Steps for Converting Intensities
from the JPL (or CDMS) Catalog to HITRAN Intensities

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This short guide is written to provide users with the steps needed for the conversion of intensities between the HITRAN database [1] and the Jet Propulsion Laboratory (JPL) [2] or Cologne Database for Molecular Spectroscopy (CDMS) [3] spectral databases. The JPL and CDMS lists, which are identical in their intensity formalisms, provide base 10 logarithms of the integrated intensity at 300 K (in nm^2MHz), while HITRAN gives the intensity at 296 K [in cm^{-1}/(molecule/cm^2)]. Apart from these differences, there are certain differences in the formalism of intensities and this guide provides steps for the most accurate conversion. If accuracy better than 2% is not required, it is fairly safe to use an approximation given in Section 5 below. Some other intensity unit conversions are described in the textbook of Bernath [4]. An appendix is also provided at the end of this guide that gives definitions of some of the quantities in the databases.

1.   Unit conversion

The JPL [2] and CDMS [3] catalogs use nm^2MHz as units of intensity. In order to convert to HITRAN [1] units [cm^{-1}/(molecule/cm^2)], one has to divide the JPL intensity (*not its logarithm*) by a factor related to the speed of light, namely $2.99792458 \times 10^{18}$. It should be recalled that the HITRAN units were constructed with application to atmospheric transmission calculations in mind, hence the emphasis on writing the units as *wavenumber per column density* and not simplifying it to the equivalent cm/molecule.

$$I_{JPL}(cm^{-1}/molecule \times cm^{-2}) = \frac{I_{JPL}(nm^2MHz)}{2.99792458 \times 10^{18}} ,$$

(1)

2.   Isotopic abundance

The JPL and CDMS catalogs assume 100% abundance of every isotopologue, whereas the HITRAN database incorporates a terrestrial abundance scaling. Therefore one has to multiply the JPL (CDMS) intensity by the isotopologue abundance value (I_a) assumed by HITRAN. For the isotopic abundances used in HITRAN, see for example Table 1 in Ref. [5].

$$S_{JPL} = I_a \frac{I_{JPL}(nm^2MHz)}{2.99792458 \times 10^{18}} ,$$

(2)

3.   Scaling of the partition sum

After conversion to cm^{-1}/(molecule/cm^2) and scaling by isotopic abundance, one needs to consider the intensity defined in the JPL catalog, S_{JPL}, which is given by:

$$S_{JPL}(T) = \frac{g'_{JPL}}{Q_{JPL}(T)} \frac{A}{8\pi c v_0^2} e^{-\frac{hcE''}{k_BT}} (1 - e^{-\frac{hcv_0}{k_BT}}),$$

(3)

where g' is a statistical weight of the upper level and $Q(T)$ is a total partition sum. The other terms in Eq. (3) are defined in the appendix of Ref. [6]. The labels "*JPL*" refer to the fact that in some cases in the JPL and CDMS catalogs the common factors are factored out in g' and $Q(T)$. This common factor is a state-independent statistical weight g_i, which is not ignored in the HITRAN database. Nevertheless it is obvious that

$$\frac{g'_{JPL}}{Q_{JPL}(T)} \approx \frac{g'_{HIT}}{Q_{HIT}(T)} . \tag{4}$$

The use of the "$\approx$" refers to the fact that partition sums are not calculated exactly the same way in JPL and HITRAN. Unlike HITRAN, the partition sums in the JPL catalog do not include the "vibrational" contribution in most cases. However this contribution may be significant for molecules possessing low vibrational modes. Therefore it is recommended that one scale the JPL intensities to HITRAN formalism in the following manner:

$$S_{HIT}(T) = S_{JPL}(T) \frac{Q_{JPL}(T)}{Q_{HIT}(T)} \frac{g'_{HIT}}{g'_{JPL}} . \tag{5}$$

For 300K, which is the reference temperature in the JPL and CDMS databases,

$$S_{HIT}(300) = I_a \frac{I_{JPL}(nm^2MHz)}{2.99792458\times10^{18}} \frac{Q_{JPL}(300)}{Q_{HIT}(300)} \frac{g'_{HIT}}{g'_{JPL}} . \tag{6}$$

It is not always immediately obvious whether or not $g'_{JPL} = g'_{HIT}$. Therefore it is always useful to obtain a ratio between partition sums in JPL and HITRAN at the same temperature and then round that ratio to an integer, which will be the ratio between statistical weights in HITRAN and JPL.

The partition sums for HITRAN database are available in the file parsum.dat that is distributed with the database. The partition sums for 296K are also listed in Table 1 of Ref. [5]. The partition sums (or their logarithms) for the JPL and CDMS catalogs are provided in the following websites:

http://spec.jpl.nasa.gov/ftp/pub/catalog/catdir.cat

and

http://www.ph1.uni-koeln.de/vorhersagen/catalog/partition_function.html

4. Temperature adjustment

All intensities in the JPL and CDMS catalogs are calculated at 300 K, whereas HITRAN gives intensities at 296 K.

