112	626	0.00375	-0.00015	-0.082	0.	0.	3	52
2290.4998	20013	20003	628	0.0181	-0.00012	-0.019	0.	0.	3	
2290.6123	20012	20002	628	0.0103	-0.00013	-0.047	0.	0.	3	
2290.6805	13312	13302	626	0.252	-0.00011	0.002	0.	0.	3	46
2290.9719	10011	10001	828	0.00487	0.	0.	0.	0.		56
2293.4089	21112	21102	626	0.151	-0.00011	-0.004	0.	0.	3	
2293.6104	21113	21103	626	0.333	0.	0.	0.	0.	3	
2294.8793	10012	10002	828	0.00796	0.	0.	0.	0.		56
2295.0411	01121	01111	628	0.00720	-0.00013	0.005	0.	0.	3	
2295.0453	03311	03301	628	0.452	-0.00011	0.019	0.	0.	3	70
2296.8471	11111	11101	628	0.330	-0.00012	0.016	0.	0.	3	70
2299.2137	04411	04401	626	4.06	-0.00011	0.006	0.	0.	3	46
2299.2398	02221	02211	626	0.0666	-0.00013	0.014	0.	0.	3	46,28
2299.2519	00031	00021	626	0.00037	0.	0.	0.	0.	@	28
2299.4138	11112	11102	628	0.679	-0.00013	-0.027	0.	0.	3	70
2301.0534	12211	12201	626	2.58	-0.00012	-0.004	0.	0.	3	46
2301.7996	01111	01101	828	0.31	0.	0.	0.	0.		56
2301.9081	10021	10011	626	0.0250	-0.00014	0.028	0.	0.	3	52
2302.3714	10022	10012	626	0.0414	-0.00014	-0.006	0.	0.	3	46,52
2302.5246	20011	20001	626	1.07	-0.00012	0.029	0.	0.	3	46
2302.9628	12212	12202	626	6.13	0.00005	0.243	0.	0.	3	
2305.2563	20013	20003	626	3.64	-0.00013	-0.02	0.	0.	3	46
2306.6919	20012	20002	626	1.96	-0.00014	-0.058	0.	0.	3	46
2306.7409	11112	11102	627	0.116	0.	0.	0.	0.		

[*continued*...]

Table 2—*continued*

ν_0	v'	v''	ISO	S_ν^0	a_1	a_2	a_3	b_2	Ref-*S*	Ref-ν
2307.3832	02211	02201	628	11.4	-0.00012	0.016	0.	0.	3	56
2307.3893	00021	00011	628	0.0856	-0.00014	-0.002	0.	0.	3	70
2309.2893	10011	10001	628	4.62	-0.00012	0.031	0.	0.	3	56
2311.6676	03311	03301	626	105.	-0.00012	0.015	0.	0.	3	46,28
2311.7010	01121	01111	626	1.62	-0.00015	0.003	0.	0.	3	46,28
2311.7150	10012	10002	628	7.75	-0.00013	-0.003	0.	0.	3	56
2313.7726	11111	11101	626	72.3	-0.00014	-0.002	0.	0.	3	46,52
2314.0483	00011	00001	828	3.60	0.	0.	0.	0.		9,56
2315.1470	02211	02201	627	1.91	0.	0.	0.	0.		
2315.2348	11112	11102	626	147.	-0.00017	-0.144	0.	0.	3	46,52
2317.3185	10011	10001	627	0.805	0.	0.	0.	0.		
2318.9644	10012	10002	627	1.29	0.	0.	0.	0.		
2319.7377	01111	01101	628	289.	-0.00013	0.006	0.	0.	3	56
2322.4360	00011	00001	728	1.35	0.	0.	0.	0.		
2324.1406	02211	02201	626	2632.	-0.00015	0.	0.	0.	10	46,28
2324.1826	00021	00011	626	19.8	-0.00015	0.009	0.	0.	3	46,28
2326.5976	10011	10001	626	1021.	-0.00015	0.	0.	0.	10	46,52
2327.4325	10012	10002	626	1717.	-0.00008	0.	0.	0.	10	46,52
2327.5809	01111	01101	627	49.7	0.	0.	0.	0.		
2332.1123	00011	00001	628	3686.	-0.00032	0.	0.	0.	10,87	56,59
2336.6324	01111	01101	626	70417.	-0.00026	0.	0.	0.	10	46,28
2340.0137	00011	00001	627	679.	-0.00022	0.	0.	0.	10	28
2349.1429	00011	00001	626	916076.	-0.00014	0.	0.	0.	10	46,27,28
2367.0824	10011	10002	636	0.00459	-0.00078	-0.415	0.	0.	3	
2415.7075	10011	10002	628	0.00325	0.	0.	0.	0.	61	61
2428.5174	20011	20002	626	0.00085	0.	0.	0.	0.	61 @	61
2429.3736	10011	10002	626	0.6635	-0.001667	-1.67	0.	0.	61,90	61
2429.4679	20012	20003	626	0.00137	0.	0.	0.	0.	61	61
2458.1584	11111	11102	626	0.0159	-0.00247	0.	0.	0.	61	61
2464.9808	21103	01101	628	0.0115	0.	0.	0.	0.	61	61
2500.7600	20003	00001	628	0.1391	0.0000069	0.69	0.	0.	61	61
2524.2481	20003	00001	627	0.00507	0.	0.	0.	0.	61	61
2588.1821	20002	00001	638	0.00242	0.	0.	0.	0.	61	61
2614.2477	20002	00001	628	0.231	-0.0000103	-1.03	0.	0.	61	61
2618.6436	21102	01101	628	0.0162	0.	0.	0.	0.	61	61
2641.2404	20002	00001	627	0.0114	0.	0.	0.	0.	61	61
2757.1777	20001	00001	628	0.033	0.	0.	0.	0.	73	
2775.5577	20001	00001	627	0.00214	0.	0.	0.	0.	73	
2791.6377	21101	01101	628	0.00255	0.	0.	0.	0.	73 @	
3125.3044	30004	01101	626	0.00016	0.4	0.	0.	0.	4	4
3154.6318	22203	01101	626	0.00015	0.4	0.	0.	0.	4	4
3181.4640	21103	00001	626	0.00159	0.5084	8.	1.35	43.	4	4
3275.1633	30003	01101	626	0.00842	0.0715	0.	0.	0.	4	4
3281.0169	21102	00001	628	0.00066	0.14	0.	0.	0.	4	4
3289.7012	21102	00001	636	0.00067	0.212	0.	0.	0.	4	4
3305.7084	31103	10002	626	0.00097	0.129	0.	0.	0.	4	4
3339.3560	21102	00001	626	0.1219	0.1615	0.	0.14	0.	4	4
3340.5345	22202	01101	626	0.00553	0.22	0.	0.23	0.	4	4
3341.6589	23302	02201	626	0.00007	0.53	0.	0.	0.	4	4
3365.2691	31102	10001	626	0.00035	0.19	0.	0.	0.	4	4
3396.8949	30002	01101	626	0.00185	0.3	0.	0.	0.		
3398.2186	21113	11101	626	0.00429	0.	0.	0.	0.	3	
3450.9018	13312	03301	636	0.0107	-0.00073	-1.24	0.	0.	3	23
3460.4664	21113	11102	636	0.0234	0.	0.	0.	0.	3	23
3465.4391	20013	10001	626	0.174	-0.00016	1.21	0.	0.	3	
3473.7120	12212	02201	636	0.246	0.00001	1.29	0.	0.	3	23
3482.2379	20013	10002	636	0.217	-0.00009	1.43	0.	0.	3	23
3482.6933	10022	00011	636	0.00153	-0.00008	2.2	0.	0.	3	23
3482.8307	21112	11101	636	0.00883	0.00011	0.943	0.	0.	3	23
3490.3956	10012	00001	638	0.463	0.	0.	0.	0.		23
3496.1413	23313	13302	626	0.00498	-0.00002	0.977	0.	0.	3	
3497.2886	30001	01101	636	0.	0.	0.	0.	0.	⋆	23
3498.7540	11112	01101	636	5.51	0.	0.	0.	0.	3 ⋆	23

[*continued*...]

