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, and in conjunction with Dr. Iouli Gordon and Dr. Roman Kochanov of the Harvard-Smithsonian Center for Astrophysics and under advisement of SUNY Oswego professor Bastian Tenbergen and SUNY Oswego Professors and Head of Physics Department Shashi Kanbur. HAPIEST functions as a GUI for HAPI.

1.1 Program Overview

The goal of HAPIEST is to simplify the use of the HITRAN Application Programming Interface (HAPI) for all users. Currently, HAPI requires some knowledge of Python and use of the command line. HAPIEST should retain as much of the funtionality HAPI as is possible in a simple GUI, while making it easier to access and use for the user. HAPIEST currently allows users the capability to fetch/download and locally store data from the HITRAN database, edit local data, and also to generate and plot spectral functions. In it's current form, HAPIEST is split up into 3 windows, one window for data management and editing, and two windows for graphing/graph display.

2 Installation

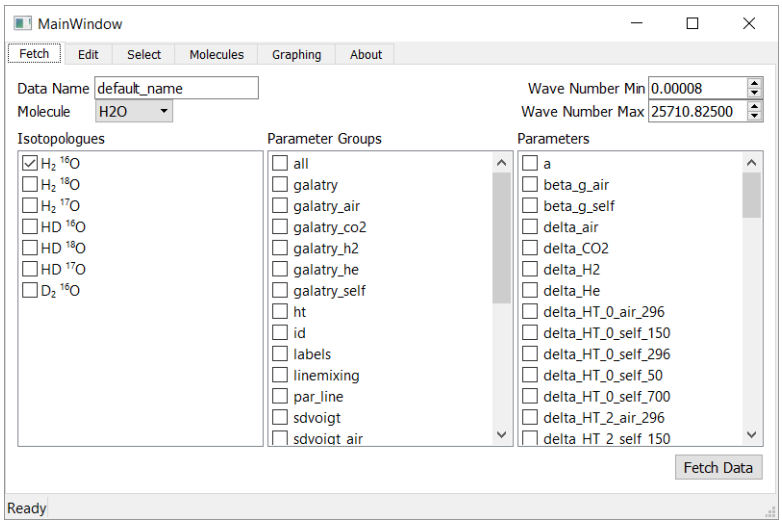
HAPIEST is available to follow and download on our github. A distrobution is also available on Windows, and will be coming to Linux and Mac. https://github.com/hitranonline/hapiest

3 Main Window

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

3.1 Fetch Tab

The Fetch tab allows the user to download data from HITRAN onto their local disk for the available molecules and their supported isotopologues. Further, the user can select from the Parameter Groups list and Parameters list to download more specific data. This window is the users primary method of obtaining data.

