

NASA Ames Research Center
The Astrophysics & Astrochemistry Laboratory



The NASA Ames PAH IR Spectroscopic Database

WEBSITE MANUAL

version 1.00

By

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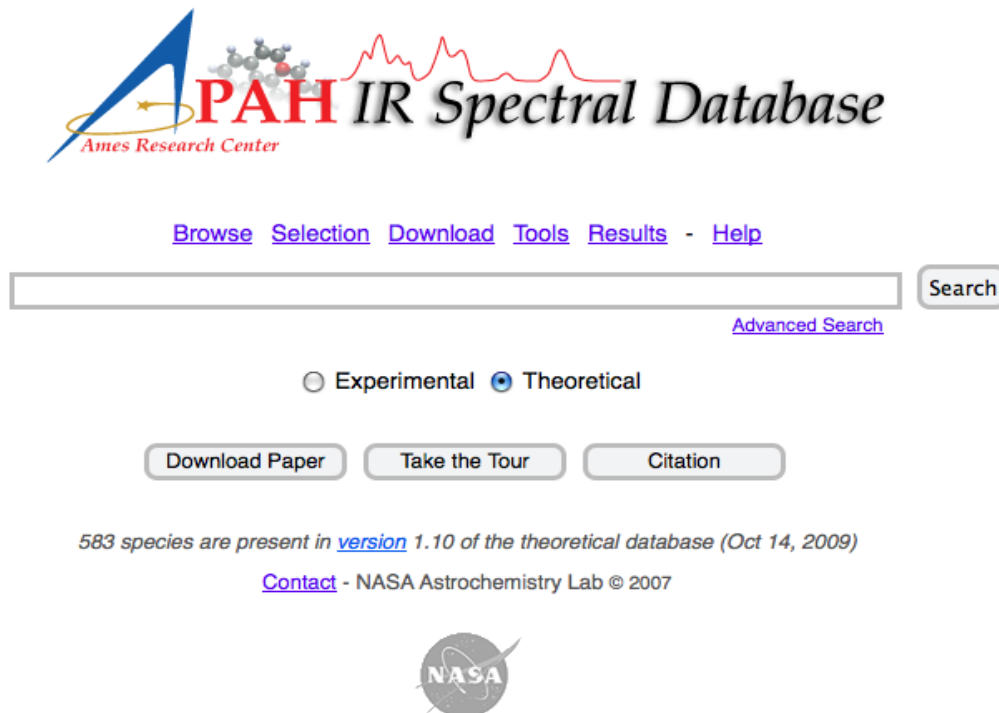
Dr. Christiaan Boersma

Updated October 2013

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

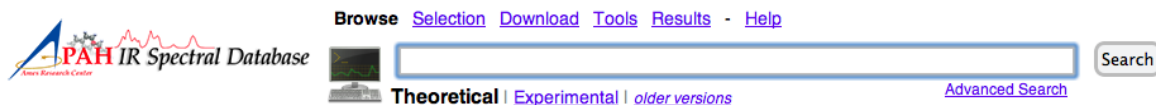
1 INTRODUCTION

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

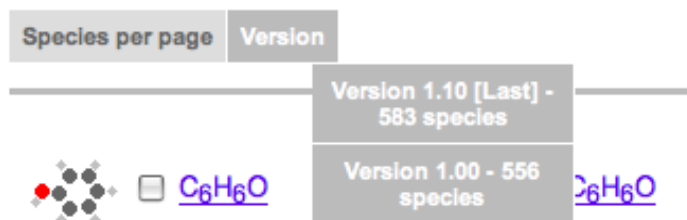
If you want to see more species you just have to click on the number page you want in the navigation menu.

1 2 3 4 5 6 7 8 9 10 11 12 Next »

Navigation menu in Browse section

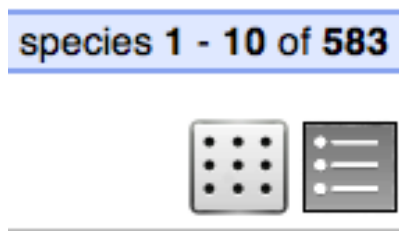
On the left side of the page you may change the species per page that you wish to display and you can browse earlier versions of the database.

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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.



Use the select/deselect buttons to update your selection.



Browsing theoretical database. Showing species 1 - 10 of 583

Species per page Version

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 ... 59 Next »

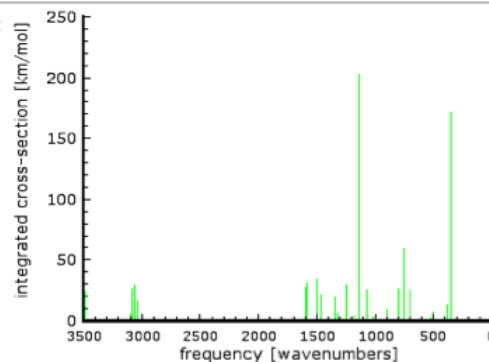


Unique id 428

solo	0	duo	0
trio	0	quartet	0
quintet	5	ch2	0
chx	0	symmetry	C_s

Full info

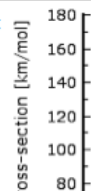
« select



Unique id 430

solo	0	duo	0
trio	0	quartet	4
quintet	0	ch2	2







« select



Detailed view of the species of the theoretical database

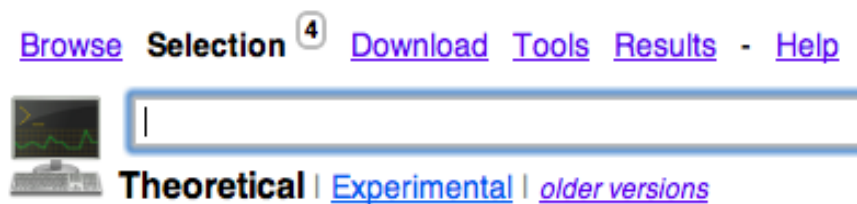
In any of the views that the application provides, you can select the species of interest, just click checkboxes.

