exciting input reference

exciting developers team
(C. Ambrosch-Draxl, Zohreh Basirat, Thomas Dengg,
Rostam Golesorkhtabar, Christian Meisenbichler, Dmitrii Nabok,
Weine Olovsson, Pasquale Pavone, Stephan Sagmeister, Jürgen Spitaler)

July 31, 2012

About this Document

In order to perform an **exciting** calculation an XML input file called **input.xml** must be provided.

This web page lists all elements and attributes that can be used in the input file of an **exciting** calculation:

- elements are defined according to the general XML conventions (http://en.wikipedia.org/wiki/XML#Key_terminology). *Example:* The element groundstate is used to set up a self-consistent calculation of the ground-state energy.
- attributes are defined according to the general XML conventions (http://en.wikipedia.org/wiki/XML#Key_terminology). An attribute is always connected to an element. In **exciting** an attribute generally specifies a parameter or a set of parameters which are connected to the corresponding element. *Example:* The attribute xctype of the element groundstate defines which exchange-correlation potential is used in the self-consistent calculation.

The input file of an **exciting** calculation is named **input.xml**. A simple example for an input file can be found here (http://exciting-code.org/input-file-format-overview). The input file **input.xml** must be a valid XML file and it must contain the root element input.

Unless explicitly stated otherwise, **exciting** uses atomic units ($\hbar = m_e = e = 1$):

- Energies are given in Hartree:
  $1\ \text{Ha} = 2\ \text{Ry} = 27.21138386(68)\ \text{eV} = 4.35926 \cdot 10^{-18}\ \text{J}$
- Lengths are given in Bohr:
  $1\ a_{\text{Bohr}} = 0.52917720859(36)\ \text{Å} = 0.52917720859(36) \cdot 10^{-10}\ \text{m}$
- Magnetic fields are given in units of
  $1\ \text{a.u.} = \dfrac{e}{a_{\text{Bohr}}^2} = 1717.2445320376\ \text{Tesla}.$

Note: The electron charge is positive, so that the atomic numbers Z are negative.

Part I
Input Elements

1 Element: input

The XML element input is the root element of the **exciting** input file. It must contain at least the elements title, structure, and groundstate, each

of them must be present only one time.

Contains:	`title` (1 times) `structure` (1 times) `groundstate` (1 times) `structureoptimization` (optional) `properties` (optional) `phonons` (optional) `xs` (optional) `keywords` (optional)
XPath:	`/input`

This element allows for specification of the following attributes:

`scratchpath`

1.1 Attribute: scratchpath

The path to the scratch space where the eigenvector related files, **`EVECFV.OUT`**, **`EVECSV.OUT`**, and **`OCCSV.OUT`** will be written. If the local directory is accessed via a network then `scratchpath` can be set to a directory on a local disk. The default value is the working directory, *i.e.*, the directory where the program is started.

Type:	anyURI
Default:	"`./`"
Use:	optional
XPath:	`/input/@scratchpath`

2 Element: title

The title of the input file, *e.g.*, "Ground-State Calculation for Aluminum".

Type:	string
XPath:	`/input/title`

3 Element: keywords

The keywords tag can contain a space separated list of keywords classifying the calculation for archiving purposes. It is not used by the **`exciting`** program.

Type:	string
XPath:	`/input/keywords`

4 Element: structure

This element contains all structural information, such as unit-cell parameters as well as type and position of each atom. The presence of the subelement species is necessary unless one wants to perform an empty-lattice calculation. The attribute speciespath must be specified.

Contains:	crystal (1 times)
	species (zero or more)
XPath:	/input/structure

This element allows for specification of the following attributes:

speciespath (required), autormt, epslat, molecule, primcell, rmtapm, tshift, vacuum

4.1 Attribute: autormt

If "true", the muffin-tin radius of each species is automatically set according to the variables specified by the attribute rmtapm.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/structure/@autormt

4.2 Attribute: epslat

This attribute defines the accuracy up to which two vectors can be considered numerically identical. Vectors with lengths less than this are considered zero.

Type:	fortrandouble (74.1)
Default:	"1.0d-6"
Use:	optional
Unit:	Bohr
XPath:	/input/structure/@epslat

4.3 Attribute: molecule

If "true", a calculation for an isolated molecule is performed. In this case, the atomic positions specified by the atom subelement of the species element must be given in cartesian coordinates. The lattice vectors are set up automatically as

$$\mathbf{A}^{(i)} = A_i \, \hat{\mathbf{e}}^{(i)} \qquad i = 1, 2, 3 \tag{1}$$

with

$$A_i = \max_{\alpha,\beta} \left| a_i^{(\alpha)} - a_i^{(\beta)} \right| + d_{\text{vac}} \tag{2}$$

where $a_i^{(\alpha)}$ is the catesian component of the atom labeled by α in the i-th direction specified by the unit vector $\hat{\mathbf{e}}^{(i)}$. Furthermore, d_{vac} represents the size of the vacuum around the molecule as defined by the attribute vacuum.

Type: boolean
Default: "false"
Use: optional
XPath: /input/structure/@molecule

4.4 Attribute: primcell

If "true", the primitive unit cell is determined automatically from the conventional cell defined by the basis vectors given by the basevect elements. The primitive unit cell is determined by searching for lattice vectors among all vectors connecting atomic sites and choosing the three shortest ones which produce a unit cell with non-zero volume.

Type: boolean
Default: "false"
Use: optional
XPath: /input/structure/@primcell

4.5 Attribute: rmtapm

This attribute assigns the two parameters governing the automatic generation of the muffin-tin radii. When the attribute autormt is set to "true", the muffin-tin radii are determined according to the following expression

$$R_i \propto 1 + \zeta |Z_i|^{1/3}, \tag{3}$$

where Z_i is the atomic number of the i th species, ζ is stored in rmtapm(1). The distance between the muffin-tin speheres is determined by the value of rmtapm(2): When rmtapm(2)=1, the closest muffin-tin spheres will touch each other.

Type: vect2d (74.5)
Default: "0.25d0 0.95d0"
Use: optional
XPath: /input/structure/@rmtapm

4.6 Attribute: speciespath

The path to the directory containing the species files. Alternatively, it can be defined as an HTTP URL, in this case the wget (http://exciting-code.org/wget) utility must be installed.

Type: anyURI
Use: required
XPath: /input/structure/@speciespath

4.7 Attribute: tshift

If "true", the crystal is shifted such that the atom closest to the origin is exactly at the origin.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/structure/@tshift

4.8 Attribute: vacuum

Determines the size of the vacuum around the molecule, see the molecule attribute.

Type:	fortrandouble (74.1)
Default:	"10.0d0"
Use:	optional
Unit:	Bohr
XPath:	/input/structure/@vacuum

5 Element: crystal

Defines the unit cell of the crystal via the 3 basis vectors.

Contains:	basevect (3 times)
XPath:	/input/structure/crystal

This element allows for specification of the following attributes:

scale, stretch

5.1 Attribute: scale

Scales all the lattice vectors by the same factor. This is useful for varying the volume.

Type:	fortrandouble (74.1)
Default:	"1.0d0"
Use:	optional
Unit:	1
XPath:	/input/structure/crystal/@scale

5.2 Attribute: stretch

Allows for an individual scaling of each lattice vector separately. "1 1 1" means no scaling.

Type: vect3d (74.4)
Default: "1.0d0 1.0d0 1.0d0 "
Use: optional
XPath: /input/structure/crystal/@stretch

6 Element: basevect

Defines one basis vector in Cartesian coordinates.

Type: vect3d (74.4)
Unit: Bohr
XPath: /input/structure/crystal/basevect

7 Element: species

Defines the atomic species, *i.e.*, the chemical element. Aatomic coordinates and, optionally, quantities relevant for magnetic calculations are defined in the subelement(s) atom.

Contains: atom (1 times or more)
LDAplusU (optional)
XPath: /input/structure/species

This element allows for specification of the following attributes:

speciesfile (required), rmt

7.1 Attribute: rmt

Defines the muffin-tin radius. This optional parameter allows to override the value either specified in the species file or generated by automatic determination. The muffin-tin radius defines the region around the atomic nucleus where the wave function is expanded in terms of atomic-like functions. In contrast, the interstitial region, *i.e.*, the region not belonging to any muffin-tin sphere, is described by planewaves.

Type: fortrandouble (74.1)
Default: "-1.0d0"
Use: optional
Unit: Bohr
XPath: /input/structure/species/@rmt

7.2 Attribute: speciesfile

Defines the file that contains the species definition. It is looked up in the species directory specified by speciespath. By default, the name of the file is *element*.xml, *e.g.*, Ag.xml.

Type: anyURI
Use: required
XPath: /input/structure/species/@speciesfile

8 Element: atom

Defines the position and other attributes of one atom in the unit cell.

Type: no content
XPath: /input/structure/species/atom

This element allows for specification of the following attributes:

coord (required), bfcmt, mommtfix

8.1 Attribute: bfcmt

Muffin-tin external magnetic field in Cartesian coordinates.

Type: vect3d (74.4)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/structure/species/atom/@bfcmt

8.2 Attribute: coord

Atom position in lattice coordinates.

Type: vect3d (74.4)
Use: required
Unit: lattice coordinates
XPath: /input/structure/species/atom/@coord

8.3 Attribute: mommtfix

The desired muffin-tin moment for a Fixed Spin Moment (FSM) calculation.

