

AFGL trace gas compilation: 1982 version

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The new edition of the AFGL trace gas compilation is described. The latest version provides the necessary parameters for the computation of absorption or emission spectra of major bands of twenty-one gases in the region from 0 to 10,000 cm^{-1} . Emphasis on this edition has been on the addition of numerous millimeter and submillimeter transitions, the inclusion of bands of significance in upper atmospheric processes, and strong IR bands of trace constituents likely to be used for remote detection. The sources for the additions and modifications of the absorption parameters are summarized.

I. Introduction

Two years have elapsed since the second edition of the AFGL Trace Gas Compilation.¹ This compilation is a data bank of molecular absorption parameters appropriate to a broad spectrum of applications including calculation of high-resolution transmission and emission in planetary atmospheres, comparison with laboratory absorption cell measurements, and remote sensing and retrieval of profiles in the atmosphere. The Trace Gas Compilation is an extension to minor terrestrial infrared active atmospheric absorbers of the main AFGL Atmospheric Absorption Line Parameters Compilation² that contains analogous data for the seven most significant atmospheric absorbers. As with the previous edition,¹ several new molecular species have been added as well as additional bands and updates of the existing species. The major efforts incorporated into this new version include pure rotational transitions,³ trace absorbers significant in the far infrared, and sequence bands of significance in upper atmospheric photochemistry. The new edition now encompasses twenty-one molecules summarized in Table I. The parameters and format of the compilation remain as before, i.e., each transition being cataloged in terms of

the resonant frequency in vacuum cm^{-1} , the line intensity in $\text{cm}^{-1}/\text{molecule cm}^{-2}$ at 296 K, the air-broadened halfwidth (HWHM) in $\text{cm}^{-1}/\text{atm}$, the lower-state energy in cm^{-1} , the quantum identifications (vibrational, rotational, electronic level, hyperfine, and splitting designation if necessary to uniquely specify the transition), and the entry date, isotope, and molecule codes. Representative examples of the card image format of transitions are shown in Table II.

The data presently available on the compilation (edition of Sept. 1982) are summarized in Table III. The discussion in Sec. II outlines the additions and modifications that have been made for this latest edition. Primary sources are given for the new or modified parameters on the compilation, and it is requested that these be referenced when the data are used.

II. Discussion of New or Updated Data

The ground $^2\Pi$ state of **nitric oxide** (NO) pure rotation data from Ref. 3 have replaced the previous microwave transitions on the atlas. The molecular constants for NO were determined by fitting the spectrum of NO to the fine structure Hamiltonian of Amiot *et al.*⁴ along with the hyperfine Hamiltonian of Meerts.⁵ The observed radio frequency lines used in the fit are from Ref. 6, and the observed millimeter lines used in the fit are from Jet Propulsion Laboratory measurements³ by Pickett and Cohen. The accuracy of the line positions is generally better than 0.0005 cm^{-1} , and the line intensities are accurate to $\sim 1\%$. The self-broadened halfwidths of Abels and Shaw⁷ have been added to the data. Because nitrogen has nuclear spin = 1, the data contain quantum numbers describing the hyperfine interaction. To specify these transitions, a branch letter (*P, Q, R*) was chosen to indicate the change in nuclear spin quantum numbers along with the nuclear spin F'' of the lower state. These appear before the

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Table I. Natural Isotopic Abundances of Compilation Constituents

Molecule	Isotope	Relative Natural Abundance	Molecule	Isotope	Relative Natural Abundance
NO (8)	46	0.99390	OCS (19)	622	0.93719
	56	0.00369		624	0.04163
	48	0.00203		632	0.01052
		822		0.00192	
SO ₂ (9)	626	0.94543	H ₂ CO(20)	126	0.98622
	646	0.04200		136	0.01107
NO ₂ (10)	646	0.99150		128	0.00202
NH ₃ (11)	4111	0.99585	HOCl(21)	165	0.75337
	5111	0.00370		167	0.24407
HNO ₃ (12)	146	0.98897	N ₂ (22)	44	0.99261
OH (13)	61	0.99744	HCN (23)	124	0.98509
	81	0.00204		134	0.01106
	62	0.00015		125	0.00366
HF (14)	19	0.99985	CH ₃ Cl(24)	215	0.74658
HCl (15)	15	0.75519		217	0.24187
	17	0.24466	H ₂ O ₂ (25)	1661	0.99489
HBr (16)	19	0.50532	C ₂ H ₂ (26)	1221	0.97763
	11	0.49452	C ₂ H ₆ (27)	1221	0.97704
HI (17)	17	0.99985	PH ₃ (28)	1111	0.99955
ClO (18)	56	0.75438			
	76	0.24411			

rotational branch and J'' quantum number in each line when hyperfine effects are present in a level [see Table II(c)].

On this edition of the atlas, bands of both nitric oxide and the hydroxyl radical (see below) have been added that are expected to be seen in emission in the upper atmosphere in nonlocal thermodynamic equilibrium conditions. The intensities have been calculated for equilibrium distribution at the 296 K standard; as a result, some intensities appear with very small exponents prior to scaling by subsequent upper atmospheric emission codes. A word of caution is thus in order for users of the compilations with computers incorporating small bit capacity/word—the intensity field should perhaps be read in a F6.3,1X,I3 format rather than the usual E10.3 and a decision made on the size of the exponent (I3).

The $X^2\Pi \leftarrow X^2\Pi\Delta v = 1$ sequence bands from (1-0) through (5-4) and the $\Delta v = 2$ series from (2-0) through (6-4) of the principal isotope of nitric oxide have been calculated by Gillis and Goldman.⁸ Hamiltonian con-

stants are from Refs. 4, 9, and 10. In addition, the fundamental bands of $^{15}\text{N}^{16}\text{O}$ and $^{14}\text{N}^{18}\text{O}$ have been added to the compilation. Hamiltonian constants for the isotopic bands are from Refs. 11 and 4, respectively. The eigenvectors were used to compute the intensities, and all bands involving $v' \leq 2$ include Λ -doubling. The intensity of the fundamental of the principal isotope is based on the high-resolution measurements of Mandin *et al.*¹² Intensities for other $^{14}\text{N}^{16}\text{O}$ bands were formed using Billingsley's Einstein A coefficients¹³ scaled so that his (1-0) band Einstein A coefficient yields the intensity derived from Ref. 12. This scaling should be valid since Green *et al.*¹⁴ show that ratios of Billingsley's band Einstein A coefficients¹³ ending in the same upper state agree with experimental observations for the bands of interest, with the exception of the (2-0) band, whose intensity has been taken from Ref. 15. Intensities for the isotopic bands were derived by multiplying the principal isotope fundamental by the abundance ratios of Table I. The halfwidths used previously on the compilation were assumed for all bands.⁷

