Psithon Documentation

Release 4.01

Psi4 Project

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CONTENTS

Note: Boolean arguments can be specified by `yes`, `on`, `true`, or `1` for affirmative and `no`, `off`, `false`, or `0` for negative, all irrespective of case.

CHAPTER

ONE

DATABASE

wrappers2.**database**(*name*, *db_name*[, *mode*, *subset*, *benchmark*, *tabulate*, *cp*, *rlxd*, *symm*, *zpe*])

Wrapper to access the molecule objects and reference energies of popular chemical databases.

Returns Mean absolute deviation of the database in kcal/mol

Required Arguments:

Parameters

- **name** (*string*) – First argument, usually unlabeled. Indicates the computational method to be applied to the database. May be any valid argument to `energy()`.
- **db_name** (*string*) – Second argument, usually unlabeled. Indicates the requested database name, matching the name of a python file in `psi4/lib/databases`. Consult that directory for available databases and literature citations.

Optional Arguments:

Parameters

- **mode** (*string*) – {*'continuous'*, 'sow', 'reap'} Indicates whether the calculation required to complete the database are to be run in one file (`'continuous'`) or are to be farmed out in an embarrassingly parallel fashion (`'sow'`/`'reap'`). For the latter, run an initial job with `'sow'` and follow instructions in its output file.
- **cp** (*bool*) – {*'off'*, 'on'} Indicates whether counterpoise correction is employed in computing interaction energies. Use this option and NOT the `cp()` wrapper for BSSE correction in the `database()` wrapper. Option valid only for databases consisting of bimolecular complexes.
- **rlxd** (*bool*) – {*'off'*, 'on'} Indicates whether correction for the deformation energy is employed in computing interaction energies. Option valid only for databases consisting of bimolecular complexes with non-frozen monomers, e.g., HBC6
- **symm** (*bool*) – {*'on'*, 'off'} Indicates whether the native symmetry of the database molecules is employed (`'on'`) or whether it is forced to c1 symmetry (`'off'`). Some computational methods (e.g., SAPT) require no symmetry, and this will be set by the database() wrapper.
- **zpe** (*bool*) – {*'off'*, 'on'} Indicates whether zero-point-energy corrections are appended to single-point energy values. Option valid only for certain thermochemical databases. Disabled until Hessians ready.
- **benchmark** (*string*) – {*'default'*, 'S22A', etc.} Indicates whether a non-default set of reference energies, if available, are employed for the calculation of error statistics.

- **tabulate** (*array of strings*) – {*[]*, ['scf total energy', 'natom'], etc.} Indicates whether to form tables of variables other than the primary requested energy. Available for any PSI variable.
- **subset** (*string or array of strings*) – Indicates a subset of the full database to run. This is a very flexible option and can be used in three distinct ways, outlined below. Note that two take a string and the last takes an array.
  - **subset = {'small', 'large', 'equilibrium'}** Calls predefined subsets of the requested database, either `'small'`, a few of the smallest database members, `'large'`, the largest of the database members, or `'equilibrium'`, the equilibrium geometries for a database composed of dissociation curves.
  - **subset = {'BzBz_S', 'FaOOFaON', 'ArNe', etc.}** For databases composed of dissociation curves, individual curves can be called by name. Consult the database python files for available molecular systems. The choices for this keyword are case sensitive and must match the database python file
  - **subset = {[1,2,5], ['1','2','5'], ['BzMe-3.5', 'MeMe-5.0'], etc.}** Specify a list of database members to run. Consult the database python files for available molecular systems. The choices for this keyword are case sensitive and must match the database python file

Todo Make local options write to the generated input files in sow/reap mode.

Example:

```
>>> # [1] Two-stage SCF calculation on short, equilibrium, and long helium dimer
>>> db('scf','RGC10',cast_up='sto-3g',subset=['HeHe-0.85','HeHe-1.0','HeHe-1.5'], tabulate=['scf

>>> # [2] Counterpoise-corrected interaction energies for three complexes in S22
>>> #     Error statistics computed wrt an old benchmark, S22A
>>> database('dfmp2','S22',cp=1,subset=[16,17,8],benchmark='S22A')

>>> # [3] SAPT0 on the neon dimer dissociation curve
>>> db('sapt0',subset='NeNe',cp=0,symm=0,db_name='RGC10')

>>> # [4] Optimize system 1 in database S22, producing tables of scf and mp2 energy
>>> db('mp2','S22',db_func=optimize,subset=[1], tabulate=['mp2 total energy','current energy'])

>>> # [5] CCSD on the smallest systems of HTBH, a hydrogen-transfer database
>>> database('ccsd','HTBH',subset='small', tabulate=['ccsd total energy', 'mp2 total energy'])
```

CHAPTER

TWO

MISC

wrappers2.**corl_xtpl_helgaker_2**(**_largs_)

Extrapolation scheme for correlation energies with two adjacent zeta-level bases.

$$E_{corl}^{X} = E_{corl}^{\infty} + \beta X^{-3}$$

CHAPTER

THREE

INDICES AND TABLES

- *genindex*
- *modindex*
- *search*

PYTHON MODULE INDEX

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