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Calculation of Spectroscopic Parameters for
Diatomic Molecules of Atmospheric Interest

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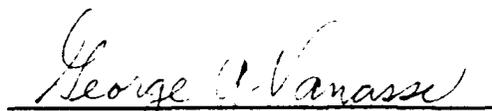
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13 ABSTRACT (Maximum 200 words)
A complete recalculation of fundamental spectroscopic parameters, in particular transitional frequency and line intensity, has been accomplished for the diatomic molecules carbon monoxide (CO), and the hydrogen halides (HF, HCl, HBr, and HI). The results have been cast into the form of the 1986 edition of the HITRAN molecular database. A primary goal of this effort was to produce parameters sufficient for the high temperature database, HITEMP, so that additional isotopic variants and additional hot and overtone bands for these species are included, also extending the bands to higher rotational levels than previously available. The spectral coverage is from the submillimeter region (pure rotational lines) through the visible (higher overtones).

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CONTENTS

I. Introduction	1
II. Procedure	2
III. Results	3
(A) Hydrogen Halides	4
(B) Carbon Monoxide	8
References	11

TABLE

1. Total Number of Lines Per Band and Total Band Intensities	12
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I. INTRODUCTION

For many years the Air Force Geophysics Laboratory has been compiling spectroscopic data for molecules of importance in the Earth's atmosphere.¹ This data, now known as the HITRAN database, is very useful for many applications, and its scope has increased dramatically in recent years, both in the number of transitions for each molecule and in the number of molecular species.² Periodically a new edition of the database is issued which incorporates new and/or improved values of the various molecular parameters. Because of additional parameters presently required to characterize accurately and completely a given transition for a specific molecule, a new format was adopted in 1986.³

The work summarized in this report constitutes a complete recalculation using the best available data for the appropriate molecular parameters of various isotopes for the following diatomic molecules: HF, HCl, HBr, HI, and CO. After a brief description of the method used, the extent of the current data (the number of vibration-rotational bands included, the maximum value of the rotational quantum number J, the cut-off value for the strength parameter S, etc.) are given together with a bibliography of the sources used for all the species. The results in the 1986 HITRAN format have been delivered to AFGL on floppy disks, and will be incorporated in the next HITRAN update. A more extensive compilation for CO appropriate for higher temperature applications has also been generated, and this data is being validated for incorporation into the "hot gas" database.

II. PROCEDURE

The method used to obtain the important parameters characterizing each transition has been described in the Proceedings of the HITRAN Database Conference⁴ held at the Geophysics Laboratory, Hanscom AFB on 8-9 June, 1989, but will be outlined here for completeness. The parameters of interest for a given transition of a specific isotopic species are: the frequency ν_{if} , the transition moment R and the corresponding strength S , and the energy level of the initial state $E_{v,J} \equiv E''$. Other parameters characterizing a transition such as the self-broadened halfwidth γ_s , air-broadened halfwidth γ_a , temperature-dependence of the air-broadened halfwidth n , pressure shift γ , and accuracy indices can be obtained directly or indirectly from the existing experimental data.

The first step is to use the most accurate available Dunham parameters, $Y_{k,l}$ obtained from analyses of transition frequencies in order to calculate the initial state energies $E_{v,J}$ and the frequencies ν_{if} for the transitions specified by the vibrational and rotational quantum numbers $i = \{v,J\}$ and $f = \{v',J'\}$ of the initial and final states of the transition, respectively; viz.

$$\nu_{if} = E_{v',J'} - E_{v,J} \quad , \quad (1)$$

where the energy levels are given by

$$E_{v,J} = \sum_{k,l} Y_{k,l} (v + \frac{1}{2})^k [J(J+1)]^l \quad . \quad (2)$$