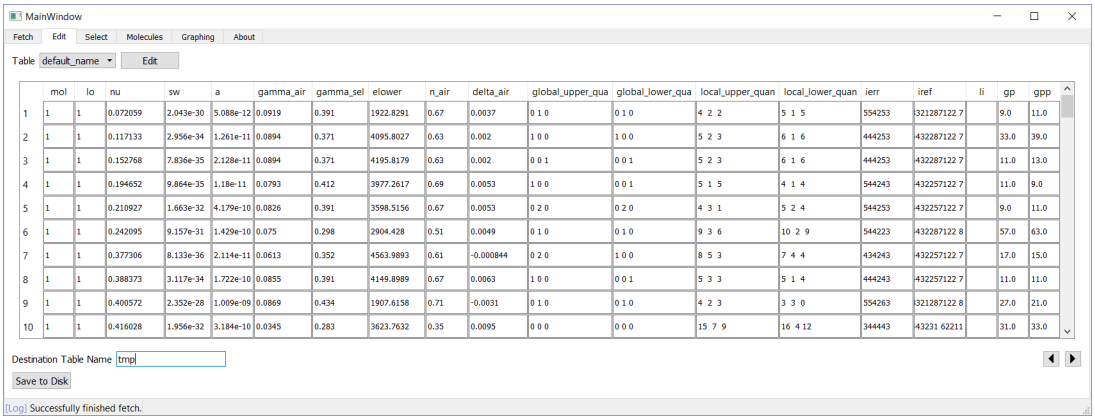


3.1.1 Fetch Dictionary

- Data Name - Local file name of data being downloaded.
- Molecule - List of molecules to select which Isotopologues to fetch data for, updates the Isotopologues list when a molecule is selected.
- Wave Numer Min - Lower threshold to fetch data (from).
- Wave Number Max - Upper threshold to fetch data (to).
- Isotopologues - List of Isotopologues for the selected molecule. This is what you are fetching data for.
- Parameter Groups - List containing groups of spectral line parameters.
- Parameters - List of individual spectral line parameters to fetch for selected isotopologues.

3.2 Edit Tab

The edit tab allows users 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.



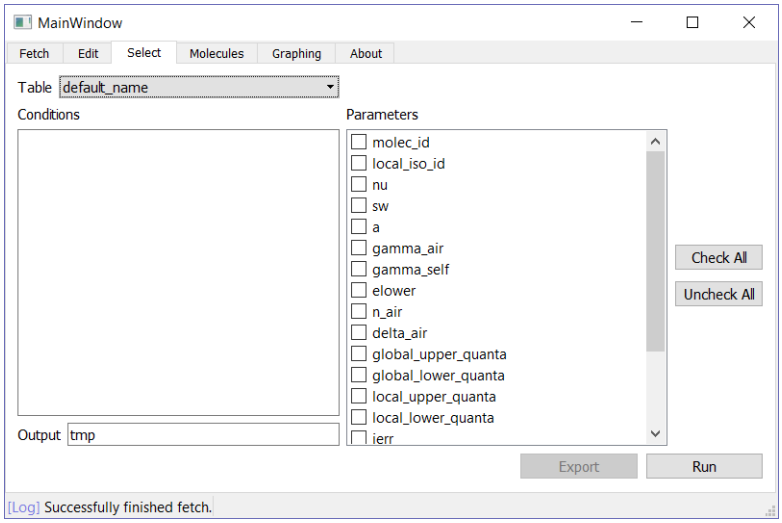
	mol	Io	nu	sw	a	gamma_air	gamma_sel	elower	n_air	delta_air	global_upper_qua	global_lower_qua	local_upper_quan	local_lower_quan	ierr	iref	li	gp	gpp
1	1	1	0.072059	2.043e-30	5.088e-12	0.0919	0.391	1922.8291	0.67	0.0037	0 1 0	0 1 0	4 2 2	5 1 5	554253	321287122 7		9.0	11.0
2	1	1	0.117133	2.956e-34	1.261e-11	0.0894	0.371	4095.8027	0.63	0.002	1 0 0	1 0 0	5 2 3	6 1 6	444253	432287122 7		33.0	39.0
3	1	1	0.152768	7.836e-35	2.128e-11	0.0894	0.371	4195.8179	0.63	0.002	0 0 1	0 0 1	5 2 3	6 1 6	444253	432287122 7		11.0	13.0
4	1	1	0.194652	9.864e-35	1.18e-11	0.0793	0.412	3977.2617	0.69	0.0053	1 0 0	0 0 1	5 1 5	4 1 4	544243	432257122 7		11.0	9.0
5	1	1	0.210927	1.663e-32	4.179e-10	0.0826	0.391	3598.5156	0.67	0.0053	0 2 0	0 2 0	4 3 1	5 2 4	544253	432257122 7		9.0	11.0
6	1	1	0.242095	9.157e-31	1.429e-10	0.075	0.298	2904.428	0.51	0.0049	0 1 0	0 1 0	9 3 6	10 2 9	544223	432287122 8		57.0	63.0
7	1	1	0.377306	8.133e-36	2.114e-11	0.0613	0.352	4563.9893	0.61	-0.000844	0 2 0	1 0 0	8 5 3	7 4 4	434243	432257122 7		17.0	15.0
8	1	1	0.388373	3.117e-34	1.722e-10	0.0855	0.391	4149.8989	0.67	0.0063	1 0 0	0 0 1	5 3 3	5 1 4	444243	432257122 7		11.0	11.0
9	1	1	0.400572	2.352e-28	1.009e-09	0.0869	0.434	1907.6158	0.71	-0.0031	0 1 0	0 1 0	4 2 3	3 3 0	554263	321287122 8		27.0	21.0
10	1	1	0.416028	1.956e-32	3.184e-10	0.0345	0.283	3623.7632	0.35	0.0095	0 0 0	0 0 0	15 7 9	16 4 12	344443	43231 62211		31.0	33.0

