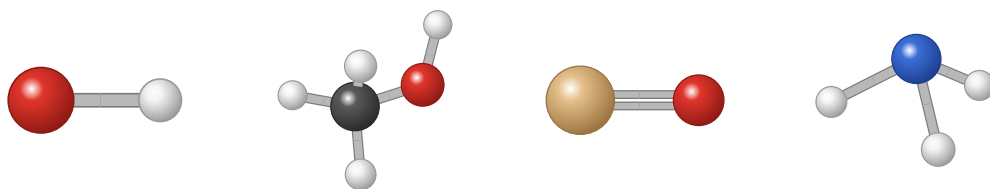


linecat

Viewer for CDMS spectral line catalogs



User Guide

Version 0.13.0

Vahid Anari

vahid.anari8@gmail.com

<https://github.com/vahid-anari/linecat>

Contents

1	Getting started	2
1.1	Installing	2
1.2	Starting with a double-click	2
1.3	Updating	2
1.4	First start and the built-in catalogs	2
2	The main window	3
2.1	Molecule	3
2.2	Quantum-number filters	4
2.3	Frequency range	4
2.4	The table	4
3	The energy-level diagram	4
3.1	Levels, transitions and the transition table	5
3.2	Tabs and secondary transitions	5
3.3	Zoom and real scale	6
3.4	L ^A T _E X rendering	6
3.5	Saving	6
4	Converting CDMS catalogs	7
5	Command line	7
6	Adding a species	7
	References	8
A	Equations	9
A.1	Constants and conversion factors	9
A.2	Conversion relations (Section A.6)	9
A.3	Intensity	9
A.4	Spontaneous emission rate	9
A.5	Transition dipole moment	10
A.6	Derivation of the conversion relations	10
A.7	Derivation of the radiative quantities	10

1 Getting started

linecat (Line Catalog Explorer) shows the spectral line catalogs of the Cologne Database for Molecular Spectroscopy (CDMS) as a table you can filter by quantum numbers and frequency, and draws the energy levels and transitions of any selection as a diagram that can be saved as PDF or exported as L^AT_EX commands.

1.1 Installing

linecat needs Python 3.10 or newer. Install it from PyPI with `pipx`, which gives it an environment of its own,

```
pipx install linecat
```

or with `pip install linecat` in an environment of your choice, and start it with `linecat`. For development, clone the repository and run `pip install -e .` in it.

L^AT_EX is optional: with a L^AT_EX installation the filter labels and the diagram can be rendered with real L^AT_EX (Section 3.4); without it linecat uses Matplotlib's built-in math rendering.

1.2 Starting with a double-click

Run once

```
linecat install-app
```

This adds *Line Catalog Explorer* with its icon to the Applications folder (`~/Applications`, also in Launchpad and Spotlight; drag it to the Dock to keep it there), to the Start menu on Windows or to the applications menu on Linux. It starts the linecat of the Python the command was run with, and keeps the `PATH` of that terminal so that L^AT_EX is found as from the terminal. After an update linecat refreshes the launcher by itself. `linecat install-app --remove` removes it; run `linecat install-app` again if you move or replace that Python.

1.3 Updating

A couple of seconds after it starts, linecat asks PyPI in the background whether a newer version exists; if so it shows what is new (from the release notes) and offers **Update Now**, which runs `pipx upgrade linecat` or `pip install -U linecat`, whichever matches the installation, and then offers a restart. Without an internet connection nothing is shown. **Help** **Check for Updates...** (`Cmd+U`) checks on request and also reports when linecat is up to date. In a terminal, `linecat update --check` shows whether there is a newer version, and `linecat update` installs it (it asks first). A copy installed from a clone with `pip install -e` is updated with `git pull` instead.

1.4 First start and the built-in catalogs

linecat ships the CDMS catalog files of four molecules: OH, CH₃OH, SiO and NH₃. On the first start, and after every update of linecat, it converts them into CSV catalogs; this takes about a second. The CSV files are written read-only to the application-data folder (on macOS `~/Library/Application Support/linecat/catalogs/`); if one goes missing it is rebuilt at the next start.