[Clear selection](#)[1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#) [10](#) [11](#) [12](#) [Next »](#)

 <input checked="" type="checkbox"/> C6H6O	 <input type="checkbox"/> C6H6O⁺	 <input checked="" type="checkbox"/> C6H6O⁺
 <input checked="" type="checkbox"/> C9H7⁺	 <input checked="" type="checkbox"/> C9H7N	 <input type="checkbox"/> C9H7N

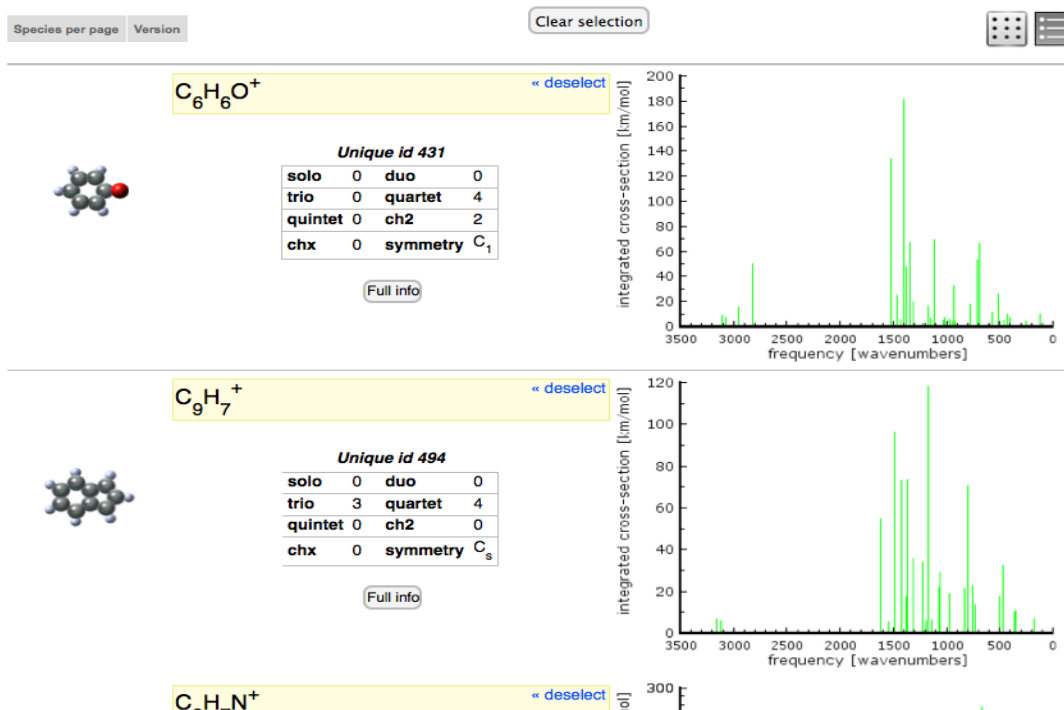
In yellow boxes the species selected

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.



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.



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 with experimental/theoretical data in the database, transition tables and molecular characteristics.



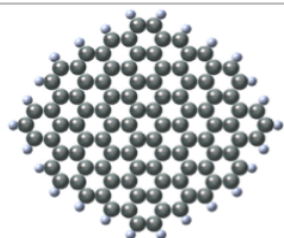
c 102 h 26x

Search

[Theoretical](#) | [Experimental](#) | [older versions](#)

[Advanced Search](#)

[« Back](#)

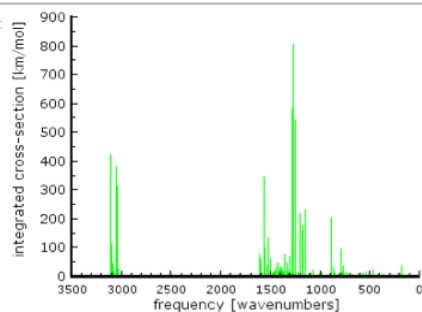


$C_{102}H_{26}$

[« select](#)

Unique id 179

solo	8	duo	12
trio	6	quartet	0
quintet	0	ch2	0
chx	0	symmetry	D_{2h}



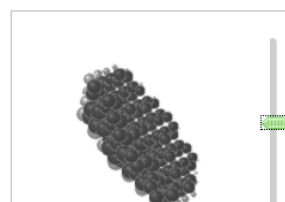
[Details](#)

[Transitions](#)

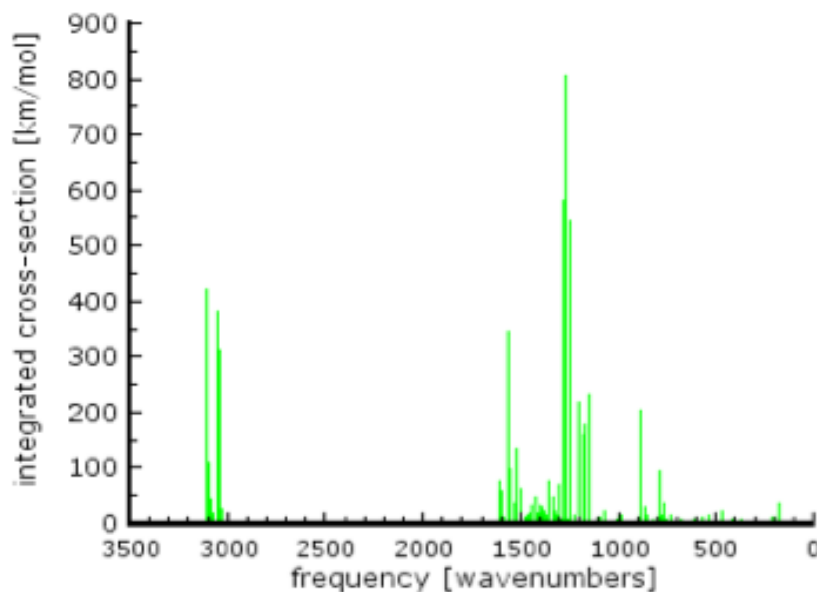
[Zoom](#)