By definition

$$S_{HIT}(300) = \frac{g'_{HIT}}{Q_{HIT}(300)} \frac{A}{8\pi c v_0^2} e^{-\frac{hcE''}{k_B 300}}(1 - e^{-\frac{hcv_0}{k_B 300}}) \tag{7}$$

and

$$S_{HIT}(296) = \frac{g'_{HIT}}{Q_{HIT}(296)} \frac{A}{8\pi c v_0^2} e^{-\frac{hcE''}{k_B 296}}(1 - e^{-\frac{hcv_0}{k_B 296}}). \tag{8}$$

Combining the last two equations one obtains

$$S_{HIT}(296) = S_{HIT}(300) \exp\left[\frac{hcE''}{k_B}\left(\frac{1}{300} - \frac{1}{296}\right)\right]\left[\frac{1 - e^{-\frac{hcv_0}{k_B 296}}}{1 - e^{-\frac{hcv_0}{k_B 300}}}\right]\frac{Q_{HIT}(300)}{Q_{HIT}(296)}, \tag{9}$$

or using Eq. (5)

$$S_{HIT}(296) = I_a \frac{I_{JPL}\,(nm^2 MHz)}{2.99792458\times10^{18}} \frac{Q_{JPL}(300)}{Q_{HIT}(300)} \frac{g'_{HIT}}{g'_{JPL}} \exp\left[\frac{hcE''}{k_B}\left(\frac{1}{300} - \frac{1}{296}\right)\right]\left[\frac{1 - e^{-\frac{hcv_0}{k_B 296}}}{1 - e^{-\frac{hcv_0}{k_B 300}}}\right]\frac{Q_{HIT}(300)}{Q_{HIT}(296)}$$

$$= I_a \frac{I_{JPL}\,(nm^2 MHz)}{2.99792458\times10^{18}} \exp\left[\frac{hcE''}{k_B}\left(\frac{1}{300} - \frac{1}{296}\right)\right]\left[\frac{1 - e^{-\frac{hcv_0}{k_B 296}}}{1 - e^{-\frac{hcv_0}{k_B 300}}}\right]\frac{Q_{JPL}(300)}{Q_{HIT}(296)} \frac{g'_{HIT}}{g'_{JPL}}. \tag{10}$$

5.   Approximate temperature adjustment

It should be noted that in the majority of cases in the literature, step 3 is omitted and the last equation in step 4 can be approximated by

$$S_{HIT}(296) \cong I_a \frac{I_{JPL}\,(nm^2 MHz)}{2.99792458\times10^{18}} \exp\left[\frac{hcE''}{k_B}\left(\frac{1}{300} - \frac{1}{296}\right)\right]\left[\frac{1 - e^{-\frac{hcv_0}{k_B 296}}}{1 - e^{-\frac{hcv_0}{k_B 300}}}\right]\left(\frac{300}{296}\right)^n, \tag{11}$$

where $n = 1$ for linear molecules and $n = 3/2$ for nonlinear molecules. Sometimes an even coarser approximation is used:

$$S_{HIT}(296) \cong I_a \frac{I_{JPL}\,(nm^2 MHz)}{2.99792458\times10^{18}} \exp\left[\frac{hcE''}{k_B}\left(\frac{1}{300} - \frac{1}{296}\right)\right]\left(\frac{300}{296}\right)^{n+1}. \tag{12}$$

Appendix A. Definitions and Units used in HITRAN

Variable	Definition	Units	Comments
g	**Statistical Weight**	**Unitless**	**Includes state-independent factors in HITRAN, see Ref. [5]**
Q	**Partition Sum**	**Unitless**	
S	**Intensity**	**cm^{-1}/(molecule/cm^2)**	**HITRAN units, see text**
I_a	**Isotopologue Abundance**	**Unitless**	**Based on terrestrial values of atoms given in Ref. [7]**
A	**Einstein A-coefficient**	**s^{-1}**	**See Ref. [5]**
v	**Transition wavenumber**	**cm^{-1}**	**Line position in vacuum**
E''	**Lower-state energy**	**cm^{-1}**	
h	**Planck constant**	**erg s**	**6.626069×10^{-27}**
c	**Speed of light**	**cm s^{-1}**	**$2.99792458 \times 10^{10}$**
k_B	**Boltzmann constant**	**erg K^{-1}**	**$1.3806505 \times 10^{-16}$**
T	**Temperature**	**K**	

Note: The databases do not strictly use the International System of Units (SI). The units have been chosen for historical, transmission-algorithm structure, and/or instrument-related reasons.

References

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