RAQET

RELATIVISTIC AND QUANTUM ELECTRONIC THEORY

Input Manual

Version 1.1

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Input File

The input file in RAQET consists of the following main sections:

1. Job Options	specifies general options for the calculation
2. Molecular Information	specifies molecular structure
3. Basis Sets	specifies atomic basis sets
4. Basis Sets 2	specifies atomic basis sets for initial guess (not required if GuessMethod=Hcore)
5. Core Potential	specifies options for core potentials (not mandatory)
6. $MOA, $MOB, $MOG	specifies initial MO coefficients when using MO read-in (not mandatory)

Job Options

In this section, the general calculation options are specified. A complete list of the options can be found in the Job Options section. Each section begins with *$[option name],* ends with *$end*, and can contain several keywords. Each keyword and its parameters have to be specified in a new line as shown in the following example:

```
$Run
  JobType=sp
  Mem=1000MB
$end
```

Molecular Information

The molecular structure is specified in this section. Besides the element symbols and the respective Cartesian coordinates (in Å), atom-specific basis sets and those used for the initial guess can be declared. The molecular structure section is initiated by *molecular information* in the first line. All subsequent lines follow the format

```
Element symbol  [basis set]  [basis set (2)]  x  y  z
```

Input in [] is not mandatory. The definition of atom-specific basis sets will overwrite the basis sets defined in the Basis Sets and Basis Sets 2 sections. As separator, spaces have to be used, not tabs. As an example of a minimal sample input, the molecular structure of the formaldehyde molecule is shown.

```
molecular information
C   0.000000  0.000000  0.000000
O   0.000000  1.219457  0.000000
```

```
H   0.465617 -0.542208  0.815579
H   0.465617 -0.542208 -0.815579
```

In this example, the basis set specified in the Basis Sets section is used. The same molecular structure with atom-specific basis set input (here for the case of the 6-31G(d,p) basis set) reads

```
molecular information
C  DB:/6-31G(d,p)/C   0.000000  0.000000  0.000000
O  DB:/6-31G(d,p)/O   0.000000  1.219457  0.000000
H  DB:/6-31G(d,p)/H   0.465617 -0.542208  0.815579
H  DB:/6-31G(d,p)/H   0.465617 -0.542208 -0.815579
```

Note that also a mixture of atom-specific basis sets and global basis sets is possible. In this case, atoms without atom-specific basis sets will use the basis sets defined in the sections Basis Sets and Basis Sets 2, while atom-specific bases will overwrite the global definition for the other atoms.

Basis Sets

In this section, the atomic basis set is specified. The declaration of the global basis set (for all atoms) follows the format:

```
basis sets = 6-31G(d,p)
```

Element-specific basis sets overwriting the global basis set, e.g. for heavy elements, can be declared by

```
basis sets = Sapporo-DZP-2012
Rh DB:Sapporo-DKH3-DZP-2012/Rh
Ir DB:Sapporo-DKH3-DZP-2012/Ir
```

Basis sets can be also specified explicitly, i.e. the angular momentum, basis function exponents, contraction coefficients, and the number of contracted primitives are given explicitly for each shell of a specific element. In the following, you can find a sample basis set input for hydrogen and oxygen without declaring a global basis set:

```
basis sets
O
S    6    1.00
   5484.6717000     0.0018311
    825.2349500     0.0139501
    188.0469600     0.0684451
     52.9645000     0.2327143
```

4

```
      16.8975700      0.4701930
       5.7996353      0.3585209
 SP    3    1.00
      15.5396160    -0.1107775     0.0708743
       3.5999336    -0.1480263     0.3397528
       1.0137618     1.1307670     0.7271586
 SP    1    1.00
       0.2700058     1.0000000     1.0000000
 D     1    1.00
       0.8000000     1.0000000


 H
 S     3    1.00
      18.7311370      0.03349460
       2.8253937      0.23472695
       0.6401217      0.81375733
 S     1    1.00
       0.1612778      1.00000000
```

In general, the definition of the basis set follows the format:

```
basis sets
element symbol
shell symbol    contraction length    scaling factor
  exponent 1    contraction coefficient 1.1    [1.2 ···]
  exponent 2    contraction coefficient 2.1    [2.2 ···]
  ...
shell symbol    contraction length    scaling factor
  exponent 1    contraction coefficient 1.1    [1.2 ···]
  exponent 2    contraction coefficient 2.1    [2.2 ···]
  ...
 ...
                                        ← one blank line
element symbol
shell symbol    contraction length    scaling factor
  ...
 ...
```

Basis Sets 2

Apart from the atomic basis set specified in the Basis Sets section, a separate (usually smaller) basis set for the initial guess method can be declared. In the case of a core Hamiltonian guess

(*GuessMethod = Hcore* in job option $Guess), the Basis Set 2 directive is not used and thus not need to be declared. The input format is equivalent to the atomic basis set input described in the previous section.

