Psithon Documentation

Release 4.01

Psi4 Project

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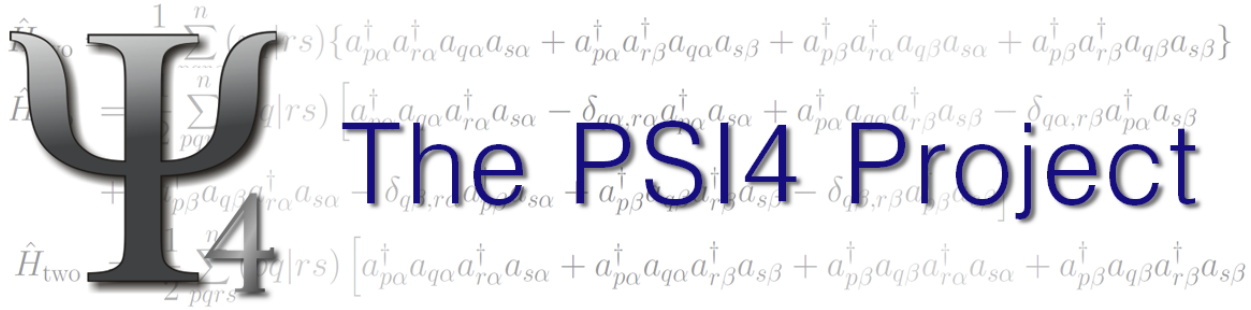

To allow arbitrarily complex computations to be performed, PSI4 was built upon the Python interpreter, with modifications termed Psithon. Chapter 3 of the User's Manual described the non-standard Python associated with molecule, basis, and option specification. This documentation addresses the Python side- what functions allow the proper, compiled code to be run, what functions post-process and interact with that output, and how the ordinary (or ambitious) user can extent PSI4's functionality.

Warning: Python naming practices of file_that_includes_function.function_name() are followed below. In psi4 input files, it is only necessary to call the function name alone. That is, use `energy('scf')`, not `driver.energy('scf')`.

Note: The options documented below are placed as arguments in the command that calls the Python function, not in the `set globals` block or with any other `set` command.

Note: Psithon keyword names and values are insensitive to case. The few exceptions are documented for the `database()` function, where case structure must match the database file.

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

CHAPTER

ONE

ENERGY

driver.**energy**(*name*, ***kwargs*)

Function to compute the single-point electronic energy.

Returns (*float*) Total electronic energy in Hartrees. SAPT returns interaction energy.

Parameters **name** (*string*) – First argument, usually unlabeled. Indicates the computational method to be computed.

Psi variables

CURRENT ENERGY
CURRENT REFERENCE ENERGY
CURRENT CORRELATION ENERGY

Keywords

Parameters **name** (*string*) – `'scf'` || `'df-mp2'` || `'ci5'` || etc.

First argument, usually unlabeled. Indicates the computational method to be applied to the system.

name	calls method
scf	Hartree–Fock (HF) or density functional theory (DFT)
mp2	2nd-order Moller-Plesset perturbation theory (MP2)
df-mp2	MP2 with density fitting
dcft	density cumulant functional theory
mcscf	multiconfigurational self consistent field (SCF)
dfcc	coupled cluster with density fitting
mp2c	coupled MP2 (MP2C)
mp2-drpa	random phase approximation?
sapt0	0th-order symmetry adapted perturbation theory (SAPT)
sapt2	2nd-order SAPT, traditional definition
sapt2+	SAPT including all 2nd-order terms
sapt2+(3)	SAPT including perturbative triples
sapt2+3	
sapt0-ct	0th-order SAPT plus charge transfer (CT) calculation
sapt2-ct	SAPT2 plus CT
sapt2+-ct	SAPT2+ plus CT
sapt2+(3)-ct	SAPT2+(3) plus CT
sapt2+3-ct	SAPT2+3 plus CT
cc2	approximate coupled cluster singles and doubles (CC2)
ccsd	coupled cluster singles and doubles (CCSD)

Continued on next page

Table 1.1 – continued from previous page

name	calls method
bccd	Brueckner coupled cluster doubles (BCCD)
cc3	approximate coupled cluster singles, doubles, and triples (CC3)
ccsd(t)	CCSD with perturbative triples
bccd(t)	BCCD with perturbative triples
ccenergy	**expert** full control over ccenergy module
mp *n*	*n* th-order Moller–Plesset perturbation theory
zapt *n*	*n* th-order z-averaged perturbation theory (ZAPT)
cisd	configuration interaction (CI) singles and doubles (CISD)
cisdt	CI singles, doubles, and triples (CISDT)
cisdtq	CI singles, doubles, triples, and quadruples (CISDTQ)
ci *n*	*n* th-order CI
fci	full configuration interaction (FCI)
detci	**expert** full control over detci module
cphf	coupled-perturbed Hartree-Fock?
cpks	coupled-perturbed Kohn-Sham?
cis	CI singles (CIS)
tda	Tamm-Dankoff approximation (TDA)
tdhf	time-dependent HF (TDHF)
tddft	time-dependent DFT (TDDFT)
adc	2nd-order algebraic diagrammatic construction (ADC)
eom-cc2	EOM-CC2
eom-ccsd	equation of motion (EOM) CCSD
eom-cc3	EOM-CC3

name	calls method in Kallay's MRCC program
mrccsd	CC through doubles
mrccsdt	CC through triples
mrccsdtq	CC through quadruples
mrccsdtqp	CC through quintuples
mrccsdtqph	CC through sextuples
mrccsd(t)	CC through doubles with perturbative triples
mrccsdt(q)	CC through triples with perturbative quadruples
mrccsdtq(p)	CC through quadruples with pertubative quintuples
mrccsdtqp(h)	CC through quintuples with pertubative sextuples
mrccsd(t)_l	
mrccsdt(q)_l	
mrccsdtq(p)_l	
mrccsdtqp(h)_l	
mrccsdt-1a	
mrccsdtq-1a	
mrccsdtqp-1a	
mrccsdtqph-1a	
mrccsdt-1b	
mrccsdtq-1b	
mrccsdtqp-1b	
mrccsdtqph-1b	
mrcc2	
mrcc3	