The Dunham $Y_{k,l}$ can also be used with a standard RKR program to compute an accurate potential energy $V(R)$ as a function of the

internuclear displacement R . This in turn can be used as input data for a computer program that numerically solves the Schrodinger equation for the vibration-rotational wavefunctions. These can then be utilized along with a dipole moment function obtained by combining the most accurate dipole moment data from intensity measurements and ab initio results⁵ to calculate the transition moments R and the corresponding strengths S . The accuracy of the frequencies and initial state energies are determined solely by the accuracy of the existing frequency data, while the accuracy of the transition moments or strengths are dependent primarily on the accuracy of the dipole moment function. We note in passing that if one is interested in transitions involving highly excited vibration-rotational states (such as those important in high-temperature CO), one cannot simply model the dipole moment function by a series expansion which, although it would reproduce the low-temperature laboratory data, would not extrapolate properly to large values of R and consequently result in incorrect results for highly excited transitions. Rather, we have modeled this function by appropriately chosen Pade approximants.⁶

III. RESULTS

In describing the new results, we will use the standard notation for the molecular parameters as specified in the 1986 edition of the HITRAN database except for the IER codes in columns 92, 93 and 94; for these, we use the following values (revised 6/13/89 at the HITRAN Database Conference):

	$\nu(92) \text{ cm}^{-1}$	$S, \gamma (93, 94)$
0	≥ 1	Default 0.05
1	$\geq 0.1 < 1$	Estimated
2	$\geq 0.01 < 0.1$	> 20%
3	$\geq 0.001 < 0.01$	10 - 20 %
4	$\geq 0.0001 < 0.001$	5 - 10 %
5	$\geq 0.00001 < 0.0001$	2 - 5 %
6	< 0.00001	1 - 2 %
7	-	< 1 %

Listed below are the vibration-rotational transitions included in the compilation together with the sources of the molecular data for HF, HCl, HBr, HI, and CO; if these data were obtained experimentally at nonstandard conditions (e.g. T different from 296 K), the method of scaling is indicated. Estimated or extrapolated values are given for some parameters, while others for which no data exist are left blank.

(A) HYDROGEN HALIDES

For the hydrogen halides, the intensity cutoff for inclusion was $S > 1.000\text{E-}26$; this is approximately two orders of magnitude less than the previous edition, resulting in a modest increase in the number of transitions considered. (See Table 1 for a summary of the transitions included.) Some higher overtone transitions of the H-halides and all transitions of DF, DCl, DBr and DI have been excluded (even if they have strengths greater than the cutoff) because these do not play a significant role in the Earth's atmosphere; results have been calculated, however, and will be made available if a need for this data exists.

HF

Pure Rotational Bands ($\Delta v = 0$)

1. ν : D. A. Jennings et al., J. Mol. Spectrosc. 122, 477 (1987).
2. S: R. H. Tipping, to be published.
3. γ_a : G. Bachet, C. R. Acad. Sci. Paris 274, 1319 (1972); J. Quant. Spectrosc. Radiat. Transfer 14, 1285 (1974).
4. γ_s : No data.
5. n: No data; default value 0.50 used.
6. y: R. Bachet and R. Coulon, Infrared Phys. 18, 585 (1978).
Values for higher J extrapolated similar to fundamental.

Fundamental and $\Delta v = 1$ Bands

1. ν : G. Guelachvili, Opt. Comm. 19, 150 (1976).
2. S: Tipping, *ibid.*
3. γ_a : A. S. Pine and J. P. Looney, J. Mol. Spectrosc. 122, 41 (1987).
4. γ_s : A. S. Pine and A. Fried, J. Mol. Spectrosc. 114, 148 (1985).
5. n: Pine and Looney, *ibid.*
6. y: Pine and Looney, *ibid.*

First Overtone Band

1. ν : Guelachvili, *ibid.*
2. S: Tipping, *ibid.*
3. γ_a : R. E. Meredith and F. G. Smith, J. Chem. Phys. 60, 3388 (1974). Measured at $T = 373$ K for N_2 ; scaled to $T = 296$ K using $n = 0.5$ and to air by $\gamma_a = 0.9 \gamma_{N_2}$.
4. γ_s : R. E. Meredith, J. Quant. Spectrosc. Radiat. Transfer 12, 485 (1972). Measured at $T = 373$ K; scaled to $T = 296$ K using $n = 0.5$.