Core Potential

In this section, the frozen core potential (FCP) is specified. Currently, the definition is restricted to one element. In order to obtain the FCP, one has to perform a calculation with *FCPmethod = potential* specified by the job option $FCP and copy the section (*core potential* and below) from the punch file (.pun) to the corresponding input file. The number of frozen core orbitals and non-frozen orbitals can be specified by the options *coreRegion* and *valRegion* in the $FCP directive, respectively. The FCP has the following format:

```
core potential
DKH3Gen
COR    1S     78
 -2.98347169E+03
 -9.99727309E-01 -2.77962103E-03  3.95750145E-03 -7.64787402E-04
   ...
COR    2S     78
 -5.31922309E+02
  4.04002299E-04 -1.00320737E+00  4.73374430E-03 -1.09011031E-03
   ...
COR    2P     78
   ...
   ...
   ...
COR    4F     78
 -3.78970260E+00
  1.68980828E-12 -7.43624793E-11  6.00973024E-10 -9.47083392E-10
   ...
```

$MOA, $MOB, $MOG

This section describes the format for the input of molecular orbital coefficients used for the initial guess in the case of *GuessMethod = MOread.* The directives $MOA, $MOB, and $MOG, containing the converged MO coefficients of the α, β, or general orbitals for the respective SCF method, are written to the punch file (.pun) at the end of a calculation. To be used for the initial guess, the respective directive has to be copied to the input file. Furthermore, one has to ensure that the employed Basis Set 2 is the same used for the representation of the MOs, i.e. the atomic orbital basis of the SCF calculation. Also, set *GuessMethod = MOread.*

The directive $MOA has the following format (equivalent for $MOB):

```
$MOA
  1  MO coeff. 1.1  MO coeff. 1.2  MO coeff. 1.3  MO coeff. 1.4
  1  MO coeff. 1.5  MO coeff. 1.6  MO coeff. 1.7  MO coeff. 1.8
  ...
  2  MO coeff. 2.1  MO coeff. 2.2  MO coeff. 2.3  MO coeff. 2.4
  ...
  ...
$end
```

The first number in each line represents the number of the molecular orbital. The directive is closed with $end in the same way as the job options. For general Hartree-Fock and DFT calculations, i.e. WavefuncType = GHF, the coefficients are specified by the $MOG directive, in which real and imaginary parts of the MO coefficients are stored continuously as follows:

```
$MOG
  1  coeff. 1.1(real)  coeff. 1.1(imag.)  coeff. 1.2(real)  ···
  1  coeff. 1.5(real)  coeff. 1.5(imag.)  coeff. 1.6(real)  ···
  ...
  2  coeff. 2.1(real)  coeff. 2.1(imag.)  coeff. 2.2(real)  ···
  2  coeff. 2.5(real)  coeff. 2.5(imag.)  coeff. 2.6(real)  ···
  ...
$end
```

Job Options

$Run
Basic settings of the calculation

JobType	type of calculation to be executed	
	Energy [sp]	single-point energy calculation (default)
	Gradient [grad]	energy gradient calculation
	Optimization [opt]	geometry optimization
	Property [prop]	property calculation
Mem	maximum amount of memory used in calculation (default: 1024MB) unit: KB, MB, GB, KW, MW, GW	
wayDiag	type of Lapack diagonalization routine	
	1	*syevd (divide-and-conquer algorithm)
	2	*syev (standard algorithm; default)

$Wavefunction

WavefuncType	selection of wavefunction theory or treatment of spin in DFT		DFT
	RHF	restricted Hartree-Fock and DFT (default)	✓
	UHF	unrestricted open-shell Hartree-Fock and DFT	✓
	ROHF	restricted open-shell Hartree-Fock and DFT	✓
	GHF	generalized Hartree-Fock and DFT	✓
	RMP2	restricted second-order Møller-Plesset perturbation theory	✕
	GMP2	general second-order Møller-Plesset perturbation theory	✕