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



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

Species 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

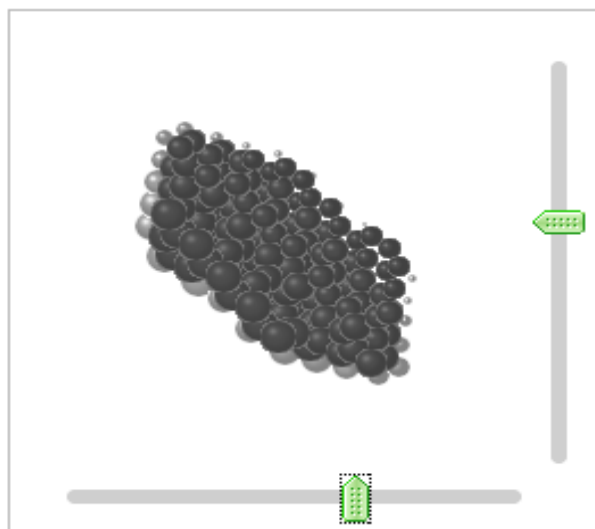
- SDT with sym

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)

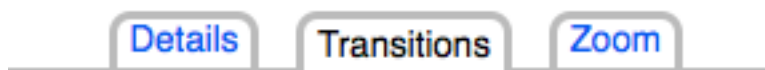
Details section of the specie $C_{102}H_{26}$

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.



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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[Details](#)[Transitions](#)[Zoom](#)

Transitions

Frequency (wavenumbers)	Intensity (km/mol)	Symmetry
3102.8	0.00	AG
3102.7	420.94	B1U
3099.3	107.52	B2U
3099.3	0.00	B3G
3081.6	0.00	AG
3081.6	43.06	B1U
3078.2	0.00	B3G
3078.2	16.68	B2U
3056.1	0.00	AG
3055.9	382.62	B2U
3044.8	0.00	AG
3044.7	310.94	B1U
3044.0	0.00	B3G

Data download

All data in the PAH Database is freely available for download. All we ask you is to provide a valid e-mail address so that we are able to track who is using the data.

E-Mail

If it's **the first time** you use this download form, please provide your full name and company. If you have downloaded data before, just leave these fields blank.

Name

Company

I agree to reference Bauschlicher et al. (2010) and Hudgins & Mattioda et al. (2010) when using any form of the data provided here. In addition, in those cases for which specific references are provided with the data, I also agree to reference those papers.

☐ Accept the usage agreement

[Download data in XML format](#)

[Download data in ASCII format](#)

Transition section of the specie C₁₀₂H₂₆

I agree to reference Bauschlicher et al. (2010) and Hudgins & Mattioda et al. (2010) when using any form of the data provided here. In addition, in those cases for which specific references are provided with the data, I also agree to reference those papers.

☐ Accept the usage agreement

Download data in XML format

Download data in ASCII format

Detail of the usage agreement

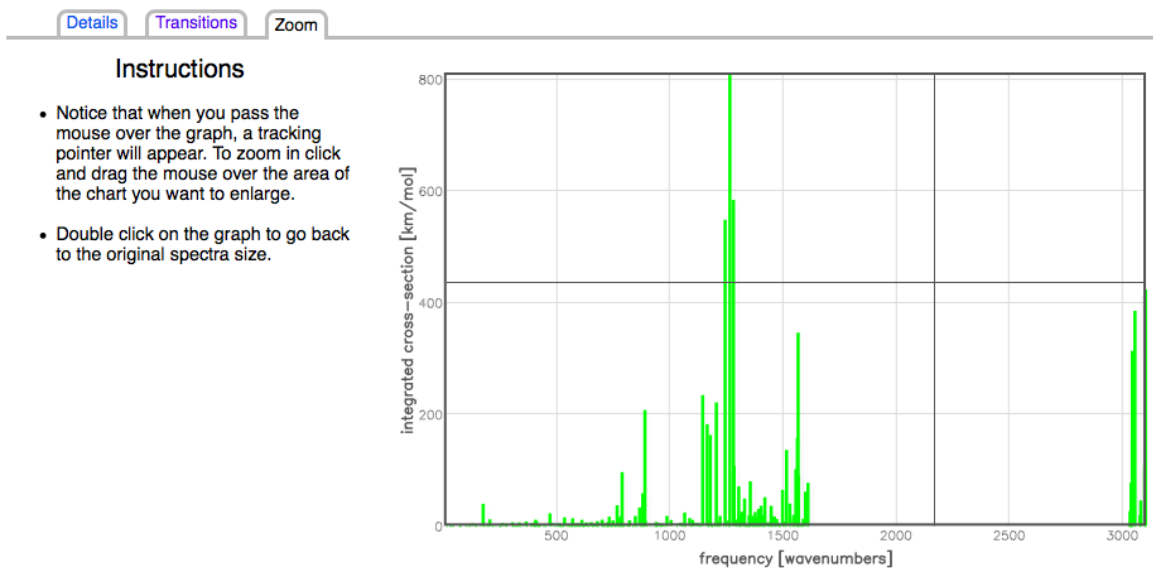
Returning to the navigation submenu, there is a tag called zoom. If you click this tag you will go to the Zoom section where you may zoom the spectrum of the species.