Table 2—*continued*

ν_0	v'	v''	ISO	S_v^0	a_1	a_2	a_3	b_2	Ref-S	Ref-ν
3500.6721	21101	00001	626	0.124	0.128	-15.71	0.	0.	3	
3504.3331	21113	11102	628	0.0162	-0.00010	0.763	0.	0.	3	
3504.9867	14412	04401	626	0.0417	-0.00029	0.018	0.	0.	3	
3506.7130	31114	21103	626	0.00899	-0.00021	0.429	0.	0.	3	
3508.3760	10012	00001	637	0.0771	0.	0.	0.	0.		
3509.2272	21112	11101	628	0.00499	-0.00007	0.361	0.	0.	3	
3511.4177	12212	02201	628	0.144	0.	0.	0.	0.	3	58
3517.3286	20012	10001	636	0.128	-0.00013	1.51	0.	0.	3	23
3518.6639	22213	12202	626	0.120	0.	1.08	0.	0.	3	
3524.2004	31113	21102	626	0.00378	0.00003	0.731	0.	0.	3	
3525.2035	10012	00001	828	0.0588	0.	0.	0.	0.		58
3527.6133	30014	20003	626	0.0900	-0.00008	1.19	0.	0.	3	
3527.7375	10012	00001	636	56.1	-0.00009	2.1	0.	0.	3	23
3527.8078	22212	12201	626	0.0323	-0.00007	0.695	0.	0.	3	
3528.0571	13312	03301	626	1.09	-0.00003	0.988	0.	0.	3	
3529.9812	22201	01101	626	0.0113	0.112	-38.06	0.	0.	3	
3531.8346	20013	10002	628	0.185	-0.00009	1.23	0.	0.	3	58
3533.9465	11122	01111	626	0.0163	-0.00010	1.23	0.	0.	3	
3538.7774	11112	01101	628	3.81	-0.00009	0.781	0.	0.	3	58
3539.0167	20012	10001	628	0.0775	-0.00009	0.354	0.	0.	3	58
3542.6043	21113	11102	626	2.83	0.	0.	0.	0.	3 *	
3543.0949	40002	11102	626	0.	0.	0.	0.	0.	*	
3549.2284	20013	10002	627	0.0224	0.	0.	0.	0.		
3550.7156	30012	20001	626	0.0167	-0.00007	0.229	0.	0.	3	
3552.8534	12212	02201	626	28.6	0.00019	1.38	0.	0.	3	58
3555.9090	21112	11101	626	0.969	-0.00004	0.598	0.	0.	3	
3556.7739	30013	20002	626	0.0537	-0.00013	1.16	0.	0.	3	
3557.7167	30001	01101	626	0.00536	0.214	-23.05	0.	0.	3	
3558.7049	11112	01101	627	0.668	0.	0.	0.	0.		
3563.3235	20012	10001	627	0.0135	0.	0.	0.	0.		
3566.0693	10022	00011	626	0.197	-0.00011	1.81	0.	0.	3	
3568.2151	20013	10002	626	30.7	-0.00008	1.52	0.	0.	3	58
3571.1402	10012	00001	628	52.5	-0.00011	1.06	0.	0.	3	58
3580.3249	11112	01101	626	729.	0.0001	1.57	0.	0.	10	58
3587.5496	10011	00001	638	0.703	0.	0.	0.	0.		23
3589.0641	10021	00011	636	0.00582	-0.00016	-0.63	0.	0.	3	23
3589.6507	20012	10001	626	16.1	-0.00012	0.641	0.	0.	3	58
3591.2510	10012	00001	627	8.41	0.	0.	0.	0.		
3608.5590	10011	00001	637	0.126	0.	0.	0.	0.		
3612.8408	10012	00001	626	9861.	0.00010	1.57	0.	0.	10,88	58
3621.2910	20011	10001	636	0.413	-0.00017	-0.952	0.	0.	3	23
3621.5629	20012	10002	636	0.422	-0.00017	-0.331	0.	0.	3	23
3623.3862	21112	11102	636	0.0381	-0.00004	-0.223	0.	0.	3	23
3625.1648	21111	11101	636	0.0330	-0.00017	-0.69	0.	0.	3	23
3632.9103	10011	00001	636	190.	-0.00016	-0.684	0.	0.	3	23
3638.0646	10011	00001	828	0.0392	0.	0.	0.	0.		58
3639.2199	11111	01101	636	15.6	-0.00016	-0.516	0.	0.	3	23
3641.5714	12211	02201	636	0.657	-0.00016	-0.551	0.	0.	3	23
3641.6762	13311	03301	636	0.0279	-0.00016	-0.553	0.	0.	3	23
3645.4349	20012	10002	628	0.146	-0.00019	-1.01	0.	0.	3	58
3656.8291	21112	11102	628	0.0120	-0.00014	-0.625	0.	0.	3	
3659.2723	02211	00001	626	0.	0.	0.	0.	0.	*	
3667.0644	20012	10002	627	0.0333	0.	0.	0.	0.		
3667.5471	10021	00011	626	0.349	-0.00017	-1.12	0.	0.	3	
3675.1327	10011	00001	628	47.3	-0.00015	-1.32	0.	0.	3	58
3675.6934	11121	01111	626	0.0290	-0.00015	-0.707	0.	0.	3	
3676.7083	30012	20002	626	0.0740	-0.00018	-1.08	0.	0.	3	
3676.7390	20011	10001	628	0.108	-0.00017	-1.03	0.	0.	3	58
3677.7082	21111	11101	628	0.00898	-0.00029	-1.18	0.	0.	3	
3679.5500	30013	20003	626	0.0797	-0.00018	-0.365	0.	0.	3	
3682.0925	31113	21103	626	0.00705	-0.00008	-0.311	0.	0.	3	
3683.8125	11111	01101	628	4.17	-0.00014	-0.764	0.	0.	3	58
3684.3193	31112	21102	626	0.00565	-0.00017	-0.753	0.	0.	3	

[*continued*...]