$Hamiltonian

Hamiltonian settings

HamilType	Hamiltonian types Infinite-order Douglas-Kroll-Hess (IODKH) is a synonym of infinite-order two-component (IOTC).		Gradient
	NR	non-relativistic Hamiltonian (default)	✓
	FW [DKH1]	[Foldy-Wouthuysen transformation](#) for one-electron Hamiltonian + non-relativistic two-electron Hamiltonian	✗
	IOTC [IODKH]	[infinite-order two-component one-electron Hamiltonian](#) + non-relativistic two-electron Hamiltonian	✗
	LUT-IOTC [LUT-IODKH]	[infinite-order two-component one-electron Hamiltonian with local unitary transformation](#) + non-relativistic two-electron Hamiltonian	✓
	IOTC-IOTC [IODKH-IODKH]	[infinite-order two-component Hamiltonian](#)	✗
SD1e	calculation of one-electron spin-dependent terms to incorporate spin-orbit coupling (default: false) effective for WavefuncType=GHF Analytic gradient is available for the Hartree-Fock calculation with the LUT-IOTC Hamiltonian.		
ConvY	convergence threshold for the iterative determination of the decoupling matrix in IOTC calculations (default: 1.0d-09)		
tolHess	threshold for linear dependency screening in calculation of Hess' transformation matrix (default: 1.0d-10)		
tolLUTtau	cutoff radius in the local unitary transformation (default: 3.5 Å)		
tolRelTEI	cutoff value for relativistic transformation of two-electron integrals (default: 1.0d-10)		
Nucleus	model of nuclei		
	point	point-charge model (default)	
	finite	finite-size nucleus based on the Gaussian model [parametrized by Visscher and Dyall](#) applied to the electron-nucleus attraction in energy	

		calculations, meaning that the nuclear repulsion is calculated based on the point-charge model

$Mol
Additional molecular information

mcharge	molecular charge (default: 0)
multiplicity	spin multiplicity (default: 1)

$Basis
Additional basis set settings

BasType	format conversion of the atomic basis set	
	None	no conversion
	GC	conversion to general contraction (default)
	SC	conversion to segmented contraction
	UC	conversion to uncontracted basis
BasTypeSmall	format conversion of the basis set specified in the Basis Sets 2 section (if not specified, same as BasType)	
	None	no conversion
	GC	conversion to general contraction (default)
	SC	conversion to segmented contraction
	UC	conversion to uncontracted basis
OrbitalShape	shape of the orbitals	
	Cartesian [xyz]	Cartesian basis functions (default)
	Spherical [SH]	spherical harmonic basis functions (only for energy calculations of Hartree-Fock and MP2 methods)

$Integral
Molecular integral settings

Method_TEI	algorithm for two-electron integral calculation Note that direct SCF is performed based on "Hybrid" algorithm.	
	Gauss-Rys	Gauss-Rys quadrature
	PHMD	combination of the Pople-Hehre and McMurchie-Davidson methods
	ACE-TRR [SC-ACE-TRR]	accompanying coordinate expansion and recurrence relation method
	GC-ACE-TRR	general contraction accompanying coordinate expansion and recurrence relation method
	Hybrid	combination of the above methods (default)
Cutoff_OEI	one-electron integral cutoff (default: 1.0d-20)	
Cutoff_TEI	two-electron integral cutoff (default: 1.0d-20)	
Cutoff_TEIout	cutoff for two-electron integrals to be saved on disk, not used in direct SCF (default: 1.0d-12)	
Cutoff_preExp	integral cutoff based on exponents of basis functions (default: 20.0 * log(10.0))	
isSchwarz	use Schwarz inequality to reduce computational cost of two-electron integrals (default: true)	
Method_DTEI	algorithm for two-electron integral gradients	
	Gauss-Rys	Gauss-Rys quadrature
	ACE-TRR [SC-ACE-TRR]	accompanying coordinate expansion and recurrence relation method
	GC-ACE-TRR	general contraction accompanying coordinate expansion and recurrence relation method
	Hybrid	combination of the above methods (default)
Cutoff_DOEI	cutoff for one-electron integral gradient (default: 1.0d-15)	
Cutoff_DTEI	cutoff for two-electron integral gradient (default: 1.0d-10)	

$Guess

Settings for the initial guess method

GuessMethod	initial guess method	
	Hcore	core Hamiltonian guess
	Huckel	extended-Hückel guess with basis set 2 (definition is required; default) available up to atom number 103 DKH3minimal is recommended as basis set 2.
	Atomic	atomic Hartree-Fock calculation with basis set 2 (definition is required) and projection to basis set
	Small	full Hartree-Fock calculation with basis set 2 (definition required) and projection to basis set
	MOread	read MO coefficients from directives $MOA, $MOB, or $MOG
GuessWavefuncType	wavefunction type for initial guess (default: WavefuncType)	
	RHF	restricted Hartree-Fock (default)
	UHF	unrestricted open-shell Hartree-Fock
	ROHF	restricted open-shell Hartree-Fock
	GHF	generalized Hartree-Fock
GuessMix	for open-shell singlet UHF and UDFT calculations: mix HOMO and LUMO of α- and β- spin (default: false)	

