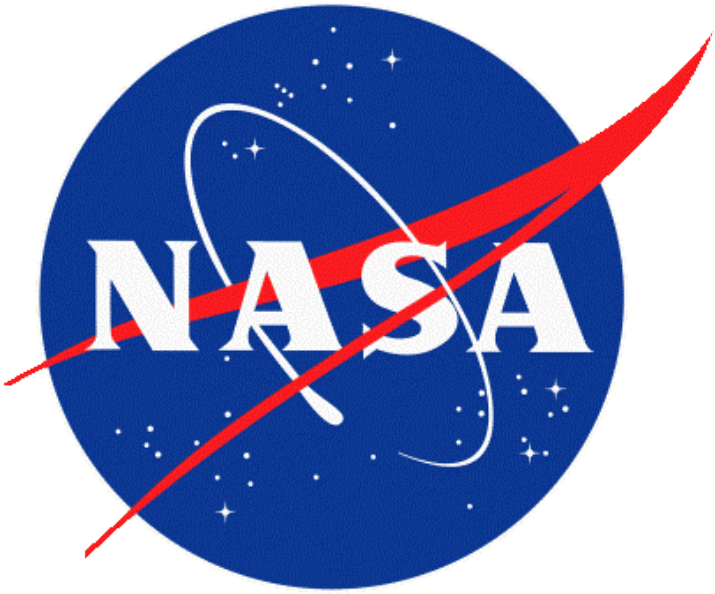


NASA Ames Research Center

The Astrophysics & Astrochemistry Laboratory

The NASA Ames PAH IR Spectroscopic Database

WEBSITE MANUAL

version 1.00

By

Gerardo Puerta Saborido

Fernando Sánchez de Armas

Directed by

Dr. Alessandra Ricca

Dr. Louis Allamandola

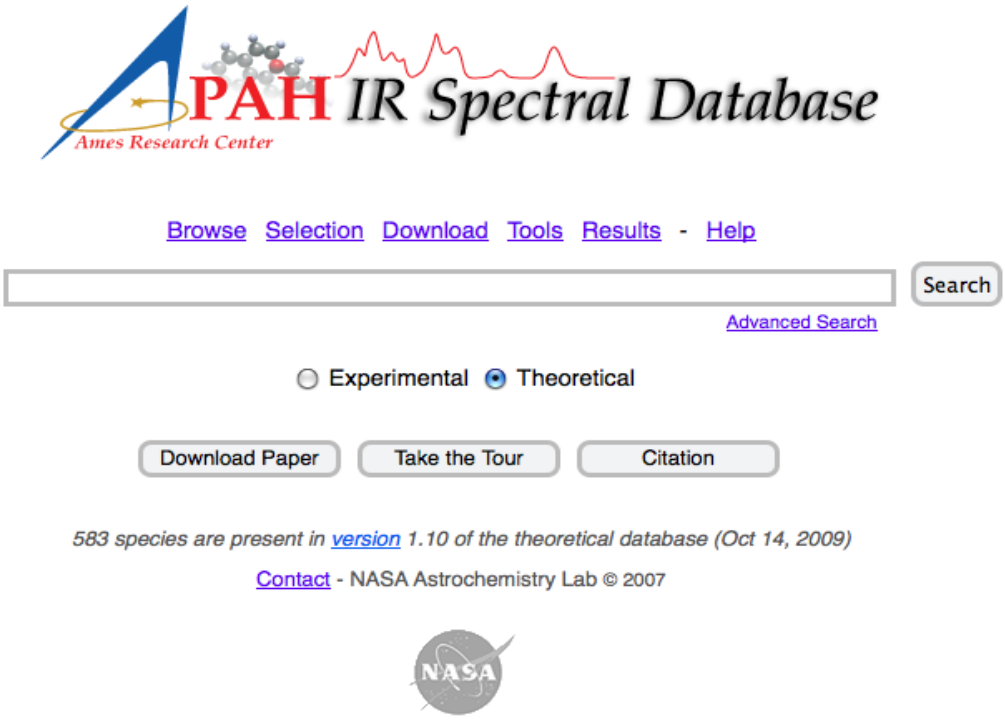
Dr. Christiaan Boersma

Updated October 2013

This manual has not yet been updated for version 2.00 of the website

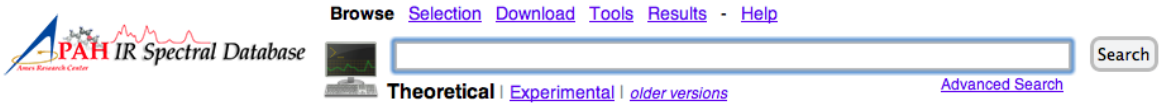
1 Introduction

The home page of our website is aimed to be simple. It basically shows a search bar where we can start searching species in the database and a menu to navigate the different sections.



2 Browse and selection

Browser and Selection are the main part of the application. They are primarily intended to facilitate the location of the species in the database. Once you access the Browse section you will find the search bar and the menu with links to the different sections of the application.



Main menu and search bar

This part, along with the logo, will appear on all pages for a better usability regarding navigation. An important part of this area is the ability to toggle between the theoretical database and the experimental database, as well as gaining access to the advanced search. The main page displays

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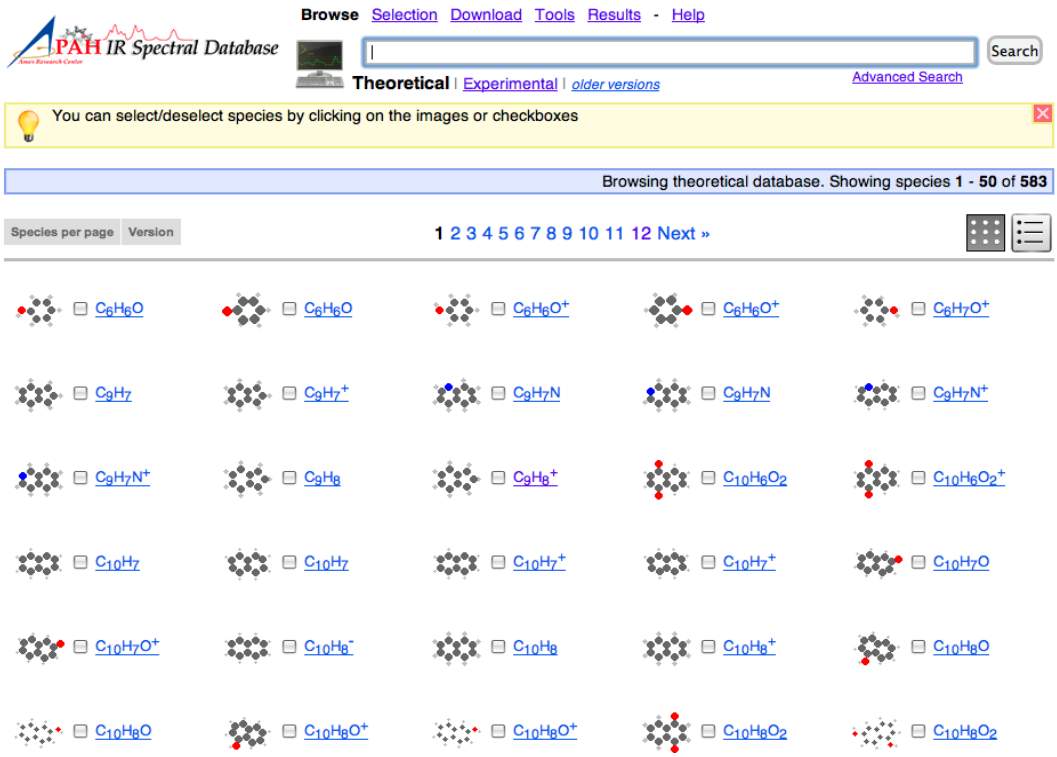
the Browse section of the top 50 species in the theoretical database as icons and a link to access them.



Main page of the Browse section

If you want to see more species you just have to click on the number page you want in the navigation menu.

Navigation menu in Browse section

On the left side of the page you may change the species per page that you wish to display and you can browse earlier versions of the database.

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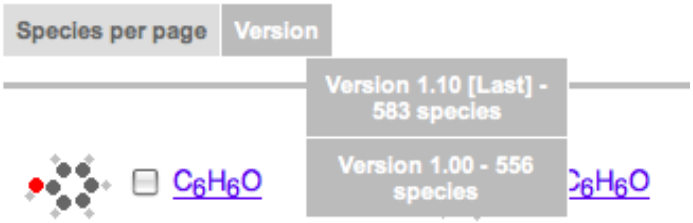
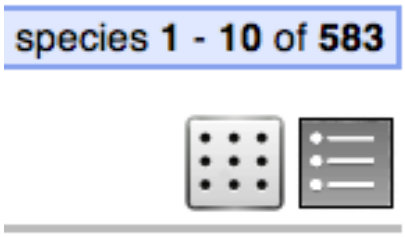


To change species per page and navigate in older versions

On the right side of the page you find two icons to change the way you want to show the species in the Browse. If you click on view details it will change to a view where more data will appear on the species in a list form.



To toggle the view between icons or list

A detailed view includes a representation of the molecule in 2D, basic data of the specie and the representation of their transitions in a spectrum. Also, it shows a link to a page with extensive information about the species selected.