Table II. Examples of Line Format on Compilation

A) General Format													
F ^a	I ^b	H ^c	E ^d	Transition Quantum Designation				D ^e	A ^f	M ^g			
				Vibrational Assignment		Electronic Rotational							
F10.4- F10.6	E10.3	F5.3	F10.3	V' A8	V'' A8	Hyperfine, Splitting A9 A10		I3	I4	I3			
B) Coalescing Rotational Multiplets (Example for HNO ₃)													
Four parent lines (only K' _a and K'' _a differ)													
F	I	H	E''	Vib Assignment	J'	K' _a	K' _c	J''	K'' _a	K'' _c	D	A	M
17.753332	6.494E-23	.130	292.087	ROT	29	13	16	28	14	15	382	146	12
17.753332	3.852E-22	.130	292.087	ROT	29	14	16	28	14	15	382	146	12
17.753332	6.494E-23	.130	292.087	ROT	29	14	16	28	13	15	382	146	12
17.753332	3.852E-22	.130	292.087	ROT	29	13	16	28	13	15	382	146	12
Resulting line from coalescing													
17.753332	9.003E-21	.130	292.087	ROT	29	16	28	15	382	146	12		
C) Hyperfine Transition Designation (Example for ClO)													
F	I	H	E''	Vib Assignment	ET ^h	B ⁱ P ^j B ^j J ^k S ^k	D	A	M				
34.046537	9.720E-25	.085	770.941	0	0	1/2-1/2 Q2R	26.5+382	56	18				

- a. line frequency, cm⁻¹
 b. line intensity, cm⁻¹/molec cm⁻²
 c. half-width at half maximum, cm⁻¹/atm
 d. lower state energy, cm⁻¹
 e. AFGL date code
 f. AFGL isotope code
 g. AFGL molecule code
 h. electronic transition
 i. hyperfine branch letter
 j. rotational branch letter
 k. symmetry label (A-doubling)

For this edition, the combination band of **sulfur dioxide** (SO₂) was updated, and the hot band of the main isotope and combination band of the second most abundant isotope in the 4- μ m region were added. The line positions and intensities for these bands were calculated by Pine and Dang-Nhu.¹⁶ Their line positions have a precision of ~ 0.0005 cm⁻¹, and the accuracy of the intensities is of the order of 1%.

Recent diode laser measurements¹⁷ of intensities of the ν_2 band of **nitrogen dioxide** (NO₂) led to an improved value of the total band intensity. The line intensities of this band were normalized in the latest atlas to the calculation of Devi *et al.*¹⁷

Pure rotation and rotation-inversion bands in the far infrared for **ammonia** (NH₃) were added to the compilation.

The pure rotation transitions in the ground state of ¹⁴NH₃ and ¹⁵NH₃ and the rotation-inversion transitions in the ν_2 level of ¹⁴NH₃ were completely reinvestigated. The absolute intensity formulation was reviewed in the case of rotation and rotation-inversion lines of molecules with C_{3v} symmetry. A reliable set of spectroscopic parameters was computed for more than 2000 lines between 0.2 and 0.5 cm⁻¹ in the microwave region³ and beyond 0.5 cm⁻¹ from a subset of the GEISA catalog¹⁸ that met the intensity cutoff criterion (see Appendix A). The details concerning the far-infrared study are given in Ref. 19.

Recently, Urban *et al.*²⁰ remeasured the far-infrared spectrum of ¹⁴NH₃ with 0.010-cm⁻¹ resolution in the 35-278-cm⁻¹ range using a Fourier transform spectrometer. They were able to assign the ground-state

inversion-rotation transitions of $^{14}\text{NH}_3$ up to $J'' = 13$ and the lines of the inversion-rotation transitions in the ν_2 excited state up to $J'' = 11$. We used their data up to $J'' = 13$ and $J'' = 11$ in the ground and ν_2 states, respectively, to improve the line positions given in Ref. 19.

In the region from 8 to $32\ \mu\text{m}$ a systematic study up to $J'' = 20$ of the line parameters of the ν_2 band of $^{14}\text{NH}_3$ and $^{15}\text{NH}_3$ and the $2\nu_2-\nu_2$ band of $^{14}\text{NH}_3$ was undertaken.²¹ (The ν_2 parameters of the main isotope, however, were not altered from the 1980 version).¹ The recent results of Urban *et al.*,²² combined with those of

Table III. Absorption Bands Present on Compilation

Molecule/ isotope	ν'	Band ν''	Origin (cm^{-1})	Range (cm^{-1})	No. of lines	$\sum S_i^a$
NO						
46	0	0		0-99	599	3.441
46	5	4	1763.8766	1463-2020	416	7.7E-33
46	4	3	1791.8403	1488-2051	416	3.8E-29
46	3	2	1819.8392	1514-2081	416	2.0E-25
48	1	0	1827.2844	1601-2039	679	1.054
56	1	0	1842.9177	1609-2061	699	1.917
46	2	1	1847.8808	1540-2112	831	0.108
46	1	0	1875.9711	1566-2142	833	500.284
46	6	4	3499.8115	3177-3733	416	3.3E-34
46	5	3	3555.7169	3231-3791	416	1.3E-30
46	4	2	3611.6795	3285-3849	416	5.4E-27
46	3	1	3667.7198	3339-3908	416	1.4E-23
46	2	0	3723.8526	3392-3967	832	8.079
SO ₂						
626	000	000		0-175	4132	238.984
626	010	000	517.75	433-617	3326	389.914
626	100	000	1151.7135	1047-1262	5812	351.914
626	001	000	1362.0295	1316-1394	2075	3080.023
646	101	000	2475.8300	2463-2497	287	0.603
626	111	010	2492.4438	2463-2516	654	2.110
626	101	000	2499.8701	2463-2527	1883	39.542
NO ₂						
646	010	000	749.6541	599-900	4594	52.989
646	001	000	1616.852	1550-1657	3276	6112.775
646	101	000	2906.0691	2833-2938	1586	257.910
NH ₃						
4111	0000	0000		0-415	490	1773.197
4111	0100	0100		4-477	593	29.063
5111	0000	0000		0-408	377	6.563
4111	0200	0100	789.537	309-1244	655	23.462
5111	0100	0000	945.282 ^b	637-1244	584	7.967
4111	0100	0000	949.878 ^b	608-1266	721	2151.304
4111	0001	0000	1630.165	1263-2056	1523	410.065
4111	0200	0000	1739.425	1239-2154	613	4.168
HNO ₃						
146	Pure rot.			0-43	4182	58.191
146	2 ν_9		896.4187	891-899	1079	189.975
146	ν_4		1324.9	1326-1336	24	2744.290
146	ν_2		1709.5676	1670-1750	7492	2014.242

Continued

Ref. 23 for the hot band, were used to improve the line positions. Further studies on these bands are in progress at the Laboratoire de Météorologie Dynamique and at the Jet Propulsion Laboratory²⁴ and will be incorporated in the compilations in the future.

The perpendicular ν_4 and the parallel $2\nu_2$ bands of ammonia from 5 to 8 μm were also added to the compilation. Theoretical details of these and the above bands can be found in Refs. 21 and 25.