$SCF

Settings for self-consistent-field (SCF) calculations

maxSCFcycle	maximum number of SCF iterations (default: 50)	
convSCF	SCF energy convergence threshold (default: 1.0d-09)	
convDen	SCF density matrix convergence threshold (default: 1.0d-05)	
convTech	SCF convergence acceleration technique (different methods can be combined by using '+' as separator)	
	C1-DIIS [DIIS, C-DIIS]	direct inversion in the iterative subspace (DIIS) method
	C2-DIIS	C2-DIIS method, valid for large values of maxDIIS
	EDIIS	energy-based DIIS method
	EDIIS+DIIS	combination of DIIS and EDIIS (default)
	SOSCF	approximate second-order SCF (SOSCF) method
	sDamp	static damping
	FON	non-integer occupation numbers during SCF based on Fermi distribution function, integer occupation for converged orbitals, known as Fermi smearing
QmtE_Cutoff	threshold for determination of linear dependencies in canonical orthogonalization of atomic orbitals (default: 1.0d-06)	
isDirectSCF	switch off storage of two-electron integrals on disc, i.e. recalculation of integrals for each SCF step, known as direct SCF (default: false)	
isFockDiff	use difference density matrix algorithm in direct-SCF calculations (default: true)	
Couple	coupling coefficients used for linear combination of Fock matrix in ROHF calculations, where $F_{XX} = A_{XX} \times F^\alpha + B_{XX} \times F^\beta$ (X = C, O, V)	
	Davidson	$A_{CC}=1/2$, $A_{OO}=1$, $A_{VV}=1$, $B_{CC}=1/2$, $B_{OO}=0$, $B_{VV}=0$ (default)
	C2006	Plakhutin et al (2006), which fulfills Koopmans' theorem ($A_{CC}=0$, $A_{OO}=1$, $A_{VV}=1$, $B_{CC}=1$, $B_{OO}=0$, $B_{VV}=0$)
	Manual	Acc, Aoo, Avv, Bcc, Boo, Bvv are specified in $SCF

	[Man, Input]	
maxDIIS	number of previous iterations used in DIIS (default: 10)	
iDIISerrVec	method for calculation of DIIS error vector	
	1	conventional (default)
	2	Anderson type (default for complex MO coefficients)
maxEDIIS	number of previous iterations used in EDIIS (default: 10)	
maxIterEDIIS	maximum number of iterations in EDIIS method (default: 200)	
maxSOSCF	number of previous iterations used in SOSCF (default: 20)	
tolSOSCFini	threshold for slope, below which SOSCF is started (default: 0.25)	
tolSOSCFgrad	threshold for convergence of SOSCF gradient (default: 1.0d-8)	
SCFdampFac	static damping coefficient in sDamp, weight of previous density matrix between 0.0 and 1.0 (default: 0.75)	

$MP2

Settings for second-order Møller-Plesset (MP2) calculations

nFrzA	number of frozen inner-shell α electrons in RMP2 calculations (default: 0)
nFrz	number of frozen inner-shell electrons in GMP2 calculations (default: 0)
SCSFacS	coefficient for antiparallel spin term used in SCS-MP2 calculations (default: 1.2d+00)
SCSFacT	coefficient for parallel spin term used in SCS-MP2 calculations (default: 0.3333333333d+00)
Cutoff_MP2	molecular integral threshold for MP2 calculations (default: 1.0d-09)

$DFT
Settings for density functional theory (DFT) calculations

DensfuncType	type of exchange-correlation functional	
	None	wavefunction theory (default)
	exchange only	
	Slater	Slater-Dirac (LDA) exchange
	Becke88	B88 exchange by Becke
	PBEX	Perdew-Burke-Ernzerhof (PBE) exchange
	Hartree-Fock + DFT correlation	
	VWN	Vosko-Wilk-Nusair (VWN) LDA correlation VWN5 parameterization
	VWN3	VWN3 parameterization
	PW92	Perdew-Wang (PW92) LDA correlation
	LYP	Lee-Yang-Parr (LYP) correlation
	PBEC	Perdew-Burke-Ernzerhof (PBE) correlation
	Pure (semi-)local density functionals	
	SVWN	Slater + VWN5
	SVWN3	Slater + VWN3
	SPW92	Slater + PW92
	BLYP	Becke88 + LYP
	PBE	PBEX + PBEC
	revPBE	revised PBEX + PBEC
	VS98	meta-GGA by van Voorhis and Scuseria
	M06-L	meta-GGA by Zhao and Truhlar (2006)