5. n: No data; default value 0.50 used.

6. y: No data.

Second Overtone Band

1. ν : Guelachvili, *ibid.*

2. S: Tipping, *ibid.*

3. γ_a : Assumed to be the same as the 2-0 band.

4. γ_s : Assumed to be the same as the 2-0 band.

5. n: No data; default value 0.50 used.

6. y: No data.

HCl

1. ν : J. Coxon and J. F. Ogilvie, *J. Chem. Soc. Faraday Trans. 2*, 78, 1345 (1982) for all bands ($\Delta v = 0, 1, 2, 3, 4, 5$).

2. S: J. F. Ogilvie et al., *J. Chem. Phys.* 73, 5221 (1980); A. S. Pine et al., *J. Mol. Spectrosc.* 109, 30 (1985) for all bands.

3. γ_a : J. Pourcin et al., *J. Mol. Spectrosc.* 90, 43 (1981) for $\Delta v = 0$ transitions; A. S. Pine and A. Fried, *J. Mol. Spectrosc.* 114, 148 (1985) for all vibrational bands.

4. γ_s : M. Sergent-Rozey et al., *J. Mol. Spectrosc.* 120, 403 (1986) for $\Delta v = 0$; A. S. Pine and J. P. Looney, *J. Mol. Spectrosc.* 122, 41 (1987) for $\Delta v = 1$ and 2 bands; and A. C. Stanton and J. Silver, *Appl. Optics.* 27, 5009 (1988) for $\Delta v = 3$ bands.

5. n: C. Chackerian et al., *J. Mol. Spectrosc.* 113, 373 (1985) and A. S. Pine and J. P. Looney, *J. Mol. Spectrosc.* 122, 41 (1987) for the 1-0 band; no data available for other bands.

6. γ : A. S. Pine and J. P. Looney, J. Mol. Spectrosc. 122, 41 (1987) for the 1-0 band; G. Guelachvili and M. A. H. Smith, J. Quant. Spectrosc. Radiat. Transfer 20, 35 (1978) for the 2-0 band; no data available for other bands.

HBr

All Bands ($\Delta v = 0, 1, 2, 3, 4$)

1. ν : P. Bernage and P. Niay, J. Mol. Spectrosc. 63, 317 (1977); P. Bernage, thesis, University of Lille, 1976.
2. S: C. B. Carlisle et al., J. Mol. Spectrosc. 130, 395 (1988).
3. γ_a : Estimated; the values used are the same as those on the last AFGL tape.
4. γ_s : B. Seoudi et al., J. Mol. Spectrosc. 112, 88 (1985). Values for lines having $|m| > 12$ are extrapolated. No vibrational dependence is included.
5. n: No data.
6. γ : No data.

HI

All Bands ($\Delta v = 0, 1, 2, 3, 4$)

1. ν : G. Guelachvili, P. Niay and P. Bernage, J. Mol. Spectrosc. 85, 253 (1981).
2. S: H. Riris et al., to be published.
3. γ_a : No data; default value of 0.05.
4. γ_s : G. Ameer and W. Benesch, J. Chem. Phys. 37, 2699 (1962); P. Niay et al., Can. J. Phys. 56, 727 (1978). No vibrational dependence included.
5. n: No data.
6. γ : No data.

(B) Carbon Monoxide

For CO, two distinct data sets were compiled. The first set appropriate for ambient atmospheric temperatures consists of data for the 5 most abundant isotopes and includes R and P transitions in the 0-0, 1-1, 1-0, 2-1, 2-0, 3-1, 3-0 and 4-1 bands for $J = 0$ to 50, independent of their strength. (For the most abundant isotope, $^{12}\text{C}^{16}\text{O}$, transitions in the 4-0 band are also included.) The second more extensive set appropriate for much higher temperatures (to be included in the "hot gas" compilation) consists of data for the two most abundant isotopes; for $^{12}\text{C}^{16}\text{O}$, transitions having $\Delta v \equiv v' - v = 0$ to 4 for $v = 0$ to 10 and $J = 0$ to 150 are included, while for $^{13}\text{C}^{16}\text{O}$, identical transitions except only for $v = 0$ to 8 are included.