Open one with **File** **Open Built-in Catalog** or with `Cmd+1–Cmd+4` (OH, CH₃OH, SiO, NH₃). **File** **Open Built-in Catalog** **Show Built-in Catalogs Folder** shows the folder in the Finder.

Note

Any other catalog in the same CSV format opens with File>Open Catalog... (Cmd+O); the last five are listed under File>Open Recent. Section 4 explains how to make such a CSV from a CDMS .cat file.

2 The main window

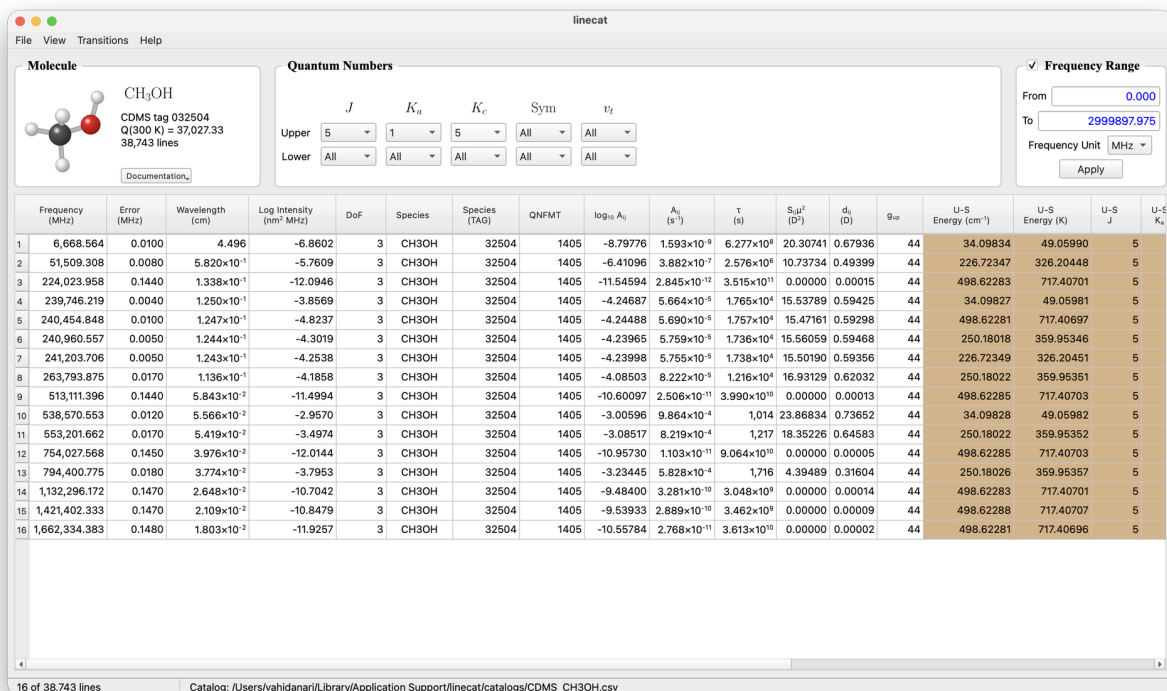


Figure 1: The main window with the built-in CH₃OH catalog, filtered to the transitions from the upper level 5_{1,5}; the first line is the 6.7 GHz methanol maser line.

The top row holds three boxes: the molecule, the quantum-number filters and the frequency range. Below them is the table of the lines that pass the filters. The status bar shows how many lines are shown out of how many in the catalog, and the path of the catalog.

2.1 Molecule

The *Molecule* box shows a picture of the molecule, its name, the CDMS tag(s) of the catalog entries, the partition function Q at 300 K used for the line strengths, and the number of lines. *Documentation* lists the CDMS documentation of the entries (for OH: $v = 0, 1$ and 2 , Figure 2); it is included with linecat and opens without an internet connection. The general CDMS documents are under Help>CDMS Documentation. The User Guide opens with Cmd+?, and Help>About Line Catalog Explorer shows the version, the CDMS credits and the libraries the app is built on.