For the compilation of the line strengths of ν_4 we adopted the value $4.10 \times 10^{-18} \text{ cm}^{-1}/\text{molecule cm}^{-2}$ at 296 K.²⁶ That value is $\sim 10\%$ lower than the experimental determination of McKean and Schatz²⁷; one can remark that these authors indicated that their experimental errors were too high by 20%. Moreover, recent determinations²⁸ of a single line strength in the ν_4 band of NH_3 using laser techniques show that the value given in Ref. 27 should be too high because of the $2\nu_2$ band,

Table III. Continued

Molecule/ isotope	ν'	Band ν''	Origin (cm^{-1})	Range (cm^{-1})	No. of lines	$\int S_i^a$
OH						
61	0	0		0-84	113	313.105
81	0	0		0-7	65	9.3E-26
62	0	0		0-2	90	1.1E-27
61	9	8	2237.0640	1287-2812	352	6.5E-68
61	8	7	2414.6890	1429-3048	352	3.8E-63
61	7	6	2585.4810	1560-3268	352	3.9E-58
61	6	5	2751.7015	1687-3482	352	6.7E-53
61	5	4	2915.2998	1810-3690	352	5.6E-47
61	4	3	3077.7771	1931-3895	352	2.5E-40
61	3	2	3240.3604	2052-4099	352	2.5E-33
61	2	1	3404.0410	2172-4303	352	4.1E-26
61	1	0	3569.6432	2293-4509	352	96.995
61	9	7	4651.7530	3503-5080	352	3.7E-63
61	8	6	5000.1700	3821-5483	352	1.0E-57
61	7	5	5337.1825	4123-5874	352	5.3E-52
61	6	4	5667.0013	4416-6253	352	5.6E-46
61	5	3	5993.0769	4703-6624	352	1.2E-39
61	4	2	6318.1375	4986-6991	352	4.7E-33
61	3	1	6644.4014	5268-7358	352	3.4E-26
61	2	0	6973.6842	5552-7726	352	36.183
61	9	6	7237.2340	5895-7582	352	2.7E-58
61	8	5	7751.8715	6384-8136	352	9.7E-53
61	7	4	8252.4823	6852-8674	352	7.0E-47
61	6	3	8744.7784	7308-9204	352	1.1E-40
61	5	2	9233.4373	7757-9730	352	3.2E-34
61	4	1	9722.1785	8202-9985	326	1.8E-27
61	3	0	10214.046	8648-9998	152	6.6E-22
HF						
19	0	0		41-589	15	5703.728
19	1	0	3961.4429	3381-4339	25	1547.412
19	2	0	7750.7949	7143-7993	22	49.615
HCl						
17	0	0		20-383	19	262.030
15	0	0		20-383	19	806.803
17	1	0	2883.8850	2486-3136	33	147.189
15	1	0	2885.9765	2459-3139	34	452.786
17	2	0	5663.9276	5303-5824	27	3.480
15	2	0	5667.9832	5271-5830	29	10.707
17	3	0	8340.9407	8124-8449	18	2.3E-22
15	3	0	8346.7771	8058-8455	21	7.1E-22

Continued

which overlaps the ν_4 and is included in the measurement of the total band strength. For this reason we did not choose the other experimentally determined value of band intensity $150 \pm 5 \text{ cm}^{-1}/\text{atm cm}$ at 299 K given in Ref. 29.

The $2\nu_2$ vibration-rotation parallel band is qualitatively similar to the ν_2 band (see Ref. 21 for theoretical details). The $S \rightarrow A$ and $A \rightarrow S$ subbands were studied as independent bands. Up to $J'' = 12$ the transition wave numbers of Urban *et al*²² were used. Higher ro-

Table III. Continued

Molecule/ isotope	Band ν'	ν''	Origin (cm^{-1})	Range (cm^{-1})	No. of lines	$\int S_i^a$
HBr						
11	0	0		16-339	21	234.581
19	0	0		16-339	21	239.782
11	1	1		64-130	5	6.7E-24
19	1	1		64-130	5	6.8E-24
11	1	0	2558.5308	2195-2773	36	72.324
19	1	0	2558.9105	2195-2773	36	73.916
11	2	0	5026.6005	4712-5160	28	0.755
19	2	0	5027.3408	4713-5161	28	0.771
11	3	0	7404.1928	7204-7495	20	1.9E-22
19	3	0	7405.2610	7205-7496	20	2.0E-22
11	4	0	9690.9914	9506-9758	18	9.5E-23
19	4	0	9692.3579	9507-9759	18	9.7E-23
HI						
17	0	0		12-286	23	106.693
17	1	1		49-137	8	1.8E-23
17	1	0	2229.5817	2117-2398	26	1.758
17	2	0	4379.2261	4117-4489	32	0.633
17	3	0	6448.0348	6176-6520	30	0.343
17	4	0	8434.7076	8190-8488	26	5.9E-22
ClO						
76	0	0		0-100	2607	18.673
56	0	0		0-100	2575	58.302
76	1	0	835.4802	763-883	402	11.861
56	1	0	842.5595	769-891	436	36.979
OCS						
622	00 ⁰ 0	00 ⁰ 0		0-40	99	8.034
624	00 ⁰ 0	00 ⁰ 0		0-40	99	0.365
632	00 ⁰ 0	00 ⁰ 0		0-38	93	9.4E-22
822	00 ⁰ 0	00 ⁰ 0		0-32	84	1.6E-22
622	10 ⁰ 0	00 ⁰ 0	858.9669	817-891	181	109.782
622	00 ⁰ 1	00 ⁰ 0	2062.2	2016-2089	181	7881.287
H ₂ CO						
126	000000	000000		0-100	610	310.095
136	000000	000000		0-73	563	5.633
128	000000	000000		0-48	367	0.694
126	000002	000000	2500	2743-2812	5	4.548
126	001100	000000	2655	2734-2735	1	0.589
126	001001	000000	2719.156	2700-2879	105	138.588
126	100000	000000	2782.457	2723-2843	424	828.793
126	000010	000000	2843.326	2703-2982	595	974.235
126	010100	000000	2905	2734-2999	28	38.133
126	010001	000000	3000.066	2896-2957	3	8.550