The values listed for the halfwidths and for the temperature-dependence of the air-broadened halfwidths are the same for all the bands (i.e., we assume that these parameters are independent of the vibrational quantum numbers and do not depend on the particular isotopic species; these assumptions are in good agreement with the limited available experimental data). The data were obtained from the following sources.

CO

All Bands

1. ν : G. Guelachvili, et al., J. Mol. Spectrosc. 98, 64 (1983);
C. R. Pollock et al., J. Mol. Spectrosc. 99, 357 (1983).
2. S: C. Chackerian and R. H. Tipping, J. Mol. Spectrosc. 99,
431 (1983).
3. γ_a : T. Nakazawa and M. Tanaka, J. Quant. Spectrosc. Radiat.
Transfer 28, 409 (1982). Values for transitions having 20

$< |m| \leq 33$ are extrapolated, while those for $|m| \geq 34$ are assumed to be constant (0.0460).

4. γ_S : J. M. Hartmann et al., Appl. Opt. 27, 3063 (1988); Hartmann et al., private communication. Values for transitions having $|m| \geq 76$ are assumed to be constant (0.0201).
5. n : Hartmann et al., ibid. Values for transitions having $|m| \geq 76$ are assumed to be constant (0.27).
6. y : No data.

This extended set of CO data contained on 7 floppy disks was provided to J. E. A. Selby for validation and eventual inclusion into the "hot gas" database; the limited data set was provided to L. S. Rothman for inclusion in the next edition of the HITRAN database.

In addition to the research described above, I would like to mention some additional work carried out primarily by one of my Ph.D. graduate students who was partially supported in the summer through this grant. This work is of interest to the HITRAN/FASCODE program in that it concerns the continuous absorption of radiation by H_2O (the so-called water "continuum").

We have extended the statistical theory proposed by Rosenkranz⁷ for the calculation of the absorption in the 300 - 1100 cm^{-1} spectral region by improving some of the approximations that were made and by eliminating others. For $H_2O - H_2O$ collisions, we can attain good agreement with the best experimental results using only known values of the dipole moment and two Lennard-Jones potential parameters describing the

isotropic interaction. This absorption exhibits a strong negative dependence in agreement with experiment. On the other hand, for $\text{H}_2\text{O} - \text{N}_2$ collisions the absorption is much less temperature dependent, but this dependence varies significantly as a function of frequency. For the lower frequencies in the spectral range considered, the dependence is again negative (i.e., as the temperature increases, the absorption decreases). However, for the higher frequencies, the temperature dependence is positive. To the best of my knowledge, this complex temperature dependence as a function of frequency is not modeled correctly in the empirical continuum presently used in the atmospheric transmission codes. Similar comments obtain for the spectral window around 2400 cm^{-1} occurring on the high-frequency wing of the fundamental band.

In addition to calculating the continuous absorption in the infrared as outlined above, we have formulated a new theory to describe the continuous absorption in the millimeter spectral region due to $\text{H}_2\text{O} - \text{H}_2\text{O}$ collisions. This is the first successful theory for calculating the absorption in this spectral region; and again using only the known values of the dipole moment and two Lennard-Jones potential parameters, we were able to get quantitative agreement both with the magnitude and the strong negative temperature dependence of the continuous absorption as determined by experiment. By combining the theoretical predictions together with the available measurements, one should be able to model more correctly the magnitude and more importantly the temperature dependence of the continuous absorption by H_2O in the Earth's atmosphere.

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Table 1. Total number of lines per band and total band intensities.