Type: vect3d (74.4)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/structure/species/atom/@mommtfix

9 Element: LDAplusU

The LADplusU element is used to specify the J, U, and l parameters of an atomic species. To switch on the LDAplusU feature one needs to set the ldapu attribute of the groundstate element.

Type: no content
XPath: /input/structure/species/LDAplusU

This element allows for specification of the following attributes:

J, U, l

9.1 Attribute: J

Type: fortrandouble (74.1)
Default: "0.0d0"
Use: optional
XPath: /input/structure/species/LDAplusU/@J

9.2 Attribute: U

Type: fortrandouble (74.1)
Default: "0.0d0"
Use: optional
XPath: /input/structure/species/LDAplusU/@U

9.3 Attribute: l

Type: integer
Default: "-1"
Use: optional
XPath: /input/structure/species/LDAplusU/@l

10 Element: groundstate

The groundstate element is required for any calculation. Its attributes are the parameters and methods used to calculate the ground-state density.

Contains: spin (optional)
solver (optional)
output (optional)
libxc (optional)
XPath: /input/groundstate

This element allows for specification of the following attributes:

ngridk (required), autokpt, beta0, betadec, betainc, cfdamp, chgexs, deband, dlinengyfermi, do, epsband, epschg, epsengy, epsforce, epsocc, epspot, fermilinengy, findlinentype, fracinr, frozencore, gmaxvr, isgkmax, ldapu, lmaxapw, lmaxinr, lmaxmat, lmaxvr, lradstep, maxscl, mixer, nempty, nktot, nosource, nosym, nprad, npsden, nwrite, ptnucl, radkpt, reducek, rgkmax, stype, swidth, symmorph, tevecsv, tfibs, tforce, vkloff, xctype

10.1 Attribute: autokpt

If "true", the set of **k**-points is determined automatically according to the total number of required **k**-points given by nktot.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@autokpt

10.2 Attribute: beta0

Initial value for mixing parameter. Used in linear mixing as choosen with mixer.

Type: fortrandouble (74.1)
Default: "0.4d0"
Use: optional
XPath: /input/groundstate/@beta0

10.3 Attribute: betadec

Mixing parameter decrease. Used in linear mixing.

Type: fortrandouble (74.1)
Default: "0.6d0"
Use: optional
XPath: /input/groundstate/@betadec

10.4 Attribute: betainc

Mixing parameter increase. Used in linear mixing.

Type: fortrandouble (74.1)
Default: "1.1d0"
Use: optional
XPath: /input/groundstate/@betainc

10.5 Attribute: cfdamp

Damping coefficient for characteristic function.

Type: fortrandouble (74.1)
Default: "0.0d0"
Use: optional
XPath: /input/groundstate/@cfdamp

10.6 Attribute: chgexs

This controls the amount of charge in the unit cell beyond that required to maintain neutrality. It can be set positive or negative depending on whether electron or hole doping is required.

Type: fortrandouble (74.1)
Default: "0.0d0"
Use: optional
XPath: /input/groundstate/@chgexs

10.7 Attribute: deband

Initial band energy step size The initial step length used when searching for the band energy, which is used as the APW linearisation energy. This is done by first searching upwards in energy until the radial wave-function at the muffin-tin radius is zero. This is the energy at the top of the band, denoted E_{t}. A downward search is now performed from E_{t} until the slope of the radial wave-function at the muffin-tin radius is zero. This energy, E_{b}, is at the bottom of the band. The band energy is taken as $(E_{\mathrm{t}}+E_{\mathrm{b}})/2$. If either E_{t} or E_{b} cannot be found then the band energy is set to the default value.

Type: fortrandouble (74.1)
Default: "0.0025d0"
Use: optional
Unit: Hartree
XPath: /input/groundstate/@deband

10.8 Attribute: dlinengyfermi

Energy difference between linearisation and Fermi energy.

Type: fortrandouble (74.1)
Default: "-0.1d0"
Use: optional
Unit: Hartree
XPath: /input/groundstate/@dlinengyfermi

10.9 Attribute: do

Decides if the ground state is calculated starting from scratch, using the densities from file or if it is skipped and only its associated input parameters are read in. Also applies fo structural optimization run.

Type:	**choose from:**
	`fromscratch`
	`fromfile`
	`skip`
Default:	"`fromscratch`"
Use:	optional
XPath:	`/input/groundstate/@do`

10.10 Attribute: epsband

Energy tolerance for search of linearisation energies.

Type:	fortrandouble (74.1)
Default:	"`1.0d-6`"
Use:	optional
Unit:	Hartree
XPath:	`/input/groundstate/@epsband`

10.11 Attribute: epschg

Maximum allowed error in the calculated total charge beyond which a warning message will be issued.

Type:	fortrandouble (74.1)
Default:	"`1.0d-3`"
Use:	optional
XPath:	`/input/groundstate/@epschg`

10.12 Attribute: epsengy

Energy convergence tolerance.

Type:	fortrandouble (74.1)
Default:	"`1.0d-4`"
Use:	optional
Unit:	Hartree
XPath:	`/input/groundstate/@epsengy`

10.13 Attribute: epsforce

Convergence tolerance for the forces during the SCF run.

Type:	fortrandouble (74.1)
Default:	"`5.0d-5`"
Use:	optional
XPath:	`/input/groundstate/@epsforce`

10.14 Attribute: epsocc

smallest occupancy for which a state will contribute to the density.

Type:	fortrandouble (74.1)
Default:	"1.0d-8"
Use:	optional
XPath:	/input/groundstate/@epsocc

10.15 Attribute: epspot

If the RMS change in the effective potential and magnetic field is smaller than epspot, then the self-consistent loop is considered converged and exited. For structural optimization runs this results in the forces being calculated, the atomic positions updated and the loop restarted. See also maxscl.

Type:	fortrandouble (74.1)
Default:	"1.0d-6"
Use:	optional
XPath:	/input/groundstate/@epspot

10.16 Attribute: fermilinengy

If "true" the linearization energies marked as non-varying are set to the Fermi level plus dlinengyfermi.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/groundstate/@fermilinengy

10.17 Attribute: findlinentype

Select method to determine the linearisation energies.

Type:	**choose from:**
	simple
	advanced
Default:	"advanced"
Use:	optional
XPath:	/input/groundstate/@findlinentype

10.18 Attribute: fracinr

Fraction of the muffin-tin radius up to which lmaxinr is used as the angular momentum cut-off.

Type: fortrandouble (74.1)
Default: "0.25d0"
Use: optional
XPath: /input/groundstate/@fracinr

10.19 Attribute: frozencore

When set to "true" the frozen core approximation is applied, i.e., the core states are fixed to the atomic states.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@frozencore

10.20 Attribute: gmaxvr

Maximum length of —G— for expanding the interstitial density and potential.

Type: fortrandouble (74.1)
Default: "12.0d0"
Use: optional
XPath: /input/groundstate/@gmaxvr

10.21 Attribute: isgkmax

Species for which the muffin-tin radius will be used for calculating gkmax.

Type: integer
Default: "-1"
Use: optional
XPath: /input/groundstate/@isgkmax

10.22 Attribute: ldapu

Type of LDA+U method to be used.

Type: **choose from:**
none
FullyLocalisedLimit
AroundMeanField
FFL-AMF-interpolation
Default: "none"
Use: optional
XPath: /input/groundstate/@ldapu

10.23 Attribute: lmaxapw

Angular momentum cut-off for the APW functions.

Type: integer
Default: "10"
Use: optional
XPath: /input/groundstate/@lmaxapw

10.24 Attribute: lmaxinr

Close to the nucleus, the density and potential is almost spherical and therefore the spherical harmonic expansion can be truncated a low angular momentum. See also fracinr.

Type: integer
Default: "2"
Use: optional
XPath: /input/groundstate/@lmaxinr

10.25 Attribute: lmaxmat

Angular momentum cut-off for the outer-most loop in the hamiltonian and overlap matrix setup.

Type: integer
Default: "5"
Use: optional
XPath: /input/groundstate/@lmaxmat

10.26 Attribute: lmaxvr

Angular momentum cut-off for the muffin-tin density and potential.

Type: integer
Default: "6"
Use: optional
XPath: /input/groundstate/@lmaxvr

10.27 Attribute: lradstep

Some muffin-tin functions (such as the density) are calculated on a coarse radial mesh and then interpolated onto a fine mesh. This is done for the sake of efficiency. lradstp defines the step size in going from the fine to the coarse radial mesh. If it is too large, loss of precision may occur.

Type: integer
Default: "4"
Use: optional
XPath: /input/groundstate/@lradstep

10.28 Attribute: maxscl

Upper limit for te self-consistency loop.

Type:	integer
Default:	"200"
Use:	optional
XPath:	/input/groundstate/@maxscl

10.29 Attribute: mixer

Select the mixing (relaxation) scheme for the SCF loop. One has the folloeing options:

Linear mixer ("lin")

Given the input μ^i and output ν^i vectors of the ith iteration, the next input vector to the $(i+1)$th iteration is generated using an adaptive mixing scheme. The jth component of the output vector is mixed with a fraction of the same component of the input vector:

$$\mu_j^{i+1} = \beta_j^i \nu_j^i + (1-\beta_j^i)\mu_j^i, \tag{4}$$

where β_j^i is set to β_0 at initialisation and increased by scaling with $\beta_{\rm inc}$ (>1) if $f_j^i \equiv \nu_j^i - \mu_j^i$ does not change sign between loops. If f_j^i does change sign, then β_j^i is scaled by $\beta_{\rm dec}$ (>1). Note that the array `nu` serves for both input and output, and the arrays `mu`, `beta` and `f` are used internally and should not be changed between calls. The routine is initialised at the first iteration and is thread-safe so long as each thread has its own independent work array. Complex arrays may be passed as real arrays with n doubled.

