pyPAHdb Documentation

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This is the Nasa Ames…

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PYPAHDB PACKAGE

2.1 Subpackages

2.1.1 pypahdb.tests package

Submodules

pypahdb.tests.test_observation module

test_observation.py: unit tests for class observation.

class pypahdb.tests.test_observation.**SpectrumTestCase**(*methodName='runTest'*)
Bases: unittest.case.TestCase

Unit tests for *observation.py*

test_is_instance()
Can we create an instance of observation?

pypahdb.tests.test_spectrum module

test_spectrum.py: unit tests for class spectrum.

class pypahdb.tests.test_spectrum.**SpectrumTestCase**(*methodName='runTest'*)
Bases: unittest.case.TestCase

Unit tests for *spectrum.py*

test_convert_units_micron_to_wavenumber()
Can we correctly convert micron to wavenumber?

test_is_instance()
Can we create an instance of spectrum?

pypahdb.tests.test_writer module

test_writer.py: unit tests for class writer.

class pypahdb.tests.test_writer.**WriterTestCase**(*methodName='runTest'*)
Bases: unittest.case.TestCase

Unit tests for *writer.py*

test_is_instance()
Can we create an instance of writer?

Module contents

unit tests for pypahdb

2.2 Submodules

2.3 pypahdb.decomposer module

decomposer.py: Using a precomputed matrix of theoretically calculated PAH emission spectra a spectrum is decomposed into contribution PAH subclasses using a nnls-approach.

This file is part of pypahdb - see the module docs for more information.

class pypahdb.decomposer.**decomposer**(*spectrum*)
Bases: object

Decomposes a spectrum with PAHdb.

spectrum
The decomposed spectrum.

fit
Return the fitted spectra.

Returns returns array

ionized_fraction
Return the ionized fraction.

Returns returns array

large_fraction
Return the large fraction.

Returns returns array

2.4 pypahdb.observation module

observation.py: Holds and astronomical observation

This file is part of pypahdb - see the module docs for more information.

class pypahdb.observation.**observation**(*file_path*)
Bases: object

Create an observation object for later analysis.

Currently setup to read ASCII data.

spectrum
spectrum – contains loaded spectrum

2.5 pypahdb.spectrum module

spectrum.py: Holds a spectrum

This file is part of pypahdb - see the module docs for more information.

class pypahdb.spectrum.**spectrum**(*abscissa*, *ordinate*, *uncertainties*, *units*)
Bases: object

Create a spectrum object.

abscissa
numpy.ndarray – The abscissa values.

ordinate
numpy.ndarray – The ordinate values.

uncertainties
numpy.ndarray – Uncertainties on the ordinate.

units
list – The units.

convertunitsto(***keywords*)
Convert units.

Parameters

- **aunits** (*str*) – The new abscissa units.
- **ounits** (*str*) – The new ordinate units.

Returns Nothing.

2.6 pypahdb.writer module

writer.py: Writes decomposer results to file

This file is part of pypahdb - see the module docs for more information.

class pypahdb.writer.**writer**(*result*, *header=''*, *basename=''*)
Bases: object

Creates a writer object.

Writes PDF and FITS files.

Attributes:

2.7 Module contents

The pyPAHdb module: Using a precomputed matrix of theoretically calculated PAH emission spectra from the NASA Ames PAH IR Spectroscopic Database a spectrum is decomposed into contribution PAH subclasses using a nnls-approach.

pyPAHdb uses a precomputed matrix of theoretically calculated PAH emission spectra from version 3.00 of the library of computed spectra. This matrix has been constructed from a collection of "astronomical" PAHs, which meet the following critera and include the fullerenes C60 and C70:

'magnesium=0 oxygen=0 iron=0 silicium=0 chx=0 ch2=0 c>20 hydrogen>0'

The PAH emission spectra have been calculated with the following parameters:

- A calculated vibrational temperature upon the absorption of a 7 eV photon
- Blackbody emission at the calculated vibrational temperature
- A redshift of 15 /cm to mimic some anharmonic effect
- Gaussian emission profile with a FWHM of 15 /cm

The NASA Ames PAH IR Spectroscopic Database website is located at www.astrochemistry.org/pahdb/.

You are kindly asked to cite the following papers when using pyPAHdb:

- C. Boersma, C.W. Bauschlicher, Jr., A. Ricca, A.L. Mattioda, J. Cami, E. Peeters, F. Sanchez de Armas, G. Puerta Saborido, D.M. Hudgins, and L.J. Allamandola, "THE NASA AMES PAH IR SPECTROSCOPIC DATABASE VERSION 2.00: UPDATED CONTENT, WEBSITE AND ON/OFFLINE TOOLS", The Astrophysical Journal Supplement Series, 211, 8, 2014 10.1088/0067-0049/211/1/8
- C.W. Bauschlicher, Jr., C. Boersma, A. Ricca, A.L. Mattioda, J. Cami, E. Peeters, F. Sanchez de Armas, G. Puerta Saborido, D.M. Hudgins, and L.J. Allamandola, "THE NASA AMES PAH IR SPECTROSCOPIC DATABASE: THE COMPUTED SPECTRA", The Astrophysical Journal Supplement Series, 189, 341, 2010 10.1088/0067-0049/189/2/341
- Mattioda, A. L., Hudgins, D. M., Boersma, C., Ricca, A., Peeters, E., Cami, J., Sanchez de Armas, F., Puerta Saborido, G., Bauschlicher, C. W., J., and Allamandola, L. J. "THE NASA AMES PAH IR SPECTROSCOPIC DATABASE: THE LABORATORY SPECTRA", The Astrophysical Journal Supplement Series, XXX, 201X (in preparation)

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