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 $C_{102}H_{26}$

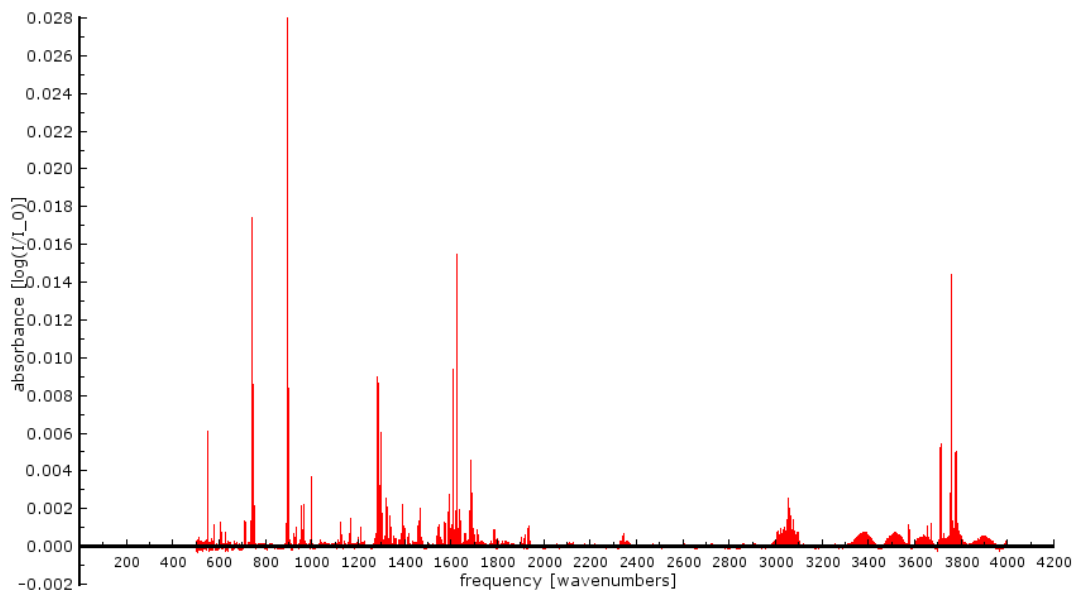
Finally, and only in the experimental database, you can find a label named Laboratory, which will show you the raw laboratory spectrum of the species. This data is not yet available for all species of experimental database.



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.

Experimental transitions image



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

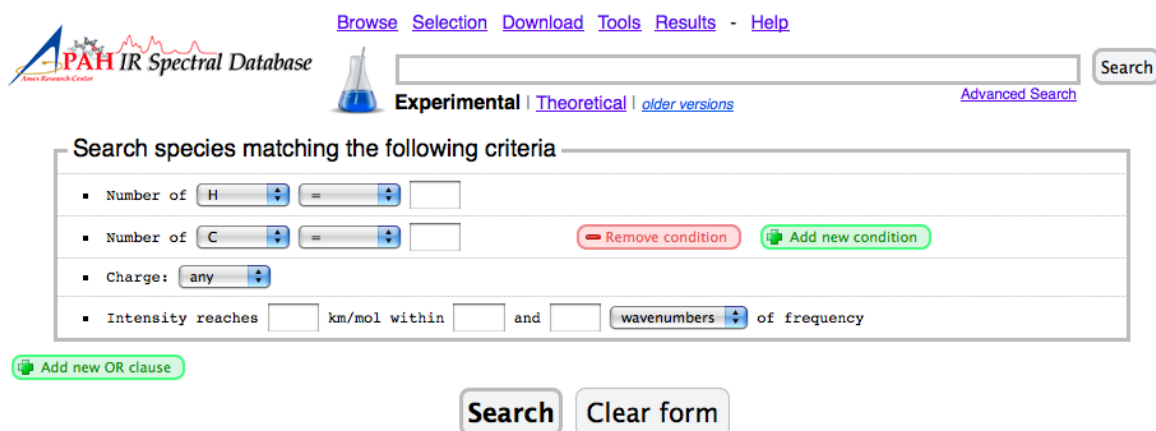
The user can search in the database at any time. That is why the search bar is always available. You also can find a link, below the search bar, where you can access the advanced search.

Search

Advanced Search

[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.



The screenshot shows the PAH IR Spectral Database search interface. At the top, there is a navigation bar with links: [Browse](#), [Selection](#), [Download](#), [Tools](#), [Results](#), and [Help](#). Below this is a search bar with a [Search](#) button and a [Advanced Search](#) link. The main search area is titled "Search species matching the following criteria" and contains several input fields: "Number of H", "Number of C", "Charge" (set to "any"), and "Intensity reaches" (with units "km/mol within" and "and"). There are also buttons for "Remove condition" and "Add new condition". At the bottom, there are buttons for "Search" and "Clear form".

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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[Browse](#)
[Selection](#) ⁴
[Download](#)
[Tools](#)
[Results](#)
[Help](#)



[Theoretical](#) | [Experimental](#) | [older versions](#)
[Advanced Search](#)


 These tools will apply to your current selection of **4 species**. Start by filling the general settings and then press any of the **Go!** buttons below

General settings

These settings are common to all tools.


- Select all transitions between and
- With an applied full width at half maximum of wavenumbers
- ☐ Multiply all intensities with a blackbody at a temperature of Kelvin

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.