Type:	**choose from:**
	lin
	msec
	pulay
Default:	"msec"
Use:	optional
XPath:	/input/groundstate/@mixer

10.30 Attribute: nempty

Defines the number of eigenstates beyond that required for charge neutrality. When running metals it is not known *a priori* how many states will be below the Fermi energy for each **k**-point. Setting nempty greater than zero allows the additional states to act as a buffer in such cases. Furthermore, magnetic calculations use the first-variational eigenstates as a basis for setting up the second-variational Hamiltonian, and thus nempty will determine the size of this basis set. Convergence with respect to this quantity should be checked.

Type: integer
Default: "5"
Use: optional
XPath: /input/groundstate/@nempty

10.31 Attribute: ngridk

Number of k grid points along the basis vector directions.

Type: integertriple (74.6)
Use: required
XPath: /input/groundstate/@ngridk

10.32 Attribute: nktot

Used for the automatic determination of the **k**-point mesh from the total number of **k**-points. If nktot is set, then the mesh will be determined in such a way that the number of **k**-points is proportional to the length of the reciprocal lattice vector in each direction and that the total number of **k**-points is less than or equal to nktot.

Type: integer
Default: "0"
Use: optional
XPath: /input/groundstate/@nktot

10.33 Attribute: nosource

When set to "true", source fields are projected out of the exchange-correlation magnetic field. experimental feature.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@nosource

10.34 Attribute: nosym

When set to "true" no symmetries, apart from the identity, are used anywhere in the code.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@nosym

10.35 Attribute: nprad

Smallest occupancy for which a state will contribute to the density.

Type: integer
Default: "4"
Use: optional
XPath: /input/groundstate/@nprad

10.36 Attribute: npsden

oOrder of polynomial for pseudo-charge density.

Type: integer
Default: "9"
Use: optional
XPath: /input/groundstate/@npsden

10.37 Attribute: nwrite

Normally, the density and potentials are written to the file STATE.OUT only after com- pletion of the self-consistent loop. By setting nwrite to a positive integer the file will be written during the loop every nwrite iterations.

Type: integer
Default: "0"
Use: optional
XPath: /input/groundstate/@nwrite

10.38 Attribute: ptnucl

The attrubute ptnucl is "true" if the nuclei are to be treated as point charges, if "false" the nuclei have a finite spherical distribution.

Type: boolean
Default: "true"
Use: optional
XPath: /input/groundstate/@ptnucl

10.39 Attribute: radkpt

Used for the automatic determination of the **k**-point mesh. If autokpt is set to "true" then the mesh sizes will be determined by $n_i = \lambda/|\mathbf{A}_i| + 1$.

Type: fortrandouble (74.1)
Default: "40.0d0"
Use: optional
XPath: /input/groundstate/@radkpt

10.40 Attribute: reducek

If the attribute `reducek` is `"true"` the **k**-point set is reduced with the crystal symmetries.

Type:	boolean
Default:	"`true`"
Use:	optional
XPath:	`/input/groundstate/@reducek`

10.41 Attribute: rgkmax

The parameter `rgkmax` implicitly determines the number of basis functions and is one of the crucial parameters for the accuracy of the calculation. It represents the product of two quantities: $R_{MT,\,Min}$, the smallest of all muffin-tin radii, and $|\mathbf{G}+\mathbf{k}|_{max}$, the maximum length for the **G**+**k** vectors. Because each **G**+**k** vector represents one basis function, `rgkmax` gives the number of basis functions used for solving the Kohn-Sham equations. Typical values of `rgkmax` are between 6 and 9. However, for systems with very short bond-lengths, significantly smaller values may be sufficient. This may especially be the case for materials containing carbon, where `rgkmax` may be 4.5-5, or hydrogen, where even values between 3 and 4 may be sufficient. In any case, a convergence check is indispensible for a proper choice of this parameter for your system!

Type:	fortrandouble (74.1)
Default:	"`7.0d0`"
Use:	optional
XPath:	`/input/groundstate/@rgkmax`

10.42 Attribute: stype

A smooth approximation to the Dirac delta function is needed to compute the occupancies of the Kohn-Sham states. The attribute `swidth` determines the width of the approximate delta function.

Type:	**choose from:**
	`Gaussian`
	`Methfessel-Paxton 1`
	`Methfessel-Paxton 2`
	`Fermi Dirac`
	`Square-wave impulse`
Default:	"`Gaussian`"
Use:	optional
XPath:	`/input/groundstate/@stype`

10.43 Attribute: swidth

Width of the smooth approximation to the Dirac delta function (must be greater than zero).

Type:	fortrandouble (74.1)
Default:	"0.001d0"
Use:	optional
Unit:	Hartree
XPath:	/input/groundstate/@swidth

10.44 Attribute: symmorph

When set to "true" only symmorphic space-group operations are to be considered, i.e. only symmetries without non-primitive translations are used anywhere in the code.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/groundstate/@symmorph

10.45 Attribute: tevecsv

The attribute tevecsv is "true" if second-variational eigenvectors are calculated.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/groundstate/@tevecsv

10.46 Attribute: tfibs

Because calculation of the incomplete basis set (IBS) correction to the force is fairly time- consuming, it can be switched off by setting tfibs to "false" This correction can then be included only when necessary, i.e. when the atoms are close to equilibrium in a structural relaxation run.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/groundstate/@tfibs

10.47 Attribute: tforce

Decides if the force should be calculated at the end of the self-consistent cycle.

Type: boolean
Default: "`false`"
Use: optional
XPath: `/input/groundstate/@tforce`

10.48 Attribute: vkloff

The **k**-point offset vector in lattice coordinates.

Type: vect3d (74.4)
Default: "`0.0d0 0.0d0 0.0d0`"
Use: optional
XPath: `/input/groundstate/@vkloff`

10.49 Attribute: xctype

Type of exchange-correlation functional to be used

- No exchange-correlation funtional ($E_{\rm xc} \equiv 0$)
- LDA, Perdew-Zunger/Ceperley-Alder, *Phys. Rev. B* **23**, 5048 (1981)
- LSDA, Perdew-Wang/Ceperley-Alder, *Phys. Rev. B* **45**, 13244 (1992)
- LDA, X-alpha approximation, J. C. Slater, *Phys. Rev.* **81**, 385 (1951)
- LSDA, von Barth-Hedin, *J. Phys. C* **5**, 1629 (1972)
- GGA, Perdew-Burke-Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996)
- GGA, Revised PBE, Zhang-Yang, *Phys. Rev. Lett.* **80**, 890 (1998)
- GGA, PBEsol, arXiv:0707.2088v1 (2007)
- GGA, Wu-Cohen exchange (WC06) with PBE correlation, *Phys. Rev. B* **73**, 235116 (2006)
- GGA, Armiento-Mattsson (AM05) spin-unpolarised functional, *Phys. Rev. B* **72**, 085108 (2005)

Type:	**choose from:**
	LDAPerdew-Zunger
	LSDAPerdew-Wang
	LDA-X-alpha
	LSDA-Barth-Hedin
	GGAPerdew-Burke-Ernzerhof
	GGArevPBE
	GGAPBEsol
	GGA-Wu-Cohen
	GGAArmiento-Mattsson
	EXX
	none
Default:	"LSDAPerdew-Wang"
Use:	optional
XPath:	/input/groundstate/@xctype

11 Element: spin

If the spin element is present calculation is done with spin polarization.

Type:	no content
XPath:	/input/groundstate/spin

This element allows for specification of the following attributes:

bfieldc, fixspin, momfix, reducebf, spinorb, spinsprl, taufsm, vqlss

11.1 Attribute: bfieldc

Allows to apply a constant B field This is a constant magnetic field applied throughout the entire unit cell and enters the second-variational Hamiltonian as

$$\frac{g_e \alpha}{4} \vec{\sigma} \cdot \mathbf{B}_{\text{ext}}, \tag{5}$$

where g_e is the electron g-factor (2.0023193043718). This field is normally used to break spin symmetry for spin-polarised calculations and considered to be infinitesimal with no direct contribution to the total energy. In cases where the magnetic field is finite (for example when computing magnetic response) the external **B**-field energy reported in INFO.OUT should be added to the total by hand. This field is applied throughout the entire unit cell. To apply magnetic fields in particular muffin-tins use the bfcmt vectors in the atom elements. Collinear calculations are more efficient if the field is applied in the z-direction.

Type:	vect3d (74.4)
Default:	"0.0d0 0.0d0 0.0d0 "
Use:	optional
XPath:	/input/groundstate/spin/@bfieldc

11.2 Attribute: fixspin

Type:	**choose from:**
	`none`
	`total FSM`
	`localmt FSM`
	`both`

Default:	"`none`"
Use:	optional
XPath:	`/input/groundstate/spin/@fixspin`

11.3 Attribute: momfix

The desired total moment for a FSM calculation.

Type:	vect3d (74.4)
Default:	"`0.0d0 0.0d0 0.0d0`"
Use:	optional
XPath:	`/input/groundstate/spin/@momfix`

11.4 Attribute: reducebf

After each iteration the external magnetic fields are multiplied with reducebf. This al- lows for a large external magnetic field at the start of the self-consistent loop to break spin symmetry, while at the end of the loop the field will be effectively zero, i.e. infinitesimal. See `bfieldc` and atom element.

