pyPAHdb Documentation

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ONE

INTRODUCTION

This is the Nasa Ames. . .

CHAPTER

TWO

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, an input spectrum is fitted and decomposed into contributions from 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

Fits and decomposes a spectrum.

spectrum
The spectrum to fit and decompose.

charge
Return the spectral charge breakdown.

Returns returns associative array with keys 'anion', 'neutral' and 'cation'

fit
Return the fit.

Returns returns array

ionized_fraction
Return the ionized fraction.

Returns returns array

large_fraction
Return the large fraction.

Returns returns array

size
Return the spectral size breakdown.

Returns returns associative array with keys 'large' and 'small'

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

Creates an observation object.

Currently reads ASCII data and Spitzer-IRS data cubes.

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=''*, *opdf=True*, *ofits=True*)
Bases: object

Creates a writer object.

Writes PDF and FITS files.

result
pypahdb.decomposer – Decomposer object.

header
fits.header.Header – FITS header (normally).

basename
str – Base string, used for saving files.

2.7 Module contents

The pyPAHdb package is being developed as part of the awarded James Webb Space Telescope (JWST) Early Release Science (ERS) program "Radiative Feedback from Massive Stars as Traced by Multiband Imaging and Spectroscopic Mosaics" (ID: 1288). The entire program is coordinated by an international "Core team" of 19 scientists and supported by 119 "science collaborators". pyPAHdb is developed by the NASA Ames PAH IR Spectroscopic Database team, asscociated with the Astrophysics & Astrochemistry Laboratory at NASA Ames Research Center.

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.W. Bauschlicher, Jr., A. Ricca, C. Boersma, and L.J. Allamandola, "THE NASA AMES PAH IR SPECTROSCOPIC DATABASE: COMPUTATIONAL VERSION 3.00 WITH UPDATED CONTENT AND THE INTRODUCTION OF MULTIPLE SCALING FACTORS", The Astrophysical Journal Supplement Series, 234, 32, 2018 10.3847/1538-4365/aaa019
- 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
- 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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THREE

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