	Global hybrid functionals	
	B3LYP	three-parameter hybrid functional by Becke 20% exact exchange (EXX)
	B3LYP3	B3LYP with VWN3 parameterization
	BHHLYP	50% Becke88 + 50% EXX + LYP
	PBE0	75% PBEX + 25% EXX + PBEC
	M05	hybrid meta-GGA by Zhao, Schultz and Truhlar (2005, 28% EXX)
	M05-2X	hybrid meta-GGA by Zhao, Schultz and Truhlar (2005, 56% EXX)
	M06	hybrid meta-GGA by Zhao and Truhlar (2006, 27% EXX)
	M06-2X	hybrid meta-GGA by Zhao and Truhlar (2006, 54% EXX)
	M06-HF	hybrid meta-GGA by Zhao and Truhlar (2006, 100% EXX)
	Double hybrid functionals	
	B2PLYP	47% Becke88 + 53% EXX + 73% LYP + 27% MP2
	B2GPPLYP	35% Becke88 + 65% EXX + 64% LYP + 36% MP2
	PBE0-DH	50% PBEX + 50% EXX + 87.5% PBEC + 12.5% MP2
	PBE0-2	20.6299% PBEX + 79.3701% EXX + 50% PBEC + 50% MP2
nRad	number of radial grid points in molecular integration grid (default: 96)	
nLeb	number of spherical grid points in molecular integration grid (Gauss-Lebedev quadrature) allowed values: 6, 14, 26, 38, 50, 74, 86, 110, 146, 170, 194, 230, 266, 302, 350, 434, 590, 770, 974, 1202, 1454 (default: 302)	
sdCol	axis of collinear spin density in spin-dependent calculation	
	X	x axis
	Y	y axis

	Z	z axis
	None	no specific axis, meaning DFT calculation with non-collinear spin density (default)
isRelPC	picture-change correction based on IOTC (IODKH) transformation for exchange-correlation terms in relativistic DFT and TDDFT (default: false) available for WavefuncType=RHF, UHF, ROHF with HamilType=IOTC-IOTC	
isRelFun	replace Slater-Dirac and Becke 88 exchange functional with relativistic counterparts (default: false) effective for DensfuncType=SVWN, BLYP, B3LYP, B2PLYP, etc. HamilType=IOTC-IOTC and isRelPC=.true. is recommended. valid for ground-state calculations, meaning that coupling matrix of TDDFT is calculated using a non-relativistic functional	

$TDDFT

Settings for excited-state calculation based on linear-response time-dependent DFT

isExcited	perform an excited-state calculation based on linear-response TDDFT using the exchange-correlation functional specified by DensfuncType in $DFT (default: false) available for WavefuncType=RHF and GHF	
isTDA	Tamm-Dancoff approximation (default: false) For WavefuncType=GHF, this keyword is forced to be true.	
wayDiag	diagonalization method (eigenvalue solver)	
	Davidson	Davidson method (for few eigenvalues; default)
	QR	all eigenvalues by QR method
nEigen	number of eigenvalues (excitation energies) with the Davidson method (default: 10)	
maxVec	keyword regarding the maximum value of the subspace extension with the Davidson method (default: 100) maximum size of subspace = nEigen × maxVec	
TDmulti	spin multiplicity of excited states for WavefuncType=RHF	
	1	singlet excited states (default)
	3	triplet excited states
TDnRad	number of radial grid points in molecular integration grid (default: 48)	
TDnLeb	number of spherical grid points in molecular integration grid (Gauss-Lebedev quadrature) allowed values: 6, 14, 26, 38, 50, 74, 86, 110, 146, 170, 194, 230, 266, 302, 350, 434, 590, 770, 974, 1202, 1454 (default: 110)	

$DFT (new routine)

Settings for density functional theory (DFT) calculations using newly implemented routine

isExCorDM	switch on newly implemented density-matrix-based routine for exchange-correlation energy and potential (default: false)	
isRelPC	picture-change transformation based on the IOTC (IODKH) method for Coulomb repulsion and exchange-correlation terms in relativistic DFT (default: false) available for WavefuncType=RHF, UHF, ROHF with HamilType=IOTC-IOTC	
isRelFun	replace Slater-Dirac and Becke 88 exchange functional with relativistic counterparts (default: false) effective for DensfuncType=SVWN, BLYP, B3LYP, B2PLYP, etc and local hybrid functionals listed below HamilType=IOTC-IOTC and isRelPC=.true. is recommended.	
DensfuncType	type of exchange-correlation functional In addition to the same functionals implemented in the old routine except meta-GGA, local hybrid functionals are available.	
	local hybrid functional	
	Lh07t-SVWN	local mixing of exact exchange and Slater exchange with mixing function of kinetic energy density and VWN correlation
	Lh07s-SVWN	local mixing of exact exchange and Slater exchange with mixing function of dimensionless density gradient and VWN correlation
	Lh12ct-SVWN	local mixing of exact exchange and Slater exchange with mixing function of kinetic energy density and VWN correlation
	Lh12ct-SsirPW92	local hybrid functional with self-interaction-reduced PW92 correlation
	Lh12ct-SsifPW92	local hybrid functional with self-interaction-free PW92 correlation