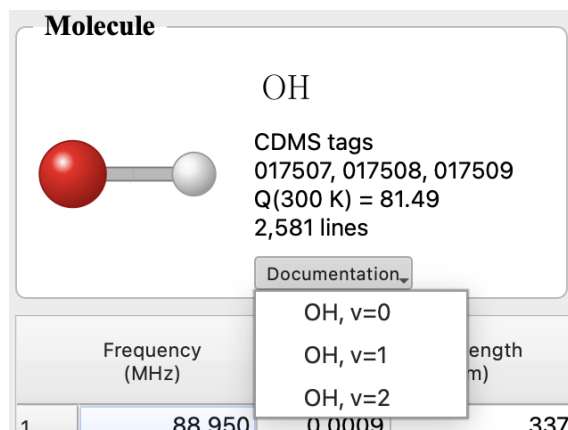


Figure 2: The Molecule box of the OH catalog with its documentation menu.

2.2 Quantum-number filters

Quantum Numbers has one column per quantum number of the molecule and two rows, for the upper and the lower state. Each list offers the values that still occur among the lines that pass the other filters, so the choices narrow as you select. All switches a filter off. **View**▷**Reset Filters** sets every filter back to All and the frequency range back to the whole catalog.

2.3 Frequency range

From and *To* set the range in the unit chosen under *Frequency Unit*: Hz, KHz, MHz, GHz or THz, or a wavelength in Å, nm, µm, mm or m. **Apply** applies the range. The check box in the title switches the range off without losing the values typed in.

2.4 The table

Click a column header to sort by that column; click again to reverse the order. Right-click a header for the column menu:

- Column Color... , No Column Color, Default Column Color;
- Text Color... , Default Text Color;
- Alignment (left, centre, right or the default);
- Hide This Column, Choose Columns... (also in View);
- Reset Colors;
- Font... , Default Font.

These settings are remembered between sessions. **File**▷**Export Table as CSV...** (Cmd+E) writes the filtered lines in the current sort order with all columns, hidden ones included, so the file opens again in linecat as a catalog of its own.

3 The energy-level diagram

Transitions▷**Show Energy-Level Diagram** (Cmd+D) draws the lines shown in the table as a diagram of their energy levels and transitions. Above 50 transitions linecat asks before drawing, since large diagrams take longer to draw; **View**▷**Large Diagram Warning...** in the main window changes the number or switches the question off.