Type:	fortrandouble (74.1)
Default:	"`1.0d0`"
Use:	optional
XPath:	`/input/groundstate/spin/@reducebf`

11.5 Attribute: spinorb

If `spinorb` is `"true"`, then a $\boldsymbol{\sigma} \cdot \mathbf{L}$ term is added to the second-variational Hamiltonian.

Type:	boolean
Use:	optional
XPath:	`/input/groundstate/spin/@spinorb`

11.6 Attribute: spinsprl

Set to `"true"` if a spin-spiral calculation is required. Experimental feature for the calculation of spin-spiral states. See `vqlss` for details.

Type:	boolean
Default:	"`false`"
Use:	optional
XPath:	`/input/groundstate/spin/@spinsprl`

11.7 Attribute: taufsm

Type: fortrandouble (74.1)
Default: "0.01d0"
Use: optional
XPath: /input/groundstate/spin/@taufsm

11.8 Attribute: vqlss

Is the **q**-vector of the spin-spiral state in lattice coordinates. Spin-spirals arise from spinor states assumed to be of the form

$$\Psi_{\mathbf{k}}^{\mathbf{q}}(\mathbf{r}) = \begin{pmatrix} U_{\mathbf{k}}^{\mathbf{q}\uparrow}(\mathbf{r}) e^{i(\mathbf{k}+\mathbf{q}/2)\cdot\mathbf{r}} \\ U_{\mathbf{k}}^{\mathbf{q}\downarrow}(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{q}/2)\cdot\mathbf{r}} \end{pmatrix}. \tag{6}$$

These are determined using a second-variational approach, and give rise to a magnetization density of the form

$$\mathbf{m}^{\mathbf{q}}(\mathbf{r}) = (m_x(\mathbf{r})\cos(\mathbf{q}\cdot\mathbf{r}), m_y(\mathbf{r})\sin(\mathbf{q}\cdot\mathbf{r}), m_z(\mathbf{r})), \tag{7}$$

where m_x, m_y and m_z are lattice periodic. See also spinsprl.

Type: vect3d (74.4)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/groundstate/spin/@vqlss

12 Element: solver

Optional configuration options for eigenvector solver.

Type: no content
XPath: /input/groundstate/solver

This element allows for specification of the following attributes:

epsarpack, evaltol, packedmatrixstorage, type

12.1 Attribute: epsarpack

Tolerance parameter for the ARPACK shift invert solver

Type: fortrandouble (74.1)
Default: "1.0d-8"
Use: optional
XPath: /input/groundstate/solver/@epsarpack

12.2 Attribute: evaltol

Error tolerance for the first-variational eigenvalues using the LAPACK Solver

Type:	fortrandouble (74.1)
Default:	"1.0d-8"
Use:	optional
Unit:	Hartree
XPath:	/input/groundstate/solver/@evaltol

12.3 Attribute: packedmatrixstorage

In the default calculation the matrix is sored in packed form. When using multi-threaded BLAS setting this parameter to "false" increases efficiency.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/groundstate/solver/@packedmatrixstorage

12.4 Attribute: type

Selects the eigenvalue solver for the first variational equation

Type:	**choose from:**
	Lapack
	Arpack
	DIIS
Default:	"Lapack"
Use:	optional
XPath:	/input/groundstate/solver/@type

13 Element: output

Specifications on the file formats for output files.

Type:	no content
XPath:	/input/groundstate/output

This element allows for specification of the following attributes:

state

13.1 Attribute: state

Selects the file format of the STATE file.

Type:	**choose from:**
	`binary`
	`XML`
Default:	"`binary`"
Use:	optional
XPath:	`/input/groundstate/output/@state`

14 Element: libxc

Type:	no content
XPath:	`/input/groundstate/libxc`

This element allows for specification of the following attributes:

`correlation`, `exchange`, `xc`

14.1 Attribute: correlation

Type: **choose from:**
XC_LDA_C_WIGNER
XC_LDA_C_RPA
XC_LDA_C_HL
XC_LDA_C_GL
XC_LDA_C_XALPHA
XC_LDA_C_VWN
XC_LDA_C_VWN_RPA
XC_LDA_C_PZ
XC_LDA_C_PZ_MOD
XC_LDA_C_OB_PZ
XC_LDA_C_PW
XC_LDA_C_PW_MOD
XC_LDA_C_OB_PW
XC_LDA_C_2D_AMGB
XC_LDA_C_2D_PRM
XC_LDA_C_vBH
XC_LDA_C_1D_CSC
XC_GGA_C_PBE
XC_GGA_C_LYP
XC_GGA_C_P86
XC_GGA_C_PBE_SOL
XC_GGA_C_PW91
XC_GGA_C_AM05
XC_GGA_C_XPBE
XC_GGA_C_LM
XC_GGA_C_PBE_JRGX

Default: "XC_GGA_C_PBE"
Use: optional
XPath: /input/groundstate/libxc/@correlation

14.2 Attribute: exchange

Type:	**choose from:**
	XC_LDA_X
	XC_LDA_X_2D
	XC_GGA_X_PBE
	XC_GGA_X_PBE_R
	XC_GGA_X_B86
	XC_GGA_X_B86_R
	XC_GGA_X_B86_MGC
	XC_GGA_X_B88
	XC_GGA_X_G96
	XC_GGA_X_PW86
	XC_GGA_X_PW91
	XC_GGA_X_OPTX
	XC_GGA_X_DK87_R1
	XC_GGA_X_DK87_R2
	XC_GGA_X_LG93
	XC_GGA_X_FT97_A
	XC_GGA_X_FT97_B
	XC_GGA_X_PBE_SOL
	XC_GGA_X_RPBE
	XC_GGA_X_WC
	XC_GGA_X_mPW91
	XC_GGA_X_AM05
	XC_GGA_X_PBEA
	XC_GGA_X_MPBE
	XC_GGA_X_XPBE
	XC_GGA_X_2D_B86_MGC
	XC_GGA_X_BAYESIAN
	XC_GGA_X_PBE_JSJR
Default:	"XC_GGA_X_PBE"
Use:	optional
XPath:	/input/groundstate/libxc/@exchange

14.3 Attribute: xc

Combined functionals. If set it overrides the exchange and the correlation attributes. The hybrid functionals can be configured but are not supported. They may give nonsense results.

Type: **choose from:**

- none
- XC_GGA_XC_LB
- XC_GGA_XC_HCTH_93
- XC_GGA_XC_HCTH_120
- XC_GGA_XC_HCTH_147
- XC_GGA_XC_HCTH_407
- XC_GGA_XC_EDF1
- XC_GGA_XC_XLYP
- XC_GGA_XC_B97
- XC_GGA_XC_B97_1
- XC_GGA_XC_B97_2
- XC_GGA_XC_B97_D
- XC_GGA_XC_B97_K
- XC_GGA_XC_B97_3
- XC_GGA_XC_PBE1W
- XC_GGA_XC_MPWLYP1W
- XC_GGA_XC_PBELYP1W
- XC_GGA_XC_SB98_1a
- XC_GGA_XC_SB98_1b
- XC_GGA_XC_SB98_1c
- XC_GGA_XC_SB98_2a
- XC_GGA_XC_SB98_2b
- XC_GGA_XC_SB98_2c
- XC_HYB_GGA_XC_B3PW91
- XC_HYB_GGA_XC_B3LYP
- XC_HYB_GGA_XC_B3P86
- XC_HYB_GGA_XC_O3LYP
- XC_HYB_GGA_XC_mPW1K
- XC_HYB_GGA_XC_PBEH
- XC_HYB_GGA_XC_B97
- XC_HYB_GGA_XC_B97_1
- XC_HYB_GGA_XC_B97_2
- XC_HYB_GGA_XC_X3LYP
- XC_HYB_GGA_XC_B1WC
- XC_HYB_GGA_XC_B97_K
- XC_HYB_GGA_XC_B97_3
- XC_HYB_GGA_XC_mPW3PW
- XC_HYB_GGA_XC_B1LYP
- XC_HYB_GGA_XC_B1PW91
- XC_HYB_GGA_XC_mPW1PW
- XC_HYB_GGA_XC_mPW3LYP
- XC_HYB_GGA_XC_SB98_1a
- XC_HYB_GGA_XC_SB98_1b
- XC_HYB_GGA_XC_SB98_1c
- XC_HYB_GGA_XC_SB98_2a
- XC_HYB_GGA_XC_SB98_2b
- XC_HYB_GGA_XC_SB98_2c

Default: "none"

Use: optional

XPath: /input/groundstate/libxc/@xc

15 Element: structureoptimization

The element `structureoptimization` activates the optimization of atomic postions.

Type: no content
XPath: `/input/structureoptimization`

This element allows for specification of the following attributes:

`epsforce`, `resume`, `tau0atm`

15.1 Attribute: epsforce

Convergence tolerance for the forces during a structural optimization run.

Type: fortrandouble (74.1)
Default: "`5.0d-5`"
Use: optional
XPath: `/input/structureoptimization/@epsforce`

15.2 Attribute: resume

Resumption of a structural optimization run using the density in `STATE.OUT`, but with positions from `input.xml`.

Type: boolean
Default: "`false`"
Use: optional
XPath: `/input/structureoptimization/@resume`

15.3 Attribute: tau0atm

Parameter determining the step size for structural optimization.