Continued on next page

Table 1.2 – continued from previous page

name	calls method in Kallay's MRCC program
mrcc4	
mrcc5	
mrcc6	
mrccsdt-3	
mrccsdtq-3	
mrccsdtqp-3	
mrccsdtqph-3	

Examples

```
>>> # [1] Coupled-cluster singles and doubles calculation with psi code
>>> energy('ccsd')

>>> # [2] Charge-transfer SAPT calculation with scf projection from small into requested basis
>>> energy('sapt0-ct',cast_up=True)

>>> # [3] Arbitrary-order MPn calculation
>>> energy('mp4')
```

CHAPTER

TWO

OPTIMIZE

Note: The derivative level type for `optimize()` and `frequencies()` functions can be specified by `energy`, `none`, or `0` for 0th derivative, `gradient`, `first`, or `1` for 1st derivative, and `hessian`, `second`, or `2` for 2nd derivative.

`driver.`**`optimize`**(*name*, ***kwargs*)

Function to perform a geometry optimization.

Aliases opt()

Returns (*float*) Total electronic energy of optimized structure in Hartrees.

Psi variables

`CURRENT ENERGY`

Note: Analytic gradients area available for all methods in the table below. Optimizations with other methods in the energy table proceed by finite differences.

Caution: Some features are not yet implemented. Buy a developer a coffee.
•Need to check that all methods do return electronic energy. I think gradient got changed at one point.

Keywords

Parameters

- **name** (*string*) – `'scf'` || `'df-mp2'` || `'ci5'` || etc.

  First argument, usually unlabeled. Indicates the computational method to be applied to the database. May be any valid argument to `driver.energy()`.

- **func** (*function*) – ⇒ `gradient` ⇐ || `energy` || `cbs`

  Indicates the type of calculation to be performed on the molecule. The default dertype accesses‘‘’gradient’‘‘ or `'energy'`, while `'cbs'` performs a multistage finite difference calculation.

- **mode** (*string*) – `'continuous'` || `'sow'` || `'reap'`

  Indicates whether the calculation required to complete the optimization 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.

- **dertype** (*dertype*) – `'gradient' || 'energy'`

  Indicates whether analytic (if available) or finite difference optimization is to be performed.

name	calls method
scf	Hartree–Fock (HF) or density functional theory (DFT)
mp2	2nd-order Moller-Plesset perturbation theory (MP2)
ccsd	coupled cluster singles and doubles (CCSD)
ccsd(t)	CCSD with perturbative triples
eom-ccsd	equation of motion (EOM) CCSD

Examples

```
>>> # [1] Analytic scf optimization
>>> optimize('scf')

>>> # [2] Finite difference mp3 optimization
>>> opt('mp3')

>>> # [3] Forced finite difference ccsd optimization
>>> optimize('ccsd', dertype=1)
```

CHAPTER

THREE

RESPONSE

driver.**response**(*name*, ***kwargs*)

CHAPTER

FOUR

FREQUENCY

driver.**frequencies**(*name*, ***kwargs*)

CHAPTER

FIVE

COUNTERPOISE CORRECT

wrappers.**cp**(*name*[, *func*, *check_bsse*])

The cp function computes counterpoise-corrected two-body interaction energies for complexes composed of arbitrary numbers of monomers.

Aliases counterpoise_correct(), counterpoise_correction()

Returns (*float*) Counterpoise-corrected interaction energy in kcal/mol

Psi variables

CP-CORRECTED 2-BODY INTERACTION ENERGY
UNCP-CORRECTED 2-BODY INTERACTION ENERGY

Caution: Some features are not yet implemented. Buy a developer a coffee.
- No values of func besides energy have been tested.
- Table print-out needs improving. Add some PSI variables.

Keywords

Parameters

- **name** (*string*) – `'scf'` || `'ccsd(t)'` || etc.

  First argument, usually unlabeled. Indicates the computational method to be applied to the molecule. May be any valid argument to `driver.energy()`; however, SAPT is not appropriate.

- **func** (*function*) – ⇒ `energy` ⇐ || `optimize` || `cbs`

  Indicates the type of calculation to be performed on the molecule and each of its monomers. The default performs a single-point `energy('name')`, while `optimize` perfoms a geometry optimization on each system, and `cbs` performs a compound single-point energy. If a nested series of python functions is intended (see *Function Intercalls*), use keyword `cp_func` instead of `func`.

- **check_bsse** (*bool*) – ⇒ `'off'` ⇐ || `'on'`

  Indicates whether to additionally compute un-counterpoise corrected monomers and thus obtain an estimate for the basis set superposition error.

Examples

```
>>> # [1] counterpoise-corrected mp2 interaction energy
>>> cp('dfmp2')
```

CHAPTER

SIX

DATABASE

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

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

Aliases db()

Returns (*float*) Mean absolute deviation of the database in kcal/mol

Psi variables

```
db_name DATABASE MEAN SIGNED DEVIATION
db_name DATABASE MEAN ABSOLUTE DEVIATION
db_name DATABASE ROOT-MEAN-SQUARE DEVIATION
```

Note: It is very easy to make a database from a collection of xyz files using the script `$PSIDATADIR/databases/ixyz2database.pl`. See *Creating a New Database* for details.

Caution: Some features are not yet implemented. Buy a developer some coffee.

- In sow/reap mode, use only global options (e.g., the local option set by `set scf scf_type df` will not be respected).

Keywords

Parameters

- **name** (*string*) – `'scf'` || `'sapt0'` || `'ccsd(t)'` || etc.

  First argument, usually unlabeled. Indicates the computational method to be applied to the database. May be any valid argument to `driver.energy()`.

- **db_name** (*string*) – `'BASIC'` || `'S22'` || `'HTBH'` || etc.

