

Line strength + Spectra databases

Atomic vs Molecular line strengths

Degeneracy, Term levels

HITRAN, NIST - Atomic database

NIST - Chemistry Webook, MPI – catalogue

Bernath Ch. 1, 5.7, 6.3, 7.6, 9.5, 10.9

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CHEM 5161



Einstein coefficients

- Absorption:
$$B_{1\leftarrow 0} = \frac{1}{6\varepsilon_0\hbar^2}\mu_{10}^2 = \frac{2\pi^2}{3\varepsilon_0\hbar^2}\mu_{10}^2 \quad (1.52)$$

- Stimulated Emission:
$$B_{1\leftarrow 0} = B_{1\rightarrow 0} \quad (1.21)$$

- Spontaneous Emission:
$$A_{1\rightarrow 0} = \frac{8\pi h\nu_{10}^3}{c^3}B_{1\leftarrow 0} \quad (1.22)$$

- Absorption cross-section:
$$\sigma = \frac{2\pi^2\mu_{10}^2}{3\varepsilon_0\hbar c}\nu g(\nu - \nu_{10}) \quad (1.57)$$

$$\sigma = \frac{A\lambda^2 g(\nu - \nu_{10})}{8\pi} = \frac{\lambda^2 g(\nu - \nu_{10})}{8\pi\tau_{sp}} \quad (1.58)$$

Atoms

- Oscillator Strength f [unitless]:

$$f = f_{\text{abs}} = f_{J' \leftarrow J''} = \frac{8\pi^2 m_e \nu}{3hc^2} \frac{S_{J', J''}}{2J'' + 1}, \quad (5.130)$$

- Line Strength S [D^2]:

$$S_{J', J''} \equiv \sum_{M'} \sum_{M''} |\langle J' M' | \boldsymbol{\mu} | J'' M'' \rangle|^2 \quad (5.112)$$

- Einstein A [s^{-1}]:

$$A_{J' \rightarrow J''} = \frac{16\pi^3 \nu^3 S_{J', J''}}{3\varepsilon_0 hc^3 (2J' + 1)} \quad (5.113)$$

- Einstein B [$m^3 J^{-1} s^{-2}$]: $(2J'' + 1)B_{J' \leftarrow J''} = (2J' + 1)B_{J' \rightarrow J''}$ (5.123)

- Absorption cross section [m^2]:

$$\sigma = \frac{2\pi^2 \nu S_{J', J''}}{3\varepsilon_0 hc (2J'' + 1)} g(\nu - \nu_{10}) \quad (5.118)$$

$$\sigma = \frac{A_{J' \rightarrow J''} \lambda^2 g(\nu - \nu_{10})}{8\pi} \frac{2J' + 1}{2J'' + 1} \quad (5.121)$$

Spectra databases

HITRAN

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The HITRAN Database

HITRAN is an acronym for **high-resolution transmission molecular absorption database**. HITRAN is a compilation of spectroscopic parameters that a variety of computer codes use to predict and simulate the transmission and emission of light in the atmosphere. The database is a long-running project started by the Air Force Cambridge Research Laboratories (AFCLR) in the late 1960's in response to the need for detailed knowledge of the infrared properties of the atmosphere. For additional background, see [Interview](#).

The HITRAN compilation, and its analogous database HITEMP (high-temperature spectroscopic absorption parameters), are now being developed at the Atomic and Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics under the continued direction of Dr. Laurence S. Rothman.

"HITRAN is like the human genome of gasses, if you will."

HITRAN 2004 Edition

Table 2
Description of the quantities present in the 100- and 160-character records of the *HITRAN* line-by-line section

Parameter	Meaning	Field length of the (100/160) character records	Type	Comments or units
<i>M</i>	Molecule number	2/2	Integer	<i>HITRAN</i> chronological assignment
<i>I</i>	Isotopologue number	1/1	Integer	Ordering within a molecule by terrestrial abundance
<i>v</i>	Vacuum wavenumber	12/12	Real	cm ⁻¹
<i>S</i>	Intensity	10/10	Real	cm ⁻¹ /(molecule cm ⁻²) at standard 296 K
<i>ℳ</i>	Weighted square of the transition moment	10/0	Real	Debye ² (for an electric dipole transition)
<i>A</i>	Einstein <i>A</i> -coefficient	0/10	Real	s ⁻¹
γ_{air}	Air-broadened half-width	5/5	Real	HWHM at 296 K (in cm ⁻¹ atm ⁻¹)
γ_{self}	Self-broadened half-width	5/5	Real	HWHM at 296 K (in cm ⁻¹ atm ⁻¹)
<i>E^l</i>	Lower-state energy	10/10	Real	cm ⁻¹
<i>n_{air}</i>	Temperature-dependence exponent for γ_{air}	4/4	Real	unitless, with $\gamma_{air}(T) = \gamma_{air}(T_0) \times (T_0/T)^{n_{air}}$
δ_{air}	Air pressure-induced line shift	8/8	Real	cm ⁻¹ atm ⁻¹ at 296 K
<i>V^u</i>	Upper-state "global" quanta	3/15	Hollerith	see Table 3
<i>V^l</i>	Lower-state "global" quanta	3/15	Hollerith	see Table 3
<i>Q^u</i>	Upper-state "local" quanta	9/15	Hollerith	see Table 4
<i>Q^l</i>	Lower-state "local" quanta	9/15	Hollerith	see Table 4
<i>Ierr</i>	Uncertainty indices	3/6	Integer	Accuracy for 3/6 critical parameters (<i>v</i> , <i>S</i> , γ_{air} / <i>v</i> , <i>S</i> , γ_{self} , γ_{air} , <i>n_{air}</i> , δ_{air}), see Table 5
<i>Iref</i>	Reference indices	6/12	Integer	References for 3/6 critical parameters (<i>v</i> , <i>S</i> , γ_{air} / <i>v</i> , <i>S</i> , γ_{self} , γ_{air} , <i>n_{air}</i> , δ_{air})
*	Flag	0/1	Character	Availability of program and data for the case of line mixing
<i>g^u</i>	Statistical weight of the upper state	0/7	Real	See details in Ref. [3]
<i>g^l</i>	Statistical weight of the lower state	0/7	Real	See details in Ref. [3]