In each step m of a structural optimization run, atom α is displaced according to

$$\mathbf{r}_\alpha^{m+1} = \mathbf{r}_\alpha^m + \tau_\alpha^m \left(\mathbf{F}_\alpha^m + \mathbf{F}_\alpha^{m-1} \right), \tag{8}$$

i.e., the magnitude of the displacement in step m is proportional to τ_α^m. For the initial step, τ_α^0 is set to `tau0atm`. If the forces of two subsequent steps have the same sign, τ_α^m is increased by τ_α^0. Otherwise, τ_α^m is reset to τ_α^0.

Type: fortrandouble (74.1)
Default: "`0.2d0`"
Use: optional
XPath: `/input/structureoptimization/@tau0atm`

16 Element: properties

Properties listed in this element can be calculated from the groundstate. It works also from a saved state from a previous run.

Contains: bandstructure (optional)
STM (optional)
wfplot (optional)
dos (optional)
LSJ (optional)
masstensor (optional)
chargedensityplot (optional)
exccplot (optional)
elfplot (optional)
mvecfield (optional)
xcmvecfield (optional)
electricfield (optional)
gradmvecfield (optional)
fermisurfaceplot (optional)
EFG (optional)
mossbauer (optional)
momentummatrix (optional)
dielectric (optional)
moke (optional)
expiqr (optional)
elnes (optional)
eliashberg (optional)

XPath: /input/properties

17 Element: bandstructure

If present a banstructure is calculated.

Contains: plot1d
XPath: /input/properties/bandstructure

This element allows for specification of the following attributes:

character, scissor

17.1 Attribute: character

Band structure plot which includes angular momentum characters for every atom.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/bandstructure/@character

17.2 Attribute: scissor

Value to shift bandgap.

Type:	fortrandouble (74.1)
Default:	"0.0d0"
Use:	optional
Unit:	Hartree
XPath:	/input/properties/bandstructure/@scissor

18 Element: STM

Contains:	plot2d (optional)
XPath:	/input/properties/STM

19 Element: wfplot

Wavefunction plot.

Contains:	kstlist (1 times)
	plot1d (optional)
	plot2d (optional)
	plot3d (optional)
XPath:	/input/properties/wfplot

20 Element: dos

If present a DOS calculation is started.

DOS and optics plots require integrals of the kind

$$g(\omega_i) = \frac{\Omega}{(2\pi)^3} \int_{\mathrm{BZ}} f(\mathbf{k}) \delta(\omega_i - e(\mathbf{k})) d\mathbf{k}. \tag{9}$$

These are calculated by first interpolating the functions $e(\mathbf{k})$ and $f(\mathbf{k})$ with the trilinear method on a much finer mesh whose size is determined by ngrdos. Then the ω-dependent histogram of the integrand is accumulated over the fine mesh. If the output function is noisy then either ngrdos should be increased or nwdos decreased. Alternatively, the output function can be artificially smoothed up to a level given by nsmdos. This is the number of successive 3-point averages to be applied to the function g.

Type:	no content
XPath:	/input/properties/dos

This element allows for specification of the following attributes:

lmirep, ngrdos, nsmdos, nwdos, scissor, sqados, winddos

20.1 Attribute: lmirep

When lmirep is set to "true", the spherical harmonic basis is transformed into one in which the site symmetries are block diagonal. Band characters determined from the density matrix expressed in this basis correspond to irreducible representations, and allow the partial DOS to be resolved into physically relevant contributions, for example eg and t2g.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/dos/@lmirep

20.2 Attribute: ngrdos

Type: integer
Default: "100"
Use: optional
XPath: /input/properties/dos/@ngrdos

20.3 Attribute: nsmdos

Type: integer
Default: "0"
Use: optional
XPath: /input/properties/dos/@nsmdos

20.4 Attribute: nwdos

Type: integer
Default: "500"
Use: optional
XPath: /input/properties/dos/@nwdos

20.5 Attribute: scissor

Type: fortrandouble (74.1)
Default: "0.0d0"
Use: optional
Unit: Hartree
XPath: /input/properties/dos/@scissor

20.6 Attribute: sqados

Spin-quantization axis in Cartesian coordinates used when plotting the spin-resolved DOS (z-axis by default).

Type: vect3d (74.4)
Default: "0.0d0 0.0d0 1.0d0"
Use: optional
XPath: /input/properties/dos/@sqados

20.7 Attribute: winddos

Frequency/energy window for the DOS or optics plot.

Type: vect2d (74.5)
Default: "-0.5d0 0.5d0"
Use: optional
Unit: Hartree
XPath: /input/properties/dos/@winddos

21 Element: LSJ

Output L, S and J expectation values.

Contains: kstlist (optional)
XPath: /input/properties/LSJ

22 Element: masstensor

Compute the effective mass tensor at the **k**-point given by vklem.

Type: no content
XPath: /input/properties/masstensor

This element allows for specification of the following attributes:

deltaem, ndspem, vklem

22.1 Attribute: deltaem

The size of the **k**-vector displacement used when calculating numerical derivatives for the effective mass tensor.

Type: fortrandouble (74.1)
Default: "0.025d0"
Use: optional
XPath: /input/properties/masstensor/@deltaem

22.2 Attribute: ndspem

The number of **k**-vector displacements in each direction around vklem when computing the numerical derivatives for the effective mass tensor.

Type:	integer
Default:	"1"
Use:	optional
XPath:	/input/properties/masstensor/@ndspem

22.3 Attribute: vklem

The **k**-point in lattice coordinates at which to compute the effective mass tensors.

Type:	vect3d (74.4)
Default:	"0.0d0 0.0d0 0.0d0"
Use:	optional
XPath:	/input/properties/masstensor/@vklem

23 Element: chargedensityplot

Plot the charge density

Contains:	plot1d (optional) plot2d (optional) plot3d (optional)
XPath:	/input/properties/chargedensityplot

This element allows for specification of the following attributes:

plotgradient

23.1 Attribute: plotgradient

Calculate and plot the module of the density gradient

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/properties/chargedensityplot/@plotgradient

24 Element: exccplot

Exchange-correlation and Coulomb potential plots.

Contains:	plot1d (optional) plot2d (optional) plot3d (optional)
XPath:	/input/properties/exccplot

25 Element: elfplot

Electron localization function (ELF).

Contains: plot1d (optional)
plot2d (optional)
plot3d (optional)
XPath: /input/properties/elfplot

26 Element: mvecfield

Plot of magnetization vector field.

Contains: plot2d (optional)
plot3d (optional)
XPath: /input/properties/mvecfield

27 Element: xcmvecfield

Plot of exchange-correlation magnetic vector field.

Contains: plot2d (optional)
plot3d (optional)
XPath: /input/properties/xcmvecfield

28 Element: electricfield

Writes the electric field to file.

Contains: plot2d (optional)
plot3d (optional)
XPath: /input/properties/electricfield

29 Element: gradmvecfield

Plot of he gradient of the magnetic vector field.

Contains: plot1d (optional)
plot2d (optional)
plot3d (optional)
XPath: /input/properties/gradmvecfield

30 Element: fermisurfaceplot

Writes Fermi surface data to file.

Type: no content
XPath: /input/properties/fermisurfaceplot

This element allows for specification of the following attributes:

nstfsp, separate

30.1 Attribute: nstfsp

Number of states to be included in the Fermi surface plot file.

Type: integer
Default: "6"
Use: optional
XPath: /input/properties/fermisurfaceplot/@nstfsp

30.2 Attribute: separate

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/fermisurfaceplot/@separate

31 Element: EFG

Calculation of electric field gradient (EFG), contact charge.

Type: no content
XPath: /input/properties/EFG

32 Element: mossbauer

Type: no content
XPath: /input/properties/mossbauer

33 Element: momentummatrix

Matrix elements of the momentum operator (legacy version, required by dielectric-element).

Type: no content
XPath: /input/properties/momentummatrix

This element allows for specification of the following attributes:

fastpmat

33.1 Attribute: fastpmat

apply generalised DFT correction of L. Fritsche and Y. M. Gu, Phys. Rev. B 48, 4250 (1993)

Type: boolean
Default: "true"
Use: optional
XPath: /input/properties/momentummatrix/@fastpmat

34 Element: dielectric

Linear optical response (without local field effects, legacy version).

Contains: optcomp
XPath: /input/properties/dielectric

This element allows for specification of the following attributes:

intraband, scissor, usegdft

34.1 Attribute: intraband

The intraband attribute is "true" if the intraband term is to be added to the optical matrix (q=0)

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/dielectric/@intraband

34.2 Attribute: scissor

Type: fortrandouble (74.1)
Default: "0.0d0"
Use: optional
Unit: Hartree
XPath: /input/properties/dielectric/@scissor

34.3 Attribute: usegdft

apply generalised DFT correction of L. Fritsche and Y. M. Gu, Phys. Rev. B 48, 4250 (1993)

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/dielectric/@usegdft

35 Element: optcomp

The components of the first- or second-order optical tensor to be calculated.

Type: integertriple (74.6)
Default: "1 1 1"
XPath: /input/properties/dielectric/optcomp

36 Element: moke

Type: no content
XPath: /input/properties/moke

37 Element: expiqr

Contains: kstlist (optional)
XPath: /input/properties/expiqr

38 Element: elnes

Type: no content
XPath: /input/properties/elnes

This element allows for specification of the following attributes:

vecql

38.1 Attribute: vecql

Gives the q-vector in lattice coordinates for calculating ELNES.

