

ruediPy documentation

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Abstract

ruediPy is a collection of Python programs for instrument control and data acquisition using RUEDI instruments⁽¹⁾. 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⁽¹⁾.

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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⁽¹⁾.

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.

As an example, here’s a step-by-step list of terminal commands to install ruediPy on a Linux computer running Ubuntu 16.04. Other Linux distributions will be similar. The user account name in this example is “mRdemo”, and this user account is enabled for sudo operations (i.e., it has ‘admin’ rights):

1. Update system software to latest versions and install basic software requirements for ruediPy:

```
sudo apt-get update
sudo apt-get upgrade
sudo apt-get install subversion python-pip
sudo apt-get install python-serial python-matplotlib python-scipy
```

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

```
sudo pip install pydigitemp
```

2. Download ruediPy:

```
svn co https://github.com/brennmat/ruediPy.git/trunk ~/ruediPy
```

3. Set permission to access the serial ports:

```
sudo usermod -a -G dialout mRdemo
```

4. Prepare directories for ruediPy data files and measurement scripts:

```
mkdir ~/data  
mkdir ~/scripts
```

5. Permanently add ruediPy and the measurement scripts to the Python and Shell searchpaths:

```
echo export PYTHONPATH='$PYTHONPATH':~/ruediPy/python >> ~/.profile  
echo export PYTHONPATH='$PYTHONPATH':~/scripts >> ~/.profile  
echo export PATH='$PATH':~/scripts >> ~/.profile
```

Log out and log back in to make the above changes active. You should also consider setting up the computer to avoid going to ‘sleep’ mode, because this might interrupt the measurement procedure.

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
- `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)

Method `filament_on`
`rgams_SRS.filamentOn()`

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`

Turn on filament current at default current value.

INPUT:
(none)

OUTPUT:
(none)

Method get_RI

x = rgams_SRS.get_RI(x)

Get current RI parameter value (peak-position tuning at low mz range)

INPUT:
(none)

OUTPUT:
x: RI value

NOTE:

See also the SRS RGA manual, chapter 7, section "Peak Tuning Procedure"

Method get_RS

x = rgams_SRS.get_RS(x)

Get current RS parameter value (peak-position tuning at high mz range)

INPUT:
(none)

OUTPUT:
x: RS value

NOTE:

See also the SRS RGA manual, chapter 7, section "Peak Tuning Procedure"

Method get_detector

```
det = rgams_SRS.get_detector()
```

Return current detector (Faraday or electron multiplier)

INPUT:

(none)

OUTPUT:

det: detector (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,unit)

Add data to PEAKS data buffer

INPUT:

t: epoch time
mz: mz values
intens: intensity value
det: detector (char/string)
unit: unit of intensity value (char/string)

OUTPUT:
(none)

Method peakbuffer_clear
rgams_SRS.peakbuffer_clear()

Clear data in PEAKS data buffer

INPUT:
(none)

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,cumsum_mz=[],cumsum_val=[])
```

Plot scan data

INPUT:

mz: mz values (x-axis)

intens: intensity values (y-axis)

unit: intensity unit (string)

cumsum_mz,cumsum_val (optional): cumulative sum of peak data (mz and sum values), as used for peak centering

OUTPUT:

(none)

Method scan

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

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 (10...25) --> 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_RI
rgams_SRS.set_RI(x)

Set RI parameter value (peak-position tuning at low mz range)

INPUT:
x: RI voltage

OUTPUT:
(none)

NOTE:
See also the SRS RGA manual, chapter 7, section "Peak Tuning Procedure"

Method set_RS
rgams_SRS.set_RS(x)

Set RS parameter value (peak-position tuning at high mz range)

INPUT:
x: RS value

OUTPUT:
(none)

NOTE:
See also the SRS RGA manual, chapter 7, section "Peak Tuning Procedure"

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 tune_peak_position

```
rgams_SRS.tune_peak_position(mz, gate, det, max_iter=10, max_delta_mz=0.05)
```

Automatically adjust peak positions in mass spectrum to make sure peaks show up at the correct mz values. This is done by scanning peaks at different mz values, and determining their offset in the mz spectrum. The mass spectrometer parameters are then adjusted to minimize the mz offsets (RI and RF, which define the peak positions at mz=0 and mz=128). This needs at least two distinct peak mz values at (one at a low and one at a high mz value). The procedure is repeated several times.

INPUT:

mz: list of mz values where peaks are scanned

gate: list of gate times used in the scans

det: list of detectors to be used in the scans ('F' or 'M')

max_iter (optional): max. number of repetitions of the tune procedure

maxdelta_mz (optional): tolerance of mz offset at mz=0 and mz=128. If the absolute offsets at mz=0 and mz=128 after tuning are less than maxdelta_mz after tuning, the tuning procedure is stopped.

OUTPUT:

(none)

EXAMPLE:

```
>>> MS = rgams_SRS ( serialport = '/dev/serial/by-id/usb-WuT_USB_Cable-  
2_WT2016234-if00-port0' , label = 'MS_MINIRUEDI_TEST', max_buffer_points  
= 1000 )  
>>> MS.filament_on()  
>>> MS.tune_peak_position([14,18,28,32,40,44,84],[0.2,0.2,0.025,0.1,0.4,0.1,2.4],[
```

NOTE:

See also the SRS RGA manual, chapter 7, section "Peak Tuning Procedure"

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 position (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(,typ='',samplename='',std_species='',std_conc='',std_mz='')
```

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

INPUT:

typ (optional): analysis type (string, default: typ = ''). The analysis type is written to the data file, and is appended to the file name. typ can be one of the following analysis types:

typ = 'SAMPLE' (for sample analyses)

typ = 'STANDARD' (for standard / calibration gas analyses)

typ = 'BLANK' (for blank analyses)

typ = 'UNKNOWN' (if analysis type is unknown)
typ = '' (if analysis type is unknown; nothing is added to the file name)
samplename (optional, only used if typ='SAMPLE'): description, name,
or ID of sample

OUTPUT:
(none)

Method warning
datafile.warning(msg)

Warn about issues related to DATAFILE object

INPUT:
msg: warning message (string)

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_sample_desc

datafile.write_sample_desc(self,desc)

Write line with sample description (e.g., name or ID of sample)

INPUT:

desc: sample description, name, or ID (string)

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_standard_conc

datafile.write_standard_conc(species,conc,mz)

Write line with standard/calibration gas information to data file: name, concentration/mixing ratio, and mz value of gas species.

INPUT:

caller: type of calling object, i.e. the "data origin" (string)
species: name of gas species (string)
conc: volumetric concentration / mixing ratio (float)
mz: mz value (integer)

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

★⁴

References

- [1] M. S. Brennwald, M. Schmidt, J. Oser, and R. Kipfer. A portable and autonomous mass spectrometric system for on-site environmental gas analysis. *Environmental Science and Technology*, 50(24):13455–13463, 2016. doi: 10.1021/acs.est.6b03669.

³TO DO: add content

⁴TO DO: add content