Table 2—*continued*

ν_0	v'	v''	ISO	S_ν^0	a_1	a_2	a_3	b_2	Ref-S	Ref-ν
3687.4743	12211	02201	628	0.175	-0.00015	-0.691	0.	0.	3	58
3692.4267	20012	10002	626	36.5	-0.00019	-0.62	0.	0.	3	58
3692.9025	20011	10001	627	0.0279	0.	0.	0.	0.		
3693.3460	10011	00001	627	10.2	0.	0.	0.	0.		
3700.2948	21112	11102	626	2.93	-0.00013	-0.499	0.	0.	3	
3702.0829	11111	01101	627	0.771	0.	0.	0.	0.		
3703.1568	31111	21101	626	0.00318	-0.0002	-1.05	0.	0.	3	
3703.5104	22212	12202	626	0.120	-0.00018	-0.621	0.	0.	3	
3704.1117	23312	13302	626	0.00489	-0.00017	-0.593	0.	0.	3	
3705.9450	30011	20001	626	0.0439	-0.00020	-1.03	0.	0.	3	
3711.4762	20011	10001	626	29.7	-0.00017	-1.09	0.	0.	3	58
3712.4120	23311	13301	626	0.00327	0.	0.	0.	0.	3	
3713.7201	21111	11101	626	2.30	-0.00017	-0.783	0.	0.	3	58
3713.8093	22211	12201	626	0.0870	-0.00017	-0.788	0.	0.	3	
3714.7819	10011	00001	626	15223.	0.00004	-1.14	0.	0.	10,88	58
3723.2486	11111	01101	626	1199.	0.00004	-1.14	0.	0.	10	58
3724.1327	15511	05501	626	0.00292	-0.00037	-1.79	0.	0.	3	
3725.5253	20011	10002	636	0.00761	-0.00040	0.181	0.	0.	3	
3726.3964	14411	04401	626	0.0746	-0.00018	-0.702	0.	0.	3	
3726.6466	12211	02201	626	48.1	-0.00016	-0.688	0.	0.	3	58
3727.3590	13311	03301	626	1.90	-0.00016	-0.627	0.	0.	3	
3799.4844	30012	20003	626	0.00211	-0.00042	-0.037	0.	0.	3	
3814.2522	20011	10002	626	0.624	-0.00034	-2.34	0.	0.	3	
3856.6580	30003	00001	628	0.0144	-0.00026	2.22	0.	0.	3	
3858.1058	21111	11102	626	0.0199	-0.00027	-1.26	0.	0.	3	
3980.5817	01121	02201	626	0.00294	0.0826	-3.49	0.	0.	3	
3987.5950	30002	00001	628	0.00625	0.00004	-0.304	0.	0.	3	
4005.9455	00021	01101	626	0.0385	0.0701	-0.479	0.	0.	3	
4416.1490	31104	00001	626	0.00024	0.144	2.9	0.97	0.	36	
4591.1167	31103	00001	626	0.00289	0.158	0.	0.	0.	37	
4614.7788	01121	01101	628	0.0104	0.	0.	0.	0.	74	
4639.5016	00021	00001	628	0.124	0.	0.	0.	0.	74	
4655.2040	00021	00001	627	0.0127	0.	0.	0.	0.		
4673.7365	22213	02201	636	0.00239	-0.00005	1.49	0.	0.	3	
4685.7762	30014	10002	636	0.00234	-0.00015	1.59	0.	0.	3	
4687.7961	30014	10001	626	0.00746	-0.00026	1.91	0.	0.	3	
4692.1790	20013	00001	638	0.0026	0.	0.	0.	0.		
4708.5263	21113	01101	636	0.0442	0.	0.	0.	0.	3	
4722.6495	32214	12202	626	0.00227	-0.00004	1.25	0.	0.	3	
4733.5180	23313	03301	626	0.0146	-0.00001	1.34	0.	0.	3	
4735.6110	40015	20003	626	0.00180	-0.00012	1.35	0.	0.	3	
4743.6967	21113	01101	628	0.0457	-0.00009	1.37	0.	0.	3	
4748.0656	20013	00001	636	0.323	-0.00009	2.84	0.	0.	3	
4753.4534	31102	00001	626	0.00412	0.146	-9.53	0.	0.	3	
4755.7069	31114	11102	626	0.0465	-0.00016	1.19	0.	0.	3	
4768.5544	22213	02201	626	0.344	-0.00003	1.42	0.	0.	3	
4784.6810	20023	00011	626	0.00154	-0.00003	3.11	0.	0.	3	
4786.7006	31113	11101	626	0.0116	0.00008	1.17	0.	0.	3	
4790.5720	30014	10002	626	0.409	-0.00008	2.03	0.	0.	3	69
4791.2598	20013	00001	628	0.531	-0.00008	2.23	0.	0.	3	
4807.6945	21113	01101	626	7.85	0.	0.	0.	0.	3 *	62
4808.1851	40002	01101	626	0.	0.	0.	0.	0.	*	
4814.5700	20012	00001	638	0.0134	0.	0.	0.	0.		
4821.5150	20013	00001	627	0.0744	0.	0.	0.	0.		
4839.7328	30013	10001	626	0.162	-0.00011	2.07	0.	0.	3	
4853.6234	20013	00001	626	78.1	0.0008	2.6	0.	0.	75	62
4871.4461	21112	01101	636	0.219	0.00003	0.54	0.	0.	3	
4887.3907	20012	00001	636	2.70	-0.00015	0.996	0.	0.	3	
4887.9850	12212	00001	626	0.	0.	0.	0.	0.	*	
4896.1927	21112	01101	628	0.0928	-0.00011	-0.3	0.	0.	3	
4904.8601	20012	00001	628	1.30	-0.00015	-0.627	0.	0.	3	
4910.6054	20022	00011	626	0.00752	-0.00016	0.157	0.	0.	3	
4912.1600	40014	20003	626	0.00361	-0.00014	0.815	0.	0.	3	

[*continued*...]