Type: vect3d (74.4)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/properties/elnes/@vecql

39 Element: eliashberg

Type: no content
XPath: /input/properties/eliashberg

This element allows for specification of the following attributes:

mustar

39.1 Attribute: mustar

Coulomb pseudopotential, $\mu*$, used in the McMillan-Allen-Dynes equation.

Type:	fortrandouble (74.1)
Default:	"0.15d0"
Use:	optional
XPath:	/input/properties/eliashberg/@mustar

40 Element: phonons

Phonon frequencies and eigen vectors for an arbitrary q-point.

Contains:	qpointset (optional)
	phonondos (optional)
	phonondispplot (optional)
	reformatdynmat (optional)
	interpolate (optional)
	parts (optional)
XPath:	/input/phonons

This element allows for specification of the following attributes:

ngridq (required), deltaph, do, phonontype, reduceq

40.1 Attribute: deltaph

Phonon calculations are performed by constructing a supercell corresponding to a particular **q**-vector and making a small periodic displacement of the atoms. The magnitude of this displacement is given by deltaph. This should not be made too large, as anharmonic terms could then become significant, neither should it be too small as this can introduce numerical error.

Type:	fortrandouble (74.1)
Default:	"0.03d0"
Use:	optional
XPath:	/input/phonons/@deltaph

40.2 Attribute: do

Decides if the phonon calculation is skipped or recalculated or continued from file.

Type:	**choose from:**
	fromscratch
	skip
Default:	"fromscratch"
Use:	optional
XPath:	/input/phonons/@do

40.3 Attribute: ngridq

Number of q grid points along the basis vector directions.

Type:	integertriple (74.6)
Use:	required
XPath:	/input/phonons/@ngridq

40.4 Attribute: phonontype

Decides which method (supercell or linear response) is used to perform the phonon calculation.

Type:	**choose from:**
	supercell
	linearresponse
Default:	"supercell"
Use:	optional
XPath:	/input/phonons/@phonontype

40.5 Attribute: reduceq

The attribute reduceq is set to "true" if the q-point set is to be reduced with the crystal symmetries.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/phonons/@reduceq

41 Element: phonondos

Phonon density of states.

Type:	no content
XPath:	/input/phonons/phonondos

This element allows for specification of the following attributes:

ngrdos, nsmdos, ntemp, nwdos

41.1 Attribute: ngrdos

Type:	integer
Default:	"100"
Use:	optional
XPath:	/input/phonons/phonondos/@ngrdos

41.2 Attribute: nsmdos

Type: integer
Default: "0"
Use: optional
XPath: /input/phonons/phonondos/@nsmdos

41.3 Attribute: ntemp

Number of temperatures points for the calculation of the thermodynamical properties from the phonon density of states.

Type: integer
Default: "10"
Use: optional
XPath: /input/phonons/phonondos/@ntemp

41.4 Attribute: nwdos

Type: integer
Default: "500"
Use: optional
XPath: /input/phonons/phonondos/@nwdos

42 Element: phonondispplot

Phonon dispersion plot.

Contains: plot1d
XPath: /input/phonons/phonondispplot

43 Element: reformatdynmat

Reads in the dynamical matrix rows from the corresponding files and outputs them in the DYNMAT*.OUT files, taking into account symmetrization and the accoustic sumrule.

Type: no content
XPath: /input/phonons/reformatdynmat

44 Element: interpolate

Interpolates the phonon frequencies on a given q-point set.

Type: no content
XPath: /input/phonons/interpolate

This element allows for specification of the following attributes:

ngridq (required), vqloff, writeeigenvectors

44.1 Attribute: ngridq

q-point grid for interpolation.

Type: integertriple (74.6)
Use: required
XPath: /input/phonons/interpolate/@ngridq

44.2 Attribute: vqloff

The q-point offset vector in lattice coordinates.

Type: vect3d (74.4)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/phonons/interpolate/@vqloff

44.3 Attribute: writeeigenvectors

Set to true if the phonon eigenvectors are to be interpolated and output in addition to the phonon frequencies.

Type: boolean
Default: "false"
Use: optional
XPath: /input/phonons/interpolate/@writeeigenvectors

45 Element: parts

Contains: dopart (zero or more)
XPath: /input/phonons/parts

46 Element: dopart

Type: no content
XPath: /input/phonons/parts/dopart

This element allows for specification of the following attributes:

id (required)

46.1 Attribute: id

This attribute is used to trigger lower-level tasks and is mainly used for testing, debugging, and the testing of new features. Do not use it unless you know what you are doing.

Type: string
Use: required
XPath: /input/phonons/parts/dopart/@id

47 Element: xs

If this element is present with valid configuration, the macroscopic dielectric function and related spectroscopic quantities in the linear regime are calculated through either time-dependent DFT (TDDFT) or the Bethe-Salpeter equation (BSE).

Contains:	tddft (optional) screening (optional) BSE (optional) transitions (optional) qpointset (1 times) tetra (optional) energywindow (1 times) plan (optional)
XPath:	/input/xs

This element allows for specification of the following attributes:

xstype (required), broad, dbglev, dfoffdiag, emattype, emaxdf, epsdfde, fastemat, fastpmat, gqmax, gqmaxtype, lmaxapw, lmaxapwwf, lmaxemat, lmaxmat, nempty, ngridk, ngridq, nosym, reducek, reduceq, rgkmax, scissor, swidth, tappinfo, tevout, vkloff

47.1 Attribute: broad

Lorentzian broadening for all spectra

Type:	fortrandouble (74.1)
Default:	"0.01d0"
Use:	optional
Unit:	Hartree
XPath:	/input/xs/@broad

47.2 Attribute: dbglev

Debugging level. Any value > 0 will produce additional debug output. The large the value, the more information is output.

Type:	integer
Default:	"0"
Use:	optional
XPath:	/input/xs/@dbglev

47.3 Attribute: dfoffdiag

"true" if also off-diagonal tensor elements for the interacting response function are to be calculated.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/@dfoffdiag

47.4 Attribute: emattype

Type of matrix element generation (band-combinations). Should only be referenced for experimental features.

Type:	integer
Default:	"1"
Use:	optional
XPath:	/input/xs/@emattype

47.5 Attribute: emaxdf

Energy cutoff for the unoccupied states in the Kohn-Sham response function and screening. This parameter ensures a cutoff at the specified energy and is defined in addition to the nempty parameter.

Type:	fortrandouble (74.1)
Default:	"1.0d10"
Use:	optional
XPath:	/input/xs/@emaxdf

47.6 Attribute: epsdfde

The smallest energy difference for which the square of its inverse will be considered in the Kohn-Sham response function.

Type:	fortrandouble (74.1)
Default:	"1.0d-8"
Use:	optional
Unit:	Hartree
XPath:	/input/xs/@epsdfde

47.7 Attribute: fastemat

If set to "true", a fast method to calculate APW-lo, lo-APW and lo-lo parts of the **q**-dependent matrix elements in the muffin-tin is used.

Type: boolean
Default: "`true`"
Use: optional
XPath: `/input/xs/@fastemat`

47.8 Attribute: fastpmat

If set to `"true"`, a fast method to calculate APW-lo, lo-APW and lo-lo parts of the momentum matrix elements in the muffin-tin is used.

Type: boolean
Default: "`true`"
Use: optional
XPath: `/input/xs/@fastpmat`

47.9 Attribute: gqmax

$|\mathbf{G}+\mathbf{q}|$ cutoff for Kohn-Sham response function, screening and for expansion of Coulomb potential

Type: fortrandouble (74.1)
Default: "`0.0d0`"
Use: optional
XPath: `/input/xs/@gqmax`

47.10 Attribute: gqmaxtype

Defines the way the gqmax cutoff is applied for the selection of the G-vectors. For "$|G+q|$" G vectors are selected such that $\mathbf{G}+\mathbf{q}$ lies within the `gqmax` cutoff. For "$|G|$" G vectors are selected such that $\mathbf{G}$ lies within the `gqmax` cutoff.

Type: **choose from:**
`|G+q|`
`|G|`
Default: "`|G+q|`"
Use: optional
XPath: `/input/xs/@gqmaxtype`

47.11 Attribute: lmaxapw

Angular momentum cut-off for the APW functions.

Type: integer
Default: "`10`"
Use: optional
XPath: `/input/xs/@lmaxapw`

47.12 Attribute: lmaxapwwf

Maximum angular momentum for APW functions for q-dependent matrix elements.

Type: integer
Default: "-1"
Use: optional
XPath: /input/xs/@lmaxapwwf

47.13 Attribute: lmaxemat

Maximum angular momentum for Rayleigh expansion of **q**-dependent plane wave factor.

Type: integer
Default: "3"
Use: optional
XPath: /input/xs/@lmaxemat

47.14 Attribute: lmaxmat

Angular momentum cut-off for the outer-most loop in the hamiltonian and overlap matrix setup.

Type: integer
Default: "5"
Use: optional
XPath: /input/xs/@lmaxmat

47.15 Attribute: nempty

Number of empty states. This parameter determines the energy cutoff for the excitation spectra. For determining the number of states related to an energy cutoff, perform one iteration of a SCF calculation, setting nempty to a higher value and check the EIGVAL.OUT.

Type: integer
Default: "5"
Use: optional
XPath: /input/xs/@nempty

47.16 Attribute: ngridk

k-point grid sizes.

Type: integertriple (74.6)
Default: "1 1 1"
Use: optional
XPath: /input/xs/@ngridk

47.17 Attribute: ngridq

q-point grid sizes.

