

HAPIEST User Manual

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1 HAPIEST

HITRAN Application Programming Interface and Efficient Spectroscopic Tools (HAPIEST) is a GUI for the HITRAN Application Programming Interface (HAPI). HAPIEST's development began at SUNY Oswego in a software engineering course by students Benji Caro, Joshua Karns, Dominik Lohmann, Wyatt Matt, Ethan Messer, and Michael Sova, in conjunction with Dr. Iouli Gordon and Dr. Roman Kochanov of the Harvard-Smithsonian Center for Astrophysics and under advisement of SUNY Oswego Professor Dr. Bastian Tenbergen and SUNY Oswego Professor and Head of the Physics Department Shashi Kanbur.

1.1 Program Overview

The goal of HAPIEST is to simplify the use of the HITRAN Application Programming Interface (HAPI). Currently, HAPI requires some knowledge of Python and use of the command line. HAPIEST retains as much of the functionality of HAPI as is possible in a simple GUI, while making it easier to learn and more accessible all users.

1.1.1 Data Retrieval

HAPIEST currently can enable you to quickly fetch line lists and cross sections from the HITRAN database, which are stored on disk for efficient access and speed. There are cross sections available for over 300 molecules, and line by line data available for 50 molecules.

1.1.2 Data Viewing

Users can view line lists they have downloaded in a spreadsheet-like fashion, and make changes to line lists. Changes can then be saved to a temporary in-memory line list, which can then be used to create graphs. In the future you will be able to save new tables to the disk, but that is not possible right now.

1.1.3 Efficient Data Processing

There is also functionality for filtering data in line lists to create new tables. This is known as the "select" functionality, and it can be used to

efficiently filter and even modify data.

1.2 Installation

A binary distribution is available on [GitHub](#)¹ for Windows. Using the distribution should be as easy as extracting the zip file and starting "hapiest.bat" or "hapiest.exe".

There is currently no binary distributions for Linux or Mac systems, but HAPIEST can easily be ran from source on those systems.

1.3 Running From Source

Running from source should only take a few commands! You must have python3 and git installed for this to work. First you must begin by cloning the github repository:

```
~/ $ git clone https://github.com/hitranonline/hapiest.git
```

If you do not have git, you can download a clone of the repository as a zip file directly from github². Extract the contents of the 'hapiest-master' folder into a folder named 'hapiest' (or rename 'hapiest-master' to 'hapiest').

This command will create a new folder named 'hapiest' which will contain all of the source code. Next, enter the 'hapiest' directory:

```
~/ $ cd hapiest
```

Then, ensure you have all of the required packages installed:

```
~/hapiest $ python3 -m pip install --user -r requirements.txt
```

You should then be able to run the program by running:

```
~/hapiest $ python3 src
```

This will launch the program. If it does not, please file an issue on our github page³ describing the problem; be sure to include any errors the program outputs.

¹The binary distribution is available for download here:
<https://github.com/hitranonline/hapiest/releases>.

²Download the repository here: <https://github.com/hitranonline/hapiest>

³You can open an issue here: <https://github.com/hitranonline/hapiest/issues>

2 Using HAPIEST

The Main Window provides the functionality of HAPI and is split into several tabs each focusing on a different feature/function.