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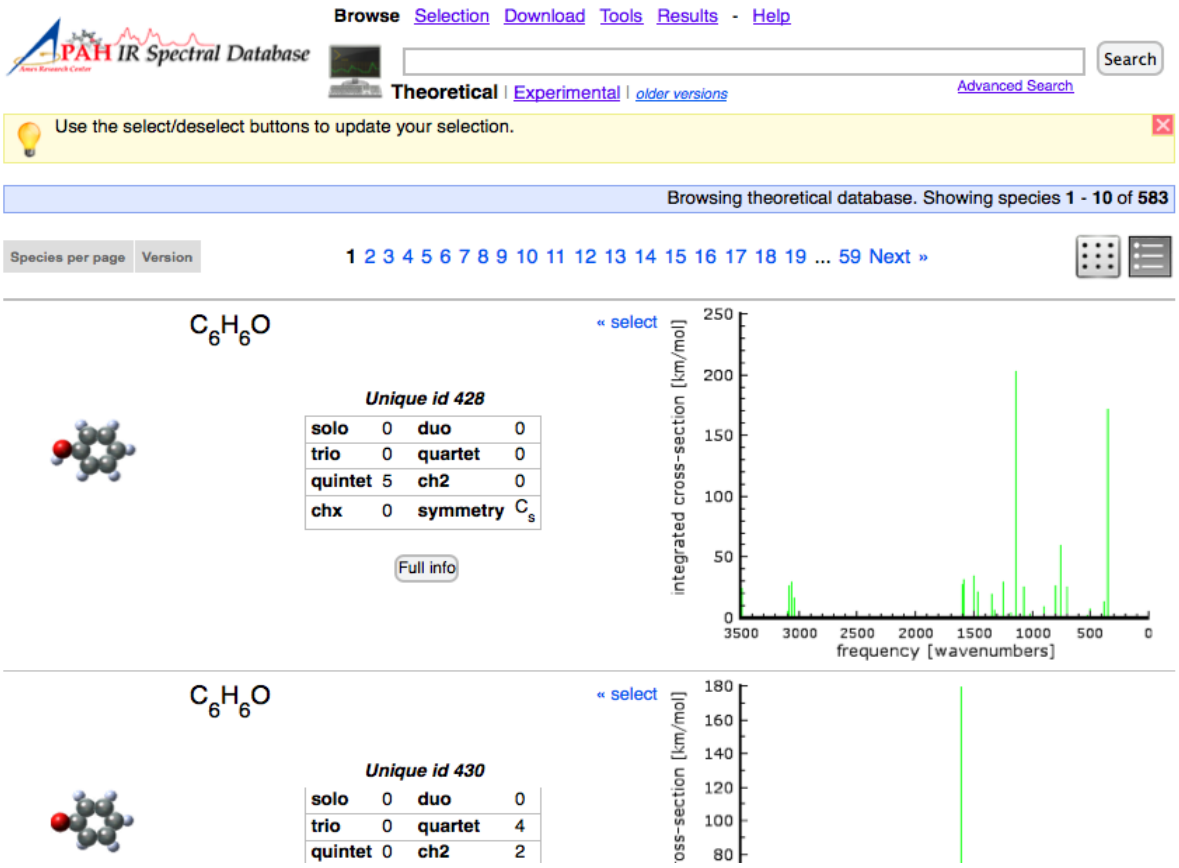

Detailed view of the species of the theoretical database

In any of the views that the application provides, you can select the species of interest, just click checkboxes.

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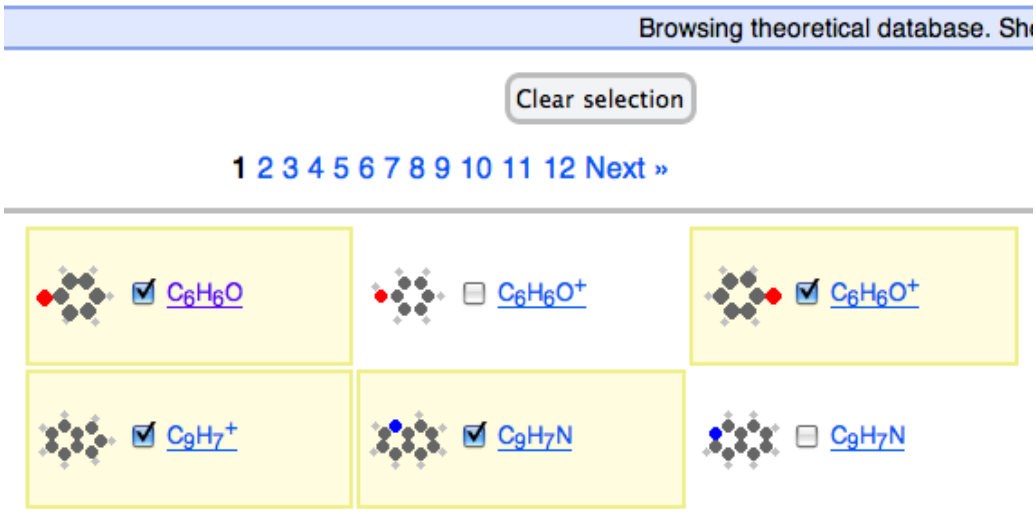

In yellow boxes the species selected

In the main menu you can see a global variable which displays the number of species selected. These species can be consulted whenever you want and mainly, to operate on them with the tools.

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Main menu with 4 species selected

The outcome of such selection would be a list of 2D molecular structures and spectra which enables one to quickly visualize individual species and their spectra. Striving for efficiency, all the available information on a species is just one click away. As you can see, there is a link *Full info* to access extensive information about the specie.

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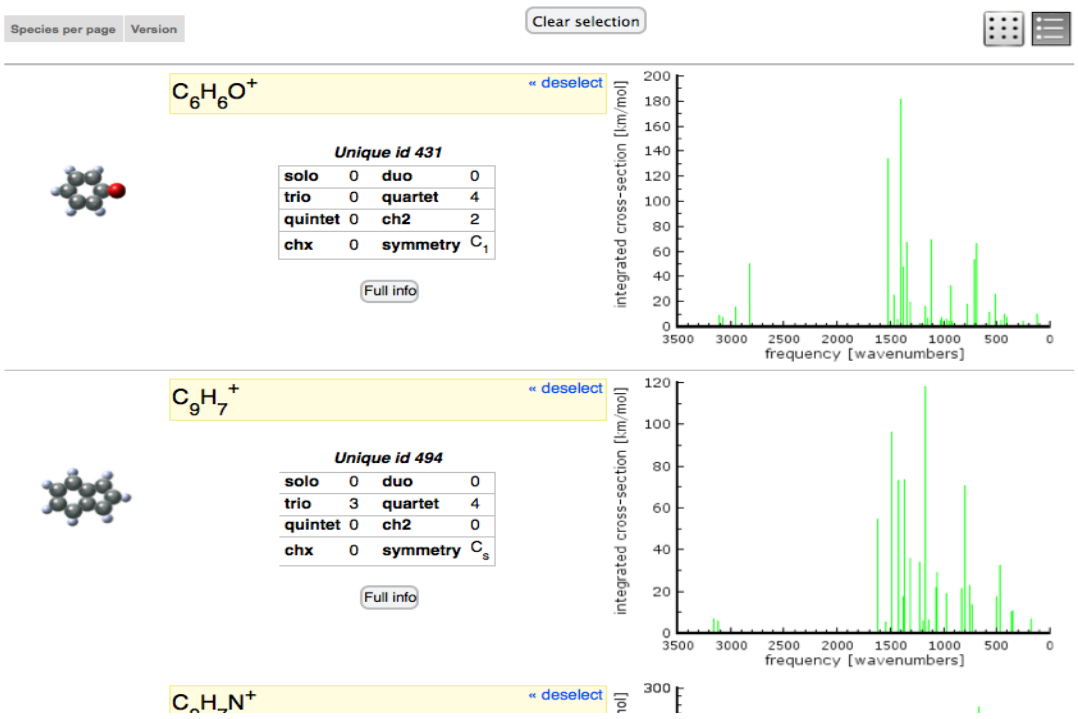

Selection section with 4 species selected

If you click on *Full info* you will go to a page with all the information on that species available in the database. Among other things, this information includes rotatable 3D structures, bibliographical references, comparisons withexperimental/theoretical data in the database, transition tables and molecular characteristics.