Type:	integertriple (74.6)
Default:	"1 1 1"
Use:	optional
XPath:	/input/xs/@ngridq

47.18 Attribute: nosym

nosym is "true" if no symmetry information should be used

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/@nosym

47.19 Attribute: reducek

reducek is "true" if **k**-points are to be reduced (with crystal symmetries).

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/@reducek

47.20 Attribute: reduceq

reducek is "true" if q-points are to be reduced (with crystal symmetries).

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/xs/@reduceq

47.21 Attribute: rgkmax

Smallest muffin-tin radius times gkmax.

Type:	fortrandouble (74.1)
Default:	"7.0d0"
Use:	optional
XPath:	/input/xs/@rgkmax

47.22 Attribute: scissor

Scissors correction to correct the conduction band energies.

Type:	fortrandouble (74.1)
Default:	"0.0d0"
Use:	optional
Unit:	Hartree
XPath:	/input/xs/@scissor

47.23 Attribute: swidth

Width of the smooth approximation to the Dirac delta function (must be ¿ 0).

Type:	fortrandouble (74.1)
Default:	"0.001d0"
Use:	optional
Unit:	Hartree
XPath:	/input/xs/@swidth

47.24 Attribute: tappinfo

"true" to append info to output file.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/@tappinfo

47.25 Attribute: tevout

"true" if energy outputs are in eV.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/@tevout

47.26 Attribute: vkloff

The **k**-point set offset. All **k**-points of a regular **k**-mesh (a mesh containing the Gamma point) are shifted by a constant vector given by $(\text{vkloff}_1/N_1, \text{vkloff}_2/N_2, \text{vkloff}_3/N_3)$, where (N_1, N_2, N_3) is the division of the **k**-point mesh. It should be selected such that all symmetries among the **k**-points from the regular (non-shifted) mesh are broken. An exception is the case of optical spectra without local field effects where symmetries among **k**-points are explicitly taken into account.

Type: vect3d (74.4)
Default: "0.0d0 0.0d0 0.0d0 "
Use: optional
XPath: /input/xs/@vkloff

47.27 Attribute: xstype

Should TDDFT be used or BSE.

Type: **choose from:**
TDDFT
BSE
Use: required
XPath: /input/xs/@xstype

48 Element: tddft

Type: no content
XPath: /input/xs/tddft

This element allows for specification of the following attributes:

acont, alphalrc, alphalrcdyn, aresdf, aresfxc, betalrcdyn, do, fxcbsesplit, fxctype, intraband, kerndiag, lindhard, lmaxalda, mdfqtype, nwacont, torddf, tordfxc

48.1 Attribute: acont

Set to "true" if analytic continuation from the imaginary axis to the real axis is to be performed.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tddft/@acont

48.2 Attribute: alphalrc

α-parameter for the static long range contribution (LRC) model xc kernel.

Type: fortrandouble (74.1)
Default: "0.0d0"
Use: optional
XPath: /input/xs/tddft/@alphalrc

48.3 Attribute: alphalrcdyn

α-parameter for the dynamical long range contribution (LRC) model xc kernel.

Type:	fortrandouble (74.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/xs/tddft/@alphalrcdyn

48.4 Attribute: aresdf

Set to "true" if to consider the anti-resonant part for the dielectric function.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/xs/tddft/@aresdf

48.5 Attribute: aresfxc

Set to "true" if to consider the anti-resonant part for the MBPT derived xc-kernels.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/xs/tddft/@aresfxc

48.6 Attribute: betalrcdyn

β-parameter for the dynamical long range contribution (LRC) model xc kernel.

Type:	fortrandouble (74.1)
Use:	optional
XPath:	/input/xs/tddft/@betalrcdyn

48.7 Attribute: do

Decides if the TDDFT calculation is to be resumed starting from a new xc kernel or is to be skipped.

Type:	**choose from:**
	fromscratch
	fromkernel
Default:	"fromscratch"
Use:	optional
XPath:	/input/xs/tddft/@do

48.8 Attribute: fxcbsesplit

Split parameter for degeneracy in energy differences of MBPT derived xc kernels. See A. Marini, Phys. Rev. Lett., 91, (2003) 256402.

Type:	fortrandouble (74.1)
Default:	"1.0d-5"
Use:	optional
Unit:	Hartree
XPath:	/input/xs/tddft/@fxcbsesplit

48.9 Attribute: fxctype

Defines which xc kernel is to be used.

Type:	**choose from:**
	RPA
	LRCstatic_NLF
	LRCstatic
	LRCdyn_NLF
	LRCdyn
	ALDA
	MB1_NLF
	MB1
Default:	"RPA"
Use:	optional
XPath:	/input/xs/tddft/@fxctype

48.10 Attribute: intraband

The intraband attribute is "true" if the intraband term is to be added to the optical matrix (q=0).

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/tddft/@intraband

48.11 Attribute: kerndiag

Set to "true" if only diagonal part of xc-kernel is to be used.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/tddft/@kerndiag

48.12 Attribute: lindhard

Set to "true" if Lindhard-like function is to be calculated.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tddft/@lindhard

48.13 Attribute: lmaxalda

Angular momentum cutoff for Rayleigh expansion of exponential factor for ALDA-kernel.

Type: integer
Default: "3"
Use: optional
XPath: /input/xs/tddft/@lmaxalda

48.14 Attribute: mdfqtype

Treatment of macroscopic dielectric function for **Q**-point outside of Brillouin zone. A value of 0 uses the full **Q** and the $(\mathbf{0},\mathbf{0})$ component of the microscopic dielectric matrix is used. A value of 1 invokes a decomposition $\mathbf{Q}=\mathbf{q}+\mathbf{G_q}$ and the $(\mathbf{Q_q},\mathbf{Q_q})$ component of the microscopic dielectric matrix is used.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/tddft/@mdfqtype

48.15 Attribute: nwacont

Number of energy intervals (on imaginary axis) for analytic continuation.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/tddft/@nwacont

48.16 Attribute: torddf

Set to "true" if to consider the time-ordered version of the dielectric function.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tddft/@torddf

48.17 Attribute: tordfxc

Set to "true" if to consider the time-ordered version of xc kernel (MBPT derived kernels only).

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/tddft/@tordfxc

49 Element: screening

Type:	no content
XPath:	/input/xs/screening

This element allows for specification of the following attributes:

do, nempty, ngridk, nosym, reducek, rgkmax, screentype, vkloff

49.1 Attribute: do

Decides if the calculation of the screening is done from scratch or is to be skipped.

Type:	**choose from:**
	fromscratch
	skip
Default:	"fromscratch"
Use:	optional
XPath:	/input/xs/screening/@do

49.2 Attribute: nempty

Number of empty states.

Type:	integer
Default:	"0"
Use:	optional
XPath:	/input/xs/screening/@nempty

49.3 Attribute: ngridk

k-point grid sizes for screening.

Type:	integertriple (74.6)
Default:	"0 0 0"
Use:	optional
XPath:	/input/xs/screening/@ngridk

49.4 Attribute: nosym

nosym is "true" if no symmetry information should be used for screening.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/screening/@nosym

49.5 Attribute: reducek

reducek is "true" if **k**-points are to be reduced with crystal symmetries for screening.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/screening/@reducek

49.6 Attribute: rgkmax

The smallest muffin-tin radius times gkmax for screening.

Type:	fortrandouble (74.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/xs/screening/@rgkmax

49.7 Attribute: screentype

Defines which type of screening is to be used.

Type:	**choose from:**
	full
	diag
	noinvdiag
	longrange
Default:	"full"
Use:	optional
XPath:	/input/xs/screening/@screentype

49.8 Attribute: vkloff

k-point offset for screening.

Type:	vect3d (74.4)
Default:	"-1.0d0 -1.0d0 -1.0d0"
Use:	optional
XPath:	/input/xs/screening/@vkloff

50 Element: BSE

Type: no content
XPath: /input/xs/BSE

This element allows for specification of the following attributes:

aresbse, bsedirsing, bsetype, fbzq, lmaxdielt, nexcitmax, nleblaik, nosym, nstlbse, nstlbsemat, reducek, rgkmax, sciavbd, sciavqbd, sciavqhd, sciavqwg, sciavtype, scrherm, vkloff

50.1 Attribute: aresbse

Is set to "true" if to consider the anti-resonant part for the BSE spectrum.

Type: boolean
Default: "true"
Use: optional
XPath: /input/xs/BSE/@aresbse

50.2 Attribute: bsedirsing

"true" if effective singular part of direct term of BSE Hamiltonian is to be used.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@bsedirsing

50.3 Attribute: bsetype

Defines which parts of the BSE Hamiltonian are to be considered.

Type: **choose from:**
IP
RPA
singlet
triplet
Default: "singlet"
Use: optional
XPath: /input/xs/BSE/@bsetype

50.4 Attribute: fbzq

Set to "true" if q-point set is to be taken from the first Brillouin zone.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@fbzq

50.5 Attribute: lmaxdielt

Angular momentum cutoff of the spherical harmonics expansion of the dielectric matrix.

Type: integer
Default: "14"
Use: optional
XPath: /input/xs/BSE/@lmaxdielt

50.6 Attribute: nexcitmax

Maximum number of excitons to be considered in a BSE calculation.

Type: integer
Default: "100"
Use: optional
XPath: /input/xs/BSE/@nexcitmax

50.7 Attribute: nleblaik

Number of points used for the Lebedev-Laikov grids must be selected according to V.I. Lebedev, and D.N. Laikov, Doklady Mathematics, 59 (1999) 477.