Table 2—*continued*

ν_0	v'	v"	ISO	S^0_v	a_1	a_2	a_3	b_2	Ref-S	Ref-ν
4920.2114	32213	12202	626	0.00387	-0.00008	0.332	0.	0.	3	
4922.5519	40013	20002	626	0.00358	-0.00012	-0.397	0.	0.	3	
4925.0130	20011	00001	638	0.00446	0.	0.	0.	0.		
4928.9159	21112	01101	627	0.0149	0.	0.	0.	0.		
4931.0863	31113	11102	626	0.0994	-0.00003	0.31	0.	0.	3	
4937.3120	40012	20001	626	0.00108	0.	0.	0.	0.	3	
4939.3510	20012	00001	627	0.231	0.	0.	0.	0.		
4941.4884	23312	03301	626	0.0313	-0.00011	0.007	0.	0.	3	
4942.5088	30013	10002	626	1.28	-0.00016	0.684	0.	0.	3	
4946.8194	31112	11101	626	0.0507	-0.00014	-0.491	0.	0.	3	
4953.4009	22212	02201	626	0.851	-0.00009	0.127	0.	0.	3	
4959.6672	30012	10001	626	0.802	-0.00013	-0.876	0.	0.	3	
4965.3849	21112	01101	626	23.5	-0.00009	0.02	0.	0.	3	62
4976.1442	30012	10002	636	0.00406	-0.00014	-1.29	0.	0.	3	
4977.8350	20012	00001	626	347.5	-0.00009	-0.47	0.	0.	92,76	62
4991.3531	20011	00001	636	1.97	-0.00017	-2.07	0.	0.	3	
4993.5619	30011	10001	636	0.00521	-0.00065	-3.9	0.	0.	3	
5013.7801	21111	01101	636	0.164	-0.00015	-1.38	0.	0.	3	
5028.4811	20021	00011	626	0.00266	-0.00015	-2.58	0.	0.	3	
5028.8123	22211	02201	636	0.00692	-0.00022	-1.59	0.	0.	3	
5042.5825	20011	00001	628	0.252	-0.00018	-2.54	0.	0.	3	
5061.7781	12211	00001	626	0.	0.	0.	0.	0.	*	
5062.4432	30012	10002	626	0.252	-0.00020	-2.21	0.	0.	3	
5064.6737	21111	01101	628	0.0281	-0.00021	-1.86	0.	0.	3	
5068.9300	20011	00001	627	0.0632	0.	0.	0.	0.		
5091.2052	31112	11102	626	0.0232	-0.00014	-1.49	0.	0.	3	
5099.6605	20011	00001	626	109.	0.	0.	0.	0.	77	62
5114.8966	30011	10001	626	0.293	-0.00023	-2.24	0.	0.	3	
5123.1961	21111	01101	626	10.1	-0.00014	-1.66	0.	0.	3	62
5126.9731	31111	11101	626	0.0263	-0.00018	-1.86	0.	0.	3	
5139.4024	22211	02201	626	0.422	-0.00022	-1.78	0.	0.	3	
5151.3812	23311	03301	626	0.0171	0.	0.	0.	0.	3	
5168.5989	01121	00001	636	0.00149	-0.00008	0.099	0.	0.	3	
5217.6726	30011	10002	626	0.0208	-0.00033	-4.11	0.	0.	3	
5247.8323	10022	01101	626	0.00846	0.0194	0.438	0.	0.	3	
5291.1322	02221	01101	626	0.0121	-0.00054	-1.79	0.	0.	3	
5315.7132	01121	00001	626	0.168	0.00315	0.268	0.	0.	3	62
5584.3931	00031	10001	626	0.00630	-0.00007	-0.797	0.	0.	3	
5687.1690	00031	10002	626	0.00683	-0.00005	2.07	0.	0.	3	
5858.0280	10022	00001	628	0.00410	0.00045	1.88	0.	0.	3	
5951.6040	30014	00001	636	0.00166	-0.00019	3.08	0.	0.	3	
5959.9560	10021	00001	628	0.00332	-0.00039	-0.892	0.	0.	3	
5972.5401	32214	02201	626	0.00339	-0.00013	1.53	0.	0.	3	
5993.5860	30014	00001	628	0.00400	-0.00008	3.12	0.	0.	3	
5998.5697	40015	10002	626	0.00409	-0.00016	2.19	0.	0.	3	
6020.7970	31114	01101	626	0.0665	-0.00010	2.36	0.	0.	3	
6075.9803	30014	00001	626	0.514	0.0016	2.5	0.	0.	78	57
6088.2180	31113	01101	636	0.00218	-0.00008	1.13	0.	0.	3	
6119.6230	30013	00001	636	0.0214	0.	0.	0.	0.	3	
6127.7830	30013	00001	628	0.0221	-0.00029	0.364	0.	0.	3	
6149.3647	41114	11102	626	0.00197	-0.00007	0.864	0.	0.	3	
6170.1019	32213	02201	626	0.0124	-0.00007	0.863	0.	0.	3	
6175.1187	40014	10002	626	0.0222	-0.00013	1.9	0.	0.	3	
6175.9540	30013	00001	627	0.0032	0.	0.	0.	0.		
6196.1765	31113	01101	626	0.330	-0.00001	0.831	0.	0.	3	57
6205.5107	40013	10001	626	0.0144	-0.00008	-0.078	0.	0.	3	
6227.9171	30013	00001	626	4.52	0.0009	4.2	0.	0.	79	57
6241.9720	30012	00001	636	0.0554	-0.00009	-0.492	0.	0.	3	
6243.6380	31112	01101	636	0.00411	0.	0.	0.	0.	3	
6254.5940	30012	00001	628	0.0121	-0.00014	-2.11	0.	0.	3	
6298.1160	30012	00001	627	0.00275	0.	0.	0.	0.		
6308.2867	40013	10002	626	0.0205	-0.00016	-0.835	0.	0.	3	
6346.2637	40012	10001	626	0.0130	0.	0.	0.	0.	3	

[*continued*. . .]

Table 2—*continued*

ν_0	v'	v''	ISO	S_v^0	a_1	a_2	a_3	b_2	Ref-*S*	Ref-ν
6347.8515	30012	00001	626	4.54	0.00095	3.8	0.	0.	80	57
6356.2954	31112	01101	626	0.341	-0.00014	-1.02	0.	0.	3	57
6359.2568	32212	02201	626	0.0128	-0.00015	-0.935	0.	0.	3	
6363.6240	30011	00001	636	0.0137	-0.00062	-4.81	0.	0.	3	
6387.8675	41101	00001	626	0.	0.	0.	0.	0.	★	
6503.0809	30011	00001	626	0.586	0.00115	3.8	0.	0.	78	57
6532.6537	40011	10001	626	0.00242	-0.00009	-2.96	0.	0.	3	
6536.4490	31111	01101	626	0.0725	0.00005	-2.12	0.	0.	3	
6537.9588	11122	00001	626	0.00598	0.0116	-8.18	0.	0.	3	
6562.4414	32211	02201	626	0.00353	0.	0.	0.	0.	3 ★	
6679.7056	11121	00001	626	0.0148	0.0159	0.888	0.	0.	3	
6745.1119	01131	01101	636	0.0147	0.	0.	0.	0.	3	
6780.2104	00031	00001	636	0.164	0.	0.	0.	0.	3	
6870.7999	11132	11102	626	0.00248	-0.00009	0.164	0.	0.	3	
6885.1540	01131	01101	628	0.00497	0.	0.	0.	0.	3	
6897.7525	02231	02201	626	0.0526	-0.00006	0.411	0.	0.	3	
6905.7669	10031	10001	626	0.0153	-0.00005	0.801	0.	0.	3	
6907.1424	10032	10002	626	0.0274	-0.00006	0.107	0.	0.	3	
6922.1967	00031	00001	628	0.0591	0.	0.	0.	0.	3	
6935.1340	01131	01101	626	1.29	-0.00007	0.426	0.	0.	3	57
6945.6080	00031	00001	627	0.0112	0.	0.	0.	0.		
6972.5773	00031	00001	626	15.8	-0.000215	0.	0.	0.	35,81	57
7283.9780	40015	00001	626	0.00401	-0.00019	3.71	0.	0.	3	
7414.4549	41114	01101	626	0.00445	-0.00009	1.18	0.	0.	3	
7460.5270	40014	00001	626	0.0469	-0.00014	2.82	0.	0.	3	
7583.252	41113	01101	626	0.00753	0.	0.	0.	0.	82	
7593.695	40013	00001	626	0.102	0.	0.	0.	0.	82	
7734.448	40012	00001	626	0.0281	0.00025	0.	0.	0.	83	
7757.625	41112	01101	626	0.00218	0.	0.	0.	0.	83	
7901.4790	21122	00001	626	0.00149	0.018	0.	0.	0.	★	
7920.8380	40011	00001	626	0.00175	0.00075	-2.43	0.	0.	3	
7981.1860	10032	00001	636	0.00258	-0.00002	2.52	0.	0.	3	
8089.0280	10031	00001	636	0.00805	-0.00010	-0.21	0.	0.	3	
8103.5857	20033	10002	626	0.00139	0.	0.	0.	0.	3	
8120.1090	10032	00001	628	0.00217	0.	0.	0.	0.	3	
8135.8900	11132	01101	626	0.0367	-0.00005	1.66	0.	0.	3	
8192.5507	10032	00001	626	0.431	0.	0.	0.	0.	84	
8220.3640	10031	00001	628	0.00191	0.	0.	0.	0.	3	
8231.5607	20032	10002	626	0.00139	0.	0.	0.	0.	3	
8243.1687	20031	10001	626	0.00112	-0.00012	-0.712	0.	0.	3	
8254.6874	12231	02201	626	0.00191	-0.00012	-0.38	0.	0.	3	
8276.7600	11131	01101	626	0.0485	-0.00011	-0.399	0.	0.	3	
8293.9512	10031	00001	626	0.614	0.	0.	0.	0.	84	
9388.9940	20033	00001	626	0.00424	0.	0.	0.	0.	91	
9478.1290	21132	01101	626	0.00185	0.	0.	0.	0.	3	
9516.9690	20032	00001	626	0.0252	0.	0.	0.	0.	91	
9631.353	20031	00001	626	0.00912	0.	0.	0.	0.	91	