3.2.1 Edit Dictionary

- Table - List of HITRAN data files.
- Edit - Button that populates table containing information in the data file.
- Destination Table Name - Name of local file upon saving.
- (Left and Right Arrows) - Select between pages of data.
- Save to Disk - Button that saves the current table to disk.

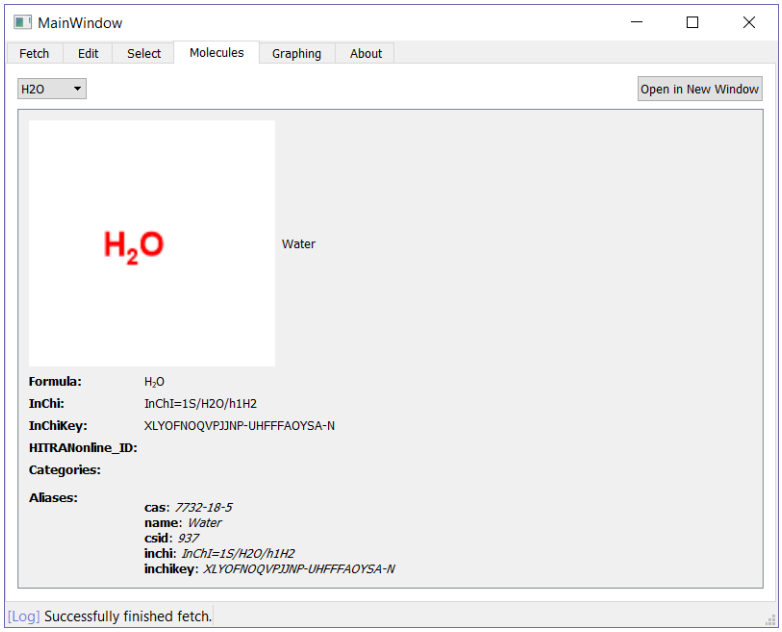
3.3 Select Tab

The select tab is dedicated to the fetch method call available in HAPI and allows users a more advanced fetch.



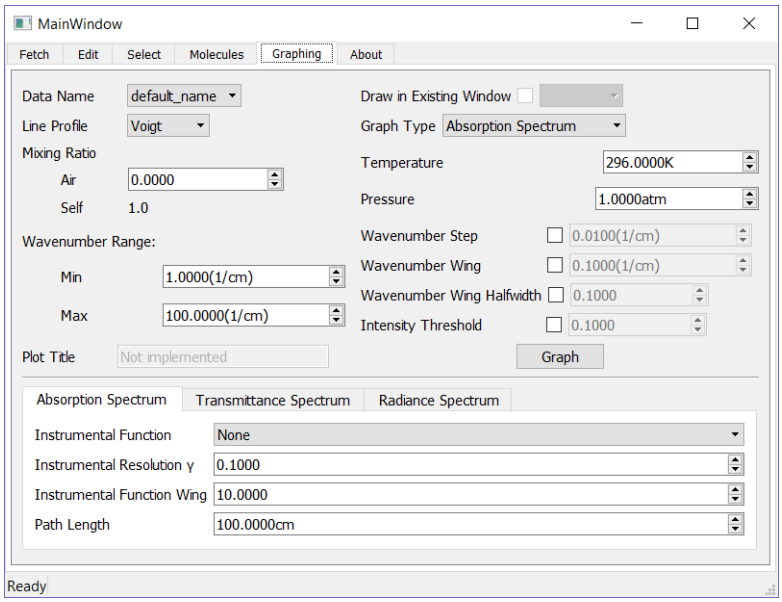
3.4 Molecules Tab

The molecules tab provides reference for the available molecules and also reference ids for each molecule.