Continued

Table III. Continued

Molecule/ isotope	Band v'	v''	Origin (cm^{-1})	Range (cm^{-1})	No. of lines	$\{S_i\}^a$
HOCl						
167	010	000	1238.1208	1179-1303	1240	291.656
165	010	000	1238.6242	1174-1311	1463	896.245
165	100	000	3609.4801	3400-3800	2675	304.351
167	100	000	3609.4851	3400-3800	2345	97.686
N ₂						
44	1	0	2329.9168	2001-2620	117	6.4E-27
HCN						
124	00 ⁰⁰	00 ⁰⁰		2-132	47	1026.457
134	00 ⁰⁰	00 ⁰⁰		2-98	34	12.226
125	00 ⁰⁰	00 ⁰⁰		2-101	35	4.036
124	02 ⁰⁰	01 ¹⁰	697.957	587-823	119	24.979
124	02 ²⁰	01 ¹⁰	713.076	595-851	232	103.278
124	01 ¹⁰	00 ⁰⁰	713.459	579-844	134	823.016
124	02 ⁰⁰	00 ⁰⁰	1426.535	1298-1537	81	139.947
124	00 ⁰¹	00 ⁰⁰	3311.4772	3158-3422	90	951.594
CH ₃ Cl						
217	v ₁		2967.745	2965-2969	229	4.919
215	v ₁		2967.777	2965-2969	255	15.432
217	v ₄		3039.1761	2986-3162	1260	20.164
215	v ₄		3039.2864	2978-3173	1844	58.776
217	3v ₆		3041.8005	2916-3128	1221	19.276
215	3v ₆		3042.8736	2907-3157	1878	66.582
H ₂ O ₂						
1661	000001	000000	1269.136	1186-1350	2389	1283.539
C ₂ H ₂						
1221	0000011	0000000	730.3341	646-811	104	2979.844
1221	0101111	0000000	3281.9020	3151-3387	101	507.407
1221	0010000	0000000	3294.8406	3162-3398	101	429.348
C ₂ H ₆						
1221	v ₉		821.737	720-933	4328	145.556
PH ₃						
1111	0100	0000	992.1301	708-1211	972	330.604
1111	0001	0000	1118.3131	828-1411	1914	411.320

^a Sum of the line intensities on the compilation in units of $\text{cm}^{-1}/\text{molecule-cm}^{-2}$ ($\times 10^{20}$ except where exponent given) at 296K.

^b In the case of sub-bands, for example NH₃, the band origins given in column 4 are the averages of the two.

= 1/2 and 3/2 states was determined by a sum over states to $F = 86$. The line intensities are accurate to 1–2%.

Because both isotopic species of chlorine have non-zero nuclear spin, the data must contain the nuclear spin quantum numbers for the states, i.e., F', F'' . These appear in the data as a branch letter for the transition (P, Q, R) given by $F' - F''$ and the nuclear spin quantum number of the lower state F'' . They occur between the vibration state quantum numbers and the branch and lower state J for the rotational transition as shown in Table II(c). In each species, lines having the same frequency to within $1 \times 10^{-5} \text{ cm}^{-1}$, the same rotational and nuclear quantum numbers but different symmetry, were coalesced into one line. For these lines the symmetry designation + or – was dropped, the frequency and lower-state energy averaged, and the line intensities added to produce the coalesced line. The frequency-dependent cutoff (Appendix A) was applied to the data; the criteria from the main isotope were $1.00 \times 10^{-26} \text{ cm}^{-1}/\text{molecule cm}^{-2}$ at 100 cm^{-1} .

The (1–0) fundamental chlorine monoxide is unchanged from the 1980 AFGL trace gas compilation,¹ except that the line positions were recalculated using the Hamiltonian constants determined from the high-resolution study of Maki *et al.*⁴⁵

Carbonyl sulfide (OCS) pure rotation bands for the isotopic species: $^{16}\text{O}^{12}\text{C}^{32}\text{S}$, $^{16}\text{O}^{13}\text{C}^{32}\text{S}$, $^{16}\text{O}^{12}\text{C}^{34}\text{S}$, and $^{18}\text{O}^{12}\text{C}^{32}\text{S}$, were added to the atlas. The frequencies and lower-state energies were calculated using the standard linear triatomic molecule formulas (for example, see Ref. 46) including the hyperfine interaction. The molecular parameters were determined by a least-squares fit to the data sets of Dubrulle *et al.*⁴⁷ and Lovas.⁴⁸ The positional accuracy is J dependent and generally better than 0.005 cm^{-1} . The line intensities were calculated using the dipole moment reported by Reinartz and Dymanus⁴⁹ for $^{16}\text{O}^{12}\text{C}^{32}\text{S}$. For the less abundant species (624, 632, and 822 in the AFGL isotopic code) the dipole moment was assumed to be the same as the parent species. The resulting intensities are accurate to ~5%. The pressure-broadened halfwidth was set at a default value $0.07 \text{ cm}^{-1}/\text{atm}$ as discussed in Ref. 44.

The new **formaldehyde (H₂CO)** data are for the pure rotation band. Three isotopic species are present in these data; $\text{H}_2^{12}\text{C}^{16}\text{O}$, the main isotope, and the minor species $\text{H}_2^{13}\text{C}^{16}\text{O}$ and $\text{H}_2^{12}\text{C}^{18}\text{O}$ (136 and 128). The experimental data are summarized in Ref. 3. Formaldehyde is an asymmetric rotor, thus the rotational energy and transitions are obtained by solving the basic rigid asymmetric rotor Hamiltonian plus terms representing centrifugal distortion. Here the Hamiltonian formulation of Kirchhoff³² was used to evaluate the rotational and centrifugal distortion constants for H_2CO . For the isotopes 126 and 136, roughly 600 lines for each are calculated in the $0\text{--}100\text{-cm}^{-1}$ region; for 128 there are ~450 lines calculated from 0 to 50 cm^{-1} . The line positions are accurate to 0.005 cm^{-1} , with the accuracy increasing to 0.00005 cm^{-1} for very low J transitions. The line intensities are accurate to ~2–5%; the

dipole moment value used in the calculation was taken from the measurement of Kondo and Oka.⁵⁰

The remaining molecular species identified as 21–28 in Table I are new to the trace gas compilation.

Two vibration–rotation bands of **hypochlorous acid (HOCl)** were considered for this atlas. The molecule is of interest in stratospheric monitoring because of its role as a chlorine sink in the atmosphere. The bending mode at 1238 cm^{-1} was investigated by Sams and Olson.⁵¹ One should consult the latter reference for the estimated precision of the line positions. Unresolvable multiplets have been coalesced as described previously in the section for nitric acid. The intensities for this band were based on measurements performed at the National Bureau of Standards.⁵²

The HOCl ν_1 band in the $2.8\text{-}\mu\text{m}$ region consists of both A and B type transitions. Both types of transition have approximately the same intensity. Strong B type transitions occur in the $3400\text{--}3800\text{-cm}^{-1}$ range, while A type transitions are strong only in the $3525\text{--}3650\text{-cm}^{-1}$ range. Line positions and intensities at 296 K were generated for the A and B type transitions of HOCl for both the 35 and 37 isotopes of Cl using the Hamiltonian constants of Wells *et al.*⁵³ The intensities for the ν_1 band of HOCl are unknown, and the following assumptions were made: (1) for isotopically pure species, the band intensities of HO^{35}Cl and HO^{37}Cl are approximately equal; (2) for a simple isotopic species, the sum of all the A type transition intensities equals the sum of all the B type transition intensities (as concluded in Ref. 53). The band intensity for both isotopic species at natural abundance (75.54% HO^{35}Cl and 24.41% HO^{37}Cl) was arbitrarily set to $\approx 100 \text{ cm}^{-1}/\text{atm cm}$ at 296 K. The final set of line parameters contains all transitions with $J' \leq 40$ and $K'_a \leq 16$ from both isotopic species in natural abundance with intensity $> 0.5\%$ that of the strongest line. Because HOCl is a very nearly prolate symmetric rotor ($\kappa \approx -0.9987$), Watson's Hamiltonian⁵⁴ is not optimum for this molecule. In addition, K'_a must be limited to ~16 to prevent the calculation of unphysical values of energy levels.