  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.

- **func** (*function*) – ⇒ `energy` ⇐ || `optimize` || `cbs`

  Indicates the type of calculation to be performed on each database member. The default performs a single-point `energy('name')`, while `optimize` perfoms a geometry optimization on each reagent, and `cbs` performs a compound single-point energy. If a nested series of python functions is intended (see *Function Intercalls*), use keyword `db_func` instead of `func`.

- **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 `wrappers.cp()` wrapper for BSSE correction in the `database()`. 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 C_1 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.

  - **`'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.

  - **`'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

  - **`[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

Examples

```
>>> # [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'])
```

6.1 Output

At the beginning of a database job is printed a listing of the individual system calculations which will be performed. The output snippet below is from the example job [1] above. It shows each reagent required for the subset of database reactions requested. Note that this is an un-counterpoise-corrected example, and the wrapper is smart enough to compute only once the monomer whose energy will be subtracted from each of the three dimers.

```
RGC1-HeHe-0.85-dimer
RGC1-He-mono-unCP
RGC1-HeHe-1.0-dimer
RGC1-HeHe-1.5-dimer
```

At the end of the job, the Requested Energy table is printed that gives the total energies for the requested model chemistry for each reagent and each reaction, as well as the stoichoimetric weights by which the reagent energies are transfromed into the reaction energy. In this case, the dimer is +1 and the monomer is -2, indicating the the interaction energy is computed from dimer less first monomer less second (identical) monomer. Error statistics are computed with respect to the reference energies stored in the database. One of these, the mean absolute deviation, is returned by the wrapper as an ordinary Python variable. (For databases without a stored reference energy, e.g., BASIC, large and meaningless numbers are printed for error.) The other two tables tabulate the PSI variables requested through :param tabulate:, in this case the total SCF energy and the number of atoms in each reagent.

```
==> Scf Total Energy <==

-------------------------------------------------------------------------------
         Reaction          Reaction Value              Reagent 1       Reagent 2
                                                        Value Wt        Value Wt
-------------------------------------------------------------------------------
   RGC1-HeHe-0.85             0.00011520         -5.71020576  1  -2.85516048 -2
    RGC1-HeHe-1.0             0.00000153         -5.71031943  1  -2.85516048 -2
    RGC1-HeHe-1.5            -0.00000000         -5.71032096  1  -2.85516048 -2
-------------------------------------------------------------------------------

==> Natom <==

-------------------------------------------------------------------------------
         Reaction          Reaction Value              Reagent 1       Reagent 2
                                                        Value Wt        Value Wt
-------------------------------------------------------------------------------
   RGC1-HeHe-0.85             0.00000000          2.00000000  1   1.00000000 -2
    RGC1-HeHe-1.0             0.00000000          2.00000000  1   1.00000000 -2
    RGC1-HeHe-1.5             0.00000000          2.00000000  1   1.00000000 -2
-------------------------------------------------------------------------------
```

```
==> Requested Energy <==

--------------------------------------------------------------------------------
         Reaction     Reaction Energy      Error       Reagent 1       Reagent 2
                         Ref     Calc [kcal/mol]          [H] Wt          [H] Wt
--------------------------------------------------------------------------------
   RGC1-HeHe-0.85     0.0376   0.0723     0.0347  -5.71020576  1  -2.85516048 -2
    RGC1-HeHe-1.0    -0.0219   0.0010     0.0228  -5.71031943  1  -2.85516048 -2
    RGC1-HeHe-1.5    -0.0029  -0.0000     0.0029  -5.71032096  1  -2.85516048 -2
--------------------------------------------------------------------------------
      Minimal Dev                         0.0029
      Maximal Dev                         0.0347
  Mean Signed Dev                         0.0201
Mean Absolute Dev                         0.0201
          RMS Dev                         0.0240
--------------------------------------------------------------------------------
```

CHAPTER

SEVEN

COMPLETE BASIS SET

wrappers.**complete_basis_set**(*name*[, *scf_basis*, *scf_scheme*, *corl_wfn*, *corl_basis*, *corl_scheme*, *delta_wfn*, *delta_wfn_lesser*, *delta_basis*, *delta_scheme*, *delta2_wfn*, *delta2_wfn_lesser*, *delta2_basis*, *delta2_scheme*])

Function to define a multistage energy method from combinations of basis set extrapolations and delta corrections, and condenses the components into a minimum number of calculations.

Aliases cbs()

Returns (*float*) – Total electronic energy in Hartrees

Psi variables

CBS TOTAL ENERGY
CBS REFERENCE ENERGY
CBS CORRELATION ENERGY
CURRENT ENERGY
CURRENT REFERENCE ENERGY
CURRENT CORRELATION ENERGY

Caution: Some features are not yet implemented. Buy a developer a coffee.

- Methods beyond basic scf, mp2, ccsd, ccsd(t) not yet hooked in through PSI variables, df-mp2 in particular.
- No scheme defaults for given basis zeta number, so scheme must be specified explicitly.
- No way to tell function to boost fitting basis size for all calculations.

As represented in the equation below, a CBS energy method is defined in four sequential stages (scf, corl, delta, delta2) covering treatment of the reference total energy, the correlation energy, a delta correction to the correlation energy, and a second delta correction. Each is activated by its stage_wfn keyword and is only allowed if all preceding stages are active.

$$E_{total}^{\text{CBS}} = \mathcal{F}_{\textbf{scf_scheme}}\left(E_{total,\,\text{SCF}}^{\textbf{scf_basis}}\right) + \mathcal{F}_{\textbf{corl_scheme}}\left(E_{corl,\,\textbf{corl_wfn}}^{\textbf{corl_basis}}\right) + \delta_{\textbf{delta_wfn_lesser}}^{\textbf{delta_wfn}} + \delta_{\textbf{delta2_wfn_lesser}}^{\textbf{delta2_wfn}}$$

Here, $\mathcal{F}$ is an energy or energy extrapolation scheme, and the following also hold.