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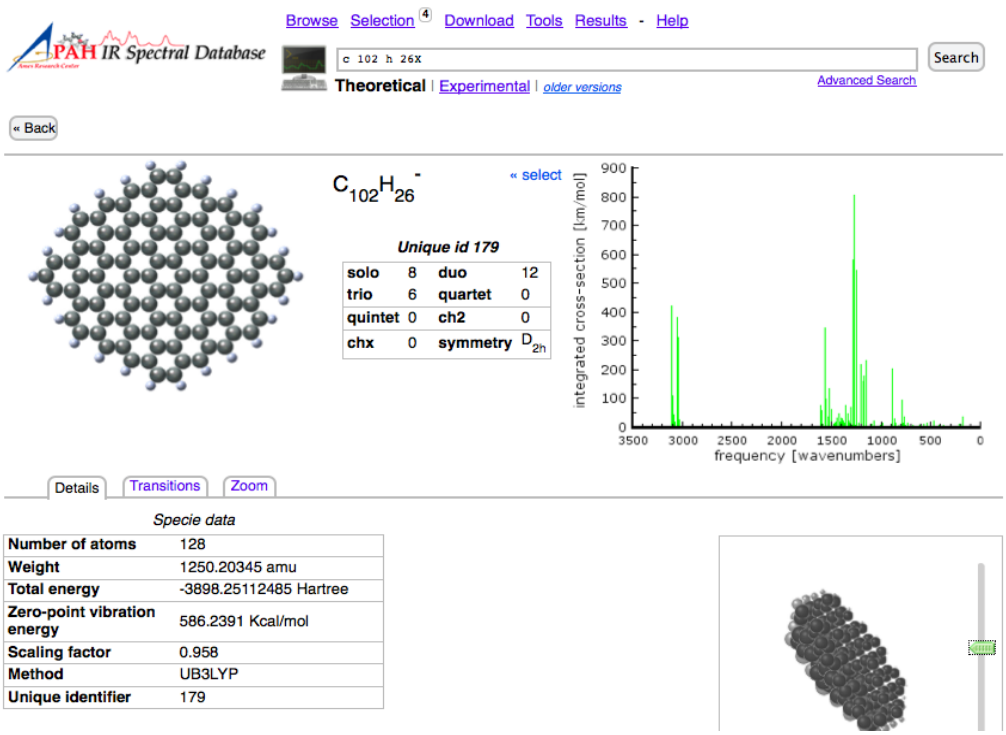
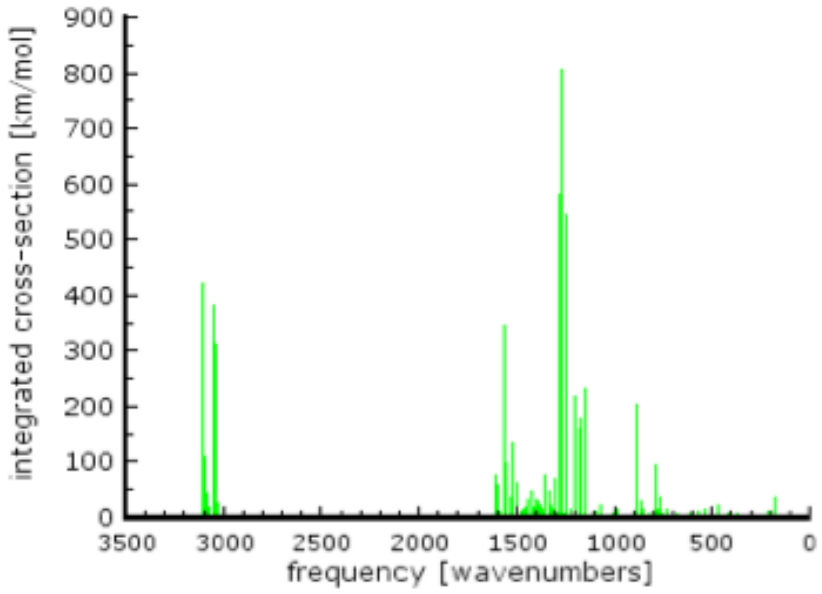


Full info page of the specie $C_{102}H_{26}$



Detail of the Spectrum of the specie $C_{102}H_{26}$

In the *Details* section you can see all the information available about the species, its bibliographical reference, comments and a complete version history.

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Details | Transitions | Zoom

Specie data

Number of atoms	128
Weight	1250.20345 amu
Total energy	-3898.25112485 Hartree
Zero-point vibration energy	586.2391 Kcal/mol
Scaling factor	0.958
Method	UB3LYP
Unique identifier	179

Reference

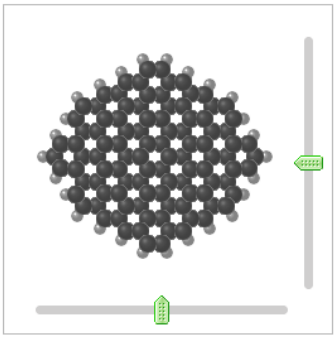
- Bauschlicher, C. W., Peeters, E., Allamandola, L. J. (2008) "The Infrared Spectra of Very Large Irregular Polycyclic Aromatic Hydrocarbons (PAHs): Observational Probes of Astronomical PAH Geometry, Size and Charge", submitted to ApJ.

Comment

- SDT with sym

History

- This specie was added on version 1 of theoretical database (December 02, 2008)
- This specie was updated on version 2 of theoretical database (October 14, 2009)



Details section of the specie $C_{102}H_{26}$

As you can see in the image below, the *details* section includes a rotatable 3D structure. Thanks to 3Dhtml it is really easy to manipulate 3D species animations in the database.

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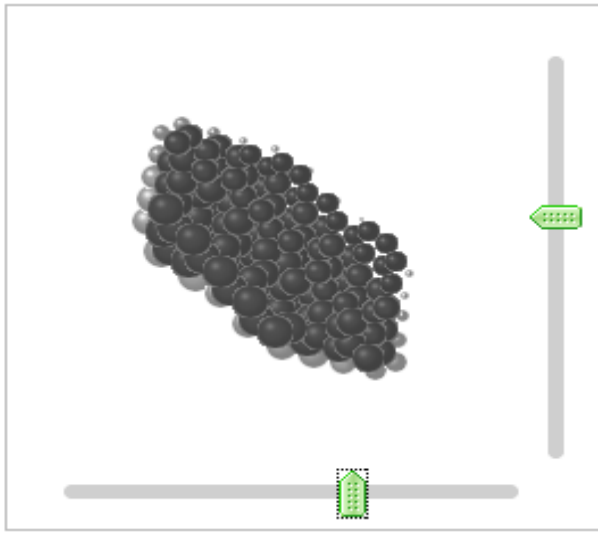
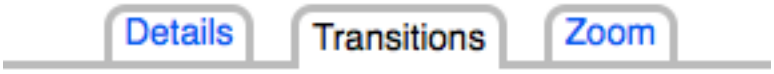


Details of the rotatable 3D structure of the specie $C_{102}H_{26}$

There is a submenu where you can go that will link you to more information about the species you are studying.



Submenu for the information of the species

For example, in the subsection of *transitions* you will find all the information available in the database about the transitions of the species. You can also download the transitions data. Just enter your e-mail address and accept the usage agreement.

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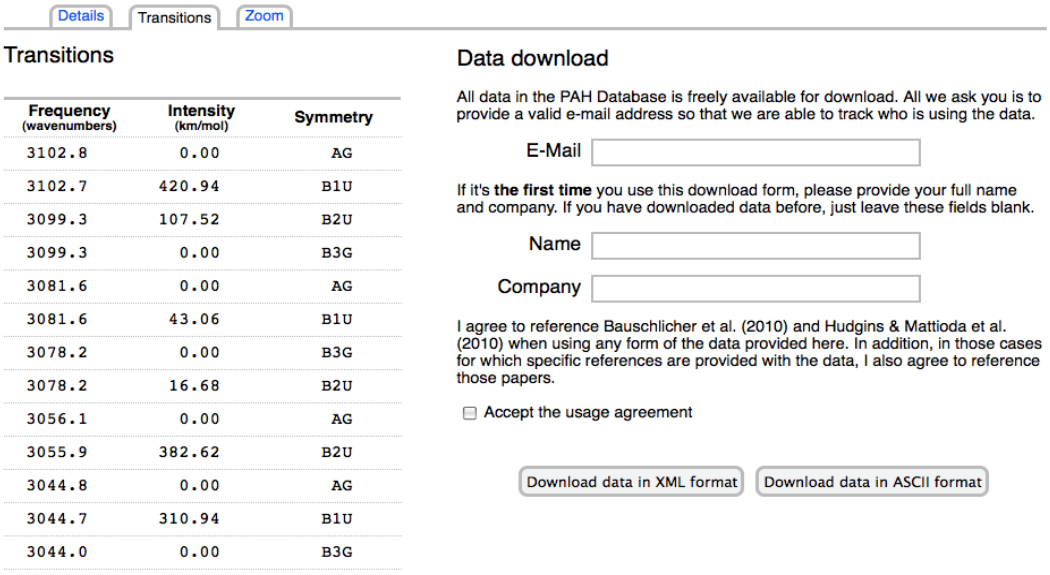
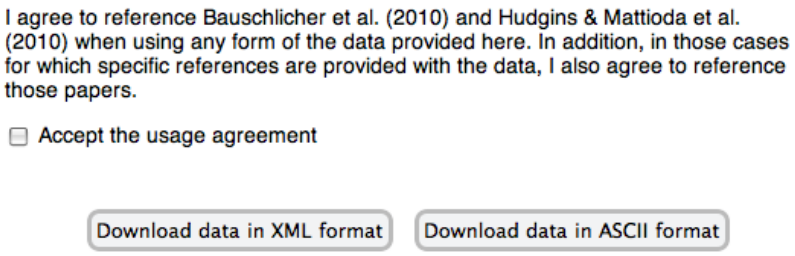


Transition section of the specie $C_{102}H_{26}$

This manual has not yet been updated for version 2.00 of the website



Detail of the usage agreement

Returning to the navigation submenu, there is a tag called zoom. If you click this tag you will go to the Zoom section where you may zoom the spectrum of the species.

Submenu for the information of the species

Once you access the Zoom section, you can move the mouse, tracking over the plot to select the area where you want to zoom in. If you double click you will come back to the initial zoom level .