2.1 Molecules Tab

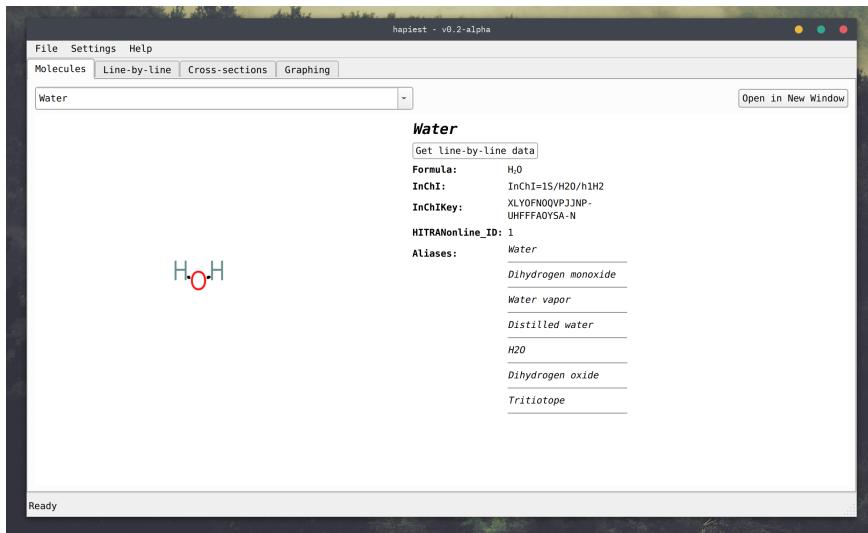


Figure 1: The molecules tab showing some information about H_2O .

The molecules tab was created for ease of use. After selecting one of over 300 molecules HAPIEST can retrieve data for, you can click the buttons presented to retrieve said data. If you select a molecule that only has line-by-line data available, only the "Get line-by-line data" button will appear. Likewise, if you select a molecule that only has cross section data available, only the "Get cross sections" button will appear. There are a few molecules for which HITRAN has line lists and cross sections, in such a case both buttons will be shown. Figure 1 is an example of how the molecules tab looks.

2.2 Line-by-line Tab

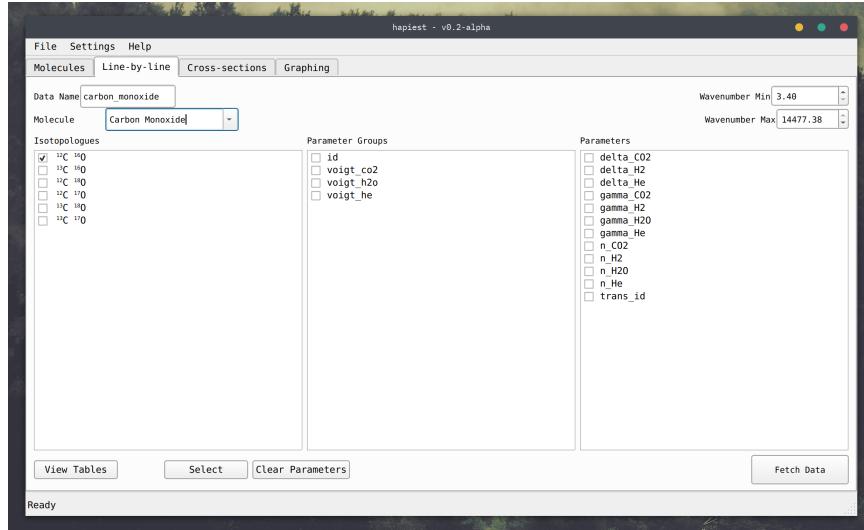


Figure 2: The line by line tab showing the available parameters for Carbon Monoxide.

The Line-by-line tab (shown in Figure 2) allows you to download line lists from HITRAN onto their local disk for the available molecules and their isotopologues. There are also extra parameters available for some molecules to allow the calculation of the SD Voigt and Galatry line profiles, and for broadening by H_2O , CO_2 , H_2 , and He . These parameters are not available for all molecules, so only the parameters that are actually available for the selected molecule will be offered as options.

