

Molecular linelists for stellar spectra Manual

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1 Introduction

This website <http://www.astro.ulb.ac.be/~spectrotools> is intended to gather the molecular linelists useful for stellar spectroscopists. Although there are already several websites collecting many molecules (e.g., HITRAN), few of them include electronic transitions useful in the optical and NIR. The other goal of the "spectrotools" website is to achieve an homogeneous and high-quality set of data compatible with stellar-spectroscopy standards, but still providing useful information for chemists, including extensive compilations of laboratory measurements. Actually, the laboratory measurements having a better precision than what the best astronomical spectrographs can achieve, the line positions provided are from laboratory measurements whenever they are available.

Currently only diatomic molecules are included, but we provide some useful links to other datasets at the bottom of the homepage.

2 How to download the data

1. Select one or more molecules in the "molecules" field.
2. Select the requested output values and their corresponding units in the "output format" field.
3. Possibly apply some selection criteria in the "filter" field. The unit automatically matches the one chosen in the "output format" field. Accepted values are numerical (1, 2593.5, 10e6...) or logical (=, != ...). Note that "0" values should always be written as float like "0."
4. Click the "send query" button.

A partial line list is displayed but the full list is downloadable as a tarball including a ReadMe file. The ReadMe file contains the reference of the linelist, the version of the linelist downloaded (for future reference) and recommended values for the dissociation energy and partition function. WARNING: It is crucial for spectrum synthesis that partition functions are compatible with the line lists are used. Note that the tarball file is named after the date of query, so that any version of the linelist can be tracked.

3 Description of the columns

Molecule molecule identification

Isotopomer isotopomer identification

Line Position position of the transition in air; the laboratory measurement is preferred to the calculated one whenever available.

Strength line strength value. It can be provided as either Einstein coefficient (A_{ij} in s), oscillator strength (gf , no unit), or log of oscillator strength ($\log gf$, no unit)

Lower Level energy of the lower level in cm^{-1} , eV or *Hartree*

v'' vibrational quantum number of the lower level

J'' rotational angular momentum quantum number of the lower level

N'' rotational angular momentum number of the lower level

Lower parity symmetry of the lower level (e or f)

Upper Level energy of the upper level in cm^{-1} , eV or *Hartree*

v' vibrational quantum number of the upper level

J' rotational angular momentum number of the upper level

N' rotational angular momentum number of the upper level

Upper parity symmetry of the upper level (*e* or *f*)

Γ_{rad} or $1/\Gamma_{rad}$ radiative broadening of the transition in s^{-1} or radiative lifetime of the upper level in *s*.

Lower state lower electronic state identification (X, A, B, a ,b ...)

Upper state upper electronic state identification (X, A, B, a ,b ...)

Branch branch of the transition (P, Q, or R)

obs-calc whenever a laboratory measurement exists, difference between measurement and calculation

Reference whenever a laboratory measurement exists, short reference of the laboratory measurement. The full reference is detailed in each molecule section.

4 Conversion formulae used

Most of the formulae can be found in Larsson, M. 1983, A&A, 128, 291 and the conversion factors can be found on the web. Here is a summary of the ones employed in the database.

- energy levels

$$1 \text{ cm}^{-1} = 4.5563352528 \times 10^{-6} \text{ Hartree} = 1.23984193 \times 10^{-4} \text{ eV}$$

- line positions

The line positions in vacuum are simply obtained by subtracting the energy of the upper level by the energy of the lower level. The conversion from vacuum to air is given by

$$\lambda_{\text{air}}(\text{\AA}) = \frac{\lambda_{\text{vacuum}}(\text{\AA})}{\text{nindex}}$$

with

$$\begin{aligned} \text{nindex} = & 1.0 + 10^{-8} \times (8342.13 + 2406030/(130 - ((1/\lambda) \times 10^{-4})^2) \\ & + 15997/(38.9 - ((1/\lambda) \times 10^{-4})^2)) \end{aligned}$$

Reminder:

1 Å = 10 nm

1 Å = 100,000,000/cm⁻¹

- intensities

$$gf = (2J'' + 1) \times f_{J''J'} = \frac{m_e \epsilon_0 c}{2\pi e^2 \nu^2} (2J'' + 1) A_{J''J'},$$

$f_{J''J'}$ being the absorption oscillator strength and ν the line position in vacuum in cm⁻¹.

- lifetime or Γ_{rad}

It is only provided for a level for which all the possible transitions are known. Otherwise a dummy value is given.

$$\Gamma_{\text{rad}} = 1/\tau_{v'J'}^{\text{rad}},$$

where $\tau_{v'J'}^{\text{rad}}$ is obtained via

$$\tau_{v'J'} = \left(\sum_{v''J''} A_{v'J'v''J''} \right)^{-1},$$

where $A_{v'J'v''J''}$ is the Einstein coefficient of a transition.

Note that for some molecules like CH, predissociation may occur for some levels. In this case, the Γ_{rad} value provided corresponds to

$$\Gamma_{\text{rad}} = 1/\tau_{v'J'}^{\text{rad}} + 1/\tau_{v'J'}^{\text{predissoc}},$$

5 Contact

In case of questions or problems, please contact: Thomas Masseron (tpm40 at ast.cam.ac.uk) or Alain Jorissen (alain.jorissen at ulb.ac.be)

6 Molecule(s) currently available

6.1 CH

This list encompasses the transitions of the four lowest states of the molecule, i.e., A-X, B-X, C-X and the rovibrational transitions X-X.

Reference: "CH in stellar atmospheres: an extensive linelist", Masseron, T., Plez, B., Van Eck, S., Colin, R., Daoutidis, I., Godefroid, M., Coheur, P.-F.,

Bernath, P., Jorissen, A., and Christlieb, N. 2014, A&A, accepted

Following the formula $\ln(Q) = \sum_0^2 a_i \ln(T)^i$, the recommended coefficients for the partition function are $a_0 = 11.00608809$, $a_1 = -2.68892131$ and $a_2 = 0.27091654$.

Recommended dissociation energy : $D00$ (CH) = 3.466 eV (Kumar et al. 1997, JCP 109, 10, 3824)

Full references for laboratory measurements:

Bembenek, Z., Ke, R., & Rytel, M. 1997, Journal of Molecular Spectroscopy, 183, 1

Bernath, P. F., Brazier, C. R., Olsen, T., et al. 1991, Journal of Molecular Spectroscopy, 147, 16

Colin, R. & Bernath, P. F. 2010, Journal of Molecular Spectroscopy, 263, Heimer, T. 1932, Zeitschrift fur Physik, 78, 771

Herzberg, G. & Johns, J. W. C. 1969, ApJ, 158, 399

Kepa, R. 1996, Journal of Molecular Spectroscopy, 178, 189

Kumar, A., Hsiao, C.-C., Hung, W.-C., & Lee, Y.-P. 1998, JCP, 109, 3824

Li, X., Kumar, A., Hsiao, C.-C., & Lee, Y.-P. 1999, The Journal of Physical Chemistry A, 103, 6162

Melen, F., Grevesse, N., Sauval, A. J., et al. 1989, Journal of Molecular Spectroscopy, 134, 305

Para, A. 1996, Journal of Physics B Atomic Molecular Physics, 29, 5765

Ubachs, W., Meyer, G., Ter Meulen, J. J., & Dymanus, A. 1986, JCP, 84, 3032

Zachwieja, M. 1995, Journal of Molecular Spectroscopy, 170, 285

Zachwieja, M. 1997, Journal of Molecular Spectroscopy, 182, 18

7 Acknowledgments

Please use as reference the paper listed in the section referring to the corresponding molecule.