Co-add

*This tool will co-add the spectra in the provided frequency range of the species you selected with equal weights and divide the result by the number of species. At the given temperature, the bands are convolved with Lorentzian emission profiles with chosen width. This is then the **average emission** spectrum from the selected mixture of PAHs.*



Stack


*This tool will stack the spectra in the provided frequency range of the first **ten** species you selected. At the given temperature, the bands are convolved with Lorentzian emission profiles with chosen width. This then allows for the direct comparison of the **individual emission** spectra of the first **ten** PAHs selected. **This tool is limited to 10 species***



Temperature stack

*This tool will stack the spectrum in the provided frequency range from **one** of the species you selected at **one-to-five** different temperatures. Which species can be chosen below. The bands are convolved with Lorentzian emission profiles with chosen width. This then allows for the direct comparison of the spectrum from **one** of the PAHs selected at different **emission** temperatures.*

- Choose a specie from your current selection:
- Choose up to 5 different blackbody temperatures (in Kelvin)



All the tools available in the application

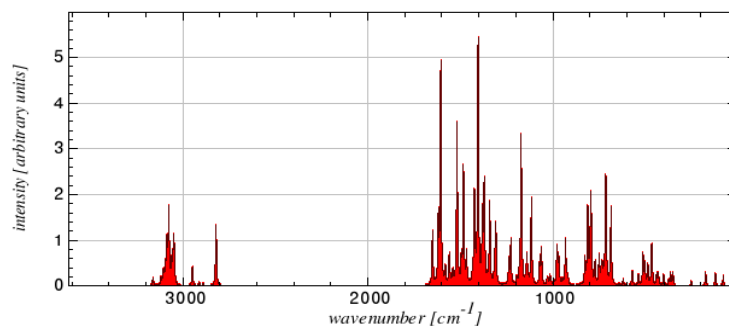
The first tool is capable of comparing up to 10 different PAH spectra directly and the second allows one to compute up to 5 different emission spectra, corresponding to 5 different emission temperatures for a single species.

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#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.

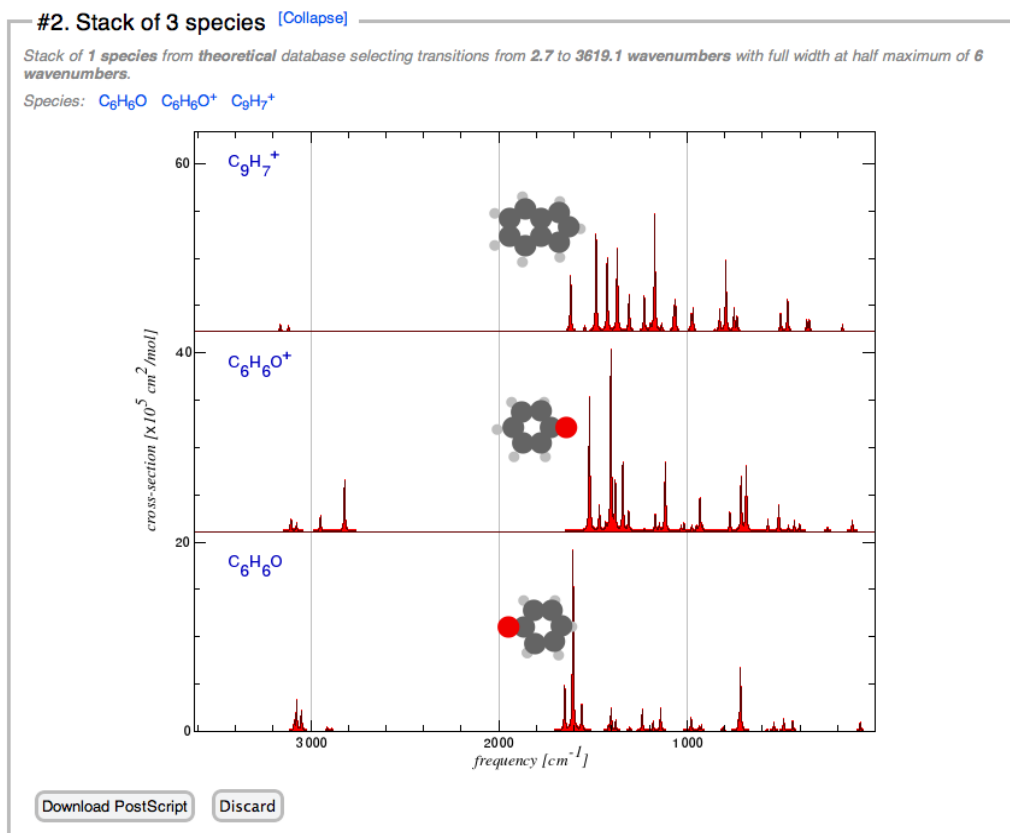
Species: $\text{C}_6\text{H}_6\text{O}$ $\text{C}_6\text{H}_6\text{O}^+$ C_9H_7^+ $\text{C}_9\text{H}_7\text{N}$



[Download PostScript](#)


[Discard](#)


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.