$$\delta_{\textbf{delta_wfn_lesser}}^{\textbf{delta_wfn}} = \mathcal{F}_{\textbf{delta_scheme}}\left(E_{corl,\,\textbf{delta_wfn}}^{\textbf{delta_basis}}\right) - \mathcal{F}_{\textbf{delta_scheme}}\left(E_{corl,\,\textbf{delta_wfn_lesser}}^{\textbf{delta_basis}}\right)$$

$$\delta_{\textbf{delta2_wfn_lesser}}^{\textbf{delta2_wfn}} = \mathcal{F}_{\textbf{delta2_scheme}}\left(E_{corl,\,\textbf{delta2_wfn}}^{\textbf{delta2_basis}}\right) - \mathcal{F}_{\textbf{delta2_scheme}}\left(E_{corl,\,\textbf{delta2_wfn_lesser}}^{\textbf{delta2_basis}}\right)$$

A translation of this ungainly equation to example [5] below is as follows. In words, this is a double- and triple-zeta 2-point Helgaker-extrapolated CCSD(T) coupled-cluster correlation correction appended to a triple- and quadruple-zeta 2-point Helgaker-extrapolated MP2 correlation energy appended to a SCF/aug-cc-pVQZ reference energy.

$$E_{total}^{\text{CBS}} = \mathcal{F}_{\text{highest_1}}\left(E_{total,\ \text{SCF}}^{\text{aug-cc-pVQZ}}\right) + \mathcal{F}_{\text{corl_xtpl_helgaker_2}}\left(E_{corl,\ \text{MP2}}^{\text{aug-cc-pV[TQ]Z}}\right) + \delta_{\text{MP2}}^{\text{CCSD(T)}}$$

$$\delta_{\text{MP2}}^{\text{CCSD(T)}} = \mathcal{F}_{\text{corl_xtpl_helgaker_2}}\left(E_{corl,\ \text{CCSD(T)}}^{\text{aug-cc-pV[DT]Z}}\right) - \mathcal{F}_{\text{corl_xtpl_helgaker_2}}\left(E_{corl,\ \text{MP2}}^{\text{aug-cc-pV[DT]Z}}\right)$$

Keywords

The cbs() function requires, at a minimum, `name='scf'` and `scf_basis` keywords to be specified for reference-step only jobs and `name` and `corl_basis` keywords for correlated jobs.

Parameters **name** (*string*) – `'scf'` || `'ccsd'` || etc.

First argument, usually unlabeled. Indicates the computational method for the correlation energy, unless only reference step to be performed, in which case should be `'scf'`. Overruled if stage_wfn keywords supplied.

Energy Methods The presence of a stage_wfn keyword is the indicator to incorporate (and check for stage_basis and stage_scheme keywords) and compute that stage in defining the CBS energy.

Parameters

- **corl_wfn** (*string*) – `'mp2'` || `'ccsd(t)'` || etc.

  Indicates the energy method for which the correlation energy is to be obtained. Can also be specified with `name` or as the unlabeled first argument to the function.

- **delta_wfn** (*string*) – `'ccsd'` || `'ccsd(t)'` || etc.

  Indicates the (superior) energy method for which a delta correction to the correlation energy is to be obtained.

- **delta_wfn_lesser** (*string*) – ⇒ `'mp2'` ⇐ || `'ccsd'` || etc.

  Indicates the inferior energy method for which a delta correction to the correlation energy is to be obtained.

- **delta2_wfn** (*string*) – `'ccsd'` || `'ccsd(t)'` || etc.

  Indicates the (superior) energy method for which a second delta correction to the correlation energy is to be obtained.

- **delta2_wfn_lesser** (*string*) – ⇒ `'mp2'` ⇐ || `'ccsd(t)'` || etc.

  Indicates the inferior energy method for which a second delta correction to the correlation energy is to be obtained.

•**Basis Sets** Currently, the basis set set through `set` commands have no influence on a cbs calculation.

Parameters

- **scf_basis** (*string*) – ⇒ `corl_basis` ⇐ ‖ `'cc-pV[TQ]Z'` ‖ `'jun-cc-pv[tq5]z'` ‖ `'6-31G*'` ‖ etc.

  Indicates the sequence of basis sets employed for the reference energy. If any correlation method is specified, `scf_basis` can default to `corl_basis`.

- **corl_basis** (*string*) – `'cc-pV[TQ]Z'` ‖ `'jun-cc-pv[tq5]z'` ‖ `'6-31G*'` ‖ etc.

  Indicates the sequence of basis sets employed for the correlation energy.

- **delta_basis** (*string*) – `'cc-pV[TQ]Z'` ‖ `'jun-cc-pv[tq5]z'` ‖ `'6-31G*'` ‖ etc.

  Indicates the sequence of basis sets employed for the delta correction to the correlation energy.

- **delta2_basis** (*string*) – `'cc-pV[TQ]Z'` ‖ `'jun-cc-pv[tq5]z'` ‖ `'6-31G*'` ‖ etc.

  Indicates the sequence of basis sets employed for the second delta correction to the correlation energy.

•**Schemes** Transformations of the energy through basis set extrapolation for each stage of the CBS definition. A complaint is generated if number of basis sets in stage_basis does not exactly satisfy requirements of stage_scheme. An exception is the default, `'highest_1'`, which uses the best basis set available. See *Extrapolation Schemes* for all available schemes.

Parameters

- **scf_scheme** (*function*) – ⇒ `highest_1` ⇐ ‖ `scf_xtpl_helgaker_3` ‖ etc.

  Indicates the basis set extrapolation scheme to be applied to the reference energy.

- **corl_scheme** (*function*) – ⇒ `highest_1` ⇐ ‖ `corl_xtpl_helgaker_2` ‖ etc.

  Indicates the basis set extrapolation scheme to be applied to the correlation energy.

- **delta_scheme** (*function*) – ⇒ `highest_1` ⇐ ‖ `corl_xtpl_helgaker_2` ‖ etc.