Notes: For the field-length column, the notation A/B corresponds to the number of characters respectively in the 100- and 160-character records. For example, concerning the weighted square of the transition moment, the number of characters for *ℳ* is 10 in the case of the *HITRAN* 2000 edition [1], and 0 in the case of the *HITRAN* 2004 edition since this parameter has been replaced by the Einstein *A*-coefficient.

39 molecules, including isotopologues, several 100k lines

Rothman et al (2005) J. Quant. Spec. & Rad. Trans. 96, 139-204

Table 6
Summary of isotopologues represented in *HITRAN*

No.	Molecule	Isotopologue (AFGL notation)	Fractional abundance	Spectral coverage (cm ⁻¹)	Number of lines
1	H ₂ O	161	0.997317	0-25233	36114
		181	0.00199983	0-14519	9548
		171	0.000372	10-11335	6120
		162	0.00031069	0-7514	9628
		182	0.00000623	0-3825	161
		172	0.00000116	1234-1599	175
2	CO ₂	626	0.98420	442-12785	27979
		636	0.01106	497-8105	8836
		628	0.0039471	0-8133	13445
		627	0.000734	0-6962	7739
		638	0.0004434	567-4947	2312
		637	0.0000825	584-3642	1593
		828	0.000039573	615-3670	72
		728	0.0000147	626-2359	288
3	O ₃	666	0.992901	0-4061	183785
		668	0.00398194	0-2114	21718
		686	0.00199097	1-2075	8937
		667	0.000740	0-2122	65106
		676	0.000370	0-2101	31935
4	N ₂ O	446	0.990333	0-7797	33066
		456	0.0036409	5-5086	4222
		546	0.0036409	4-4704	4592
		448	0.00198582	542-4672	4250
		447	0.000369	550-4430	1705
5	CO	26	0.98654	3-8465	917
		36	0.01108	3-6279	780
		28	0.0019782	3-6267	760

NIST: Atomic Spectra Database - home page - Microsoft Internet Explorer

Address: <http://physics.nist.gov/PhysRefData/ASD/index.html>

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Physical Reference Data

NIST ATOMIC SPECTRA DATABASE

Version 3

Welcome to the NIST Atomic Spectra Database, NIST Standard Reference Database #78. The spectroscopic data may be selected and displayed according to wavelengths or energy levels by choosing one of the following options:

LINES Spectral lines and associated energy levels displayed in wavelength order with all selected spectra intermixed or in multiplet order. Transition probabilities for the lines are also displayed where available.

LEVELS Energy levels of a particular atom or ion displayed in order of energy above the ground state.

NIST Chemistry webbook

<http://webbook.nist.gov/chemistry/>

Search for Species Data by Chemical Name

Please follow the steps below to conduct your search ([Help](#)):

1. Enter a chemical species name or pattern (e.g., methane, *2-hexene)
2. Select the desired units for thermodynamic data:
 SI calorie-based
3. Select the desired type(s) of data:

Thermodynamic Data	Other Data
<input type="checkbox"/> Gas phase	<input type="checkbox"/> IR spectrum
<input type="checkbox"/> Condensed phase	<input type="checkbox"/> THz IR spectrum
<input type="checkbox"/> Phase change	<input type="checkbox"/> Mass spectrum
<input type="checkbox"/> Reaction	<input type="checkbox"/> UV/Vis spectrum
<input type="checkbox"/> Ion energetics	<input type="checkbox"/> Gas Chromatography
<input type="checkbox"/> Ion cluster	<input type="checkbox"/> Vibrational & electronic energy levels
	<input type="checkbox"/> Constants of diatomic molecules
	<input type="checkbox"/> Henry's Law
4. Press here to search:

The screenshot shows a Microsoft Internet Explorer browser window with the following details:

- Title Bar:** UV-VIS Absorption Spectra of Gaseous Molecules and Radicals: Introduction - Microsoft Internet Explorer
- Address Bar:** http://www.atmosphere.mpg.de/enid/2295
- Page Content:**
 - Header:** MPI-Mainz-UV-VIS Spectral Atlas of Gaseous Molecules. A Database of Atmospherically Relevant Species, Including Numerical Data and Graphical Representations. Hannelore Keller-Rudek, Geert K. Moortgat. Max-Planck-Institut für Chemie, Atmospheric Chemistry Division, Mainz, Germany.
 - Left Navigation Menu:** Introduction (selected), Presentation, Catalogue, Quick Search, Contact, Impressum.
 - Main Content:**
 - Introduction**
 - Scientific background**
 - Database at MPI-Mainz**
- Status Bar:** Done, Internet