2.3 Select

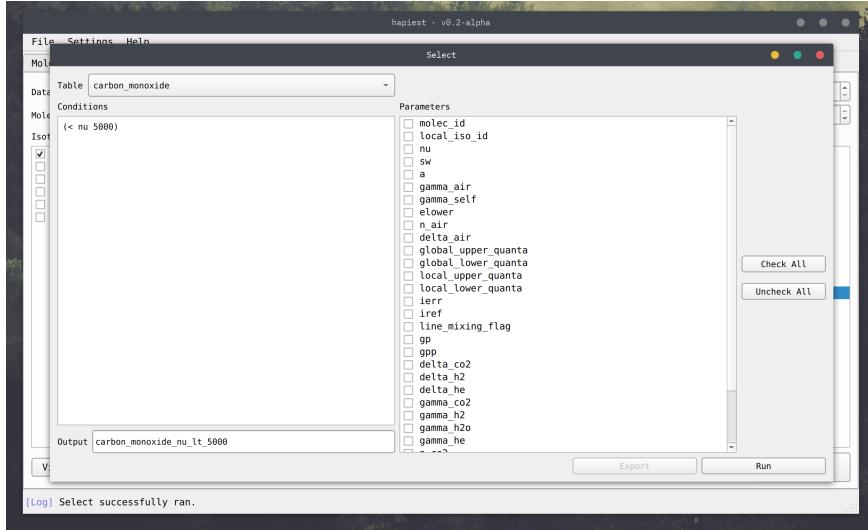


Figure 3: An example usage of the select functionality.

The select functionality comes from HAPI, and it behaves in a way similar to SQL queries. As an example of when it may be useful, if you downloaded all of the water lines HITRAN has to offer you would have data in the range of $0 < \tilde{\nu} < 24000$. If you only wanted data for the first 500 wavenumbers, you could easily filter out any data with $\tilde{\nu} > 500$ with this simple condition: $(< \text{nu } 500)$. A query to do such a thing is depicted in Figure 3.

2.4 View Windows

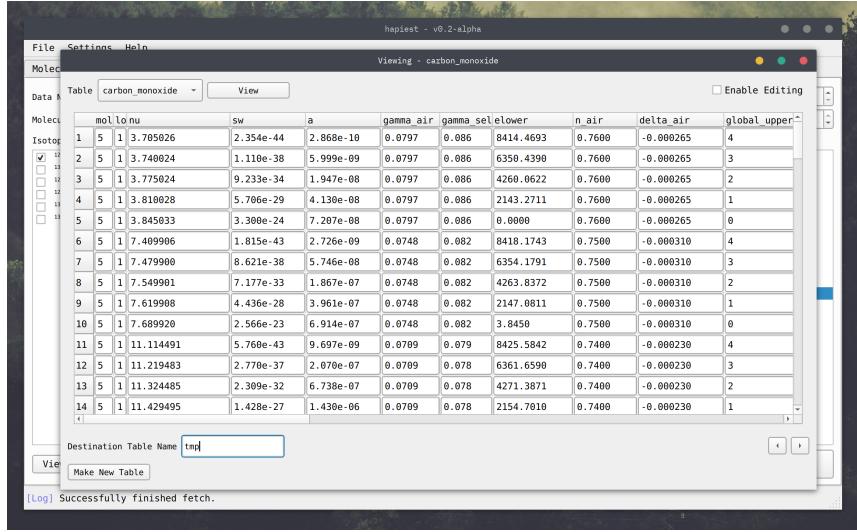


Figure 4: A view window looking at a Carbon Monoxide line lists.

View windows allow you to view and edit local data that has been downloaded through HAPIEST. It offers a table view of all parameters and values, and can be saved to disk. Figure 4 is an example of a view window looking at a line list.