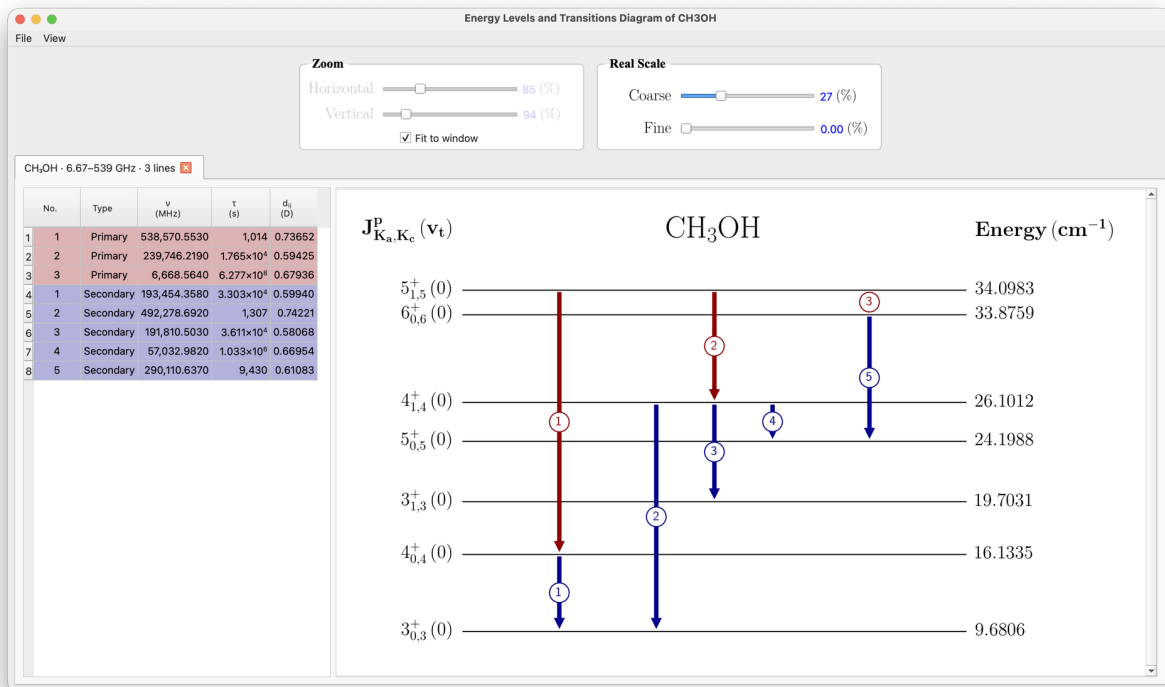


Figure 3: The diagram window: transition table on the left, diagram on the right. CH_3OH , three primary transitions (red) with their secondary transitions (blue), drawn with $\text{\LaTeX}$ at 27 % real scale.

3.1 Levels, transitions and the transition table

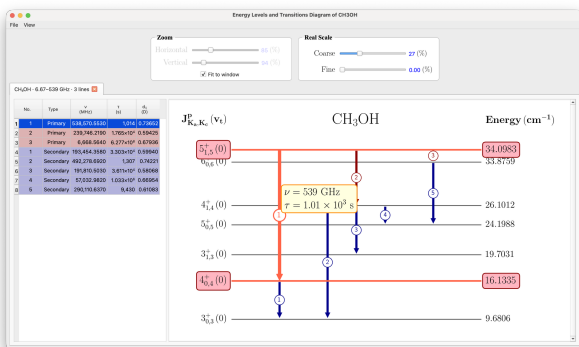
Each level is a horizontal line, labelled with its quantum numbers on the left and its energy (cm^{-1}) on the right; each transition is a numbered arrow from the upper to the lower level. The table on the left lists the same transitions with their frequency ν , lifetime τ and transition dipole moment d_{ij} ; rows are coloured by type.

The diagram is as large as its content needs: every level gets at least one line of text, and transitions that would touch are moved apart. Groups of transitions that lie at different heights share a column, so a large selection grows downwards rather than sideways.

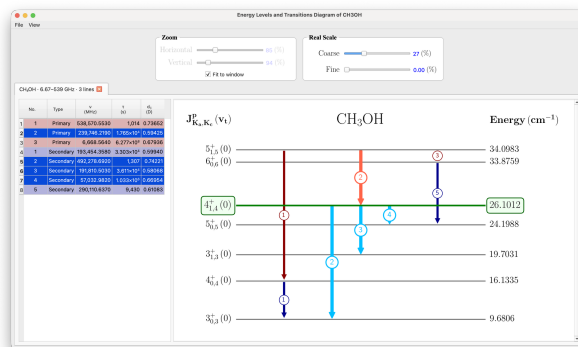
Hovering over an arrow highlights it, its two levels and its row in the table, and shows ν and τ next to the pointer, on the side towards the middle of the diagram; hovering over a level highlights the transitions that start or end on it (Figure 4). The other way round, selecting rows in the table highlights their arrows.

3.2 Tabs and secondary transitions

The first tab is named after the selection, e.g. $\text{NH}_3 \cdot 18.4\text{--}22.2 \text{ GHz} \cdot 70 \text{ lines}$. Double-click an arrow to open a new tab, *From (level)*, with all transitions that start from its lower level. **View** $\triangleright$ **Secondary Transitions** adds to the current tab the transitions that leave the lower levels of the primary ones (drawn in blue). Each tab keeps its own settings; the first tab cannot be closed.



(a) over an arrow



(b) over a level

Figure 4: Hovering. (a) The arrow, its two levels and its table row light up, with ν and τ beside the pointer. (b) Every transition that starts or ends on the level lights up, in the diagram and in the table.

3.3 Zoom and real scale

Fit to window (check box under the zoom sliders, or View▷Fit to Window, Cmd+0) scales the diagram to the space beside the table and follows the window when it is resized, but never below the size at which the labels stay apart: a larger diagram scrolls instead. Switch it off to set the *Horizontal* and *Vertical* zoom by hand.

