

ruediPy documentaion

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Abstract

ruediPy is a collection of Python programs for instrument control and data acquisition using RUEDI instruments^(?). ruediPy also includes some GNU Octave (or Matlab) tools to load, process, and manipulate RUEDI data acquired with ruediPy Python classes.

ruediPy is distributed as free software under the GNU General Public License (see LICENSE.txt).

This document describes the ruediPy software only. The RUEDI instrument is described in a separate document^(?).

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1 Overview

ruediPy is a collection of Python programs for instrument control and data acquisition using RUEDI instruments. ruediPy also includes some GNU Octave (or Matlab) tools to load, process, and manipulate RUEDI data acquired with ruediPy Python classes. The RUEDI instrument itself is described in a separate document^(?).

The Python classes for instrument control and data acquisition are designed to reflect the different hardware units of a RUEDI instrument, such as the mass spectrometer, selector valve, or probes for total gas pressure or temperature. These classes, combined with additional helper classes (e.g., for data file handling), allow writing simple Python scripts that perform user-defined procedures for a specific analysis task.

The GNU Octave tools (m-files) are designed to work hand-in-hand with the data files produced by the data acquisition parts of the Python classes. ★¹

ruediPy is developed on Linux and Mac OS X systems, but should also work on any other system that run Python and GNU Octave.

2 Obtaining and installing ruediPy

ruediPy can be downloaded from <http://brennmat.github.io/ruediPy> either as a compressed archive file, or using Subversion or Git version control systems. ruediPy can be installed to just about any directory on the computer that is used for instrument control – but the user home directory (`~/ruediPy`) may seem like a sensible choice, and that's what is assumed throughout the examples shown in this manual.

3 Python classes

3.1 Overview

The Python classes are used to control the various hardware units of the RUEDI instruments, to acquire measurement data, and to write these data to well-formatted and structured data files.

Currently, the following classes are implemented:

- `rgams_SRS.py`: control and data acquisition from the SRS mass spectrometer

¹TO DO: expand this: load raw data, process / calibrate data, etc.

- `selectorvalve_VICI.py`: control of the VICI inlet valve
- `pressuresensor_WIKA.py`: control and data acquisition from the WIKA pressure sensor
- `datafile.py`: data file handling
- `misc.py`: helper functions

The Python class files are located at `~/ruediPy/python/classes/`. To make sure Python knows where to find the ruediPy Python classes, set your `PYTHONPATH` environment variable accordingly.²

These classes are continuously expanded and new classes are added to ruediPy as required by new needs or developments of the RUEDI instruments. The various methods / functions included are documented in the class files. Due to the ongoing development of the code, it seems futile to keep an up-to-date copy of the methods / functions documentation in this manual. Please refer to the detailed documentation in the class files directly.

3.2 Python classes reference

3.2.1 Class `rgams_SRS`

`ruediPy/python/classes/rgams_SRS.py`

ruediPy class for SRS RGA-MS control.

Method `filament_off`
`rgams_SRS.filament_off()`

Turn off filament current.

INPUT:
 (none)

OUTPUT:
 (none)

²A convenient method to achieve this on Linux or similar UNIXy systems is to put the following line to the `.profile` file: `export PYTHONPATH=~/ruediPy/python`

Method filament_on
rgams_SRS.filamenOn()

Turn on filament current at default current value.

INPUT:
(none)

OUTPUT:
(none)

Method get_detector
det = rgams_SRS.get_detector()

Return current detector (Faraday or electron multiplier)

INPUT:
(none)

OUTPUT:
det: detecor (string):
det='F' for Faraday
det='M' for electron Multiplier

Method get_electron_energy
val = rgams_SRS.get_electron_energy()

Return electron energy of the ionizer (in eV).