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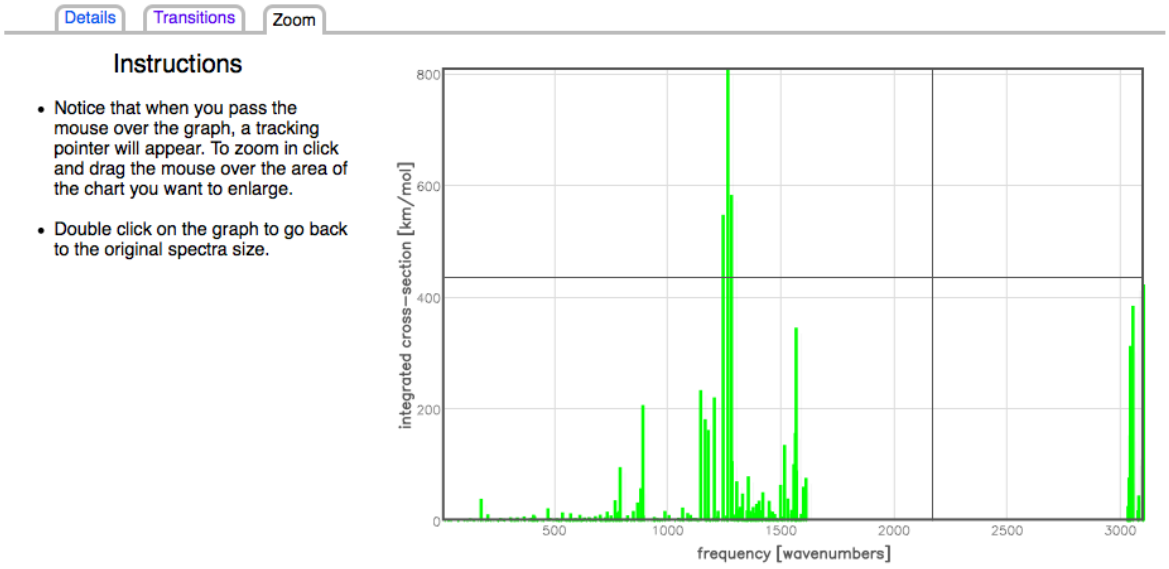

Zoom section of the specie $C_{102}H_{26}$

Finally, and only in the experimental database, you can find a label named Laboratory, which will show you the raw laboratory spectrum of the species. This data is not yet available for all species of experimental database.

Submenu for the information of the species

Browser and Selection are the main part of the application. They are primarily intended to facilitate the location of the species in the database. This will offer alternatives that will allow a selection process to lead the user in a quick and efficient way to view the species.

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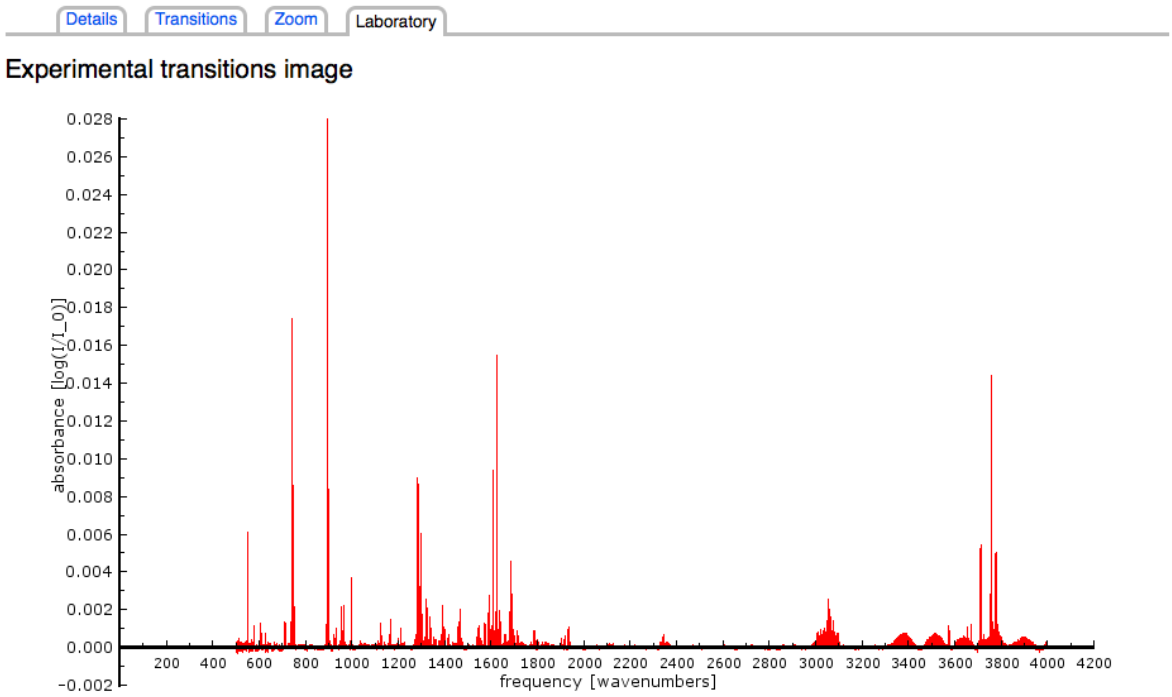

Spectrum with the experimental transitions of the species $C_{18}H_{12}$

As you can see in the image above, there is a download form like in the transitions section that will let you download the experimental transitions of the species.

4.3 Search engine

The user can search in the database at any time. That is why the search bar is always available. You also can find a link, below the search bar, where you can access the advanced search.

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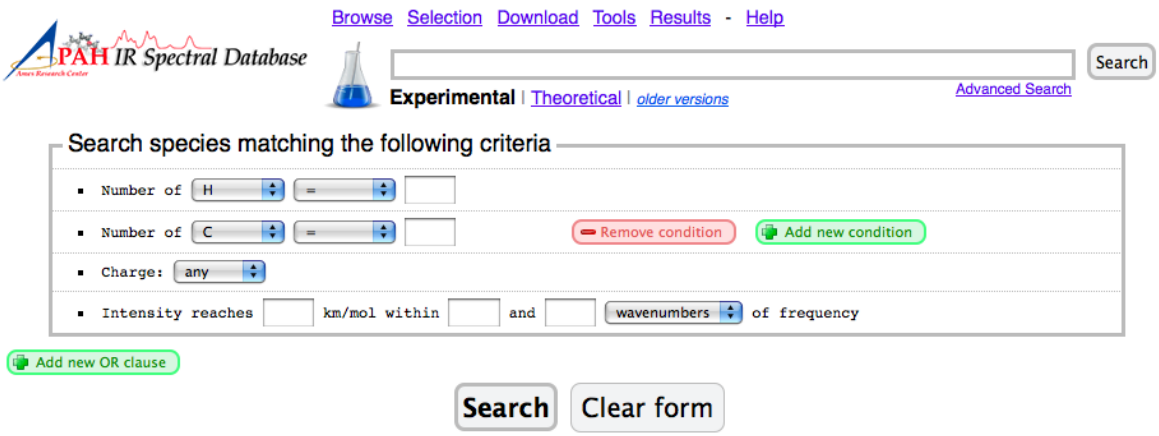
Advanced search link

The web-portal implements a powerful search engine that allows you to find and select data using simplified queries. In this section you can specify what you want to find. Also, you can add or remove conditions and OR clauses for narrower search.



Advanced search page

Detail of the buttons to add or to remove conditions

4.4 Tools and results

Once a set of species is selected, several tools are available for you to work with the data. In the general settings you can specify parameters such as frequency (in wavenumbers) or wavelength (in micron), which FWHM to apply for the Lorentzian emission profiles and also specify the emission temperature in terms of a blackbody at *x* kelvin.