Molecule	Code	v'	v	Total # lines	Total S
HF	141	0	0	16	5.705×10^{-17}
		1	0	29	1.764×10^{-17}
		2	0	26	4.963×10^{-19}
		3	0	23	1.232×10^{-20}
		1	1	6	2.481×10^{-25}
		2	1	7	1.041×10^{-25}
		HCl	151	0	0
1	0			39	4.750×10^{-18}
2	0			35	1.077×10^{-19}
3	0			29	7.180×10^{-22}
4	0			19	3.188×10^{-24}
5	0			12	2.276×10^{-25}
1	1			13	6.902×10^{-24}
2	1			21	7.419×10^{-24}
3	1			13	2.738×10^{-25}
HCl	152			0	0
		1	0	38	1.517×10^{-18}
		2	0	33	3.434×10^{-20}
		3	0	27	2.288×10^{-22}
		4	0	16	9.936×10^{-25}
		1	1	12	2.220×10^{-24}
		2	1	19	2.382×10^{-24}
		3	1	2	2.068×10^{-26}

HBr	161	0	0	24	2.405×10^{-18}		
		1	0	42	7.232×10^{-19}		
		2	0	36	7.909×10^{-21}		
		3	0	29	1.976×10^{-22}		
		4	0	28	1.014×10^{-22}		
		1	1	15	9.921×10^{-24}		
		2	1	23	5.575×10^{-24}		
		3	1	3	3.380×10^{-26}		
		HBr	162	0	0	24	2.339×10^{-18}
				1	0	41	7.033×10^{-19}
2	0			35	7.690×10^{-21}		
3	0			29	1.921×10^{-22}		
4	0			28	9.858×10^{-23}		
1	1			15	9.667×10^{-24}		
2	1			23	5.432×10^{-24}		
3	1			3	3.293×10^{-26}		
HI	171	0	0	26	1.067×10^{-18}		
		1	0	40	1.934×10^{-20}		
		2	0	39	6.018×10^{-21}		
		3	0	39	3.375×10^{-21}		
		4	0	36	5.571×10^{-22}		
		1	1	18	2.099×10^{-23}		
		2	1	18	8.340×10^{-25}		
		3	1	9	1.396×10^{-25}		
4	1	12	1.723×10^{-25}				

CO	051	0	0	50	1.817×10^{-20}
		1	0	100	1.036×10^{-17}
		2	0	100	7.692×10^{-20}
		3	0	100	4.909×10^{-22}
		4	0	100	1.531×10^{-24}
		1	1	50	3.129×10^{-25}
		2	1	100	6.164×10^{-22}
		3	1	100	7.032×10^{-24}
		4	1	100	6.216×10^{-26}
CO	052	0	0	50	1.943×10^{-22}
		1	0	100	1.102×10^{-19}
		2	0	100	7.992×10^{-22}
		3	0	100	4.976×10^{-24}
		1	1	50	4.274×10^{-27}
		2	1	100	8.246×10^{-24}
		3	1	100	9.186×10^{-26}
		4	1	100	7.918×10^{-28}

CO	053	0	0	50	3.490×10^{-23}		
		1	0	100	1.979×10^{-20}		
		2	0	100	1.432×10^{-22}		
		3	0	100	8.900×10^{-25}		
		1	1	50	7.837×10^{-28}		
		2	1	100	1.509×10^{-24}		
		3	1	100	1.678×10^{-26}		
		4	1	100	1.443×10^{-28}		
		CO	054	0	0	50	6.771×10^{-24}
				1	0	100	3.849×10^{-21}
2	0			100	2.820×10^{-23}		
3	0			100	1.775×10^{-25}		
1	1			50	1.341×10^{-28}		
2	1			100	2.611×10^{-25}		
3	1			100	2.938×10^{-27}		
4	1			100	2.561×10^{-29}		
CO	055	0	0	50	3.723×10^{-25}		
		1	0	100	2.099×10^{-22}		
		2	0	100	1.483×10^{-24}		
		3	0	100	8.980×10^{-27}		
		1	1	50	1.075×10^{-29}		
		2	1	100	2.027×10^{-26}		
		3	1	100	2.198×10^{-28}		
		4	1	100	1.841×10^{-30}		