An arbitrary halfwidth of $0.06 \text{ cm}^{-1}/\text{atm}$ was assumed for both bands.

Nitrogen (N₂) is included on this edition of the compilation owing to its contribution to atmospheric absorption through electric quadrupole transitions.⁵⁵ The vibration–rotation band at 2330 cm^{-1} consists of O , Q , and S transitions. An estimated air-broadening coefficient of $0.06 \text{ cm}^{-1}/\text{atm}$ at 296 K was assumed.⁵⁶ (The O_2 quadrupole lines have been included in the Main compilation.²)

Hydrogen cyanide (HCN) has been detected in both the troposphere⁵⁷ and stratosphere.⁵⁸ This molecule is known to contribute in certain spectral regions to temperature profile retrieval.⁵⁹

The pure rotation bands of $\text{H}^{13}\text{C}^{14}\text{N}$ and $\text{H}^{12}\text{C}^{15}\text{N}$ from the JPL catalog,³ edition 2, have been added to the atlas. Because of the nonzero nuclear spin of ^{13}C , ^{14}N , and ^{15}N , the hyperfine interaction between the nuclear electronic quadrupole and spin rotation is included in the calculations. The molecular constants were de-

tational transitions were calculated using the constants of Gille and Lee.³⁰ The ground-state energy levels are the same as those calculated for ν_4 (see Ref. 25).

Absolute line intensities have never been measured in the $2\nu_2$ band. An analysis of the atmosphere of Jupiter gives the value of $1.03 \text{ cm}^{-1}/\text{atm cm}$ at 296 K for the $2\nu_2$ band, and this value has been adopted. This band intensity is not applied to the *R*-branch individual line intensities. Indeed, the relatively large intensity (for an overtone band) of the $2\nu_2$ *R*-branch is to be contrasted to the weak *Q*- and *P*-branches. This anomalous intensity pattern is a result of the Coriolis interaction between the $2\nu_2^S$ and the ν_4 rotational levels, since these two vibrations are only 29 cm^{-1} apart. As for the ν_4 band, we must take into account the influence of those interactions in the intensity expressions. Thus the line intensities we give must be considered at best as preliminary results, and more theoretical and analytical works remain to be done.

A halfwidth value of $0.075 \text{ cm}^{-1}/\text{atm}$ at 296 K has been adopted for all updated NH_3 bands on this edition.

The rotational spectrum of **nitric acid** ($\text{H}^{14}\text{N}^{16}\text{O}_3$) was replaced on the atlas. The data are from the revised JPL catalog³ and consist of lines generated by constants obtained by fitting to lines with $J \leq 40$ from the observed nitric acid data of Cazzoli and DeLucia.³¹ The fit to the data was in terms of Kirchhoff's³² formulation of the asymmetric rotor Hamiltonian of Kivelson and Wilson.³³ The accuracy of the rotational transitions is generally better than 0.0001 cm^{-1} . The dipole moment was taken from the measurements of Cox and Riveros,³⁴ and the partition function was determined by a sum over states to $J = 40$. The resulting line intensities are accurate to 3–5%. Because of the small separation between many groups of lines for this molecule, the spectra are very dense (7259 lines in the 0–41- cm^{-1} range). Many of the lines differ in frequency by an amount not observable in field and some laboratory experiments. To facilitate the use of the atlas we coalesced some groups of lines into single lines. The criterion for coalescing is: a pair or group of lines separated in frequency by $< 1 \times 10^{-5} \text{ cm}^{-1}$ has been coalesced if the lines have the same rotational quantum numbers, $J' = J''$ and $K'_c = K''_c$, with $K'_a \neq K''_a$, or $K'_a = K''_a$, with $K'_c \neq K''_c$. This occurs in the data for groups of 2, 3, and 4 lines. The resulting line is composed of the average of the frequencies and lower-state energies of the parent lines (these are usually the same as in the individual lines), and the line intensity is the sum of the individual line intensities of the parent lines. The quantum numbers that differed in the parent line (either K_a or K_c) are replaced by a blank, thus allowing lines resulting from coalescing to be identified in the atlas. An example of coalescing is given in Table II(b). The data were reduced to 4186 lines by coalescing.

A frequency-dependent intensity cutoff (see Appendix A) was applied to the data. The criteria used were $1.02 \times 10^{-22} \text{ cm}^{-1}/\text{molecule cm}^{-2}$ at 41.15 cm^{-1} . The cutoff procedure reduced the data to 4182 lines, to

which a constant halfwidth of $0.13 \text{ cm}^{-1}/\text{atm}$ as reported by Brockman *et al.*³⁵ was added.

Line parameters for the ν_2 band at $5.8 \mu\text{m}$ were recalculated using the Hamiltonian constants of Maki and Wells.³⁶ The set of rovibrational constants for the upper state have been fit to a standard deviation of 0.0012 cm^{-1} . The relative line intensities adopted are consistent with the results of Ref. 36; however, laboratory measurements³⁷ suggest that the absolute line intensities of this band in the present compilation may be too low by ~65%.

The 1982 atlas contains microwave data for the ground $^2\Pi_{3/2}$ and $^2\Pi_{1/2}$ states of the **hydroxyl radical** (OH). Data are for the main isotope OH and for the isotopic species OD and ^{18}OH . A complete description of the calculational method and microwave data is reported in Ref. 38. The procedure refitted the spectra of OH and OD to all the available data. For ^{18}OH most of the molecular parameters were estimated by isotopic scaling of the known ^{16}OH and OD parameters; the more critical molecular parameters of ^{18}OH were then fitted to observed transitions. The data account for 125 lines between 0 and 84 cm^{-1} for ^{16}OH , 235 lines between 0 and 4 cm^{-1} for ^{16}OD , and 113 lines between 0 and 10 cm^{-1} for ^{18}OH . As discussed in Ref. 1, a constant halfwidth of $0.083 \text{ cm}^{-1}/\text{atm}$ was added to the data. All lines that have a strength $> 10^{-30} \text{ cm}^{-1}/\text{molecule cm}^{-2}$ or are laboratory measurements were retained. The reported strengths are accurate to a few percent. The accuracy of the line positions is *J* dependent and is better than 0.005 cm^{-1} .

Goldman³⁹ calculated the $X^2\Pi \leftarrow X^2\Pi \Delta v = 1, 2, \text{ and } 3$ series of $^{16}\text{O}^1\text{H}$ through $v' = 9$. Hamiltonian constants are from Ref. 40. Intensities are calculated using the individual transition Einstein *A* coefficients of Mies.⁴¹ For the (1–0), (2–1), (3–2), and (4–3) bands these individual Einstein *A* coefficients were scaled to give the band Einstein *A* coefficients reported by Agrawalla *et al.*⁴² Mies' Einstein *A* coefficients⁴¹ were used directly for all other bands. Further normalization will be required for the atmospheric OH bands based on the recent work of Werner *et al.*⁴³

No modifications were made to the hydrogen halides for this edition.