On a trackpad, pinch to zoom in and out around the point between your fingers, as in a PDF viewer; with a mouse, turn the wheel while holding Cmd. Both switch Fit to window off and move the zoom sliders along; a two-finger double tap switches it on again. Two fingers dragging, or the wheel, scroll the diagram as before.

By default the levels are evenly spaced, in order of energy. The *Real Scale* sliders move them towards their true energies: *Coarse* (0–95 %) and *Fine* (0–5 %) add up to the fraction of the true spacing used, 100 % being energies to scale.

3.4 L^AT_EX rendering

View▷Use L^AT_EX for Rendering redraws the diagram with L^AT_EX. The labels are rendered in the background behind a progress dialog the first time; L^AT_EX keeps the results, so later drawings are quick. In the main window, View▷Use L^AT_EX for Labels does the same for the filter labels.

3.5 Saving

File▷Save Figure as PDF... (Cmd+S) writes a two-page PDF: the diagram, then the transition table.

File▷L^AT_EX Commands... lists the levels and transitions of the tab as two L^AT_EX commands, for drawing your own diagram; Copy puts them on the clipboard and Save... writes a .tex file. For the diagram of Figure 3:

```
% CH3OH · 6.67–539 GHz · 3 lines -- linecat 0.10.3
\Level{L1}{$3_{0, 3}\sim\{+}\,(0)$}{9.6806}
...
```

```
\Level{L7}{\$5_{1, 5}~{+}}\,(0)\${34.0983}
\Transition{pri}{1}{L7}{L2}{538570.553}{1.014e3}
...
\Transition{sec}{1}{L2}{L1}{193454.358}{3.303e4}
```

Command	Arguments
<code>\Level</code>	name, label (as in the diagram), energy in cm^{-1}
<code>\Transition</code>	type (<code>pri</code> or <code>sec</code>), number, upper and lower level, frequency in MHz, lifetime in s

Levels are named L1, L2, ... from the lowest energy up, so the transitions refer to them by name; numbers are the catalog's. linecat does not define the two commands: write them as you like, for instance with TikZ, storing each level's position under its name with `\coordinate` and drawing an arrow between two names; `\num` from `siunitx` prints the numbers. A level that the catalog lists only as an upper state gets the energy of its first line (lower energy + $h\nu$); the others get the lower-state energy as listed by CDMS.

4 Converting CDMS catalogs

The built-in catalogs cover OH, CH₃OH, SiO and NH₃. To use a newer CDMS release, download the `.cat` files of the entries from <https://cdms.astro.uni-koeln.de/> and put them in a folder per species, named as in linecat (OH/c017507.cat, ...). Then choose File▷Convert CDMS Catalogs... and select either the folder that holds the species folders or a single species folder. The CSV files are written next to the `.cat` files; a progress dialog and a short report follow. A single converted catalog opens by itself.

For each line the converter computes the wavelength, the upper-state energy, both energies in kelvin, the Einstein coefficient A_{ij} , the lifetime $\tau = 1/A_{ij}$, the line strength $S_{ij}\mu^2$ and the transition dipole moment d_{ij} , using the relations in Appendix A.

5 Command line

<code>linecat</code>	open the viewer
<code>linecat CATALOG.csv</code>	open a catalog at start
<code>linecat convert</code>	convert the built-in CDMS files (into the current folder)
<code>linecat convert OH SiO</code>	convert some species
<code>linecat convert -catalogs DIR</code>	convert your own <code>.cat</code> files in DIR
<code>... -output-dir OUT</code>	write the CSV files to OUT
<code>linecat update</code>	update from PyPI (asks first)
<code>linecat update -check</code>	only show whether a newer version exists
<code>linecat install-app</code>	add the app to Applications / the Start menu
<code>linecat install-app -remove</code>	remove it again
<code>linecat -version</code>	show the version

6 Adding a species

A species is described in `linecat/molecules.py` by a `MoleculeInfo`: its name, the `.cat` files, the partition function and temperature, the quantum numbers of the CDMS format and the filters

shown in the window. Two functions complete it: `<name>_standardize(df, prefix)`, which turns the raw quantum numbers into the ones shown (for example Ω and the parity of OH), working on whole columns of the table, and `<name>_label(df, prefix)`, which writes the level labels of the diagram. Register the species in `REGISTRY` and put its `.cat` files, the CDMS documentation PDFs of its entries and a picture `<SPECIES>.svg` in `linecat/data/molecules/<SPECIES>/.svg`.