ν_0 is in cm^{-1} and S_v^0 is in units of $cm^{-1}/(molecule\text{-}cm^{-2}) \times 10^{-22}$. The Herman–Wallis coefficients a_1, a_2, a_3 are for the *P*- and *R*-branches, while b_2 is for the *Q*-branch. The second-and third-order Herman–Wallis coefficients (a_2, a_3, and b_2) should be multiplied by 10^{-5}. The non-numeric characters in the Ref-*S* column are interpreted thus: ⊥ = HITRAN line intensity cutoff lowered for significant *Q*-branch (densely-packed lines); @ = band absent from HITRAN, but included since it was used in the least-squares determination of energy levels; ★ = a perturbed band. When there are multiple references under Ref.-*S*, the first is the one actually used in HITRAN.

(Note that, to derive $Q_R(T)$ from the $Q(T)$ given by Gamache et al,[38] one must use $Q_R(T) = Q(T)/[g_j\, Q_v(T)]$. Values of g_j are given in Ref. 38 and Q_v(296K) can be obtained by a simple summation of exponentials using the G_v in Table 1). Then the line intensity $S(T)$ at temperature T is

$$S(T) = [(8\pi^3 10^{-36})/(3hc)]\,[I_a/(g_j Q_v(T) Q_R(T)]\nu \times \exp(-G_v''/kT)\exp(-E_R''/kT)\,[1 - \exp(-h\nu/kT)]\,|R_v|^2 L(J'',\ell)F(J'') \quad (5)$$

where h is Planck's constant, c is the speed of light, I_a is the isotopic abundance, ν is the transition frequency or line position, E_R'' is the rotational energy of the lower state, and k is Boltzmann's constant. Often the factor g_j is omitted from Eq.(5) by absorbing it into $|R_v|^2$.

The rotationless band strength given in Table 2 is defined as

$$S_v^0(T) = [(8\pi^3 10^{-36})/(3hc)]\,[(\nu_0 I_a)/(g_j Q_v(T)]\,\exp(-G_v''/kT)\,|R_v|^2 \tag{6}$$

at $T = 296$K, where ν_0 is the band center $(G_v' - G_v'')$. Substituting Eq. (6) into Eq. (5), the line intensity can then be expressed

$$S(T) = (\nu/\nu_0) S_v^0(T) L(J'', \ell)\, F(J'')\,[\exp(-E_R''/kT)/Q_R(T)]\,[1 - \exp(-h\nu/kT)]. \tag{7}$$

$S(T)$ should be used as given by Eq. (7) when at least one of the upper and lower states has zero vibrational angular momentum ($\ell = 0$). When both upper and lower states have nonzero vibrational angular momentum ($\ell > 0$), the intensity is split between e and f subbands, and $S(T)$ should be divided by 2.

It should be noted that some of the S_v^0 values listed in Table 2 were determined with an additional factor, g_v, in the numerator of Eq. 6, where $g_v = 2 - \delta_{\ell 0}$. For such values, the rotational partition sum of the band in question was used to determine S_v^0. This cancels the factor of approx. 2 since for $\ell \neq 0$ bands, all rotational levels exist and Q_R ($\ell \neq 0$) = 2 × Q_R(ground state). For these bands, we have used 2 × Q_R(ground state) which introduces an error of a few percent for transitions originating from bands with ℓ larger than 0. There are not many bands on the HITRAN database where this would be a problem, e.g. starting from the Γ level ($\ell = 4$).

The Hönl–London factors for parallel bands ($\Delta\ell = 0$) are given by

$$L(J'', \ell) = (J'' + 1 + \ell)(J'' + 1 - \ell)/(J'' + 1) \quad (R\text{-branch}), \tag{8}$$

$$L(J'', \ell) = (2J'' + 1)\ell^2/[J''(J'' + 1)] \quad (Q\text{-branch}), \tag{9}$$

$$L(J'', \ell) = (J'' + \ell)(J'' - \ell)/J'' \quad (P\text{-branch}), \tag{10}$$

and for perpendicular bands ($\Delta\ell = \pm 1$)

$$L(J'', \ell) = (J'' + 2 + \ell\Delta\ell)(J'' + 1 + \ell\Delta\ell)/2(J'' + 1) \quad (R\text{-branch}), \tag{11}$$

$$L(J'', \ell) = (J'' + 1 + \ell\Delta\ell)(J'' - \ell\Delta\ell)(2J'' + 1)/[2J''(J'' + 1)] \quad (Q\text{-branch}), \tag{12}$$

$$L(J'', \ell) = (J'' - 1 - \ell\Delta\ell)(J'' - \ell\Delta\ell)/2J'' \quad (P\text{-branch}). \tag{13}$$

The Herman–Wallis factor F was assumed to be of the form

$$F(m) = (1 + a_1 m + a_2 m^2 + a_3 m^3)^2 \quad (P\text{- and } R\text{-branches}), \tag{14a}$$

$$F(m) = (1 + b_2 m^2)^2 \quad (Q\text{-branches}), \tag{14b}$$

where a_1, a_2, and a_3 are constants for a given band, and where there is potentially a separate b_2 constant for e and f lines in the Q-branch of a given band (b_2^e and b_2^f). The running index m is $m = J + 1$ in the R-branch, $m = J$ in the Q-branch, and $m = -J$ in the P-branch. The use of up to three coefficients in the P- and R-branches is a significant improvement over the single coefficient used in the 1986 edition of HITRAN. Other expressions are used to report Herman–Wallis factors in the literature. These other formulae were algebraically converted to the form of Eq. (14) for use in generating the values in Table 2.

DND has now been extensively utilized to calculate unobserved band intensities, and especially Herman–Wallis factors, for the three most abundant species (626, 636 and 628 in HITRAN notation). On the 1986 HITRAN database, the method[2] was utilized only for the parallel band intensities of the 626 isotopomer. It was decided to supercede DND calculations with experimental values where available. The DND calculations yielded first and second order coefficients for the Herman–Wallis coefficients for the P- and R-branches (a_1 and a_2). The experiments occasionally provided the third-order coefficient a_3 and the second-order coefficient for the Q-branch, b_2. In a few cases, the measurement did not supply a_1 and/or a_2.

PRESSURE BROADENING

General approach

It was assumed that the pressure broadening of CO_2 is independent of vibrational transition. Data from Johns[16] and Dana et al[12,15] were used for self-broadening. Data from Dana et al[12] provided nitrogen- and oxygen-broadening, data from Johns[16] provided air-broadening, and data from Devi et al[17] and Margottin-Maclou et al[18] provide additional nitrogen-broadening values. The calculations of Gamache and Rosenmann[19] provide a complete set in m for $1 \leqslant |m| \leqslant 121$ for nitrogen-, oxygen- and self-broadening.