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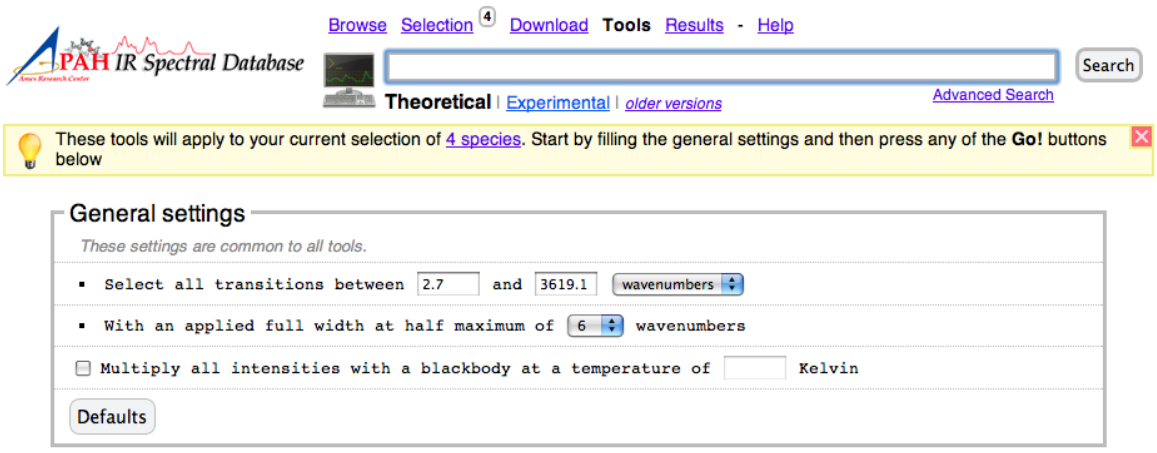
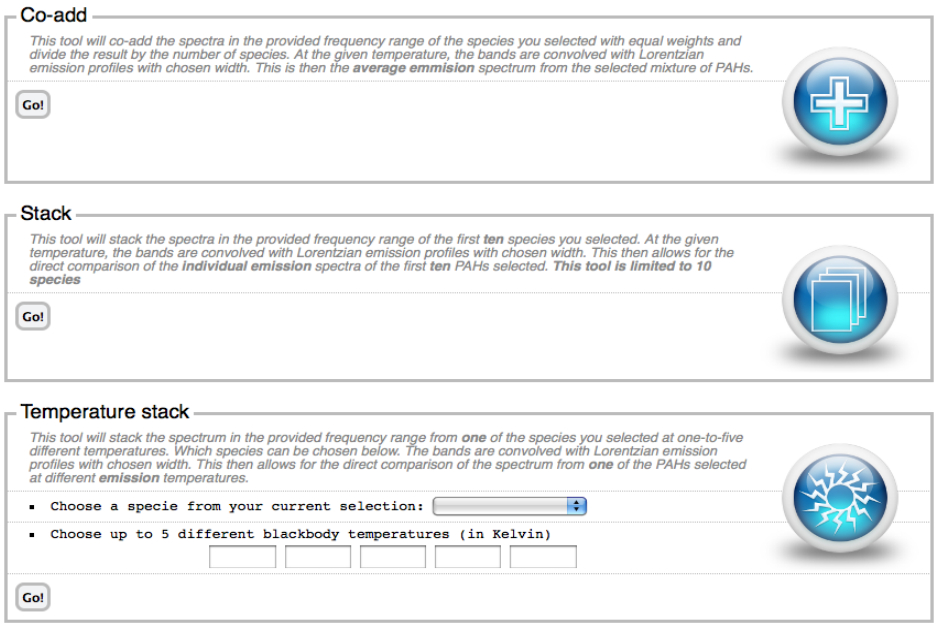


Detail of the buttons to add or to remove conditions

We have a tool that can co-add spectra and two tools that compare spectra in a stack plot by simply clicking on the corresponding Go! Button.



All the tools available in the application

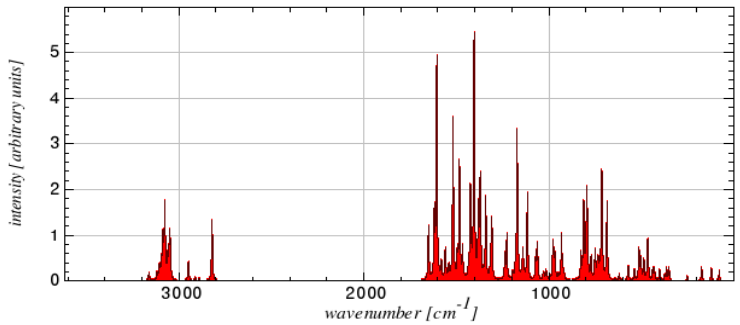
The first tool is capable of comparing up to 10 different PAH spectra directly and the second allows one to compute up to 5 different emission spectra, corresponding to 5 different emission temperatures for a single species.

This manual has not yet been updated for version 2.00 of the website

#1. Co-add of 4 species [Collapse]

*Co-add of **1 species** from **theoretical** database selecting transitions from **2.7** to **3619.1 wavenumbers** with full width at half maximum of **6 wavenumbers**.*

Species: C_6H_6O $C_6H_6O^+$ $C_9H_7^+$ C_9H_7N



Download PostScript Discard

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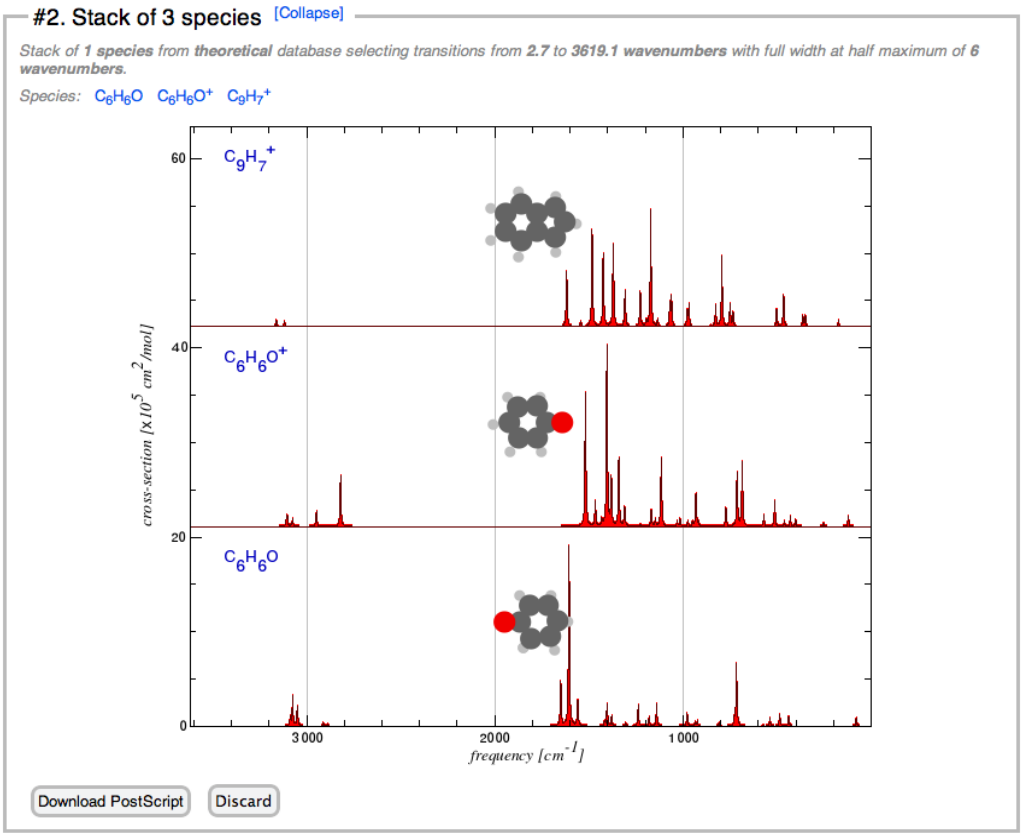
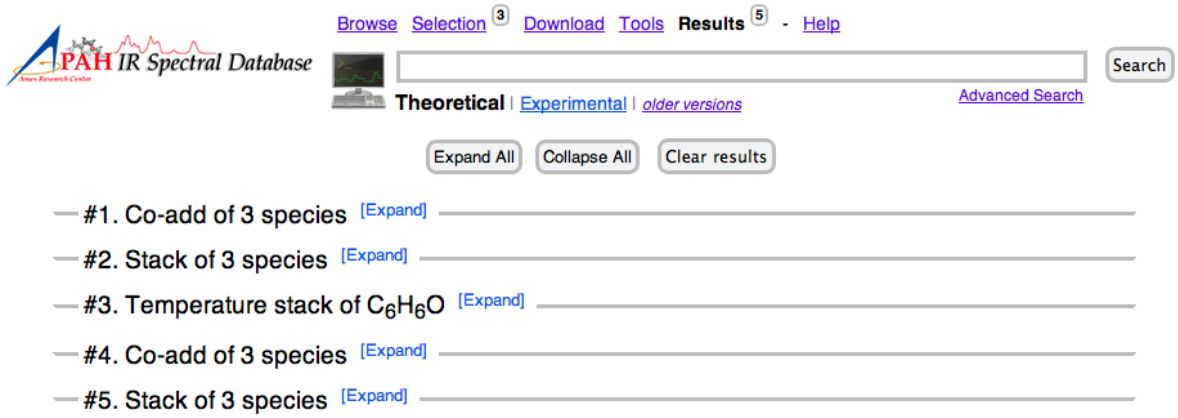
Co-add tool of three species



Stack tool of three species

The resulting spectra are presented together with those from earlier exercises to allow comparison. Use the buttons *Expand All*, *Collapse All* and *Clear results* for these tasks.



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All the results together

Detail of the buttons

It offers users the option of downloading the data from the species result in PostScript format or discarding the result.