References

The catalog data come from the Cologne Database for Molecular Spectroscopy; please cite

- H. S. P. Müller et al., 2001, *Astron. Astrophys.* 370, L49;
- H. S. P. Müller et al., 2005, *J. Mol. Struct.* 742, 215;
- C. P. Endres et al., 2016, *J. Mol. Spectrosc.* 327, 95.

The catalog format and the SPCAT program are described by H. M. Pickett et al., 1998, *J. Quant. Spectrosc. Radiat. Transfer* 60, 883. The CDMS documentation pages included with linecat are reproduced with credit to CDMS.

A Equations

These are the relations `linecat convert` uses to derive the radiative quantities of each line from the CDMS catalog entries (frequency, intensity at $T = 300$ K, lower-state energy, upper-state degeneracy and the partition function $Q_{rs}(300\text{ K})$). *All equations are in cgs units.*

A.1 Constants and conversion factors

$$\begin{aligned}
 h &= 6.62607015 \times 10^{-27} \text{ erg} \cdot \text{s} \\
 k_B &= 1.380649 \times 10^{-16} \text{ erg} \cdot \text{K}^{-1} \\
 c &= 2.99792458 \times 10^{10} \text{ cm} \cdot \text{s}^{-1} \\
 1 \text{ D} &= 10^{-18} \text{ statC} \cdot \text{cm} \\
 1 \text{ erg} &= \text{statC}^2 \cdot \text{cm}^{-1} \\
 {}^x S_{ij} \mu_x^2 &= g_i \mu_{ij}^2
 \end{aligned} \tag{1}$$

A.2 Conversion relations (Section A.6)

Frequency (MHz $\rightarrow$ cm $^{-1}$):

$$\left[\frac{\tilde{\nu}}{\text{cm}^{-1}} \right] = 3.33564095 \times 10^{-5} \left[\frac{\nu}{\text{MHz}} \right] \tag{2}$$

Energy (cm $^{-1} \rightarrow$ K):

$$\left[\frac{T}{\text{K}} \right] = 1.43877688 \left[\frac{\tilde{\nu}}{\text{cm}^{-1}} \right] \tag{3}$$

A.3 Intensity

The intensity $I(T)$ is calculated according to

$$I(T) = \frac{8\pi^3}{3hc} \nu S_g \mu_g^2 \frac{e^{-E''/kT} - e^{-E'/kT}}{Q_{rs}(T)} \tag{4}$$

with ν and S_g the line frequency and strength, μ_g the dipole moment along the molecular g -axis, E'' and E' the lower and upper state energy, and Q_{rs} the rotation-spin partition function at the temperature T . With $I(T)$ in nm ^{2} MHz, ν in MHz and μ_g in D one obtains (Section A.7)

$$I(T) = \nu S_g \mu_g^2 \frac{e^{-E''/kT} - e^{-E'/kT}}{Q_{rs}(T)} 4.16237896 \times 10^{-5} \text{ nm}^2 \text{ MHz} \tag{5}$$

A.4 Spontaneous emission rate

The average spontaneous emission rate from the upper states into the lower states is

$$A = \frac{8\pi\nu^2}{c^2} I(T) \left(\frac{Q_{rs}(T)}{g_{up}} \right) \left[e^{-E''/kT} - e^{-E'/kT} \right]^{-1} \tag{6}$$

in which g_{up} is the degeneracy of the upper state. With $I(T)$ in nm ^{2} MHz and ν in MHz one obtains (Section A.7)

$$A = I(T) \nu^2 [Q_{rs}(T)/g_{up}] \left[e^{-E''/kT} - e^{-E'/kT} \right]^{-1} 2.79639459 \times 10^{-16} \text{ s}^{-1} \tag{7}$$