3.5 Graphing Tab

In the graphing tab, the user is given a list of parameter fields to populate in order to create the specific graph they need for each graph type (Absorption Coefficient; Absorption, Transmittance, and Radiance Spectra graphs). Multiple plots of the same type may be displayed together on the same graph.



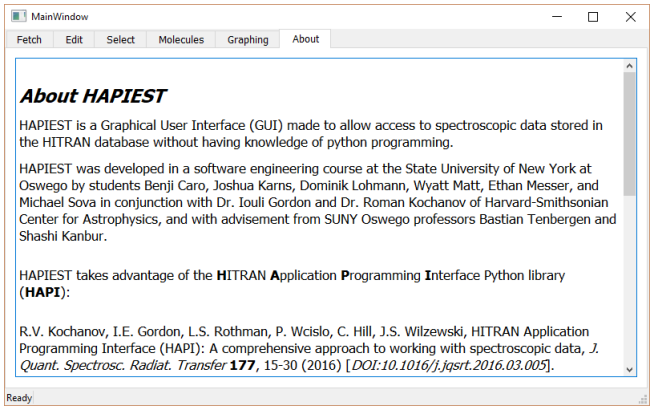
3.5.1 Graphing Dictionary

- Data Name - Data file used to calculate spectra for graphing.
- Draw in Existing Window - Checkbox to enable multiple plots on the same graph for the same Line Profiles. List of graph windows open to plot to.
- Line Profile - Line profile (lineshape) type to use in the spectra calculation..
- Graph Type - Type of the graph to plot: dependent on the spectra type (i.e. absorption, transmittance, etc...).
- Mixing Ratio - Volume mixing ratio of air in the modeled mixture.

- Temperature - Temperature (Kelvin) of the modeled gas mixture.
- Pressure - Total pressure (in atmospheres) of the modeled gas mixture.
- 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.
- Wave Number Wing Halfwidth - Relative of the size of the wing (in line halfwidths) at which line profile is not zero.
- Intensity Threshold - Minimum value of the line intensity to consider in the spectra calculation.
- Plot Title - Title of the plot.
- Graph - Button that creates a plot according to selected parameters.

3.6 About Tab

The about tab is a summary tab informing the user about the development and some information about each tab.



4 Graph Window

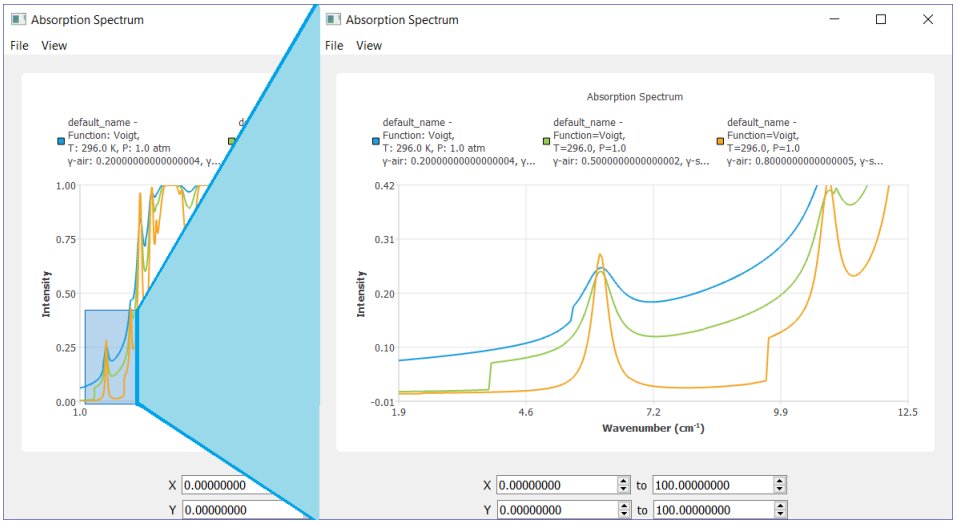
Graphs are displayed in this window. There is an option in the graphing tab to display multiple graphs in the same window.