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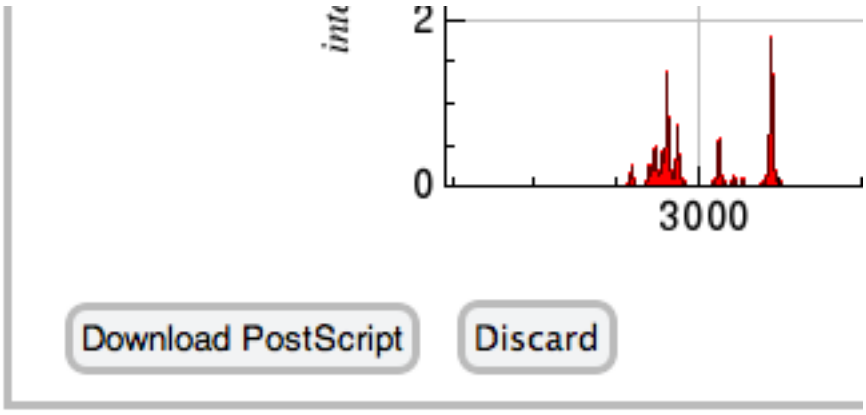
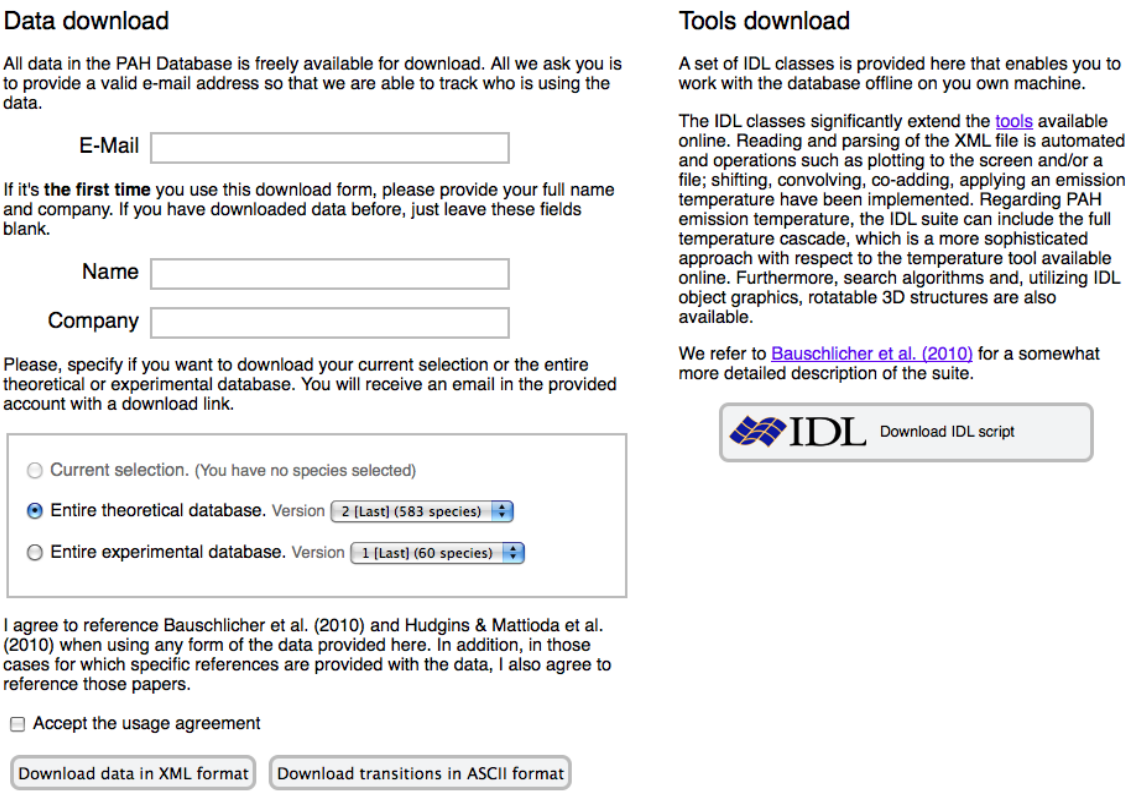


Detail of the buttons

4.5 Download

This page allows you to download all the information requested from the database. You can do this by simply filling out a form to let administrators have a record of the download volume. It offers you the option of downloading the data from the species in two formats, XML and ASCII, and also you can download the entire database or a selection of the species.



Download section in the PAHDB

Detail of the options in the download section

Let us see an example of how to download the entire database in XML format. Once you fill out the form you have to click in the Download data in XML format button. A page with information about the data that you want to download will show up.

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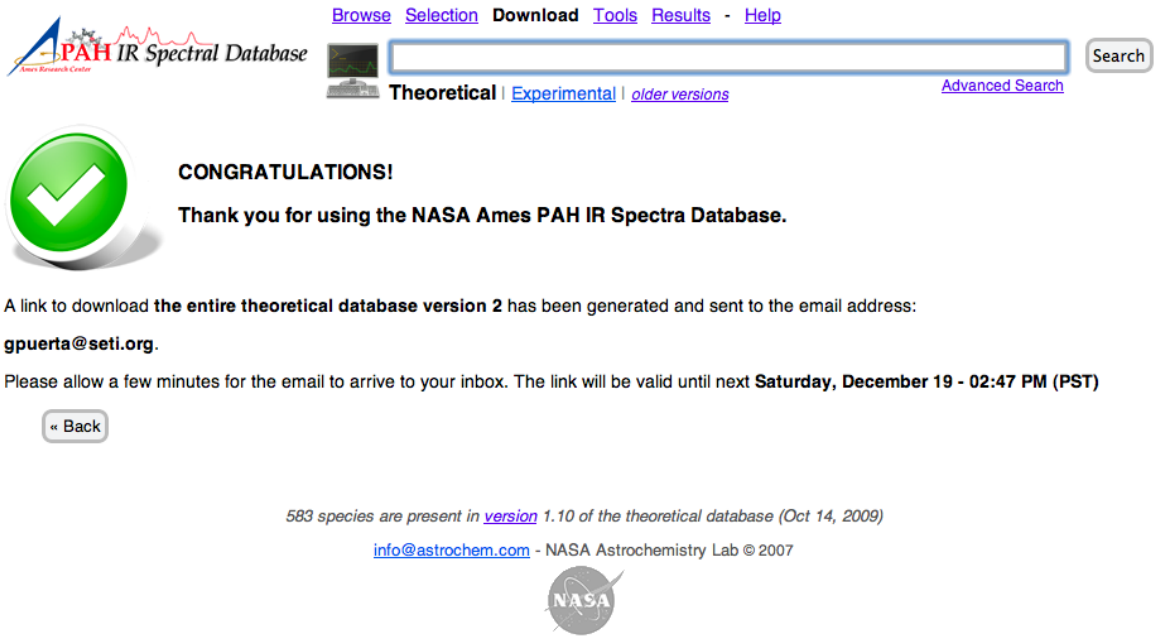
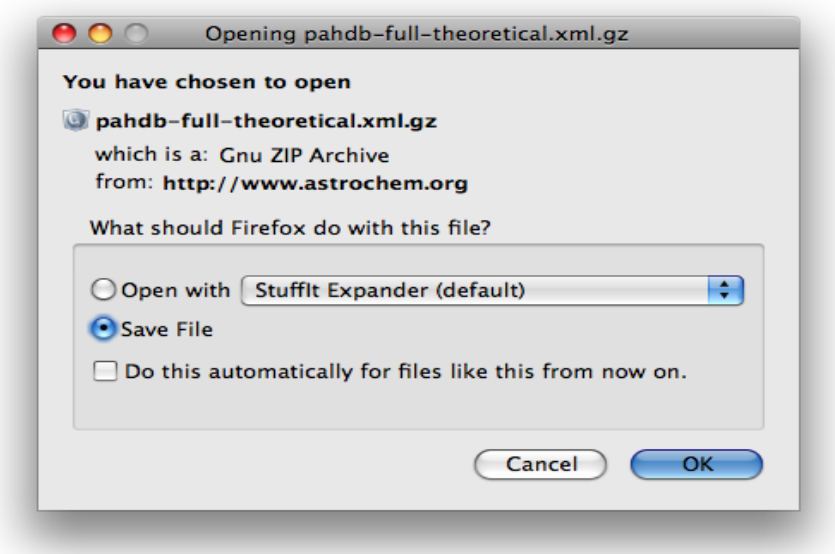


Confirmation page

Go check your email and you will find an email from PAHDB with your download link. Click on the link and you will be able to download the data.

This manual has not yet been updated for version 2.00 of the website



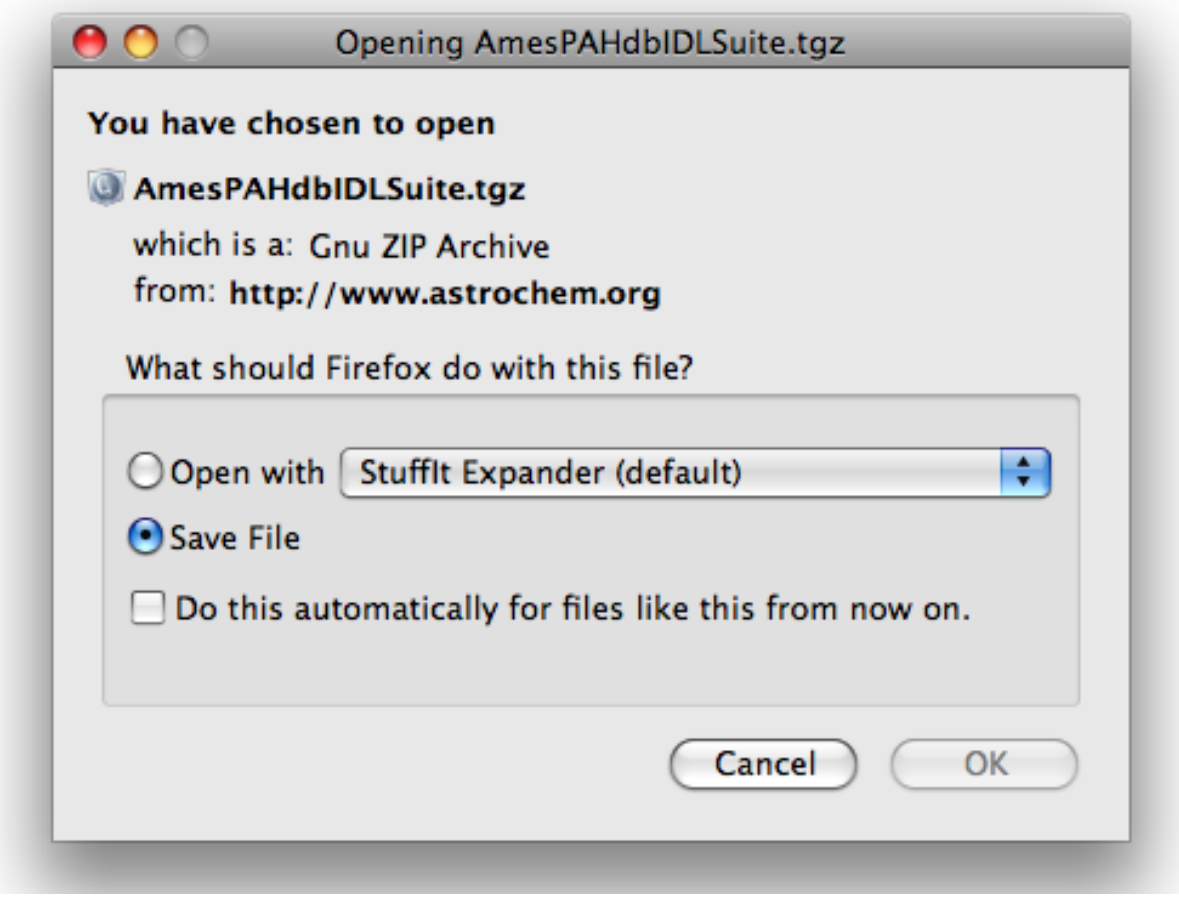
A window to accept the file you want to download