The measured broadenings $\gamma(T)$ were converted to 296K by

$$\gamma(T) = \gamma(T_0)(T/T_0)^n \tag{15}$$

setting $T_0 = 296$K and using a value for n calculated by Gamache and Rosenmann.[19] Air-broadened widths were obtained from nitrogen- and oxygen-broadened widths by

$$\gamma_{air} = 0.79\gamma_{nitrogen} + 0.21\gamma_{oxygen}. \tag{16}$$

Where only nitrogen-broadening was available, the m-dependent $\gamma_{air}/\gamma_{nitrogen}$ ratio determined from the calculations of Gamache and Rosenmann was used to convert to air-broadening. As a test, these procedures were applied to the data of Dana,[12] determining γ_{air} in two ways: by Eq. (16), and by multiplying the nitrogen broadening by the calculated ratio. The two methods agreed to better than 1% in all cases. For comparison, the measurements in the different references cited differ by as much as 6%, with an average difference of 2.7%.

Air broadening

The air-broadened line widths at 296K used in HITRAN were determined in this way: because the polynomial fit did not work well for $m = 1$, the only available experimental value[16] was used:

$$\gamma_{air}(1) = 0.09489\ \text{cm}^{-1}/\text{atm}. \tag{17}$$

For $m = 2$ to $m = 45$ inclusive,

$$\gamma_{air}(m = 2 \text{ to } 45) = 0.09259 - 1.749\ 10^{-3}m + 4.263\ 10^{-5}m^2 - 3.6793\ 10^{-7}m^3 \tag{18}$$

in cm^{-1}/atm, obtained by least-squares fitting the experimental data.

For $m = 46$ to 121 inclusive,

$$\gamma_{air}(m = 46 \text{ to } 121) = 0.039313 + 1.7806\ 10^{-3}m - 3.7746\ 10^{-5}m^2 + 2.9570\ 10^{-7}m^3 - 7.969\ 10^{-4}m^4 \tag{19}$$

in cm^{-1}/atm, obtained from the calculated widths, with the requirements that Eq. (18) match Eq. (19) at $m = 45$, and go smoothly to 0.055 at $m = 121$. However, HITRAN does not include any lines above $m = 108$. Figure 1 shows a plot of γ_{air} as a function of m chosen for HITRAN.

Self-broadening

The self-broadened widths at 296K used averages of the experimental values[15,16] for $m = 1$–4, again because of poor polynomial fits:

$$\gamma_{self}(1) = 0.1279\ \text{cm}^{-1}/\text{atm}, \tag{20}$$

$$\gamma_{self}(2) = 0.1228\ \text{cm}^{-1}/\text{atm}, \tag{21}$$

$$\gamma_{self}(3) = 0.1204\ \text{cm}^{-1}/\text{atm}, \tag{22}$$

$$\gamma_{self}(4) = 0.1190\ \text{cm}^{-1}/\text{atm}. \tag{23}$$

For $m = 5$ to 121 inclusive,

$$\gamma_{self}(m) = 0.12223 - 1.4039\ 10^{-3}m + 9.1762\ 10^{-6}m^2 - 2.0051\ 10^{-8}m^3 \tag{24}$$

in cm^{-1}/atm, obtained by least-squares fitting of the experimental data. Figure 2 illustrates the function chosen for the HITRAN database.

Related parameters

The temperature dependence of the air-broadened halfwidths, n, used for the current edition of HITRAN was taken from the calculations of Ref. 19. These calculations provide a J-dependent parameter, which is applied as in Eq. (15). Pressure shifts for the lines were only provided for the ν_3 fundamental; these data were from the work of Devi et al.[17]

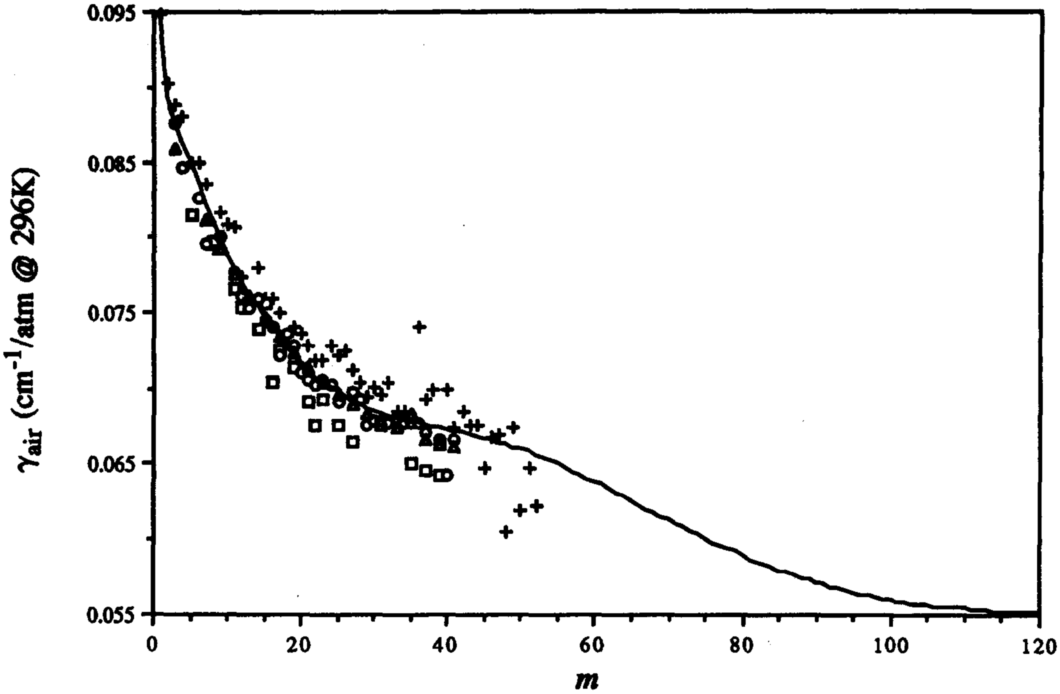

Fig. 1. Air-broadened halfwidths of carbon dixode as a function of *m*. The data are: □ Ref. 12, + Ref. 16, ○ Ref. 17, and △ Ref. 18. (——) represent the values on HITRAN92.

CONCLUSION

The improvement in the method of fitting observed CO_2 line positions did not, in general, significantly change those lines which also appeared in the 1986 edition of HITRAN. However, the global fit procedure makes full use of the experimental data, where the old method required