 [Browse](#) [Selection](#) ³ [Download](#) [Tools](#) [Results](#) ⁵ - [Help](#)

 [Theoretical](#) | [Experimental](#) | [older versions](#) [Advanced Search](#)

[Expand All](#) [Collapse All](#) [Clear results](#)

— #1. Co-add of 3 species [\[Expand\]](#)

— #2. Stack of 3 species [\[Expand\]](#)

— #3. Temperature stack of $\text{C}_6\text{H}_6\text{O}$ [\[Expand\]](#)

— #4. Co-add of 3 species [\[Expand\]](#)

— #5. Stack of 3 species [\[Expand\]](#)

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

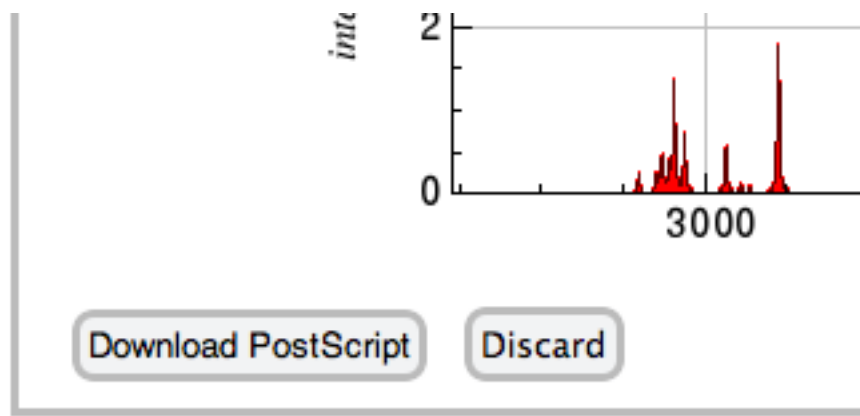
All the results together



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.

Data download

All data in the PAH Database is freely available for download. All we ask you is to provide a valid e-mail address so that we are able to track who is using the data.

E-Mail

If it's **the first time** you use this download form, please provide your full name and company. If you have downloaded data before, just leave these fields blank.

Name

Company

Please, specify if you want to download your current selection or the entire theoretical or experimental database. You will receive an email in the provided account with a download link.

☐ Current selection. (You have no species selected)

☒ Entire theoretical database. Version

☐ Entire experimental database. Version

I agree to reference Bauschlicher et al. (2010) and Hudgins & Mattioda et al. (2010) when using any form of the data provided here. In addition, in those cases for which specific references are provided with the data, I also agree to reference those papers.

☐ Accept the usage agreement

Tools download

A set of IDL classes is provided here that enables you to work with the database offline on your own machine.

The IDL classes significantly extend the [tools](#) available online. 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. Regarding PAH emission temperature, the IDL suite can include the full temperature cascade, which is a more sophisticated approach with respect to the temperature tool available online. Furthermore, search algorithms and, utilizing IDL object graphics, rotatable 3D structures are also available.

We refer to [Bauschlicher et al. \(2010\)](#) for a somewhat more detailed description of the suite.



Download section in the PAHDB

☐ Current selection. (You have no species selected)

☒ Entire theoretical database. Version

☐ Entire experimental database. Version

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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CONGRATULATIONS!

Thank you for using the NASA Ames PAH IR Spectra Database.

A link to download **the entire theoretical database version 2** has been generated and sent to the email address:

gpuerta@seti.org.

Please allow a few minutes for the email to arrive to your inbox. The link will be valid until next **Saturday, December 19 - 02:47 PM (PST)**

[« Back](#)

583 species are present in [version 1.10](#) of the theoretical database (Oct 14, 2009)

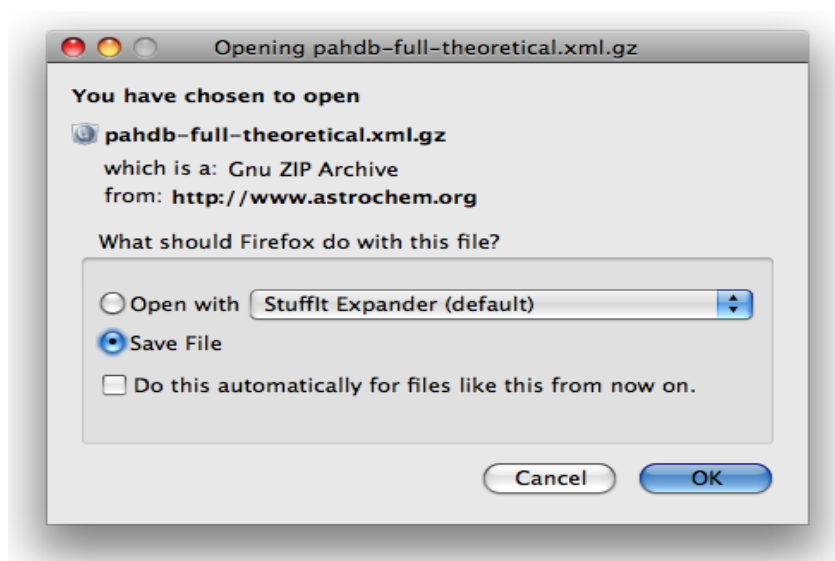
info@astrochem.com - NASA Astrochemistry Lab © 2007



Confirmation page

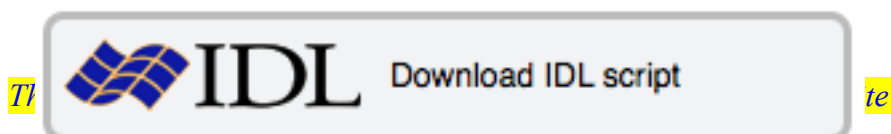
Go check your email and you will find an email from PAHDB with your download link. Click on the link and you will be able to download the data.