INPUT:

(none)

OUTPUT:

val: electron energy in eV

Method get_filament_current

val = rgams_SRS.get_filament_current()

Return filament current (in mA)

INPUT:

(none)

OUTPUT:

val: filament current in mA

Method get_noise_floor

val = rgams_SRS.get_noise_floor()

Get noise floor (NF) parameter for RGA measurements (noise floor controls gate time, i.e., noise vs. measurement speed).

INPUT:

(none)

OUTPUT:

val: NF noise floor parameter value, 0...7 (integer)

Method has_multiplier

val = rgams_SRS.has_multiplier()

Check if MS has electron multiplier installed.

INPUT:

(none)

OUTPUT:

val: result flag, val = 0 --> MS has no multiplier, val <> 0: MS has multiplier

Method label

l = rgams_SRS.label()

Return label / name of the RGAMS object.

INPUT:

(none)

OUTPUT:

l: label / name (string)

Method mz_max

val = rgams_SRS.mz_max()

Determine highest mz value supported by the MS.

INPUT:

(none)

OUTPUT:

val: max. supported mz value

Method param_IO

```
ans = rgams_SRS.param_IO(cmd,ansreq)
```

Set / read parameter value of the SRS RGA.

INPUT:

cmd: command string that is sent to RGA (see RGA manual for commands and syntax)

ansreq: flag indicating if answer from RGA is expected:

ansreq = 1: answer expected, check for answer

ansreq = 0: no answer expected, don't check for answer

OUTPUT:

ans: answer / result returned from RGA

Method peak

```
val,unit = rgams_SRS.peak(mz,gate,f)
```

Read out detector signal at single mass (m/z value).

INPUT:

mz: m/z value (integer)

gate: gate time (seconds)

f: file object for writing data (see datafile.py). If f = 'nofile', data is not written to any data file.

OUTPUT:

val: signal intensity (float)

unit: unit (string)

NOTE FROM THE SRS RGA MANUAL:

Single mass measurements are commonly performed in sets where several different masses are monitored sequentially and in a merry-go-round fashion.

For best accuracy of results, it is best to perform the consecutive mass measurements in a set with the same type of detector and at the same noise floor (NF) setting.

Fixed detector settings eliminate settling time problems in the electrometer and in the CDEM's HV power supply.

Method peakbuffer_add

rgams_SRS.peakbuffer_add(t,mz,intens)

Add data to PEAKS data buffer

INPUT:

t: epoch time

mz: mz values (x-axis)

intens: intensity values (y-axis)

det: detector (char/string)

OUTPUT:

(none)

Method plot_peakbuffer

rgams_SRS.plot_peakbuffer()

Plot trend (or update plot) of values in PEAKs data buffer (e.g. after adding data)

NOTE: plotting may be slow, and it may therefore be a good idea to keep the update interval low to avoid affecting the duty cycle.

INPUT:

(none)

OUTPUT:

(none)

Method plot_scan

rgams_SRS.plot_scan(mz,intens,unit)

Plot scan data

INPUT:

mz: mz values (x-axis)

intens: intensity values (y-axis)

unit: intensity unit (string)

OUTPUT:

(none)

Method scan

M,Y,unit = rgams_SRS.scan(low,high,step,gate,f,p)

Analog scan

INPUT:

low: low m/z value

high: high m/z value

step: scan resolution (number of mass increment steps per amu)

step = integer number --> use given number (high number equals small mass increments between steps)

step = '*' use default value (step = 10)

gate: gate time (seconds)

f: file object or 'nofile':

if f is a DATAFILE object, the scan data is written to the current data file

if f = 'nofile' (string), the scan data is not written to a datafile

OUTPUT:

M: mass values (mz, in amu)

Y: signal intensity values (float)

unit: unit of Y (string)

Method set_detector
rgams_SRS.set_detector()

Set current detector used by the MS (direct the ion beam to the Faraday or electron multiplier detector).

INPUT:
det: detector (string):
det='F' for Faraday
det='M' for electron multiplier

OUTPUT:
(none)

Method set_electron_energy
rgams_SRS.set_electron_energy(val)

Set electron energy of the ionizer.