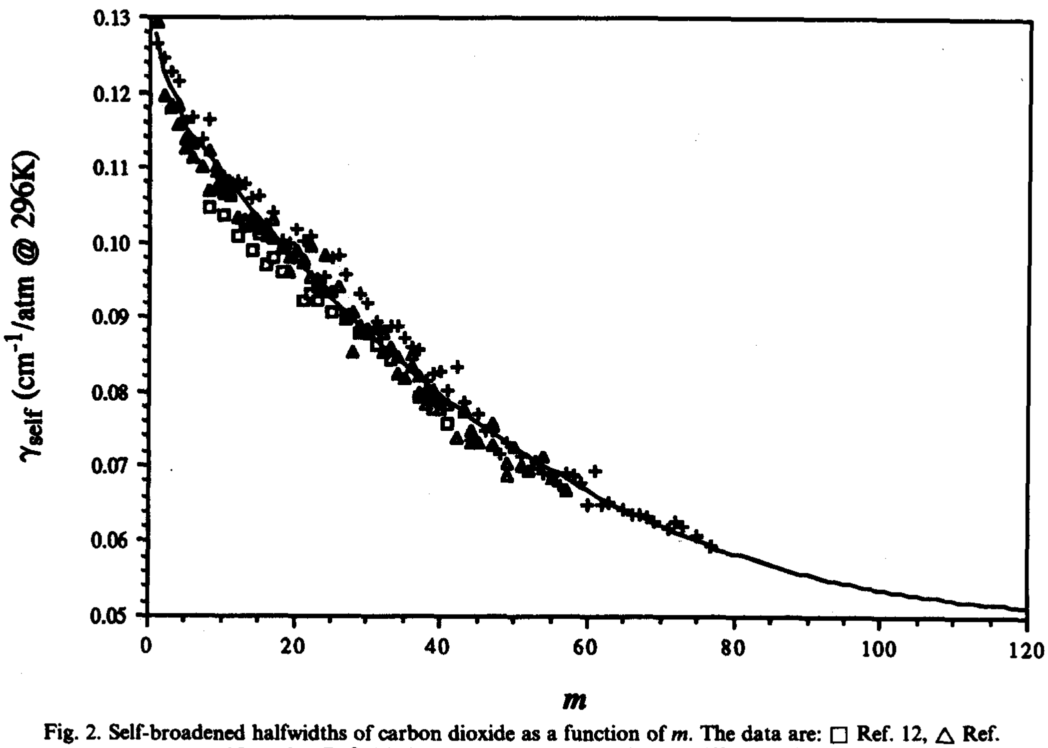

Fig. 2. Self-broadened halfwidths of carbon dioxide as a function of *m*. The data are: □ Ref. 12, △ Ref. 15, and +Ref. 16. (——) represents the values on HITRAN92.

a subset of the measured bands to be chosen. Also, it is more flexible, allowing use of information from other sources. Extrapolation to unobserved levels via DND does represent a significant improvement.

Line intensities are greatly improved, through inclusion of new measurements, and DND calculations which now include Herman–Wallis coefficients. Line broadening is improved by use of new measurements and calculations. A single m-dependence of the line broadening was used for all CO_2 bands.

There remains a fair amount of research, both experimental and theoretical, to be performed to adequately simulate carbon dioxide spectra in problems such as remote sensing and high-temperature applications. There is the need to obtain more intensity measurements of lines, especially isotopically-enriched samples. There is still a dearth of observations of the line positions of the ^{17}O isotopomers. Further advancements of the Direct Numerical Diagonalization approach will lead to better Herman–Wallis factors, but more importantly, to proper representation of perturbed bands.

Acknowledgements—Many colleagues have graciously provided their data prior to publication for this project. We wish to thank in particular J. W. C. Johns, V. Dana, M. P. Esplin, M. L. Hoke, D. C. Benner, V.M. Devi, M. A. H. Smith, C. P. Rinsland, and C. Boulet for their valuable inputs. This project has been supported by the Air Force Office of Scientific Research under Task 2310G1.

REFERENCES

1. L. S. Rothman, *Appl. Opt.* **25**, 1795 (1986).
2. R. B. Wattson and L. S. Rothman, *J. Molec. Spectrosc.* **119**, 83 (1986); R. B. Wattson, L. S. Rothman, A. Newburgh, and R. Pavelle, Paper TE9, *43rd Molecular Spectroscopy Symposium*, Ohio State University (1988).
3. R. B. Wattson and L. S. Rothman, *JQSRT* **48**, 763 (1992).
4. D. C. Benner, V. Malathy Devi, C. P. Rinsland, and P. S. Ferry-Leeper, *Appl. Opt.* **27**, 1588 (1988).
5. M. P. Esplin, private communication (1987).
6. M. P. Esplin, R. B. Wattson, M. L. Hoke, R. L. Hawkins, and L. S. Rothman, *Appl. Opt.* **28**, 409 (1989).
7. M. P. Esplin and M. L. Hoke, paper TE6, *44th Molecular Spectroscopy Symposium*, Ohio State University (1989).
8. G. Blanquet, J. Walrand, and J.-L. Teffo, *Appl. Opt.* **27**, 2098 (1988).
9. D. Bailly, Thesis, Université de Paris-Sud, France (1983).
10. J. W. C. Johns, *J. Molec. Spectrosc.* **134**, 433 (1989).
11. J. W. C. Johns and J. Vander Auwera, *J. Molec. Spectrosc.* **140**, 71 (1990).
12. V. Dana, A. Valentin, A. Hamdouni, and L. S. Rothman, *Appl. Opt.* **28**, 2562 (1989).
13. A. Hamdouni and V. Dana, *Appl. Opt.* **29**, 1570 (1990).
14. V. Dana, A. Hamdouni, R. B. Wattson, and L. S. Rothman, *Appl. Opt.* **29**, 2474 (1990).
15. V. Dana, J.-Y. Mandin, G. Guelachvili, Q. Kou, M. Morillon-Chapey, R. B. Wattson, and L. S. Rothman, *J. Molec. Spectrosc.* **152**, 328 (1992).
16. J. W. C. Johns, *J. Molec. Spectrosc.* **125**, 442 (1987).
17. V. Malathy Devi, D. C. Benner, C. P. Rinsland, and M. A. H. Smith, *JQSRT* **48**, 581 (1992).
18. M. Margottin-Maclou, P. Dahoo, A. Henry, A. Valentin, and L. Henry, *J. Molec. Spectrosc.* **131**, 21 (1988).
19. R. R. Gamache and L. Rosenmann, unpublished results.
20. L. S. Rothman and L. D. G. Young, *JQSRT* **25**, 505 (1981).
21. A. George and M. T. Heath, *Linear Algebra and Its Applications* **34**, 69 (1980); M. T. Heath, *SIAM J. Sci. Stat. Comput.* **5**, 497 (1984).
22. W. M. Gentleman, *J. Inst. Maths. Applics.* **12**, 329 (1973); W. M. Gentleman, *Appl. Stat.* **23**, 448 (1974).
23. A. Baldacci, C. P. Rinsland, M. A. H. Smith, and K. Narahari Rao, *J. Molec. Spectrosc.* **94**, 351 (1982).
24. C. P. Rinsland and D. C. Benner, *Appl. Opt.* **23**, 4523 (1984).
25. C. P. Rinsland, D. C. Benner, V. Malathy Devi, P. S. Ferry-Leeper, C. H. Sutton, and D. J. Richardson, NASA Technical Memorandum 85764 (1984).
26. G. Guelachvili, *J. Molec. Spectrosc.* **79**, 72 (1980).
27. A. S. Pine and G. Guelachvili, *J. Molec. Spectrosc.* **79**, 84 (1980).
28. D. Bailly, R. Farrenq, G. Guelachvili, and C. Rossetti, *J. Molec. Spectrosc.* **90**, 74 (1981).
29. L. R. Brown and R. A. Toth, *JOSA B* **2**, 842 (1985).
30. L. S. Rothman, R. R. Gamache, A. Goldman, L. R. Brown, R. A. Toth, H. M. Pickett, R. L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C. P. Rinsland and M. A. H. Smith, *Appl. Opt.* **26**, 4058 (1987).
31. V. Dana, private communication (1989).

