PYQCTools Documentation

Release 1.0

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PYQCTools is a collection of python scripts useful to dump quantum chemistry integrals and to perform data post-processing for different quantum chemistry methods.

PYQCTools requires the following prerequisites to work:

- Python 2.6, 2.7, 3.2, 3.3, 3.4
- Numpy 1.6.2 or higher
- Scipy 0.10 or higher (0.12.0 or higher for python 3.3, 3.4)
- PySCF for Intergrals Calculation in Integrals Dumpings.

CHAPTER

ONE

CONTENTS

1.1 Tools for Omega Space Green's Functions

`gf_trace.py()`: Calculate the Density of States (DOS) value from an ω-dependent Green's Function. It makes the trace of the Green's Function associated with a certain frequency value.

`Example :`

```
>>> python gf_trace.py /PATH/green.txt omega_value
```

`green.txt`: formatted text file containing the Green's function. `omega_value`: double frequency value.

1.2 Tools for Real-Time Green's Functions

1.3 Tools for Integrals Dumping