INPUT:
val: electron energy in eV

OUTPUT:
(none)

Method set_filament_current
rgams_SRS.set_filament_current(val)

Set filament current.

INPUT:
val: current in mA

OUTPUT:

(none)

Method set_gate_time

```
val = rgams_SRS.set_gate_time()
```

Set noi floor (NF) parameter for RGA measurements according to desired gate time (by choosing the best-match NF value).

INPUT:

gate: gate time in (fractional) seconds

OUTPUT:

(none)

NOTE (1):

FROM THE SRS RGA MANUAL:

Single mass measurements are commonly performed in sets where several different masses are monitored sequentially and in a merry-go-round fashion.

For best accuracy of results, it is best to perform the consecutive mass measurements in a set with the same type of detector and at the same noise floor (NF) setting.

Fixed detector settings eliminate settling time problems in the electrometer and in the CDEM HV power supply.

NOTE (2):

Experiment gave the following gate times vs NF parameter values:

NF gate (seconds)

0 2.4

1 1.21

2 0.48

3 0.25

4 0.163

5 0.060

6 0.043

7 0.025

Method set_noise_floor

```
val = rgams_SRS.set_noise_floor()
```

Set noise floor (NF) parameter for RGA measurements (noise floor controls gate time, i.e., noise vs. measurement speed).

INPUT:

NF: noise floor parameter value, 0...7 (integer)

OUTPUT:

(none)

Method warning

```
rgams_SRS.warning(msg)
```

Issue warning about issues related to operation of MS.

INPUT:

msg: warning message (string)

OUTPUT:

(none)

Method zero

```
val,unit = rgams_SRS.zero(mz,mz_offset,gate,f)
```

Read out detector signal at single mass with relative offset to given m/z value (this is useful to determine the baseline near a peak at a given m/z value), see rgams_SRS.peak()

The detector signal is read at $mz+mz_offset$

INPUT:

mz: m/z value (integer)

mz_offset: offset relative m/z value (integer).

gate: gate time (seconds)

f: file object for writing data (see datafile.py). If f = 'nofile', data is not written to any data file.

OUTPUT:

val: signal intensity (float)

unit: unit (string)

NOTE FROM THE SRS RGA MANUAL:

Single mass measurements are commonly performed in sets where several different masses are monitored sequentially and in a merry-go-round fashion.

For best accuracy of results, it is best to perform the consecutive mass measurements in a set with the same type of detector and at the same noise floor (NF) setting.

Fixed detector settings eliminate settling time problems in the electrometer and in the CDEM's HV power supply.

3.2.2 Class selectorvalve_VICI

ruediPy/python/classes/selectorvalve_VICI.py

ruediPy class for VICI valve control.

Method getpos

pos = selectorvalve_VICI.getpos()

Get valve position

INPUT:

(none)

OUTPUT:

pos: valve postion (integer)

Method label

label = selectorvalve_VICI.label()

Return label / name of the SELECTORVALVE object

INPUT:

(none)

OUTPUT:

label: label / name (string)

Method setpos

selectorvalve_VICI.setpos(val,f)

Set valve position

INPUT:

val: new valve position (integer)

f: datafile object for writing data (see datafile.py). If f = 'nofile', data is not written to any data file.

OUTPUT:

(none)

Method warning No method description available.

3.2.3 Class pressuresensor_WIKA

ruediPy/python/classes/pressuresensor_WIKA.py

ruediPy class for WIKA pressure sensor control.

Method label

```
label = pressuresensor_WIKA.label()
```

Return label / name of the PRESSURESENSOR object

INPUT:

(none)

OUTPUT:

label: label / name (string)

Method pressure

```
press,unit = pressuresensor_WIKA.pressure(f)
```

Read out current pressure value.

INPUT:

f: file object for writing data (see datafile.py). If f = 'nofile', data is not written to any data file.