2.5 Graphing Tab

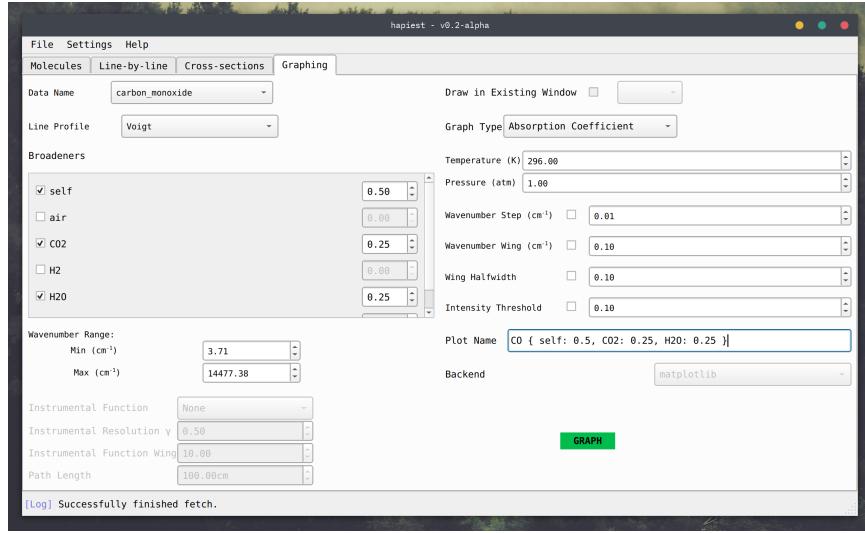


Figure 5: An example of the graphing tab, with a Carbon Monoxide table selected. In this example, the table has downloaded the appropriate parameters to allow for broadening by a few different broadeners. Without the appropriate parameters, the only available broadeners will be self and air.

In the graphing tab, you're given a list of parameter fields to fill out for the type of graph you've selected. The available types of graphs are Absorption Coefficient and Absorption, Transmittance, and Radiance spectra. It is also possible to plot the Bands of a line list. If you've selected a cross section as your data, the only graph type that is available will be "Cross Section." You may add other curves to the same graph display window, in order to compare the two.

2.6 Main Window Menu

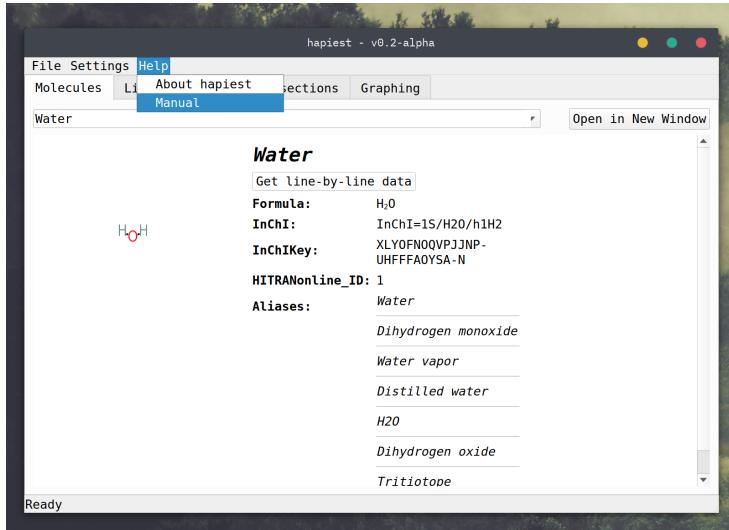


Figure 6: A demonstration of how to access the manual from the help menu.

The toolbar in the Main Window can direct you to this document, and lets you edit your settings. Accessing the help toolbar is shown in Figure 6.

The config editor allows you to change user-configurable settings. This includes:

- The data folder, the location data will be stored on disk.
- High DPI mode for people who are using high-resolution monitors (namely 4K and 2K).
- The number of lines to show per page in the view window.
- Your HAPI API key.

The config editor can be accessed through the 'Settings' tab in the menu bar, which will have 'Edit Configuration' as a choice when you hover over or click it. An example of what the configuration editor may look like is shown in Figure 7.