	[Lh14t-calPBE](#)	local mixing of exact exchange and PBE exchange with mixing function of kinetic energy density, calibration function, and PBE correlation
GridType	type of grid used in computation of exchange-correlation terms	
	SMASH	conventional Lebedev grid implemented in the [SMASH program](#) (default)
	Ahlrichs	[standard grid](#) for efficient calculation proposed by Ahlrichs
nRad	number of radial grid points in molecular integration grid for GridType=SMASH (default: 96)	
nLeb	number of spherical grid points in molecular integration grid (Gauss-Lebedev quadrature) for GridType=SMASH allowed values: 6, 14, 26, 38, 50, 74, 86, 110, 146, 170, 194, 230, 266, 302, 350, 434, 590, 770, 974, 1202, 1454 (default: 302)	
GridSize	predefined grid sizes for Ahlrichs grids	
	1	very small test grid
	2	small standard grid for fast calculation
	3	medium standard grid for standard calculation (default)
	4	large standard grid
	5	large standard grid with higher accuracy
	6	small reference grid
	7	accurate reference grid
	8	highly accurate reference grid
	9	'cheap' reference grid for accurate atomic calculations
	42	meaninglessly large grid for almost exact results, reference only

Junc	thresholds for screening in seminumerical integration of exact exchange energy density (default: 12,12,12) "Junc=s,d,f" means thresholds of 10^{-s}, 10^{-p}, and 10^{-f} for S-junction (overlap screening), P-junction (density matrix screening), and F-junctions (screening before Fock matrix build), respectively.

$Opt

Settings for molecular structure optimization

Coord	coordinates used for optimization	
	Redundant [RD, Redun]	redundant internal coordinates (default)
	Cartesian [Cart]	Cartesian coordinates
maxOptCycle	maximum number of optimization steps (default: 50)	
convOpt	convergence threshold wrt the gradient in hartree/bohr (default: 1.0d-04)	
wayDTEI	method for calculating two-electron integral gradients	
	Gauss-Rys	Gauss-Rys quadrature
	ACE-TRR	accompanying coordinate expansion and recurrence relation method
	GC-ACE-TRR	general contraction accompanying coordinate expansion and recurrence relation method
	Hybrid	combination of ACE-TRR, PHMD, and Gauss-Rys (default)
Numerical	numerical differentiation of total energy to calculate gradient (default: false)	
StepSize	displacement for numerical gradient in angstrom (default: 1.0d-04)	
numPoint	number of points for numerical differentiation	
	3	three-point formula (default)
	5	five-point formula
	7	seven-point formula
	9	nine-point formula

$FCP

Settings for [frozen core potential (FCP)](#)

FCPmethod	FCP creation/calculation settings	
	None	no FCP (default)
	Potential	creating an FCP
	FCP	execution of calculation using FCP
nCoreOut(n)	number of core shells of FCP (n = 1, 2, 3, 4 corresponds to s, p, d and f orbitals)	
CoreRegion(1)	number of shells treated as core shells	
ValRegion(1)	number of shells treated as valence shells	
isUcore	core potential obtained with UHF (default: false)	
isCorePotEx	presence of exchange integration in core potential generation (default: true)	
isValPotEx	presence of exchange integration in valence potential generation (default: true)	
doCVint	core-valence electron integration to create potential (default: true) requires false for OrbitalShape = Spherical	

$TCE

Settings for post-HF calculations implemented using [tensor contraction engine (TCE)](#)

TCEmethod	electron correlation method	
	None	do not utilize the TCE routine (default)
	MP2	second-order Møller-Plesset perturbation theory
	MP2.5	average of MP2 & MP3
	MP3	third-order Møller-Plesset perturbation theory
	LCCD	linearized coupled cluster doubles
	CCD	coupled cluster doubles
	LCCSD	linearized coupled cluster singles and doubles
	CCSD	coupled cluster singles and doubles
	CCSD[T]	coupled cluster singles and doubles with non-iterative connected triples
	CCSD(T)	coupled cluster singles and doubles with non-iterative connected triples
	CCSDT	coupled cluster singles, doubles, and triples
	CCSDTQ	coupled cluster singles, doubles, triples, and quadruples
nFrzA	number of frozen inner-shell α electrons (default: 0)	
nFrzVirA	number of frozen virtual α orbitals (default: 0)	
CutoffTransInt	molecular integral threshold for correlation calculation (default: 1.0d-09)	
maxTCEcycle	maximum number of iterations for iterative methods (default: 100)	
TCEtol	convergence threshold wrt. the amplitudes (default: 1.0d-08)	