OUTPUT:

press: pressure value in hPa (float)

unit: unit of pressure value (string)

Method serial_checksum

```
cs = pressuresensor_WIKA.serial_checksum( cmd )
```

Return checksum used for serial port communication with WIKA pressure sensor.

INPUT:

cmd: serial-port command string without checksum

OUTPUT:

cs: checksum byte

Method warning

pressuresensor_WIKA.warning(msg)

Issue warning about issues related to operation of pressure sensor.

INPUT:

msg: warning message (string)

OUTPUT:

(none)

3.2.4 Class temperaturesensor_MAXIM

ruediPy/python/classes/temperaturesensor_MAXIM.py

ruediPy class for MAXIM DS1820 type temperature sensors (wrapper class for pydig-
itemp package).

Method label

label = temperaturesensor_MAXIM.label()

Return label / name of the TEMPERATURESENSOR object

INPUT:

(none)

OUTPUT:

label: label / name (string)

Method temperature

```
temp,unit = temperaturesensor_MAXIM.temperature(f)
```

Read out current temperaure value.

INPUT:

f: file object for writing data (see datafile.py). If f = 'nofile', data is not written to any data file.

OUTPUT:

temp: temperature value (float)

unit: unit of temperature value (string)

Method warning

```
temperaturesensor_MAXIM.warning(msg)
```

Issue warning about issues related to operation of pressure sensor.

INPUT:

msg: warning message (string)

OUTPUT:

(none)

3.2.5 Class datafile

ruediPy/python/classes/datafile.py

ruediPy class for handling of data files.

Method `basepath`

```
pat = datafile.basepath()
```

Return the base path where datafiles are stored

INPUT:

(none)

OUTPUT:

pat: datafile base path (string)

Method `close`

```
datafile.close()
```

Close the currently open data file (if any)

INPUT:

(none)

OUTPUT:

(none)

Method `fid`

```
f = datafile.fid()
```

Return the file ID / object of the current file

INPUT:

(none)

OUTPUT:

f: datafile object

Method label

```
lab = datafile.label()
```

Return label / name of the DATAFILE object

INPUT:

(none)

OUTPUT:

lab: label / name (string)

Method name

```
n = datafile.name()
```

Return the name the current file (or empty string if not datafile has been created)

INPUT:

(none)

OUTPUT:

n: file name (string)

Method next

```
datafile.next()
```

Close then current data file (if it's still open) and start a new file.

INPUT:

typ (optional): string that will be appended to the file name. This may be useful to indicate 'type' of measurement data, e.g. typ = 'SAMPLE', typ = 'S', typ = 'BLANK', typ = 'B', typ = 'CAL', typ = 'C', etc.). The string can be anything. If omitted or typ = '', nothing will be appended to the file name

OUTPUT:
(none)

Method warning
datafile.warning(msg)

Warn about issues related to DATAFILE object

INPUT:
msg: warning message (string)

OUTPUT:
(none)

Method write_analysis_type
datafile.write_analysis_type(caller , typ , timestamp)

Write ANALYSIS TYPE info line to the data file.

INPUT:
caller: type of calling object, i.e. the "data origin" (string)
typ: analysis type (string / char)
timestamp: timestamp of the peak measurement (see misc.now_UNIX)

OUTPUT:
(none)

Method write_comment
datafile.write_comment(caller,cmt)

Write COMMENT line to the data file.

INPUT:

caller: label / name of the calling object (string)
cmt: comment string

OUTPUT:

(none)

Method write_peak

datafile.write_peak(caller,mz,intensity,unit,det,gate,timestamp)

Write PEAK data line to the data file.

INPUT:

caller: type of calling object, i.e. the "data origin" (string)
label: name/label of the calling object (string)
mz: mz value (integer)
intensity: peak intensity value (float)
unit: unit of peak intensity value (string)
det: detector (string), e.g., det='F' for Faraday or det='M' for multiplier
gate: gate time (float)
timestamp: timestamp of the peak measurement (see misc.now_UNIX)

OUTPUT:

(none)

Method write_pressure

datafile.write_pressure(caller,label,value,unit,timestamp)

Write PRESSURE data line to the data file.