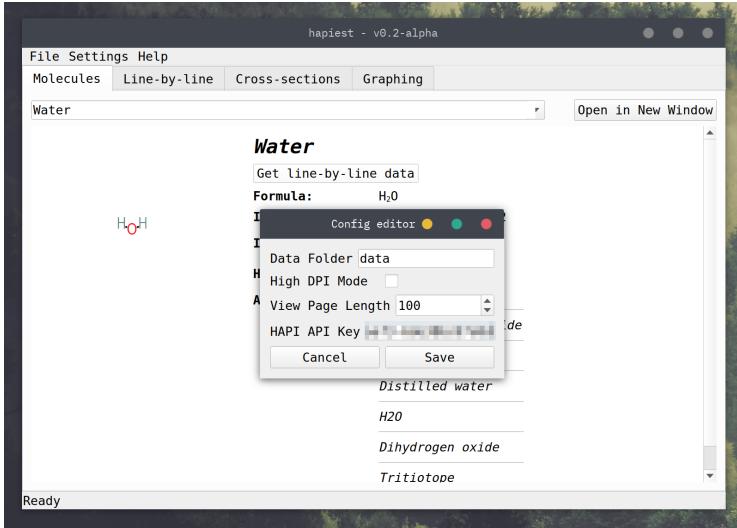


Figure 7: This is what the config editor looks like, spare the censored API key.

3 Graph Window

Graphs are displayed in a separate window from the main window. You may create an arbitrary number of these windows (so long as your computer has the resources). It is also possible for you to send multiple plots to the same window for comparison, as shown in Figure 8.

3.1 Standard Graph User Interactivity

HAPIEST uses matplotlib to display graphs, so it inherits all of the functionality offered by matplotlib. Each one of the tools laid out below is visible in Figure 8. The features inherited from matplotlib include:

- The ability to change the axis type (either log or linear) for both the x and y axis, accessible using the tool with a graph icon.
- The ability to change the style of curve you have, also offered by the graph icon. This includes the curve thickness, and symbols that should be used to indicate points. These options will apply to one of your curves at a time, so you can configure every curve separately. It is also possible to change a curve into a scatter plot with no connecting line. Hiding a curve entirely is also supported.

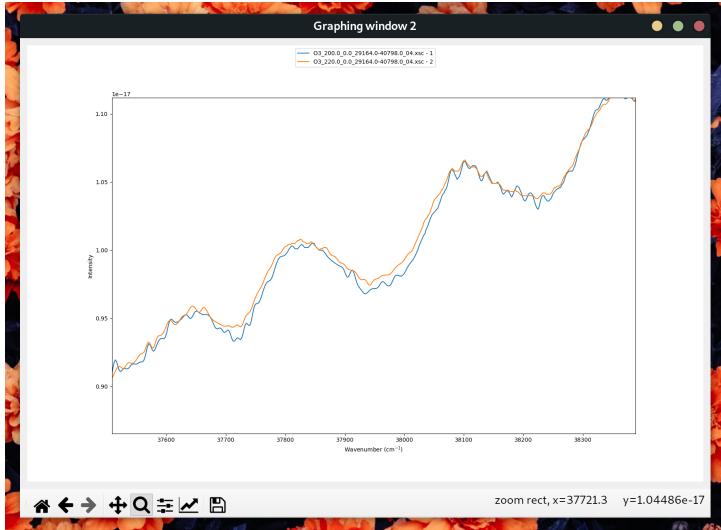


Figure 8: An example of the graph display window, comparing two different ozone cross sections.

- Rectangular zooming, offered by the hourglass tool.
- Saving images in a variety of formats (including LaTeX and postscript), offered by the floppy disk icon.
- Panning offered by the panning icon (the plus icon with arrows at each end).
- A home button, which will return the graphs view area to what it was when the graph display window was first created.
- Back and forwards buttons, corresponding to the left arrow and right arrow buttons respectively.

3.2 Band Graph User Interactivity

Band display windows are different than normal graph windows as they have an additional widget that allows you to hide or embolden individual bands. Additionally, it has all of the functionality outlined in Section 3.1.