  Indicates the basis set extrapolation scheme to be applied to the delta correction to the correlation energy.

- **delta2_scheme** (*function*) – ⇒ `highest_1` ⇐ ‖ `corl_xtpl_helgaker_2` ‖ etc.

  Indicates the basis set extrapolation scheme to be applied to the second delta correction to the correlation energy.

Examples

```
>>> # [1] replicates with cbs() the simple model chemistry scf/cc-pVDZ: set basis cc-pVDZ energy
>>> cbs('scf', scf_basis='cc-pVDZ')

>>> # [2] replicates with cbs() the simple model chemistry mp2/jun-cc-pVDZ: set basis jun-cc-pVD
>>> cbs('mp2', corl_basis='jun-cc-pVDZ')

>>> # [3] DTQ-zeta extrapolated scf reference energy
>>> cbs('scf', scf_basis='cc-pV[DTQ]Z', scf_scheme=scf_xtpl_helgaker_3)

>>> # [4] DT-zeta extrapolated mp2 correlation energy atop a T-zeta reference
>>> cbs('mp2', corl_basis='cc-pv[dt]z', corl_scheme=corl_xtpl_helgaker_2)

>>> # [5] a DT-zeta extrapolated coupled-cluster correction atop a TQ-zeta extrapolated mp2 corr
>>> cbs('mp2', corl_basis='aug-cc-pv[tq]z', corl_scheme=corl_xtpl_helgaker_2, delta_wfn='ccsd(t)
```

```
>>> # [6] a D-zeta ccsd(t) correction atop a DT-zeta extrapolated ccsd cluster correction atop a
>>> cbs('mp2', corl_basis='aug-cc-pv[tq]z', corl_scheme=corl_xtpl_helgaker_2, delta_wfn='ccsd',

>>> # [7] cbs() coupled with database()
>>> database('mp2', 'BASIC', subset=['h2o','nh3'], symm='on', func=cbs, corl_basis='cc-pV[tq]z',
```

7.1 Output

At the beginning of a cbs() job is printed a listing of the individual energy calculations which will be performed. The output snippet below is from the example job [2] above. It shows first each model chemistry needed to compute the aggregate model chemistry requested through cbs(). Then, since, for example, an `energy('ccsd(t)')` yields CCSD(T), CCSD, MP2, and SCF energy values, the wrapper condenses this task into the second list of minimum number of calculations which will actually be run.

```
Naive listing of computations required.
        scf / aug-cc-pvqz              for  SCF TOTAL ENERGY
        mp2 / aug-cc-pvtz              for  MP2 CORRELATION ENERGY
        mp2 / aug-cc-pvqz              for  MP2 CORRELATION ENERGY
    ccsd(t) / aug-cc-pvdz              for  CCSD(T) CORRELATION ENERGY
    ccsd(t) / aug-cc-pvtz              for  CCSD(T) CORRELATION ENERGY
        mp2 / aug-cc-pvdz              for  MP2 CORRELATION ENERGY
        mp2 / aug-cc-pvtz              for  MP2 CORRELATION ENERGY

Enlightened listing of computations required.
        mp2 / aug-cc-pvqz              for  MP2 CORRELATION ENERGY
    ccsd(t) / aug-cc-pvdz              for  CCSD(T) CORRELATION ENERGY
    ccsd(t) / aug-cc-pvtz              for  CCSD(T) CORRELATION ENERGY
```

At the end of a cbs() job is printed a summary section like the one below. First, in the components section, are listed the results for each model chemistry available, whether required for the cbs job (*) or not. Next, in the stages section, are listed the results for each extrapolation. The energies of this section must be dotted with the weightings in column Wt to get the total cbs energy. Finally, in the CBS section, are listed the results for each stage of the cbs procedure. The stage energies of this section sum outright to the total cbs energy.

```
==> Components <==

-------------------------------------------------------------------------------
               Method / Basis            Rqd   Energy [H]   Variable
-------------------------------------------------------------------------------
                  scf / aug-cc-pvqz        *  -1.11916375   SCF TOTAL ENERGY
                  mp2 / aug-cc-pvqz        *  -0.03407997   MP2 CORRELATION ENERGY
                  scf / aug-cc-pvdz           -1.11662884   SCF TOTAL ENERGY
                  mp2 / aug-cc-pvdz        *  -0.02881480   MP2 CORRELATION ENERGY
              ccsd(t) / aug-cc-pvdz        *  -0.03893812   CCSD(T) CORRELATION ENERGY
                 ccsd / aug-cc-pvdz           -0.03893812   CCSD CORRELATION ENERGY
                  scf / aug-cc-pvtz           -1.11881134   SCF TOTAL ENERGY
                  mp2 / aug-cc-pvtz        *  -0.03288936   MP2 CORRELATION ENERGY
              ccsd(t) / aug-cc-pvtz        *  -0.04201004   CCSD(T) CORRELATION ENERGY
                 ccsd / aug-cc-pvtz           -0.04201004   CCSD CORRELATION ENERGY
-------------------------------------------------------------------------------

==> Stages <==

-------------------------------------------------------------------------------
 Stage         Method / Basis             Wt   Energy [H]   Scheme
-------------------------------------------------------------------------------
```

```
   scf            scf / aug-cc-pvqz        1  -1.11916375   highest_1
  corl            mp2 / aug-cc-pv[tq]z     1  -0.03494879   corl_xtpl_helgaker_2
 delta        ccsd(t) / aug-cc-pv[dt]z     1  -0.04330347   corl_xtpl_helgaker_2
 delta            mp2 / aug-cc-pv[dt]z    -1  -0.03460497   corl_xtpl_helgaker_2
-------------------------------------------------------------------------------

==> CBS <==

-------------------------------------------------------------------------------
 Stage         Method / Basis                  Energy [H]   Scheme
-------------------------------------------------------------------------------
   scf            scf / aug-cc-pvqz          -1.11916375   highest_1
  corl            mp2 / aug-cc-pv[tq]z       -0.03494879   corl_xtpl_helgaker_2
 delta  ccsd(t) - mp2 / aug-cc-pv[dt]z       -0.00869851   corl_xtpl_helgaker_2
 total            CBS                        -1.16281105
-------------------------------------------------------------------------------
```