A set of IDL classes is provided here that enables you to work with the database offline on you own machine. The IDL classes significantly extend the tools available online.

Th IDL Download IDL script *te*

Detail of the Download button

Reading and parsing of the XML file is automated and operations such as plotting to the screen and/or a file; shifting, convolving, co-adding, applying an emission temperature have been implemented.



A window to accept the file you want to download

4.6 Help

This section contains useful information for users of PAHDB. A tutorial and a video tutorial are

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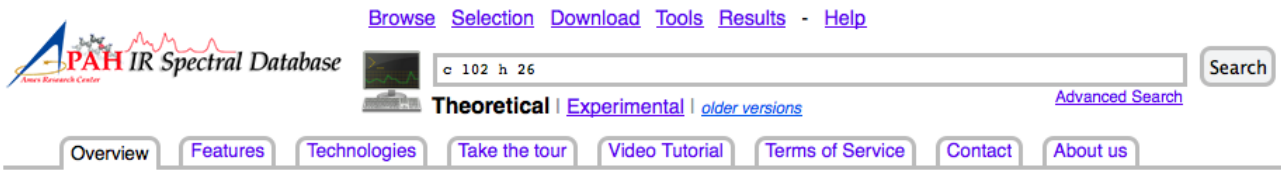
available to explain how to use the application. Also, a page with Frequently Asked Questions, mainly about the project, as a full description of application usage are in the appendix A of this documentation. It also contains an overview and an explanation of the features and technologies used for the realization of this project.

This manual has not yet been updated for version 2.00 of the website

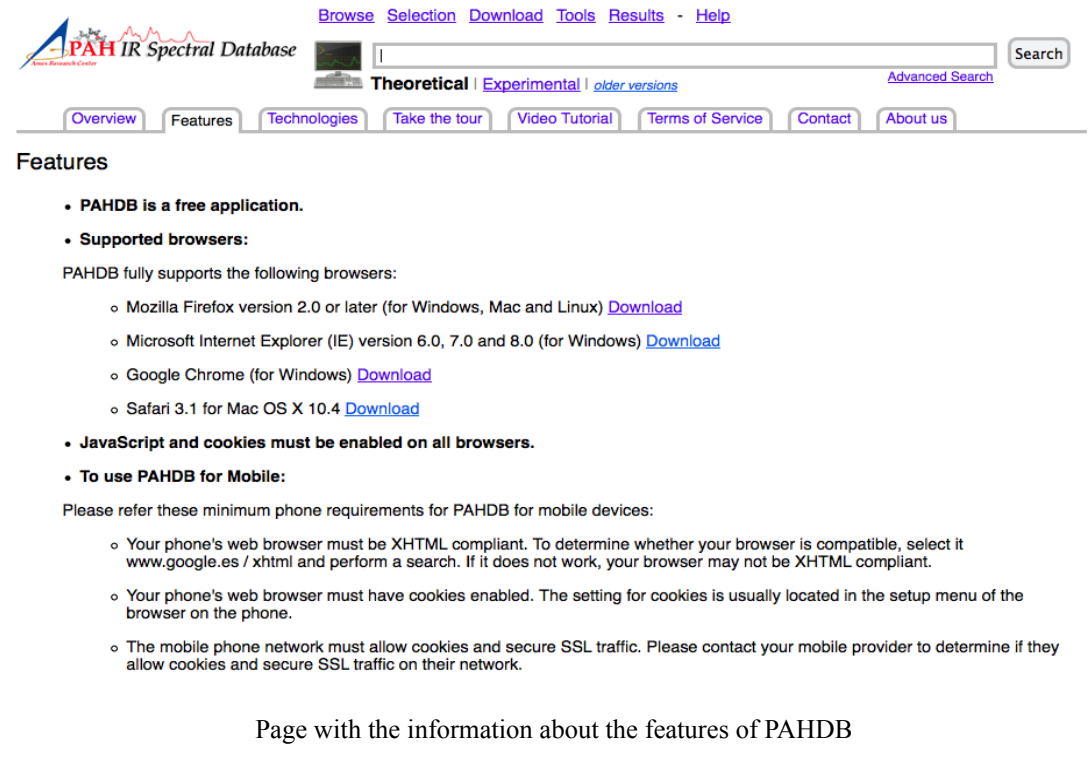
This manual has not yet been updated for version 2.00 of the website