4.1 User Interactivity

Inside the graph display windows, the user has options to box zoom on the graph, reset view, and save the graph in popular file formats.

4.1.1 Box Zoom

To box zoom, simply click the left mouse button, hold it down and drag across the area you want to zoom in on, and release. In order to reset the graph view, click View in the menu and then click Fit.



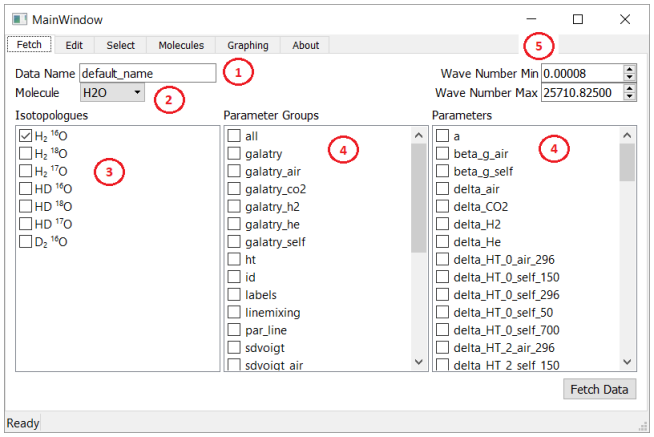
4.1.2 Save Features

Options to save graphs in image formats PNG and JPEG, or text based as Comma Separated Values (CSV), Text File (TXT), or in JSON format.

5 How to Use

5.1 Fetching Data

In order to plot/graph data, the user needs to first download data from the HITRAN database. This can be done in HAPIEST or using HAPI. To do so in HAPIEST, follow the instructions below.



1. Edit data name to change the name of the file downloaded upon fetching.

2. Select the molecule to update the Isotopologues list.

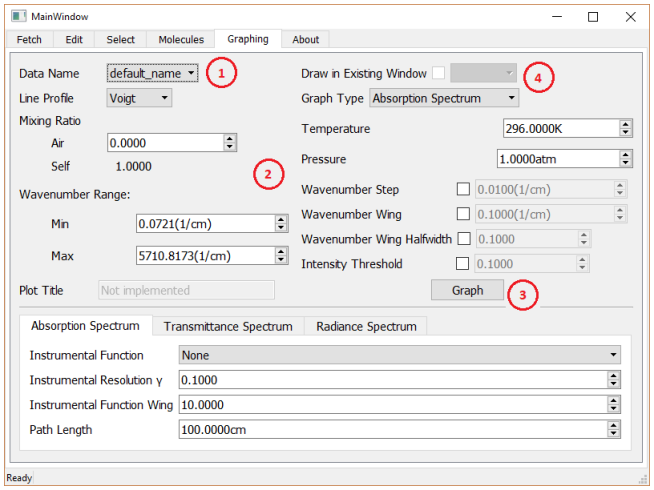
3. Select the Isotopologues you want to download data for.

4. Select from the Parameter Groups and Parameters list to download further data for the selected Isotopologues.

5. Edit the Wave Number Min and Max values to refine your download (Smaller ranges are faster to fetch and take up less space).

5.2 Graphing Data

Once you have data on your system, you can then go to the Graphing Tab to produce a graph.



1. In the Data Name list, select the data file you want to use to create a plot.

2. Skip Draw in Existing Window for now, and select the parameters of the plot.

3. Click the graph button and another window will appear to display the graph.

4. Now, if you want to plot another graph of the same type in/with a previous plot, check the Draw in Existing Window check box and select the compatible window in the drop-down list.

6 Demo