7.2 Extrapolation Schemes

wrappers.**highest_1**(**_largs_)

Scheme for total or correlation energies with a single basis or the highest zeta-level among an array of bases. Used by `complete_basis_set()`.

$$E_{total}^{X} = E_{total}^{X}$$

wrappers.**scf_xtpl_helgaker_2**(**_largs_)

Extrapolation scheme for reference energies with two adjacent zeta-level bases. Used by `complete_basis_set()`.

$$E_{total}^{X} = E_{total}^{\infty} + \beta e^{-\alpha X}, \alpha = 1.63$$

wrappers.**scf_xtpl_helgaker_3**(**_largs_)

Extrapolation scheme for reference energies with three adjacent zeta-level bases. Used by `complete_basis_set()`.

$$E_{total}^{X} = E_{total}^{\infty} + \beta e^{-\alpha X}$$

wrappers.**corl_xtpl_helgaker_2**(**_largs_)

Extrapolation scheme for correlation energies with two adjacent zeta-level bases. Used by `complete_basis_set()`.

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

CHAPTER

EIGHT

FRACTIONAL OCCUPATION

frac.**frac_nuke**(*mol*, ***kwargs*)

frac.**frac_traverse**(*mol*, ***kwargs*)

frac.**ip_fitting**(*mol*, *omega_l*, *omega_r*, ***kwargs*)

CHAPTER

NINE

BEGINNER PSITHON PROGRAMMING

Note: No recompile of the PSI program is necessary for changes made to files in `$PSIDATADIR`, including those described below.

9.1 Defining a Method Alias

Since quantum chemical methods in PSI4 are accessed through Python functions, and most important quantities are available as PSI variables, it is straightforward to create aliases to commonly run calculations or to define hybrid methods. The `$PSIDATADIR/python/aliases.py` file is intended for editing by the user for this purpose.

As an example, the MP2.5 method is the average of MP2 and MP3. The latter is available through the arbitrary order MPn code and returns all lower energies along with it in PSI variables. The following is basic code that will compute and return the MP2.5 energy.

```
def run_mp2_5(name, **kwargs):

    energy('mp3', **kwargs)
    e_scf = PsiMod.get_variable('SCF TOTAL ENERGY')
    ce_mp2 = PsiMod.get_variable('MP2 CORRELATION ENERGY')
    ce_mp3 = PsiMod.get_variable('MP3 CORRELATION ENERGY')
    e_mp2 = e_scf + ce_mp2
    e_mp3 = e_scf + ce_mp3

    ce_mp25 = 0.5 * (ce_mp2 + ce_mp3)
    e_mp25 = e_scf + ce_mp25

    print """  MP2.5 total energy:                %16.8f\n""" % (e_mp25)
    print """  MP2.5 correlation energy:          %16.8f\n""" % (ce_mp25)

    return e_mp25
```

Compare the above to the method that resides in `aliases.py`. The rationale for the changes is indicated in the comments below.

```
def run_mp2_5(name, **kwargs):
    lowername = name.lower()
    kwargs = kwargs_lower(kwargs)  # removes case sensitivity in keyword names

    # Run detci calculation and collect conventional quantities
    energy('mp3', **kwargs)
    e_scf = PsiMod.get_variable('SCF TOTAL ENERGY')
```

```
    ce_mp2 = PsiMod.get_variable('MP2 CORRELATION ENERGY')
    ce_mp3 = PsiMod.get_variable('MP3 CORRELATION ENERGY')
    e_mp2 = e_scf + ce_mp2
    e_mp3 = e_scf + ce_mp3

    # Compute quantities particular to MP2.5
    ce_mp25 = 0.5 * (ce_mp2 + ce_mp3)
    e_mp25 = e_scf + ce_mp25
    PsiMod.set_variable('MP2.5 CORRELATION ENERGY', ce_mp25)  # add new method's vitals to PSI variab
    PsiMod.set_variable('MP2.5 TOTAL ENERGY', e_mp25)
    PsiMod.set_variable('CURRENT CORRELATION ENERGY', ce_mp25)
    PsiMod.set_variable('CURRENT ENERGY', e_mp25)  # geometry optimizer tracks this variable, permits

    # build string of title banner and print results
    banners = ''
    banners += """PsiMod.print_out('\\n')\n"""
    banners += """banner(' MP2.5 ')\n"""
    banners += """PsiMod.print_out('\\n')\n\n"""
    exec banners

    tables  = ''
    tables += """  SCF total energy:                        %16.8f\n""" % (e_scf)
    tables += """  MP2 total energy:                        %16.8f\n""" % (e_mp2)
    tables += """  MP2.5 total energy:                      %16.8f\n""" % (e_mp25)
    tables += """  MP3 total energy:                        %16.8f\n\n""" % (e_mp3)
    tables += """  MP2 correlation energy:                   %16.8f\n""" % (ce_mp2)
    tables += """  MP2.5 correlation energy:                 %16.8f\n""" % (ce_mp25)
    tables += """  MP3 correlation energy:                   %16.8f\n""" % (ce_mp3)
    PsiMod.print_out(tables)  # prints nice header and table of all involved quantities to output fi

    return e_mp25
```

One final step is necessary. At the end of the `aliases.py` file, add the following line.

```
procedures['energy']['mp2.5'] = run_mp2_5
```

This permits the newly defined MP2.5 method to be called in the input file with the following command.

```
energy('mp2.5')
```

9.2 Creating a New Database

A necessary consideration in constructing a database is the distinction between reagents and reactions. A reagent is a single molecular system (may be a dimer) whose geometry you are possession of and whose electronic energy may be of interest. A reaction is a combination of one or more reagent energies whose value you are interested in and a reference value for which you may or may not be in possession of. A few examples follow. In a database of interaction energies, the reagents are dimers and their component monomers (usually derived from the dimer geometry), and the reactions are the dimer less monomers energies. In a database of barrier heights, the reagents are reactants, products, and transition-state structures, and the reactions are the transition-states less minimum-energy structures. Possibly you may have a collection of structures to simply be acted upon in parallel, in which case the structures are both the reagents and the reactions. The role of the database.py file is to collect arrays and dictionaries that define the geometries of reagents (GEOS), their combination into reactions (RXNM & ACTV), available reference values for reactions (BIND), and brief comments for reagents and reactions (TAGL). The journey from reagent geometries to functional database.py file is largely automated, in a process described below.