Data from the JPL catalog³ for the **chlorine monoxide** species $^{35}\text{Cl}^{16}\text{O}$ and $^{37}\text{Cl}^{16}\text{O}$ are now on the atlas. The data are the pure rotation band of the ground vibrational state for the $^2\Pi$ state of each chlorine monoxide species. The molecular constants were determined by fitting the observed spectrum to a fine-structure Hamiltonian and a hyperfine Hamiltonian including off-diagonal matrix elements. The observed spectrum below 6.7 cm^{-1} (200 GHz) was from the measurements of Kakar *et al.*⁴⁴; the spectrum above 6.7 cm^{-1} was from measurements of Cohen and Pickett at the Jet Propulsion Laboratory.³ The uncertainties for the transition frequencies of ^{35}ClO and ^{37}ClO are *J*-dependent and increase from 0.00001 cm^{-1} at $J = 20.5$ to 0.005 and 0.02 cm^{-1} for the isotopes, respectively, at the highest *J* listed. The partition function for both Ω

terminated by exact matrix diagonalization of the Hamiltonian fitting to the observed lines reported by Pearson *et al.*⁶⁰ Line position accuracy is J dependent ranging from $1 \times 10^{-6} \text{ cm}^{-1}$ for the $R\ 0$ line of both isotopic species at $\sim 3 \text{ cm}^{-1}$, to 0.015 cm^{-1} for the $R\ 33$ line of $\text{H}^{13}\text{C}^{14}\text{N}$ at 97 cm^{-1} and 0.003 cm^{-1} for the $R\ 34$ line of $\text{H}^{12}\text{C}^{15}\text{N}$ at 100 cm^{-1} . For the calculation of the line intensities the dipole moment was assumed to be the same as for the main isotope, 2.984 D.⁶¹ The accuracy of the intensities is $\approx 5\%$. The first fourteen lines of data for $\text{H}^{13}\text{C}^{14}\text{N}$ arise from hyperfine splitting of three lines ($R0$, $R1$, and $R2$). Because the separation of the lines is so small ($1 \times 10^{-5} \text{ cm}^{-1}$), the fourteen lines have been coalesced back to the three parent lines. Three lines for the main isotope from the JPL catalog were included in the atlas. These lines contain the hyperfine splitting, and additional quantum numbers appear before the rotational quantum numbers. The branch letter corresponding to the change in nuclear spin quantum numbers (P, Q, R) and the nuclear spin F of the lower state was added to the data. These lines were retained because their separation is observable in many laboratory and some field experiments. The remaining lines of the principal isotope were calculated by A. Goldman.

The line parameters of the ν_2 , $2\nu_2$, $2\nu_2-\nu_2$, and ν_3 bands of HCN were also added to the compilation. Line positions for $2\nu_2$ were calculated using the Hamiltonian constants of Maki.⁶² Intensities for $2\nu_2$ were calculated using rigid rotor line strengths and are normalized to the band intensity of Smith.⁶³ Line positions for ν_2 and $2\nu_2 - \nu_2$ were calculated using the Hamiltonian constants of Maki⁶² and the band origin from Wang and Overend.⁶⁴ The total band intensity of $2\nu_2-\nu_2$ was derived from scaling the ν_2 band intensity of Hyde and Hornig⁶⁵ by the 2-D harmonic oscillator matrix element and the Boltzmann factor. Line positions for ν_3 were calculated using the Hamiltonian constants of Maki.⁶² The band intensity used is the average of available published values^{63,66} for this band and is corrected for the $\sim 7\%$ contribution from the $\nu_3 + \nu_2 - \nu_2$ band. Line positions for all bands are accurate to $\pm 0.005 \text{ cm}^{-1}$. A halfwidth of $0.06 \text{ cm}^{-1}/\text{atm}$ was adopted for all bands; however, preliminary measurements by Smith⁶⁷ indicate a J dependence of the halfwidth and that an average value of $0.12 \text{ cm}^{-1}/\text{atm}$ would be more appropriate.

The parameters for the ν_1 , ν_4 , and $3\nu_6$ bands of **methyl chloride** (CH_3Cl) around $3.3 \mu\text{m}$ were provided by Dang-Nhu.⁶⁸ This molecule is considered to be a natural source for chlorine in the upper atmosphere. The ν_1 band was studied at high resolution by Dang-Nhu *et al.*⁶⁹ and is a candidate for detection since the Q branches coincide with a relative gap in the methane spectrum. The ν_4 and $3\nu_6$ bands were also studied and analyzed using a high-resolution Fourier transform spectrometer.⁷⁰ References 69 and 70 should be consulted for an understanding of the reliability of the parameters of these complex perturbed bands. A constant value of $0.08 \text{ cm}^{-1}/\text{atm}$ was assumed for the halfwidths.

Interest in **hydrogen peroxide** (H_2O_2) is related to its prominent role in atmospheric photochemistry. It is expected to be a sink species for odd hydrogen radicals. Although it has been proposed to be in higher concentration than OH, it has yet to be detected in the terrestrial atmosphere or extraterrestrially. The ν_6 band is the strongest fundamental, and the parameters on the compilation were provided by Hillman.⁷¹ The line positions for this band were calculated with a general asymmetric rotor program with a fit to some 600 observations.⁷² The ground state was constrained to the submillimeter analysis,⁷³ and the standard deviation of the fit is of the order of 0.005 cm^{-1} . Unresolvable multiplets were coalesced on the atlas. The intensities were calculated and are in general agreement with experiment.⁷² A value of $0.10 \text{ cm}^{-1}/\text{atm}$ was assumed for the Lorentz halfwidth.⁷¹

The linear molecule **acetylene** (C_2H_2) was identified in atmospheric absorption spectra.⁷⁴ Line parameters for the ν_5 band were calculated to an estimated accuracy of 0.001 cm^{-1} using the Hamiltonian constants of Hietanen and Kauppinen.⁷⁵ The band intensity is based on the value of Varanasi and Bangaru.⁷⁶

In the $3\text{-}\mu\text{m}$ region the two strongest bands of acetylene were provided by Rinsland.⁷⁷ Details of the laboratory study that measured the line positions and intensities are given in Ref. 78. A constant halfwidth of $0.08 \text{ cm}^{-1}/\text{atm}$ was applied to this molecule.

Interest in **ethane** (C_2H_6) was spurred by its detection in the atmospheres of the Jovian planets. There is also wide interest in this hydrocarbon for remote sensing in terrestrial tropospheric problems. In this edition of the atlas the ν_9 fundamental has been introduced. The transitions came from Daunt *et al.*,⁷⁹ with the relative intensities corrected to agree with recent experiments.⁸⁰ A halfwidth of $0.10 \text{ cm}^{-1}/\text{atm}$ was assumed.