$Prop
Setting for property evaluations

In addition to Mulliken atomic charge, Mulliken atomic spin density (WavefuncType=UHF, ROHF) and Mulliken atomic spin vector (WavefuncType=GHF) are obtained by a single-point calculation. For WavefuncType=RHF, UHF, and ROHF, other properties are calculated by RunType=prop and the following options:

isContact	calculate contact density, which is electron density and spin density at the position of nuclear coordinate (default: false)
isGridProperty	calculate atomic charge, dipole moment, and electric field gradient tensor using grid routine (default: false) Atomic charges are calculated using Becke's partition function and the values of covalent radii, which are also used in DFT and TDDFT routines.
isPCC	perform picture-change transformation of the density operator (default: true) valid for HamilType=IOTC, IOTC-IOTC, LUT-IOTC

Basis Set Library

RAQET provides the user with a comprehensive basis set library containing a large number of predefined common Gaussian basis sets. Each basis set is stored in a separate subdirectory of the library. Addition of new basis sets can be done by the following procedure:

1. Create a new directory for the basis set, e.g. basis/MyDZP.
2. Create basis set files for the desired elements. The format can be adapted from the existing basis set files and is similar to the format described in the section Basis Sets.
3. Different basis set names can be used by creating symbolic links.

The initially provided basis set library contains the following basis sets:

STO-nG Basis Sets

	Elements	Remarks
STO-2G	H-Ca, Sr	
STO-3G	H-Cd	
STO-6G	H-Zn	

Pople Basis Sets

	Alias	Elements	Remarks
3-21G		H-Cs	
3-21G(d)	3-21G*	Na-Ar	
3-21++G		H-Ca	
3-21++G(d)	3-21++G*	Na-Ar	
4-31G		H-Ne, P-Cl	
6-31G		H-Zn	
6-31G(d)	6-31G*	H-Zn	
6-31G(d,p)	6-31G**	H-Zn	
6-31+G		H-Ar	
6-31+G(d)	6-31+G*	H-Ca	
6-31++G		H-Ca	

6-31++G(d)	6-31++G*	H-Ca	
6-31++G(d,p)	6-31++G**	H-Ar	
6-311G		H-Ca, Ga-Kr, I	
6-311G(d)	6-311G*	H-Ca, Ga-Kr, I	
6-311G(d,p)	6-311G**	H-Ca, Ga-Kr, I	
6-311G(2df,2pd)		H-Ne, K-Ca	
6-311+G(d)	6-311+G*	H-Ca	
6-311++G(d,p)	6-311++G**	H-Ca	
6-311++G(2d,2p)		H-Ca	
6-311++G(3df,3pd)		H-Ar	

Sapporo Basis Sets

	Elements	Remarks
Sapporo-DZP	H-Xe	
Sapporo-DZP+d	H-Xe	
Sapporo-DZP-2012	H-Xe	
Sapporo-DZP-2012+d	H-Xe	
Sapporo-TZP	H-Xe	
Sapporo-TZP+d	H-Xe	
Sapporo-TZP-2012	H-Xe	
Sapporo-TZP-2012+d	H-Xe	
Sapporo-QZP	H-Xe	
Sapporo-QZP+d	H-Xe	
Sapporo-QZP-2012	H-Xe	
Sapporo-QZP-2012+d	H-Xe	
Sapporo-DKH3-DZP	K-Xe	for relativistic calculations
Sapporo-DKH3-DZP+d	K-Xe	for relativistic calculations

Sapporo-DKH3-DZP-2012	K-Rn	for relativistic calculations
Sapporo-DKH3-DZP-2012+d	K-Rn	for relativistic calculations
Sapporo-DKH3-TZP	K-Xe	for relativistic calculations
Sapporo-DKH3-TZP+d	K-Xe	for relativistic calculations
Sapporo-DKH3-TZP-2012	K-Rn	for relativistic calculations
Sapporo-DKH3-TZP-2012+d	K-Rn	for relativistic calculations
Sapporo-DKH3-QZP	K-Xe	for relativistic calculations
Sapporo-DKH3-QZP+d	K-Xe	for relativistic calculations
Sapporo-DKH3-QZP-2012	K-Rn	for relativistic calculations
Sapporo-DKH3-QZP-2012+d	K-Rn	for relativistic calculations