INPUT:

caller: type of calling object, i.e. the "data origin" (string)

label: name/label of the calling object (string)
value: pressure value (float)
unit: unit of peak intensity value (string)
timestamp: timestamp of the pressure measurement (see misc.now_UNIX)

OUTPUT:
(none)

Method write_scan

datafile.write_scan(caller,mz,intensity,unit,det,gate,timestamp)

Write PEAK data line to the data file.

INPUT:

caller: type of calling object, i.e. the "data origin" (string)
label: name/label of the calling object (string)
mz: mz values (floats)
intensity: intensity values (floats)
unit: unit of intensity values (string)
det: detector (string), e.g., det='F' for Faraday or det='M' for multiplier
gate: gate time (float)
timestamp: timestamp of the peak measurement (see misc.now_UNIX)

OUTPUT:
(none)

Method write_temperature

datafile.write_temperature(caller,label,value,unit,timestamp)

Write TEMPERATURE data line to the data file.

INPUT:

caller: type of calling object, i.e. the "data origin" (string)
label: name/label of the calling object (string)

value: temperature value (float)
unit: unit of peak intensity value (string)
timestamp: timestamp of the temperature measurement (see misc.now_UNIX)

OUTPUT:
(none)

Method write_valve_pos

datafile.write_valve_pos(caller,position,timestamp)

Write multi-port valve position data line to the data file.

INPUT:
caller: type of calling object, i.e. the "data origin" (string)
label: name/label of the calling object (string)
position: valve position (integer)
timestamp: timestamp of the peak measurement (see misc.now_UNIX)

OUTPUT:
(none)

Method write_zero

datafile.write_zero(caller,mz,mz_offset,intensity,unit,det,gate,timestamp)

Write ZERO data line to the data file.

INPUT:
caller: type of calling object, i.e. the "data origin" (string)
label: name/label of the calling object (string)
mz: mz value (integer)
mz_offset: mz offset value (integer, positive offset corresponds to higher mz value)
intensity: zero intensity value (float)
unit: unit of peak intensity value (string)

det: detector (string), e.g., det='F' for Faraday or det='M' for multiplier
gate: gate time (float)
timestamp: timestamp of the peak measurement (see misc.now_UNIX)

OUTPUT:
(none)

Method writeln

datafile.writeln(caller,identifier,data,timestamp)

Write a text line to the data file (format: TIMESTAMP CALLER[LABEL] IDENTIFIER: DATA). CALLER, LABEL, and IDENTIFIER should not contain spaces or similar white space (will be removed before writing to file). If LABEL == '' or LABEL == CALLER, the [LABEL] part is omitted.

INPUT:

caller: type of calling object, i.e. the "data origin" (string)
label: name/label of the calling object (string)
identifier: data type identifier (string)
data: data / info string
timestamp: timestamp of the data in unix time (see misc.now_UNIX)

OUTPUT:
(none)

3.2.6 Class misc

ruediPy/python/classes/misc.py

ruediPy class with helper functions.

Method now_UNIX

dt = misc.now_UNIX()

Return date/time as UNIX time / epoch (seconds after Jan 01 1970 UTC)

INPUT:

(none)

OUTPUT:

dt: date-time (UNIX / epoch time)

Method now_string

dt = misc.now_string()

Return string with current date and time

INPUT:

(none)

OUTPUT:

dt: date-time (string) in YYYY-MM-DD hh:mm:ss format

Method warnmessage

misc.warnmessage(caller,msg)

Print a warning message

INPUT:

caller: caller label / name of the calling object (string)

msg: warning message

OUTPUT:

(none)

4 GNU Octave tools

★³

5 Examples

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References

³TO DO: add content

⁴TO DO: add content