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



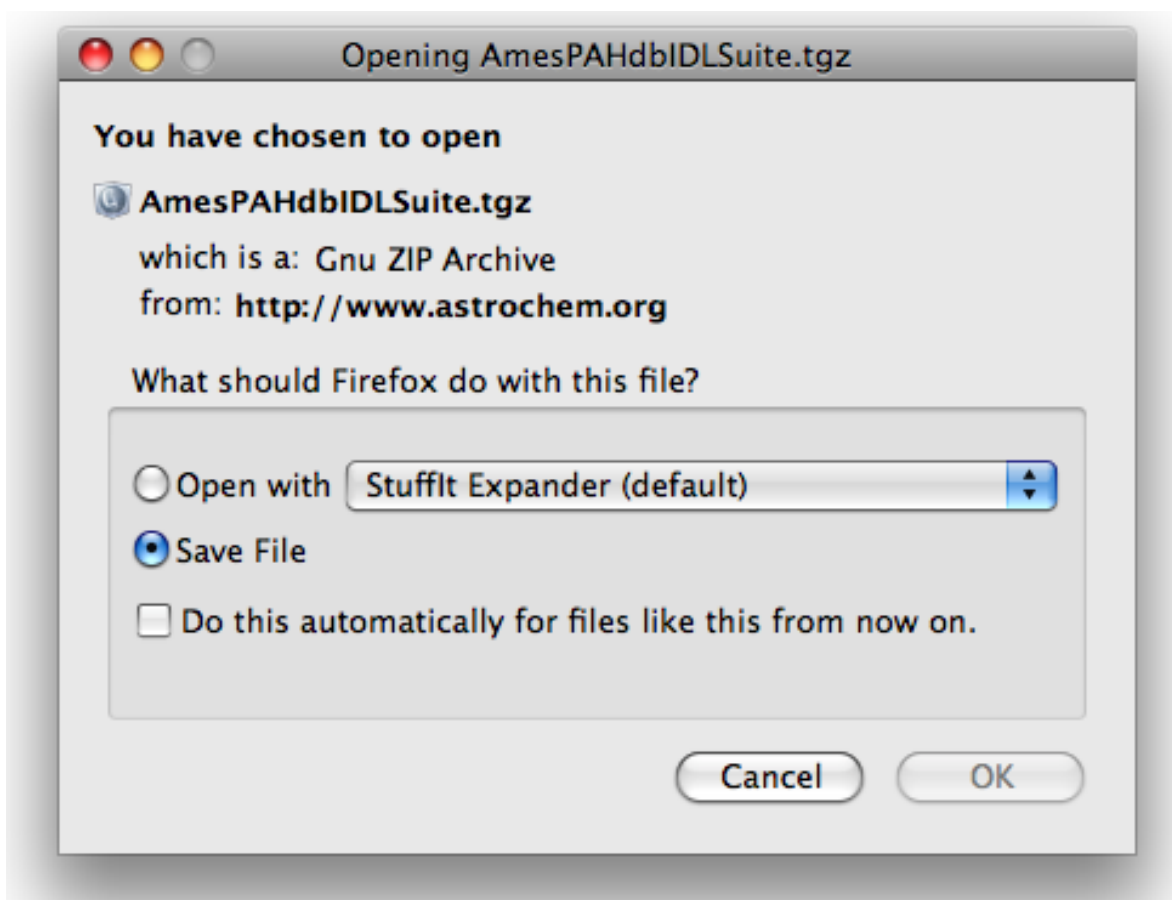
A window to accept the file you want to download

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



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.

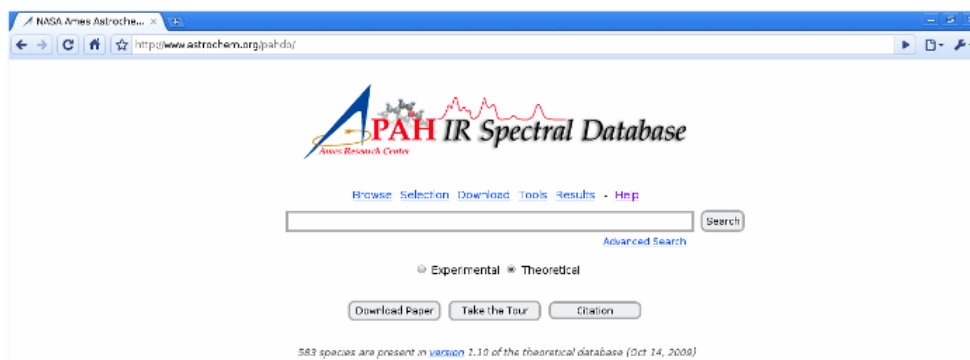


[Theoretical](#) | [Experimental](#) | [older versions](#)
[Advanced Search](#)
[Overview](#)
[Features](#)
[Technologies](#)
[Take the tour](#)
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[Contact](#)
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Welcome to PAHDB

The family of emission features formerly known as the Unidentified Infrared (UIR) bands which were discovered some thirty five years ago are now generally attributed to polycyclic aromatic hydrocarbons. The features that comprise this apparently universal spectrum contain a wealth of information about the conditions in the emitting regions and the nature of the PAH carriers. However, exploitation of these features as astrophysical and astrochemical probes has been slow in coming because the IR properties of PAHs under interstellar conditions were largely unknown for at least twenty years after the bands were discovered and the experimental and computational tools needed to provide these data were not fully developed.