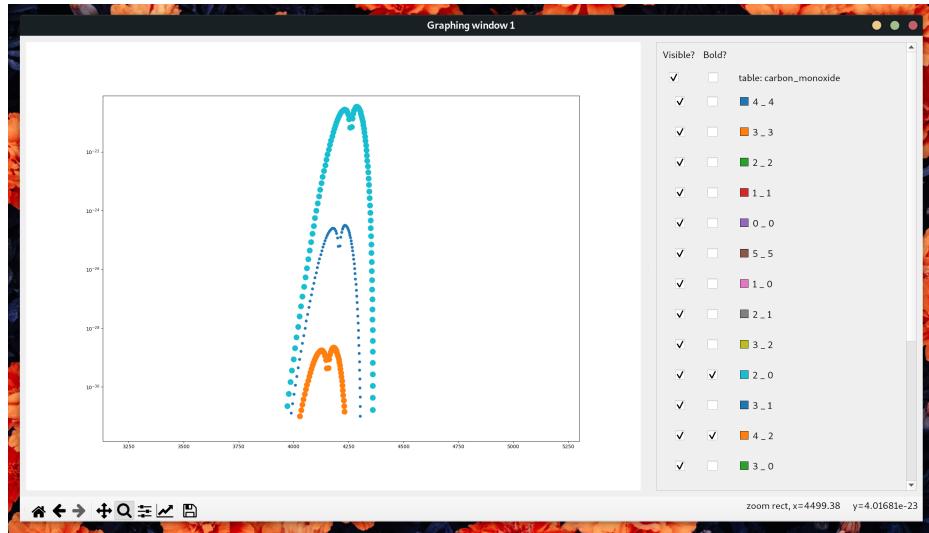


Figure 9: An example of the band display window, showing three bands of the Carbon Monoxide line list, two of which have been made bold.

4 Glossary

This is less of a tradition glossary and functions more as a reference to what various elements of the GUI describe, represent, or do.

Glossary

Backend In the future it will let you choose between the default graphing library matplotlib and VisPy, but right now matplotlib is the only supported graphing library..

Broadeners The broadeners are the group of gases that the simulated spectra will be broadened with. The sum of their proportions should be 1.0.

Clear Parameters Unchecks all Parameters and Parameter Groups.

Data Name Local data file name used to calculate spectra for graphing.

Data Name Local file name of data being downloaded.

Destination Table Name Name of of file to save changes to.

Draw in Existing Window Checkbox to enable multiple plots on the same graph display window, along with a list of graph windows that a plot can be sent to.

Edit Button that populates table containing information in the data file.

Get cross-sections Opens the Cross-sections tab to the current molecule displayed in the molecules tab.

Get line-by-line data Opens the Line-by-line tab to the current molecule displayed in the molecules tab.

Graph Button that creates a plot according to selected parameters.

Graph Type Type of the graph to plot: dependent on the spectra type (i.e. absorption, transmittance, etc.).

Instrumental Function .

Instrumental Function Wing .

Instrumental Resolution y .

Intensity Threshold Minimum value of the line intensity to consider in the spectra calculation.

Isotopologues List of Isotopologues for the selected molecule. This is what you are fetching data for.

Line Profile Line profile (line shape) type to use in the spectra calculation.

Molecule List of molecules to select which Isotopologues to fetch data for, updates the Isotopologue and Parameter lists.

Parameter Groups List containing groups of spectral line parameters to fetch. Updates available Parameter Groups per molecule. Parameters in the Parameters list reflect the parameter groups you check.

Parameters List of individual spectral line parameters to fetch. Updates available Parameters per molecule. , 13

Path Length .

Plot Title Title of the plot.

Pressure Total pressure (in atmospheres) of the modeled gas mixture.

Save to disk Saves the changes you made into your data folder.

Select Opens the Select Window which allows you access the HAPI's select function.

Table List of HITRAN data files.

Temperature Temperature (Kelvin) of the modeled gas mixture.

View Tables Opens the Edit Window which allows you to edit downloaded data files.

Wave Number Max Upper threshold to select data to.

Wave Number Min Lower threshold to fetch data from.

Wave Number Range Spectral range to be used in the simulation (in wavenumbers).

Wave Number Step Wavenumber step to be used in the simulation.

Wave Number Wing Absolute size of the wing (in wavenumbers) at which line profile is not zero.

Wing Halfwidth Relative of the size of the wing (in line halfwidths) at which line profile is not zero.