- **Prepare geometry files** Assemble xyz files for all intended reagent systems in a directory. Follow the rules

below for best results. The filename for each xyz file should be the name of the system. lowercase or MixedCase is preferable (according to Sherrill lab convention). Avoid dashes and dots in the name as python won't allow them. If you're determined to have dashes and dots, they must be replaced by other characters in the process_input line, then translated back in the GEOS section; see NBC10.py for an example.

  - The first line for each xyz file should be the number of atoms in the system.
  - The second line for each xyz file can be blank (interpreted as no comment), anything (interpreted as a comment), or two integers and anything (interpreted as charge, multiplicity, and remainder as comment).
  - The third and subsequent lines have four fields: the element symbol and the three cartesian coordinates in angstroms. The atom lines should not contain any dummy atoms (what's the use in cartesian form). For dimer systems, an algorithm is used to apportion the atoms into two fragments; thus the atoms need not be arranged with all fragmentA atoms before all fragmentB atoms. The algorithm will fail for very closely arranged fragments. For dimers, any charge and multiplicity from the second line will be applied to fragmentA (python); charge and multiplicity may need to be redistributed later in the editing step.

- Run script ixyz2database.pl

  Move into the directory where all your xyz files are located. Run the script in place, probably as `$PSIDATADIR/databases/ixyz2database.pl`. It will ask a number of questions about your intended database and generate a python file named for your database. Uppercase is preferable for database names (according to Sherrill lab convention). Note your choice for the route variable for the next step.

- Edit file database.py
  - All routes. Optionally, rearrange the order of reactions in HRXN as this will define the order for the database.
  - All routes. Optionally, add sources for geometries and any reference data to commented lines above the dbse variable.
  - All routes. Optionally, the comment lines of TAGL may be edited in plain text.
  - All routes. Optionally, fill in reference values (in kcal/mol) into BIND.
  - All routes. Optionally, define alternate sets of reference values in the array BIND_ALTREF in the database.py file to be called in a psi4 input file as benchmark='ALTREF' . See S22.py as an example.
  - All routes. Optionally, fill in the least computationally expensive 2-3 reactions into HRXN_SM and the most expensive into HRXN_LG
  - All routes. Optionally, define subsets of reactions in the array SUBSETARRAY = ['reaction', 'reaction'] in the database.py file to be called in a psi4 input file as subset='SUBSETARRAY'. See NBC10.py as an example.
  - All routes. Necessarily (if charge and multiplicity not read in through line2 = cgmp and nor all neutral singlets), assign correct charge and multiplicity to all reagents.
  - Route 3. Necessarily (if any charge and multiplicity specified for the whole reagent is not intended for fragmentA with neutral singlet fragmentB), apportion charge and multiplicity properly between fragmentA and fragmentB. This is not likely necessary if all subsystems are neutral singlets.
  - Route 2. Necessarily, define the reagents that contribute to each reaction by filling in the empty single-quotes in ACTV. Add or delete lines as necessary if for each reaction more or fewer than three reagents contribute. See NHTBH.py as an example.

- Route 2. Necessarily, define the mathematical contribution of reagents to reactions by adding a number (most often +1 or -1) for each reagent to the RXNM of each reaction. See NHTBH.py as an example.
- All routes. Necessarily, copy your new database into `$PSIDATADIR/databases`.

CHAPTER

TEN

FUNCTION INTERCALLS

table; handling func; no sow/reap

CHAPTER

ELEVEN

EMBARRASSING PARALLELISM

what functions; no intercalls; no local set; special section in parameter list

CHAPTER

TWELVE

PSITHON PROGRAMMING BEST PRACTICES

stuff that's in README;

CHAPTER

THIRTEEN

EXPERT

driver.**gradient**(*name*, ***kwargs*)

driver.**hessian**(*name*, ***kwargs*)

driver.**parse_arbitrary_order**(*name*)

driver.**response**(*name*, ***kwargs*)

wrappers.**call_function_in_1st_argument**(*funcarg*, ***kwargs*)

wrappers.**drop_duplicates**(*seq*)

wrappers.**n_body**(*name*, ***kwargs*)

wrappers.**reconstitute_bracketed_basis**(*needarray*)

wrappers.**split_menial**(*menial*)
split meial docstring

wrappers.**tblhead**(*tbl_maxrgt*, *tbl_delimit*, *ttype*)

wrappers.**validate_bracketed_basis**(*basisstring*)

wrappers.**validate_scheme_args**(*functionname*, ***largs*)
lsdkjflskld Deprecated since version old: news

aliases.**run_mp2_5**(*name*, ***kwargs*)

aliases.**run_plugin_ccsd_serial**(*name*, ***kwargs*)

aliases.**run_plugin_omega**(*name*, ***kwargs*)

aliases.**sherrillgroup_gold_standard**(*name='mp2'*, ***kwargs*)

class pubchem.**PubChemObj**(*cid*, *mf*, *iupac*)

getCartesian()

getMoleculeString()

getSDF()

getXYZFile()

name()

pubchem.**getPubChemResults**(*name*)

class qmmm.**Diffuse**(*molecule*, *basisname*, *ribasisname*)

fitGeneral()

fitScf()