Finally, two bands of **phosphine** (PH_3), ν_2 and ν_4 , were added to the atlas. This species is presently of interest in studies of planetary atmospheres. The parameters are described in Ref. 81, and a constant halfwidth of $0.075 \text{ cm}^{-1}/\text{atm}$ was assumed.

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Appendix A: Frequency-Dependent Intensity Cutoff Criterion

Intensity criteria were developed⁸² for the main IR active constituents of the terrestrial atmosphere by assuming normal concentration of a species and an extreme atmospheric path. The path was taken to be the atmospheric path tangent to the earth's surface and extending from space to space. Lines having $<10\%$ absorption at the line center were omitted from the atlas. Although an absolute line intensity cutoff was

established, exceptions were immediately necessary (see Ref. 82). For trace gas constituents of the atmosphere, similar considerations are not possible because both the notion of concentration and tangent path seemed inappropriate.

As microwave data were added to the atlases it became obvious that the intensity cutoff criterion had to account for the effect of the radiation field⁸³ in the line intensity at low frequency. The frequency-dependent cutoff developed¹ to account for this is

$$I(\nu) = \frac{I_c \nu}{\nu_c} \tanh\left(\frac{c_2 \nu}{2T_0}\right), \quad (\text{A1})$$

where I_c is the standard intensity cutoff (main gases only) at the defined frequency ν_c (e.g., $I_c = 3.0 \times 10^{-27}$ cm⁻¹/molecule cm⁻² and $\nu_c = 2000$ cm⁻¹ for H₂O), ν is the frequency of the line in vacuum wave numbers, c_2 is the second radiation constant (hc/k), and T_0 is the atlas temperature 296 K. The cutoff given by Eq. (A1) is well-defined for the main constituents of the atmosphere, where I_c and ν_c are known. To use Eq. (A1) for the trace gases a static cutoff intensity I_c and frequency ν_c must be defined. Care must be taken in defining I_c for Eq. (A1) so that $I(\nu)$ goes smoothly into I_c at the cutoff frequency.

The cutoff parameters are determined by using ν and I of the strongest intensity line of the principal isotope from the lines at high frequency in the data. The intensity cutoff is then chosen to be 2 orders of magnitude weaker than this line, and the frequency of this line is ν . Thus

$$I(\nu = \nu_c) = I_{\text{strongest line}} \times 10^{-2}, \quad (\text{A2})$$

and one solves for the static cutoff via

$$I_c = \frac{I(\nu = \nu_c)}{\tanh\left(\frac{c_2 \nu_c}{2T_0}\right)}. \quad (\text{A3})$$

Using the static intensity cutoff defined by Eq. (A3) along with ν_c gives the desired criterion for Eq. (A1) to be applied to the individual line intensities for the trace gases.

References

- L. S. Rothman *et al.*, *Appl. Opt.* **20**, 1323 (1981).
- L. S. Rothman, *Appl. Opt.* **20**, 791 (1981); for latest edition of the Main Compilation, see L. S. Rothman *et al.*, *Appl. Opt.* submitted for publication (1983).
- R. L. Poynter and H. M. Pickett, "Submillimeter, Millimeter and Microwave Spectral Line Catalogue," JPL Publication 80-23, Revision 1 (Jet Propulsion Laboratory, California Institute of Technology, Pasadena, Calif., 1981), and Edition 1 of the same catalog.
- C. Amiot, R. Bacis, and G. Guelachvili, *Can. J. Phys.* **56**, 251 (1978).
- W. L. Meerts, *Chem. Phys.* **14**, 421 (1976).
- W. L. Meerts and A. Dymanus, *J. Mol. Spectrosc.* **44**, 320 (1972).
- L. L. Abels and J. H. Shaw, *J. Mol. Spectrosc.* **20**, 11 (1966).
- J. R. Gillis and A. Goldman, *Appl. Opt.* **21**, 1161 (1982).
- L. D. G. Young, A. T. Young, S. A. Clough, and F. X. Kneizys, *J. Quant. Spectrosc. Radiat. Transfer* **20**, 317 (1978).
- C. Amiot and J. Verges, *J. Mol. Spectrosc.* **81**, 424 (1980).
- C. Amiot and G. Guelachvili, *J. Mol. Spectrosc.* **76**, 86 (1979).
- J.-Y. Mandin, C. Amiot, and G. Guelachvili, *Ann. Phys.* **5**, 91 (1980).
- F. P. Billingsley II, *J. Mol. Spectrosc.* **61**, 53 (1976).
- B. D. Green, G. E. Caledonia, and R. E. Murphy, *J. Quant. Spectrosc. Radiat. Transfer* **26**, 215 (1981).
- G. Chandraiah and C. W. Cho, *J. Mol. Spectrosc.* **47**, 134 (1973).
- A. S. Pine and M. Dang-Nhu, *J. Mol. Spectrosc.* **84**, 132 (1980).
- V. M. Devi *et al.*, *J. Mol. Spectrosc.* **88**, 251 (1981).
- N. Husson, A. Chedin, N. A. Scott, I. Cohen-Hallaleh, and A. Berroir, "La Banque de Données GEISA Mise à Jour 3," *Laboratoire de Météorologie Dynamique Note 116* (1982).
- N. Husson, A. Goldman, and G. Orton, *J. Quant. Spectrosc. Radiat. Transfer* **27**, 505 (1982).
- S. Urban *et al.*, *J. Mol. Spectrosc.* **88**, 274 (1981).
- N. Husson, A. Chedin, and N. A. Scott, "Paramètres Spectroscopiques de la Molécule d'Ammoniac dans la Région 32-7.5 μm (Bandes ν_2 et $2\nu_2-\nu_2$)," *Laboratoire de Météorologie Dynamique Note 90* (1979).
- S. Urban *et al.*, *J. Mol. Spectrosc.* **79**, 455 (1980).
- J. J. Hillman, D. E. Jennings, and J. L. Faris, *Appl. Opt.* **18**, 1808 (1979); G. Baldacchini, S. Marchetti, and V. Montelatici, *J. Mol. Spectrosc.* **86**, 115 (1981); J. P. Sattler, L. S. Miller, and T. L. Worchesky, *J. Mol. Spectrosc.* **88**, 347 (1981).
- R. L. Poynter and J. S. Margolis, *Mol. Phys.* **11**, 1 (1983).
- N. Husson and A. Chedin, "Line Parameters of Infrared Absorption Bands of Ammonia in Connection with the Voyager IRIS Mission," *Laboratoire de Météorologie Dynamique Note 115* (1982).
- R. Hanel *et al.*, *Science* **204**, 972 (1979); **206**, 952 (1979).
- D. C. McKean and P. N. Schatz, *J. Chem. Phys.* **24**, 316 (1956).
- L. A. Farrow and R. E. Richton, *J. Chem. Phys.* **70**, 2166 (1979).
- W. L. France and D. Williams, *J. Opt. Soc. Am.* **56**, 70 (1966).
- J. C. Gille and T. H. Lee, *J. Appl. Sci.* **26**, 932 (1969).
- G. Cazzoli and F. C. DeLucia, *J. Mol. Spectrosc.* **76**, 131 (1979).
- W. H. Kirchhoff, *J. Mol. Spectrosc.* **41**, 333 (1972).
- D. Kivelson and E. B. Wilson, Jr., *J. Chem. Phys.* **20**, 1575 (1952).
- A. P. Cox and J. M. Riveros, *J. Chem. Phys.* **42**, 3106 (1965).
- P. Brockman, C. H. Bair, and F. Allario, *Appl. Opt.* **17**, 91 (1978).
- A. G. Maki and J. S. Wells, *J. Mol. Spectrosc.* **82**, 427 (1980).
- A. Goldman, T. G. Kyle, and F. S. Bonomo, *Appl. Opt.* **10**, 65 (1971).
- R. A. Beaudet and R. L. Poynter, *J. Phys. Chem. Ref. Data* **7**, 311 (1978).
- A. Goldman, *Appl. Opt.* **21**, 2100 (1982).
- J. A. Coxon, *Can. J. Phys.* **58**, 933 (1980); J. A. Coxon and S. C. Foster, *Can. J. Phys.* **60**, 41 (1982).
- F. H. Mies, *J. Mol. Spectrosc.* **53**, 150 (1974).
- B. S. Agrawalla, A. S. Manocha, and D. W. Setser, *J. Phys. Chem.* **85**, 2873 (1981).
- H. J. Werner, P. Rosmus, and E. A. Reinsch, "MCSCF, MCSCF-SCEP, and SCEP-CEPA Calculations of Infrared Transition Rates for the Electronic Ground States of OH, OH⁻ and OH⁺," *J. Chem. Phys.* (1982), submitted for publication.
- R. K. Kakar, E. A. Cohen, and M. Geller, *J. Mol. Spectrosc.* **70**, 243 (1978).
- A. G. Maki, F. J. Lovas, and W. B. Olson, *J. Mol. Spectrosc.* **92**, 410 (1982).
- C. H. Townes and A. L. Schawlow, *Microwave Spectroscopy* (McGraw-Hill, New York, 1955).
- A. Dubrulle, J. Demaison, J. Burie, and D. Boucher, *Z. Naturforsch. Teil A* **35**, 471 (1980).
- F. J. Lovas, *J. Phys. Chem. Ref. Data* **7**, 1445 (1978).