[Download Paper part 1](#)

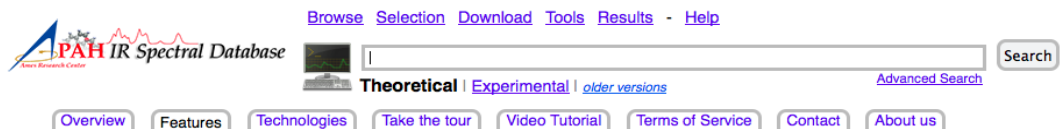
[Download Paper part 2](#)


Main page in Help section

[Overview](#)
[Features](#)
[Technologies](#)
[Take the tour](#)
[Video Tutorial](#)
[Terms of Service](#)
[Contact](#)
[About us](#)

Welcome to PAHDB

Menu to navigate in Help section



Features

- **PAHDB is a free application.**

- **Supported browsers:**

PAHDB fully supports the following browsers:

- Mozilla Firefox version 2.0 or later (for Windows, Mac and Linux) [Download](#)
- Microsoft Internet Explorer (IE) version 6.0, 7.0 and 8.0 (for Windows) [Download](#)
- Google Chrome (for Windows) [Download](#)
- Safari 3.1 for Mac OS X 10.4 [Download](#)

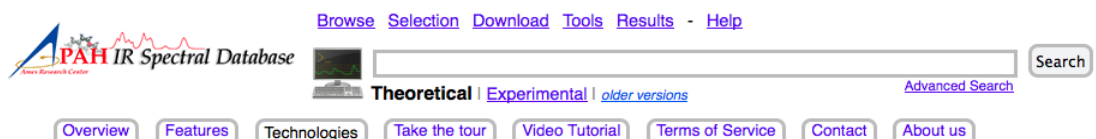
- **JavaScript and cookies must be enabled on all browsers.**

- **To use PAHDB for Mobile:**

Please refer these minimum phone requirements for PAHDB for mobile devices:

- Your phone's web browser must be XHTML compliant. To determine whether your browser is compatible, select it [www.google.es / xhtml](http://www.google.es/xhtml) and perform a search. If it does not work, your browser may not be XHTML compliant.
- Your phone's web browser must have cookies enabled. The setting for cookies is usually located in the setup menu of the browser on the phone.
- The mobile phone network must allow cookies and secure SSL traffic. Please contact your mobile provider to determine if they allow cookies and secure SSL traffic on their network.

Page with the information about the features of PAHDB



Technologies

The PAHDB basically follows the Model-View-Controller (MVC) architectural design pattern (with some exceptions). It also uses the FrontController design pattern. MVC is an architectural pattern used in software engineering. Successful use of the pattern isolates business logic from user interface considerations, resulting in an application where it is easier to modify either the visual appearance of the application or the underlying business rules without affecting the other. In MVC, the model represents the information (the data) of the application; the view corresponds to elements of the user interface such as text, checkbox items, and so forth; and the controller manages the communication of data and the business rules used to manipulate the data to and from the model. To implement this MVC we have used these technologies below, **all free and open source software**:

1. [LAMP](#)
2. [Apache 2](#)
3. [MySQL 5](#)
4. [PHP 5](#)
5. [XHTML](#)
6. [CSS 2](#)
7. [jQuery](#)
8. [C++](#)
9. [Libraries](#)

• LAMP:

The acronym LAMP refers to a solution stack of software, usually free and open source software, used to run dynamic Web sites or servers. The original expansion is as follows:

- Linux, referring to the operating system.
- Apache, the Web server.
- MySQL, the database management system (or database server).
- one of several scripting languages: Perl, PHP or Python.

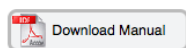
The combination of these technologies is used primarily to define a web server infrastructure, define a programming paradigm of developing software, and establish a software distribution package.

Though the originators of these open source programs did not design them all to work specifically with each other, the combination has become popular because of its low acquisition cost and because of the ubiquity of its components (which come bundled with most current Linux distributions). When used in combination they

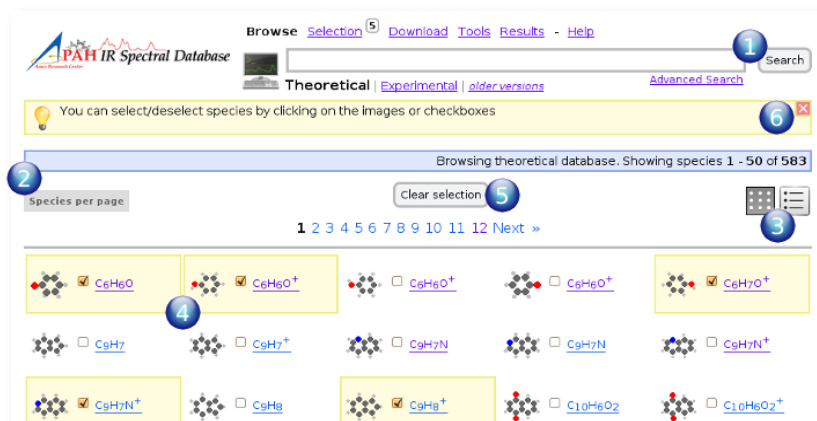
Page with the information about the technologies of PAHDB

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Getting Started



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<input checked="" type="checkbox"/> <chem>C6H6O</chem>	<input checked="" type="checkbox"/> <chem>C6H6O+</chem>	<input type="checkbox"/> <chem>C6H6O+</chem>	<input type="checkbox"/> <chem>C6H6O+</chem>	<input checked="" type="checkbox"/> <chem>C6H7O+</chem>
<input type="checkbox"/> <chem>C6H7</chem>	<input type="checkbox"/> <chem>C6H7+</chem>	<input type="checkbox"/> <chem>C6H7N</chem>	<input type="checkbox"/> <chem>C6H7N</chem>	<input type="checkbox"/> <chem>C6H7N+</chem>
<input checked="" type="checkbox"/> <chem>C6H7N+</chem>	<input type="checkbox"/> <chem>C6H8</chem>	<input checked="" type="checkbox"/> <chem>C6H8+</chem>	<input type="checkbox"/> <chem>C10H6O2</chem>	<input type="checkbox"/> <chem>C10H6O2+</chem>


Page with a tutorial of PAHDB


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A Frequently Asked Questions of PAHDB

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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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