moltools Documentation

Release 1.0.0

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Contents

moltools is a package of scripts and modules I use daily in my research as a Ph.D. student to ease setting up and analyzing calculations.

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CHAPTER 1

Requirements

For bug-free performance, and full compatability, the latest source of the core dependencies are recommended.

The only hard-requirement is that python is the 2.7 version.

- numpy 1.9.1
- scipy 0.15.1
- matplotlib 1.4.3
- python-nose 1.3.4

Optional dependencies include:

- mpl_toolkits
- h5py 2.5.0
- mayavi2 http://mayavi.sourceforge.net/
- DALTON any stable version for Alpha properties. http://www.daltonprogram.org/www/download.html
- DALTON (Development version, master branch commit 51601c2 and forward is fine) for Beta properties.

CHAPTER 2

Installation

Right now only installation on Linux is supported.

There is currently no plans to port this package to other systems.

2.1 Linux

1. Clone the repository git@github.com:fishstamp82/dalton_tools.git
2. set the PYTHONPATH environment variable to the target dalton_tools/src path.

CHAPTER 3

Modules

3.1 molecules.py

3.1.1 Atom

3.1.2 Molecule

3.1.3 Water

3.1.4 Rotator

3.1.5 Property

3.1.6 Cluster

3.2 use_generator.py

3.3 use_calculator.py

3.4 template.py

class `template.`**`Template`**

This class holds data obtained by the LoProp transformation. Each template depends on 5 variables.

Variable	Choices	Type
Model:	TIP3P / OLAV	string
Method:	HF	string
Basis:	PVDZ/ANOPVDZ/ANOPVTZ	string
LoProp:	True/False	bool
Frequency:	Field ω	string

```
>>> temp = Template().get()
>>> print temp ("O1", "charge")
0.0

>>> temp = Template().get( model = "TIP3P", method = "HF",
        basis = "ANOPVDZ", dist = True, freq = "0.0"  )
```

```
    >>> print temp ("O1", "charge")
    -0.678
```

3.5 read_dal.py

CHAPTER 4

Testing

The code uses continous testing with Travis CI.

Unit-tests can be launched by the user by running

```
$ nosetests
```

CHAPTER 5

Bugs

Bugs can appear in any shape, form or code.

If you find some bugs and want to fix them, it would be greatly appreciated!

Create a pull-request for the github repository.

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