32. T. Huet, N. Lacome, and A. Lévy, *J. Molec. Spectrosc.* **128,** 206 (1988).
33. P. Varanasi and S. Chudamani, *J. Geophys. Res.* **94,** 13069 (1989).
34. R. A. McClatchey, W. S. Benedict, S. A. Clough, D. E. Burch, R. F. Calfee, K. Fox , L. S. Rothman, and J. S. Garing, "AFCRL atmospheric absorption line parameters compilation," Tech. Report AFCRL-TR-0096 (1973).
35. C. Boulet, private communication (1991).
36. L. P. Giver and C. Chackerian Jr, *J. Molec. Spectrosc.* **148,** 80 (1991).
37. L. P. Giver and C. Chackerian Jr, Paper RF6, *46th Molecular Spectroscopy Symposium*, Ohio State University (1991).
38. R. R. Gamache, R. L. Hawkins, and L. S. Rothman, *J. Molec. Spectrosc.* **142,** 205 (1990).
39. J.-Y. Mandin, *J. Molec. Spectrosc.* **67,** 304 (1977).
40. R. Paso, J. Kauppinen, and R. Anttila, *J. Molec. Spectrosc.* **79,** 236 (1980).
41. R. Paso, U. Oulu Finland, private communication (1980).
42. V. Malathy Devi, P. Das, and K. N. Rao, *Appl. Opt.* **18,** 2918 (1979).
43. C. Freed, L. C. Bradley, and R. G. O'Donnell, *IEEE J.Q.Electronics* **16,** 1195 (1980).
44. J.-P. Monchalin, M. J. Kelly, J. E. Thomas, N. A. Kurnit, and A. Javan, *J. Molec. Spectrosc.* **64,** 491 (1977).
45. J. Dupre-Maquaire and P. Pinson, *J. Molec. Spectrosc.* **62,** 181 (1976).
46. M. P. Esplin, H. Sakai, L. S. Rothman, G. A. Vanasse, W. Barowy, and R. Huppi, Tech. Report AFGL-TR-0046 (1986).
47. F. R. Petersen, J. S. Wells, A. G. Maki, and K. J. Siemsen, *Appl. Opt.* **20,** 3635 (1981).
48. K. J. Siemsen, *Opt. Lett.* **6,** 114 (1981).
49. K. J. Siemsen and B. G. Whitford, *Opt. Commun.* **22,** 11 (1977).
50. K. J. Siemsen, *Opt. Commun.* **34,** 447 (1980).
51. H. Sakai, Paper ME7, *38th Molecular Spectroscopy Symposium*, Ohio State University (1983).
52. D. Bailly and C. Rossetti, *J. Molec. Spectrosc.* **102,** 392 (1983).
53. M. P. Esplin, R. J. Huppi, and G. A. Vanasse, *Appl. Opt.* **21,** 1681 (1982).
54. J. Kauppinen, K. Jolma, and V.-M. Horneman, *Appl. Opt.* **21,** 3332 (1982).
55. F. R. Petersen, J. S. Wells, K. J. Siemsen, A. M. Robinson, and A. G. Maki, *J. Molec. Spectrosc.* **105,** 324 (1984).
56. M. P. Esplin and L. S. Rothman, *J. Molec. Spectrosc.* **100,** 193 (1983).
57. J. P. Maillard, J. Cuisenier, Ph. Arcas, E. Arié, and C. Amiot, *Can. J. Phys.* **58,** 1560 (1980).
58. M. P. Esplin and L. S. Rothman, *J. Molec. Spectrosc.* **116,** 351 (1986).
59. D. Bailly and C. Rossetti, *J. Molec. Spectrosc.* **105,** 331 (1984).
60. K. Jolma, J. Kauppinen, and V.-M. Horneman, *J. Molec. Spectrosc.* **101,** 300 (1983).
61. V. Malathy Devi, C. P. Rinsland, and D. C. Benner, *Appl. Opt.* **23,** 4067 (1984).
62. Ph. Arcas, E. Arié, M. Cuisenier, and J. P. Maillard, *Can. J. Phys.* **61,** 857 (1983).
63. R. A. Toth, *Appl. Opt.* **24,** 261 (1985).
64. C. P. Rinsland, D. C. Benner, and V. Malathy Devi, *Appl. Opt.* **24,** 1644 (1985).
65. C. P. Rinsland, D. C. Benner, D. J. Richardson, and R. A. Toth, *Appl. Opt.* **22,** 3805 (1983).
66. D. C. Benner and C. P. Rinsland, *J. Molec. Spectrosc.* **112,** 18 (1985).
67. C. P. Rinsland, D. C. Benner, and V. Malathy Devi, *Appl. Opt.* **25,** 1204 (1986).
68. K. Jolma, *J. Molec. Spectrosc.* **111,** 211 (1985).
69. Ph. Arcas, private communication (1985).
70. M. P. Esplin, private communication (1987).
71. M. S. Abubakar and J. H. Shaw, *Appl. Opt.* **25,** 1196 (1986).
72. C. P. Rinsland, private communication (1985).
73. M. L. Hoke and J. H. Shaw, *Appl. Opt.* **22,** 328 (1983).
74. M. S. Abubakar and J. H. Shaw, *Appl. Opt.* **23,** 3310 (1984).
75. F. P. J. Valero, C. B. Suarez, and R. W. Boese, *JQSRT* **22,** 93 (1979).
76. F. P. J. Valero, C. B. Suarez, and R. W. Boese, *JQSRT* **23,** 337 (1979).
77. K. P. Vasilevskii, L. E. Danilochkina, and V. A. Kazbanov, *Opt. Spektrosk.* **38,** 871 (1975).
78. C. B. Suarez and F. P. J. Valero, *JQSRT* **19,** 569 (1978).
79. C. B. Suarez and F. P. J. Valero, *J. Molec. Spectrosc.* **71,** 46 (1978).
80. F. P. J. Valero and C. B. Suarez, *JQSRT* **19,** 579 (1978).
81. R. A. Toth, R. H. Hunt, and E. K. Plyler, *J. Molec. Spectrosc.* **38,** 107 (1975).
82. F. P. J. Valero, *J. Molec. Spectrosc.* **68,** 269 (1977).
83. F. P. J. Valero and R. W. Boese, *JQSRT* **18,** 391 (1977).
84. D. E. Burch, D. A. Gryvnak, and R. R. Patty, *JOSA* **58,** 335 (1968).
85. A. Chedin and J.-L. Teffo, *J. Molec. Spectrosc.* **107,** 333 (1984).
86. N. Papineau and M. Pealat, *Appl. Opt.* **24,** 3002 (1985).
87. V. Malathy Devi, B. Fridovich, G. D. Jones, and D. G. S. Snyder, *J. Molec. Spectrosc.* **105,** 61 (1984).
88. H. D. Dowling, L. R. Brown, and R. H. Hunt, *JQSRT* **15,** 205 (1975).
89. Y. Ouazzany and J. P. Boquillon, *Europhys. Lett.* **4,** 421 (1987); R. Saint-Loup, B. Lavorel, G. Millot, C. Wenger, and H. Berger, *J. Raman Spectrosc.* **21,** 77 (1990).

90. V. Dana and A. Valentin, *Appl. Opt.* **27**, 4450 (1988).
91. R. W. Boese, J. H. Miller, and E. C. Y. Inn, *JQSRT* **6**, 717 (1966).
92. C. B. Suarez and F. P. J. Valero, *J. Molec. Spectrosc.* **140**, 407 (1990).
93. A. Groh, D. Goddon, M. Schneider, W. Zimmermann, and W. Urban, *J. Molec. Spectrosc.* **146**, 161 (1991).