49. J. M. L. J. Reinartz and A. Dymanus, *Chem. Phys. Lett.* **24**, 346 (1974).
50. K. Kondo and T. Oka, *J. Phys. Soc. Jpn.* **15**, 307 (1960).
51. R. L. Sams and W. B. Olson, *J. Mol. Spectrosc.* **84**, 113 (1980).
52. R. L. Sams and A. G. Maki, NBS; private communication.
53. J. S. Wells, R. L. Sams, and W. J. Lafferty, *J. Mol. Spectrosc.* **77**, 349 (1979).
54. J. K. G. Watson, *Mol. Phys.* **15**, 479 (1968).
55. A. Goldman, J. Reid, and L. S. Rothman, *Geophys. Res. Lett.* **8**, 77 (1981).
56. C. Camy-Peyret, J.-M. Flaud, L. Delbouille, G. Roland, J. W. Brault, and L. Testerman, *J. Phys. Lett.* **42**, 279 (1981).
57. C. P. Rinsland, M. A. H. Smith, P. L. Rinsland, A. Goldman, J. W. Brault, and G. M. Stokes, *J. Geophys. Res.* **87**, 11119 (1982).
58. M. T. Coffey, W. G. Mankin, and R. J. Cicerone, *Science* **214**, 333 (1981).
59. M. T. Coffey and A. Goldman, *Appl. Opt.* **20**, 3480 (1981).
60. E. F. Pearson, R. A. Creswell, M. Winnewisser, and G. Winnewisser, *Z. Naturforsch. Teil A* **31**, 1394 (1976).
61. G. Tomasevich, Thesis, Harvard U. (1970).
62. A. G. Maki, *J. Mol. Spectrosc.* **58**, 308 (1975).
63. I. W. M. Smith, *J. Chem. Soc. Faraday Trans. 2* **77**, 2357 (1981).
64. V. K. Wang and J. Overend, *Spectrochim. Acta Part A* **29**, 687 (1973).
65. G. E. Hyde and D. F. Hornig, *J. Chem. Phys.* **20**, 647 (1952).
66. J. H. Jaffe, "Refraction of Gases in the Infrared," in *Advances in Spectroscopy*, H. W. Thompson, Ed. (Interscience, New York, 1961), pp. 263-291; J. Finzi, J. H. S. Wang, and F. N. Mastrup, *J. Appl. Phys.* **48**, 2681 (1977); K. Kim and W. T. King, *J. Chem. Phys.* **71**, 1967 (1979).
67. M. A. H. Smith, NASA Langley; private communication.
68. M. Dang-Nhu, CNRS, Orsay; private communication.
69. M. Dang-Nhu, M. Morillon-Chapey, G. Graner, and G. Guela-chvili, *J. Quant. Spectrosc. Radiat. Transfer* **26**, 515 (1981).
70. M. Dang-Nhu, M. Morillon-Chapey, G. Graner, and G. Guela-chvili, *Can. J. Phys.* **60**, 1328 (1982).
71. J. J. Hillman, NASA Goddard; private communication.
72. J. J. Hillman, D. E. Jennings, W. B. Olson, and A. Goldman; private communication.
73. J. J. Hillman, *J. Mol. Spectrosc.* **95**, 236 (1982).
74. A. Goldman *et al.*, *J. Geophys. Res.* **86**, 12143 (1981).
75. J. Hietanen and J. Kauppinen, *Mol. Phys.* **42**, 411 (1981).
76. P. Varanasi and B. R. P. Bangaru, *J. Quant. Spectrosc. Radiat. Transfer* **14**, 839 (1974).
77. C. P. Rinsland, NASA Langley; private communication.
78. C. P. Rinsland, A. Baldacci, and K. N. Rao, *Astrophys. J.* **49**, 487 (1982).
79. S. J. Daunt *et al.*, *J. Mol. Spectrosc.* **86**, 327 (1981).
80. G. S. Orton, JPL, and D. E. Jennings, NASA Goddard; private communication.
81. A. Goldman, G. R. Cook, and F. S. Bonomo, *J. Quant. Spectrosc. Radiat. Transfer* **24**, 211 (1980); G. Tarrago, M. Dang-Nhu, and A. Goldman, *J. Mol. Spectrosc.* **88**, 311 (1981).
82. R. A. McClatchey *et al.*, "AFCRL Atmospheric Absorption Line Parameters Compilation," AFCRL-TR-0096 (1973).
83. S. A. Clough, F. X. Kneizys, L. S. Rothman, and W. O. Gallery, *Proc. Soc. Photo. Opt. Instrum. Eng.* **277**, 152 (1981).