populateExtern(*extern*)

class qmmm.**QMMM**

addChargeAngstrom(*Q*, *x*, *y*, *z*)

addChargeBohr(*Q*, *x*, *y*, *z*)

addDiffuse(*diffuse*)

populateExtern()

class inpsight.**InPsight**(*molecule*)

atoms = []

azimuth = 0.0

bohr_per_ang = 1.8897161646320724

bond_width = 0.2

bonding_alpha = 0.65

bonds = []

colors = [[0, 0, 0], [255, 255, 255], [217, 255, 255], [204, 128, 255], [194, 255, 0], [255, 181, 181], [144, 144, 144], [48, 80, 24

defines = {'Shadows': 'false', 'Output_Alpha': 'true', 'Filepath': '/Users/loriab/linux/psi4/doc/userman/sphinx_psithon

elevation = 0.0

height = 900

light = [1.0, 0.0, 0.0]

light_color = [0.6, 0.6, 0.6]

location = [1.0, 0.0, 0.0]

look_at = [0.0, 0.0, 0.0]

position_camera()

radial_scale = 0.25

radii = [2.0, 1.001, 1.012, 0.825, 1.408, 1.485, 1.452, 1.397, 1.342, 1.287, 1.243, 1.144, 1.364, 1.639, 1.716, 1.705, 1.683, 1.63

right = [1.0, 0.0, 0.0]

save_density(*filename='rho', overlap=2.0, n=[40, 40, 40], caxis=[0.0, 1.0]*)

save_molecule(*filename*)

set_camera(*location*, *sky*, *up*, *right*, *look_at*, *light*, *light_color*)

set_color(*Z*, *color*)

set_define(*key*, *value*)

set_radius(*Z*, *radius*)

set_size(*width*, *height*)

set_view(*azimuth*, *elevation*, *zoom=0.7*)

sky = [0.0, -1.0, 0.0]

up = [0.0, 0.75, 0.0]

update_geometry()

width = 1200

zoom = 0.5

input.**bad_option_syntax**(*line*)

input.**check_parentheses_and_brackets**(*input_string*, *exit_on_error*)

input.**parse_multiline_array**(*input_list*)

input.**process_basis_block**(*matchobj*)

input.**process_basis_file**(*matchobj*)

input.**process_external_command**(*matchobj*)

input.**process_extract_command**(*matchobj*)

input.**process_input**(*raw_input*, *print_level=1*)

input.**process_memory_command**(*matchobj*)

input.**process_molecule_command**(*matchobj*)

input.**process_multiline_arrays**(*inputfile*)

input.**process_option**(*spaces*, *module*, *key*, *value*, *line*)

input.**process_print_command**(*matchobj*)

input.**process_pubchem_command**(*matchobj*)

input.**process_set_command**(*matchobj*)

input.**process_set_commands**(*matchobj*)

input.**process_word_quotes**(*matchobj*)

input.**quotify**(*string*)

proc.**run_adc**(*name*, ***kwargs*)

proc.**run_bccd**(*name*, ***kwargs*)

proc.**run_bccd_t**(*name*, ***kwargs*)

proc.**run_cc_gradient**(*name*, ***kwargs*)

proc.**run_cc_response**(*name*, ***kwargs*)

proc.**run_ccenergy**(*name*, ***kwargs*)

proc.**run_dcft**(*name*, ***kwargs*)

proc.**run_detci**(*name*, ***kwargs*)

proc.**run_dfcc**(*name*, ***kwargs*)

proc.**run_dfmp2**(*name*, ***kwargs*)

proc.**run_eom_cc**(*name*, ***kwargs*)

proc.**run_eom_cc_gradient**(*name*, ***kwargs*)

proc.**run_libfock**(*name*, ***kwargs*)

proc.**run_mcscf**(*name*, ***kwargs*)

proc.**run_mp2**(*name*, ***kwargs*)

proc.**run_mp2_gradient**(*name*, ***kwargs*)

proc.**run_mp2c**(*name*, ***kwargs*)

proc.**run_mp2drpa**(*name*, ***kwargs*)

proc.**run_mrcc**(*name*, ***kwargs*)

proc.**run_sapt**(*name*, ***kwargs*)

proc.**run_sapt_ct**(*name*, ***kwargs*)

proc.**run_scf**(*name*, ***kwargs*)

proc.**run_scf_gradient**(*name*, ***kwargs*)

proc.**scf_helper**(*name*, ***kwargs*)

procutil.**format_kwargs_for_input**(*filename*, *lmode=1*, ***kwargs*)

procutil.**format_molecule_for_input**(*mol*)

procutil.**format_options_for_input**()

procutil.**get_psifile**(*fileno*, *pidspace='54024'*)

procutil.**kwargs_lower**(*kwargs*)

exception psiexceptions.**PsiException**

exception psiexceptions.**ValidationError**(*msg*)

class text.**Table**(*rows=()*, *row_label_width=10*, *row_label_precision=4*, *cols=()*, *width=16*, *precision=10*)

absolute_to_relative(*Factor=627.5095*)

copy()

format_label()

format_values(*values*)

save(*file*)

scale(*Factor=627.5095*)

text.**banner**(*text*, *type=1*, *width=35*)

text.**print_stderr**(*stuff*)

text.**print_stdout**(*stuff*)

util.**compare_integers**(*expected*, *computed*, *label*)

util.**compare_matrices**(*expected*, *computed*, *digits*, *label*)

util.**compare_strings**(*expected*, *computed*, *label*)

util.**compare_values**(*expected*, *computed*, *digits*, *label*)

util.**compare_vectors**(*expected*, *computed*, *digits*, *label*)

util.**get_memory**()

util.**get_num_threads**()

util.**set_memory**(*bytes*)

util.**set_num_threads**(*nthread*)

util.**success**(*label*)

CHAPTER

FOURTEEN

PSIMOD METHODS

CHAPTER

FIFTEEN

MOLECULE METHODS

CHAPTER

SIXTEEN

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