Note: numerical problems may occur in this equation if the frequency ν is small with respect to the lower state energy E'' . So, if $e^{-E''/kT} - e^{-E'/kT} = 0$ numerically, we use

$$e^{-E''/kT} - e^{-E'/kT} \simeq \frac{h\nu}{kT} e^{-E''/kT} \quad (8)$$

A.5 Transition dipole moment

$$\mu^2 = \frac{3hc^3}{64\pi^4\nu^3} A \quad (9)$$

With A in s^{-1} and ν in MHz one obtains (Section A.7)

$$\mu = \sqrt{\frac{A}{\nu^3}} 9.26894 \times 10^9 \text{ D} \quad (10)$$

A.6 Derivation of the conversion relations

$$\begin{aligned} \left[\frac{\tilde{\nu}}{\text{cm}^{-1}} \right] &= \frac{1}{c} \left[\frac{\nu}{\text{Hz}} \right] = 3.33564095 \times 10^{-5} \left[\frac{\nu}{\text{MHz}} \right] \\ \left[\frac{\tilde{\nu}}{\text{cm}^{-1}} \right] &= \frac{1}{hc} \left[\frac{E}{\text{erg}} \right] = 5.03411657 \times 10^{15} \left[\frac{E}{\text{erg}} \right] \\ \left[\frac{T}{\text{K}} \right] &= \frac{1}{k_B} \left[\frac{E}{\text{erg}} \right] = \frac{hc}{k_B} \left[\frac{\tilde{\nu}}{\text{cm}^{-1}} \right] = 1.43877688 \left[\frac{\tilde{\nu}}{\text{cm}^{-1}} \right] \end{aligned}$$

A.7 Derivation of the radiative quantities

Here i is the upper and j the lower state.

Intensity

$$\begin{aligned} I_{ij}(T) &= \frac{8\pi^3}{3hc} \nu_{ij}^x S_{ij} \mu_x^2 \frac{e^{-E_j/kT} - e^{-E_i/kT}}{Q_{rs}(T)} \\ &= 4.16237896 \times 10^{17} \left(\frac{\nu_{ij}}{\text{Hz}} \right) \left(\frac{x S_{ij} \mu_x^2}{\text{statC}^2 \cdot \text{cm}^2} \right) \frac{e^{-E_j/kT} - e^{-E_i/kT}}{Q_{rs}(T)} \frac{\text{Hz} \cdot \text{statC}^2 \cdot \text{cm}^2}{\text{erg} \cdot \text{s} \cdot \text{cm} \cdot \text{s}^{-1}} \\ &= 4.16237896 \times 10^{17} \left(\frac{\nu_{ij}}{\text{Hz}} \right) \left(\frac{x S_{ij} \mu_x^2}{\text{statC}^2 \cdot \text{cm}^2} \right) \frac{e^{-E_j/kT} - e^{-E_i/kT}}{Q_{rs}(T)} \text{cm}^2 \text{Hz} \\ &= 4.16237896 \times 10^{31} \left(\frac{\nu_{ij}}{\text{MHz}} \right) \left(\frac{x S_{ij} \mu_x^2}{\text{statC}^2 \cdot \text{cm}^2} \right) \frac{e^{-E_j/kT} - e^{-E_i/kT}}{Q_{rs}(T)} \text{nm}^2 \text{MHz} \\ &= 4.16237896 \times 10^{31} \left(\frac{\nu_{ij}}{\text{MHz}} \right) \left(\frac{x S_{ij} \mu_x^2}{\text{D}^2 \text{statC}^2 \cdot \text{cm}^2} \right) \frac{e^{-E_j/kT} - e^{-E_i/kT}}{Q_{rs}(T)} \text{nm}^2 \text{MHz} \\ &= 4.16237896 \times 10^{-5} \left(\frac{\nu_{ij}}{\text{MHz}} \right) \left(\frac{x S_{ij} \mu_x^2}{\text{D}^2} \right) \frac{e^{-E_j/kT} - e^{-E_i/kT}}{Q_{rs}(T)} \text{nm}^2 \text{MHz} \\ \left[\frac{I_{ij}(T)}{\text{nm}^2 \text{MHz}} \right] &= 4.16237896 \times 10^{-5} \left(\frac{\nu_{ij}}{\text{MHz}} \right) \left(\frac{x S_{ij} \mu_x^2}{\text{D}^2} \right) \frac{e^{-E_j/kT} - e^{-E_i/kT}}{Q_{rs}(T)} \end{aligned}$$