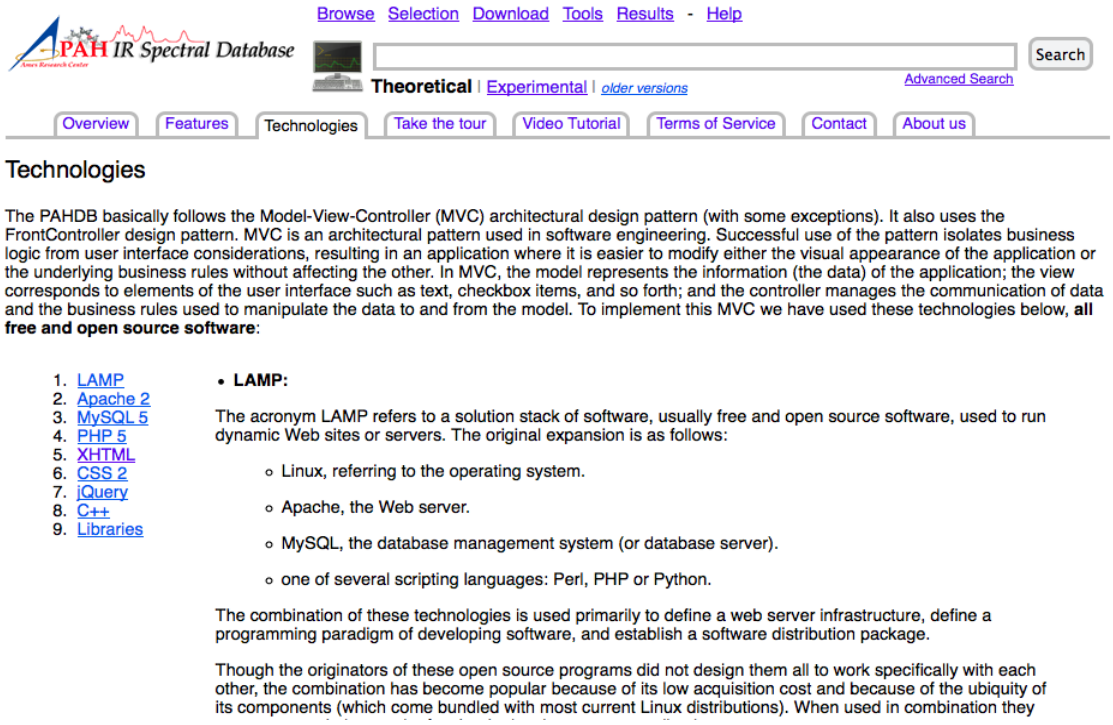
Main page in Help section

Menu to navigate in Help section

This manual has not yet been updated for version 2.00 of the website

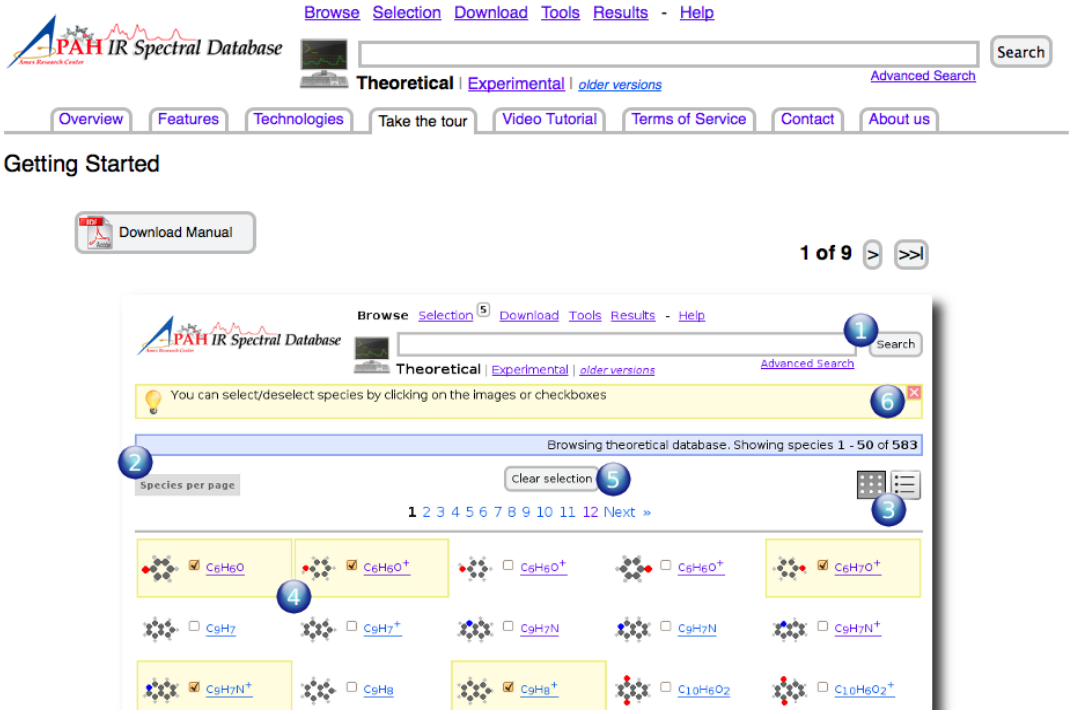


Page with the information about the features of PAHDB

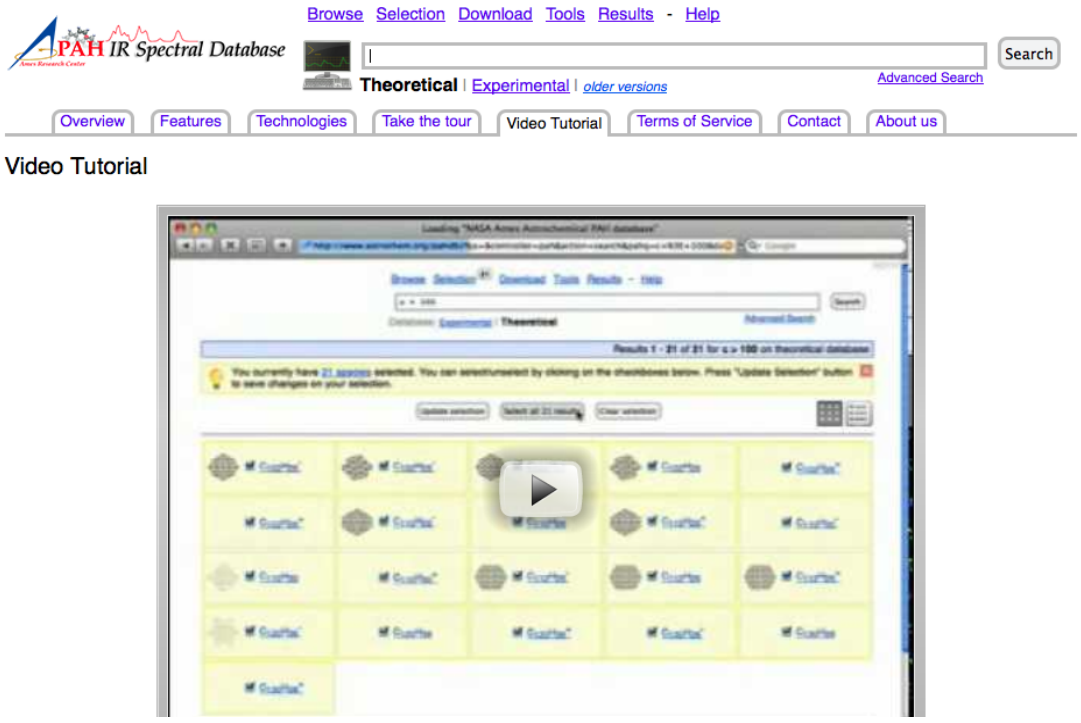


Page with the information about the technologies of PAHDB

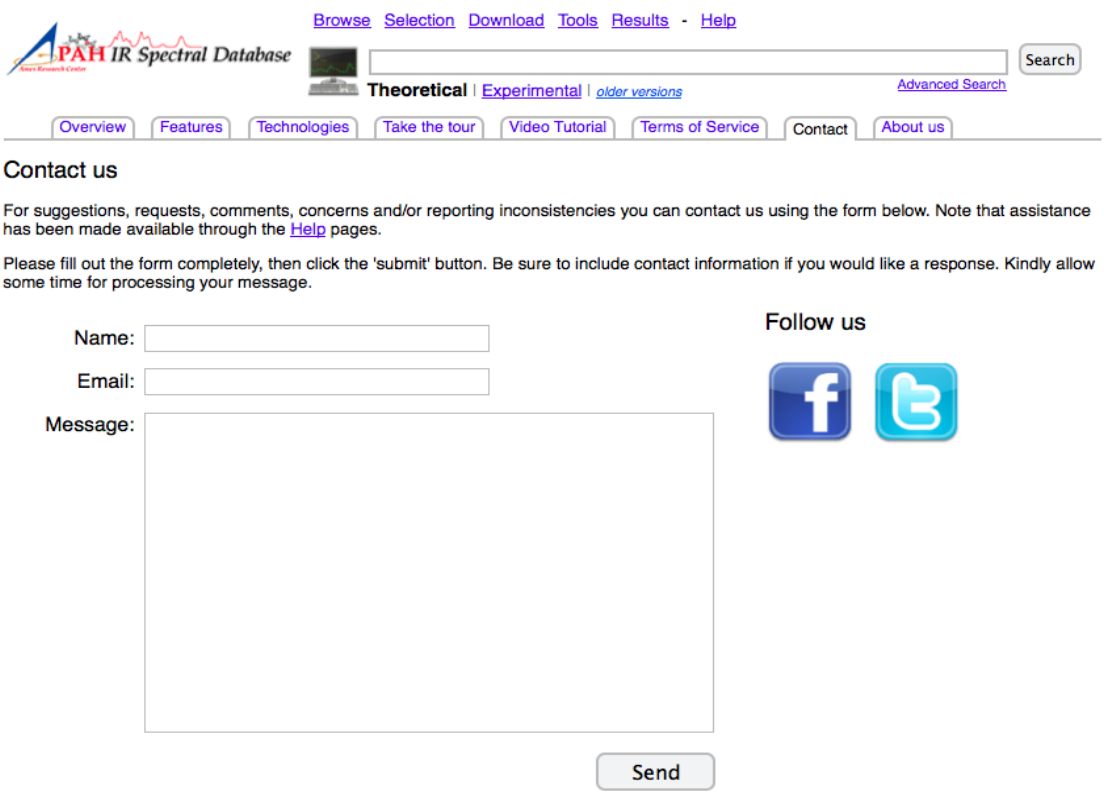
This manual has not yet been updated for version 2.00 of the website



Page with a tutorial of PAHDB



This manual has not yet been updated for version 2.00 of the website



Page with to contact with us

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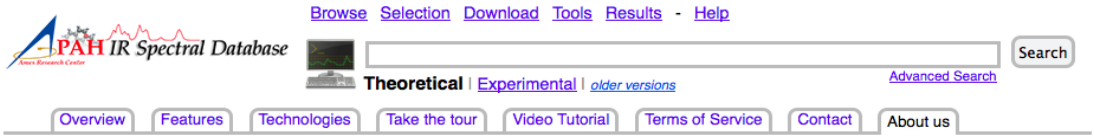

About us

A synergy between the astronomers, laboratory chemists and theoretical chemists at the facilities of NASA's Ames Research Center has resulted in the collection of PAH spectra known as *The NASA Ames PAH IR Spectroscopic Database*. Collaboration with different institutes, across several countries, helped mature the database and allowed for the construction of the web-portal, with its data and tools, you see here. Initially intended for astronomers to explain the astronomical unidentified infrared bands and to investigate the "PAH hypothesis", now the spectral data and developed paradigms prove also valuable to, e.g., chemists, environmentalists, pharmacologists and nano-technologists. Many people, across several disciplines, were involved, for which you will find a short bibliography below.

Dr. Alessandra Ricca - Principal Investigator at SETI Institute

Dr. Ricca is a computational chemist with more than 15 years of expertise in the theoretical analysis of organic molecules including the calculation of IR vibrational frequencies and ionization potentials. She is responsible for computing the harmonic frequencies and intensities compiled in the PAH IR database. More...

Dr. Christiaan Boersma - Astronomer at NASA Ames

Dr. Boersma is an astronomer and currently working as a postdoc with the Astrophysics & Astrochemistry Laboratory group at NASA's Ames Research Center, studying the role of PAHs in a multitude of astronomical environments. He conducts his research through analysing and interpreting astronomical spectra utilizing the combination of laboratory and synthesised spectroscopic data in the NASA Ames PAH IR Spectroscopic Database. More...

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