Correlation-Consistent Basis Sets

	Elements	Remarks
cc-pVDZ	H-Ar, Ca-Kr	
cc-pVTZ	H-Ar, Ca-Kr	
cc-pVQZ	H-Ar, Ca-Kr	
cc-pV5Z	H-Ar, Ca-Kr	
cc-pV6Z	H-He, B-Ne, Al-Ar	
cc-pVDZ-DK	H-He, B-Ne, Al-Ar, Sc-Kr	contractions optimized for relativistic calculations
cc-pVTZ-DK	H-He, B-Ne, Al-Ar, Sc-Kr	contractions optimized for relativistic calculations
cc-pVQZ-DK	H-He, B-Ne, Al-Ar, Sc-Kr	contractions optimized for relativistic calculations
cc-pV5Z-DK	H-He, B-Ne, Al-Ar, Sc-Kr	contractions optimized for relativistic calculations
cc-pCVDZ	H-He, B-Ar, Ca	
cc-pCVTZ	H-He, B-Ar, Ca	

cc-pCVQZ	H-He, B-Ar, Ca	
cc-pCV5Z	H-He, B-Ne	
cc-pwCVDZ	H-He, B-Ne, Al-Ar	
cc-pwCVTZ	H-He, B-Ne, Al-Ar, Sc-Zn	
cc-pwCVQZ	H-He, B-Ne, Al-Ar, Sc-Zn	
cc-pwCV5Z	H-He, B-Ne, Al-Ar, Sc-Zn	
cc-pwCVTZ-DK	B-Ne, Al-Ar, Sc-Zn	contractions optimized for relativistic calculations
cc-pwCVQZ-DK	B-Ne, Al-Ar, Sc-Zn	contractions optimized for relativistic calculations
cc-pwCV5Z-DK	B-Ne, Al-Ar, Sc-Zn	contractions optimized for relativistic calculations
cc-pV(D+d)Z	Al-Ar	
cc-pV(T+d)Z	Al-Ar	
cc-pV(Q+d)Z	Al-Ar	
cc-pV(5+d)Z	Al-Ar	
cc-pV(6+d)Z	Al-Ar	
aug-cc-pVDZ	H-Ar, Sc-Kr	
aug-cc-pVTZ	H-Ar, Sc-Kr	
aug-cc-pVQZ	H-Ar, Sc-Kr	
aug-cc-pV5Z	H-He, B-Be, Al-Ar, Sc-Kr	
aug-cc-pV6Z	H-He, B-Ne, Al-Ar	
aug-cc-pVDZ-DK	H-He, B-Ne, Al-Ar, Sc-Kr	contractions optimized for relativistic calculations
aug-cc-pVTZ-DK	H-He, B-Ne, Al-Ar, Sc-Kr	contractions optimized for relativistic calculations
aug-cc-pVQZ-DK	H-He, B-Ne, Al-Ar, Sc-Kr	contractions optimized for relativistic calculations

aug-cc-pV5Z-DK	H-He, B-Ne, Al-Ar, Sc-Kr	contractions optimized for relativistic calculations
aug-cc-pCVDZ	H-Ar	
aug-cc-pCVTZ	H-Ar	
aug-cc-pCVQZ	H-Ar	
aug-cc-pCV5Z	H-He, B-Ne, Al-Ar	
aug-cc-pV(D+d)Z	Al-Ar	
aug-cc-pV(T+d)Z	Al-Ar	
aug-cc-pV(Q+d)Z	Al-Ar	
aug-cc-pV(5+d)Z	Al-Ar	
aug-cc-pV(6+d)Z	Al-Ar	
cc-pVQZdenfit	H, B-F, Al-Cl	
aug-pV7Z	H, C-F, S	
aug-cc-pCVTZ-CTOCD-uc	H, C-F	
aug-cc-pVTZ-J	H, C-F, S	

Polarization-Consistent Basis Sets

	Elements	Remarks
pc-0	H-Ca, Ga-Kr	general contractions
pc-1	H-Kr	general contractions
pc-2	H-Kr	general contractions
pc-3	H-Kr	general contractions
pc-4	H-Kr	general contractions
pcseg-0	H-Kr	
pcseg-1	H-Kr	
pcseg-2	H-Kr	

	Elements	
pcseg-3	H-Kr	
pcseg-4	H-Kr	

Others

	Elements	Remarks
ANO-RCC	H-Cm	general contractions for relativistic calculations
DKH3minimal	H-Lr	general contractions for relativistic calculations
SARC-DKH	La-Rn, Ac-Lr	contractions for relativistic calculations
Sadlej-pol	H-Ca, Cu-Sr, Ag-Ba, Au-Fr	for polarizability calculations
Sadlej-pol-DK	H-Ca, Cu-Sr, Ag-Ba, Pt-Fr	for relativistic polarizability calculations
UGBS	H-Th, Pu-Am, Cf-Lr	General purpose minimal basis set
WTBS	He-Rn	

Nuclear Basis Set

	Elements	Remarks
N1G-VD97	H-Rn	Gaussian nucleus model parameterized by Visscher and Dyall, used with Nucleus=finite