Einstein A coefficient

$$\begin{aligned}
A_{ij} &= \frac{64\pi^4 \nu_{ij}^3}{3hc^3} \mu_{ij}^2 = \frac{64\pi^4 \nu_{ij}^3}{3hc^3} \frac{{}_x S_{ij} \mu_x^2}{g_i} \\
&= \frac{64\pi^4 \nu_{ij}^3}{3hc^3} \frac{1}{g_i} \left\{ \frac{I_{ij}(T) Q_{rs}(T)}{\frac{8\pi^3}{3hc} \nu_{ij} [e^{-E_j/kT} - e^{-E_i/kT}]} \right\} = \frac{8\pi \nu_{ij}^2}{c^2} \frac{I_{ij}(T) Q_{rs}(T)}{g_i} [e^{-E_j/kT} - e^{-E_i/kT}]^{-1} \\
&= 2.79639459 \times 10^{-20} \left[\frac{I_{ij}(T)}{\text{nm}^2 \text{MHz}} \right] \left[\frac{\nu_{ij}}{\text{Hz}} \right]^2 [Q_{rs}(T)/g_i] [e^{-E_j/kT} - e^{-E_i/kT}]^{-1} \frac{\text{nm}^2 \text{MHz} \cdot \text{Hz}^2}{\text{cm}^2 \text{s}^{-2}} \\
&= \left[\frac{I_{ij}(T)}{\text{nm}^2 \text{MHz}} \right] \left[\frac{\nu_{ij}}{\text{MHz}} \right]^2 [Q_{rs}(T)/g_i] [e^{-E_j/kT} - e^{-E_i/kT}]^{-1} 2.79639459 \times 10^{-16} \text{s}^{-1} \\
\left[\frac{A_{ij}}{\text{s}^{-1}} \right] &= 2.79639459 \times 10^{-16} \left[\frac{I_{ij}(T)}{\text{nm}^2 \text{MHz}} \right] \left[\frac{\nu_{ij}}{\text{MHz}} \right]^2 [Q_{rs}(T)/g_i] e^{E_j/kT} [1 - e^{-h\nu_{ij}/kT}]^{-1}
\end{aligned}$$

Note: if $e^{-E''/kT} - e^{-E'/kT} = 0$ numerically, we use

$$e^{-E''/kT} - e^{-E'/kT} = e^{-E''/kT} \left(1 - e^{-(E' - E'')/kT} \right) = e^{-E''/kT} \left(1 - e^{-h\nu/kT} \right) \simeq \frac{h\nu}{kT} e^{-E''/kT}$$

Transition dipole moment

$$\begin{aligned}
\mu_{ij}^2 &= \frac{3hc^3}{64\pi^4 \nu_{ij}^3} A_{ij} \\
&= 85.9132065 \left[\frac{A_{ij}}{\text{s}^{-1}} \right] \left[\frac{\nu_{ij}}{\text{Hz}} \right]^{-3} \frac{\text{erg} \cdot \text{s} \cdot \text{cm}^3 \cdot \text{s}^{-3}}{\text{s} \cdot \text{Hz}^3} = 85.9132065 \left[\frac{A_{ij}}{\text{s}^{-1}} \right] \left[\frac{\nu_{ij}}{\text{Hz}} \right]^{-3} \text{statC}^2 \cdot \text{cm}^2 \\
&= 8.59132065 \times 10^{19} \left[\frac{A_{ij}}{\text{s}^{-1}} \right] \left[\frac{\nu_{ij}}{\text{MHz}} \right]^{-3} \text{D}^2 \\
\left[\frac{\mu_{ij}}{\text{D}} \right] &= \sqrt{8.59132065 \times 10^{19} \left[\frac{A_{ij}}{\text{s}^{-1}} \right] \left[\frac{\nu_{ij}}{\text{MHz}} \right]^{-3}}
\end{aligned}$$