Type: integer
Default: "5810"
Use: optional
XPath: /input/xs/BSE/@nleblaik

50.8 Attribute: nosym

Set to "true" if no symmetry information should be used for BSE.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@nosym

50.9 Attribute: nstlbse

Range of bands included for the BSE calculation. The first pair of numbers corresponds to the band index for local orbitals and valence states (counted from the lowest eigenenergy), the second pair corresponds to the band index of the conduction states (counted from the Fermi level).

Type: integerquadrupel (74.7)
Default: "0 0 0 0"
Use: optional
XPath: /input/xs/BSE/@nstlbse

50.10 Attribute: nstlbsemat

Range of bands for calculating the screening and matrix elements needed for solving the BSE. The first pair of numbers corresponds to the band index for local orbitals and valence states (counted from the lowest eigenenergy), the second pair corresponds to the band index of the conduction states (counted from the Fermi level).

Type:	integerquadrupel (74.7)
Default:	"0 0 0 0"
Use:	optional
XPath:	/input/xs/BSE/@nstlbsemat

50.11 Attribute: reducek

reducek is "true" if **k**-points are to be reduced with crystal symmetries for BSE.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/BSE/@reducek

50.12 Attribute: rgkmax

Smallest muffin-tin radius times gkmax.

Type:	fortrandouble (74.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/xs/BSE/@rgkmax

50.13 Attribute: sciavbd

"true" if the body of the screened Coulomb interaction is to be averaged (q=0).

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/BSE/@sciavbd

50.14 Attribute: sciavqbd

"true" if the body of the screened Coulomb interaction is to be averaged (q!=0).

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/BSE/@sciavqbd

50.15 Attribute: sciavqhd

"true" if the head of the screened Coulomb interaction is to be averaged (q!=0).

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/BSE/@sciavqhd

50.16 Attribute: sciavqwg

"true" if the wings of the screened Coulomb interaction are to be averaged (q!=0).

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/BSE/@sciavqwg

50.17 Attribute: sciavtype

Defines how the screened Coulomb interaction matrix is to be averaged (important for the singular terms).

Type:	**choose from:**
	spherical
	screendiag
	invscreendiag
Default:	"spherical"
Use:	optional
XPath:	/input/xs/BSE/@sciavtype

50.18 Attribute: scrherm

Method of how an almost Hermitian matrix is inverted. A value of 0: invert full matrix (matrix is allowed to be not strictly Hermitian); a value of 1: take the Hermitian average for inversion; a value of 2: assume Hermitian and use the upper triangle; a value of 3: assume Hermitian and use the lower triangle.

Type:	integer
Default:	"0"
Use:	optional
XPath:	/input/xs/BSE/@scrherm

50.19 Attribute: vkloff

k-point offset for BSE.

Type:	vect3d (74.4)
Default:	"`-1.0d0 -1.0d0 -1.0d0`"
Use:	optional
XPath:	`/input/xs/BSE/@vkloff`

51 Element: transitions

Describe transitions between Kohn-Sham states for the calculation of the Kohn-Sham response function (and screening) here. Individual transitions as well as a range (or a list) of initial and final states can be defined.

Contains:	`individual` (optional)
	`ranges` (optional)
	`lists` (optional)
XPath:	`/input/xs/transitions`

52 Element: individual

A list of individual transitions consisting of an initial state a final state and a **k**-point is given here. If the list is empty, no transitions are considered.

Contains:	`trans` (zero or more)
XPath:	`/input/xs/transitions/individual`

53 Element: trans

An individual transition consisting of an initial state a final state and a **k**-point is given here. Values of zero correspond to the inclusion of all initial and final states and all **k**-points and can be used as "wildcards" (default). Therefore, an empty element amounts to include all transitions.

Type:	no content
XPath:	`/input/xs/transitions/individual/trans`

This element allows for specification of the following attributes:

`action`, `final`, `initial`, `kpointnumber`

53.1 Attribute: action

Select to include or exclude states. If a state is included as well as excluded several times the last definition (in the sequence of individual transitions) counts.

Type:	**choose from:**
	`include`
	`exclude`
Default:	"`include`"
Use:	optional
XPath:	`/input/xs/transitions/individual/trans/@action`

53.2 Attribute: final

Final state of individual transition. A value of zero (default) means to include all states.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/xs/transitions/individual/trans/@final`

53.3 Attribute: initial

Initial state of individual transition. A value of zero (default) means to include all states.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/xs/transitions/individual/trans/@initial`

53.4 Attribute: kpointnumber

Number of **k**-points to be considered. A value of zero (default) means to include all **k**-points.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/xs/transitions/individual/trans/@kpointnumber`

54 Element: ranges

A list of ranges of transitions (initial state as well as final state ranges) and a **k**-point are given here. An empty list amounts to no transitions at all.

Contains:	`range` (zero or more)
XPath:	`/input/xs/transitions/ranges`

55 Element: range

A range of transitions (for initial as well as final states) is given here. A range consists of a "start" and a "stop" values as well as a **k**-point. Values of zero correspond to starting at the first state and stopping at the last state and considering all **k**-points. They can be used as "wildcards" (default). Therefore, an empty element corresponds to the full initial/final state range for all **k**-points.

Type: no content
XPath: /input/xs/transitions/ranges/range

This element allows for specification of the following attributes:

statestype (required), action, kpointnumber, start, stop

55.1 Attribute: action

Select to include or exclude states. If a state is included as well as excluded several times the last definition (in the sequence of individual transitions) counts.

Type: **choose from:**
include
exclude
Default: "include"
Use: optional
XPath: /input/xs/transitions/ranges/range/@action

55.2 Attribute: kpointnumber

Number of **k**-point to be considered. A value of zero (default) means to include all **k**-point.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/transitions/ranges/range/@kpointnumber

55.3 Attribute: start

Start value (first state) for range. A value of zero (default) means to start from the first state.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/transitions/ranges/range/@start

55.4 Attribute: statestype

Select for initial or final state range.

Type:	**choose from:**
	`initialstates`
	`finalstates`
Use:	required
XPath:	`/input/xs/transitions/ranges/range/@statestype`

55.5 Attribute: stop

Stop value (last state) for range. A value of zero (default) means to stop at the last state (no upper limit).

Type:	integer
Default:	"0"
Use:	optional
XPath:	`/input/xs/transitions/ranges/range/@stop`

56 Element: lists

A list of initial and final state entries to be considered for transitions. An empty list amounts to no transitions at all.

Contains:	`istate` (zero or more)
XPath:	`/input/xs/transitions/lists`

57 Element: istate

An initial or final state and corresponding **k**-point is given here. Values of zero correspond to considering all initial/final states for all **k**-points. They can be used as "wildcards" (default). Therefore, an empty element corresponds to the full initial/final state set for all **k**-points.

Type:	no content
XPath:	`/input/xs/transitions/lists/istate`

This element allows for specification of the following attributes:

`statestype` (required), `action`, `kpointnumber`, `state`

57.1 Attribute: action

Select to include or exclude states. If a state is included as well as excluded several times the last definition (in the sequence of individual transitions) counts.

Type:	**choose from:**
	`include`
	`exclude`
Default:	"`include`"
Use:	optional
XPath:	`/input/xs/transitions/lists/istate/@action`

57.2 Attribute: kpointnumber

Number of **k**-point to be consider. A value of zero (default) means to include all **k**-point.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/xs/transitions/lists/istate/@kpointnumber`

57.3 Attribute: state

The state to be considered. A value of zero (default) means to include all states.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/xs/transitions/lists/istate/@state`

57.4 Attribute: statestype

Select for initial or final state list.

Type:	**choose from:**
	`initialstates`
	`finalstates`
Use:	required
XPath:	`/input/xs/transitions/lists/istate/@statestype`

58 Element: tetra

Type:	no content
XPath:	`/input/xs/tetra`

This element allows for specification of the following attributes:

`cw1k`, `kordexc`, `qweights`, `tetradf`, `tetraocc`

58.1 Attribute: cw1k

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tetra/@cw1k

58.2 Attribute: kordexc

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tetra/@kordexc

58.3 Attribute: qweights

Choice of weights and nodes for the tetrahedron method and non-zero Q-point.

Type: integer
Default: "1"
Use: optional
XPath: /input/xs/tetra/@qweights

58.4 Attribute: tetradf

"true" if tetrahedron method is used for the **k**-space integration in the Kohn-Sham response function.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tetra/@tetradf

58.5 Attribute: tetraocc

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tetra/@tetraocc

59 Element: plan

Contains: doonly (zero or more)
XPath: /input/xs/plan

60 Element: doonly

Type: no content
XPath: /input/xs/plan/doonly

This element allows for specification of the following attributes:

task (required)

60.1 Attribute: task

Type:	**choose from:**
	xsgeneigvec
	tetcalccw
	writepmatxs
	writeemat
	df
	df2
	idf
	scrgeneigvec
	scrtetcalccw
	scrwritepmat
	screen
	scrcoulint
	exccoulint
	bse
	kernxc_bse
	writebandgapgrid
	writepmat
	dielectric
	writepmatasc
	pmatxs2orig
	writeematasc
	writepwmat
	emattest
	x0toasc
	x0tobin
	fxc_alda_check
	kernxc_bse3
	testxs
	xsestimate
	xstiming
	testmain
	portstate(1)
	portstate(2)
	portstate(-1)
	portstate(-2)
Use:	required
XPath:	/input/xs/plan/doonly/@task

61 Element: energywindow

Type:	no content
XPath:	/input/xs/energywindow

This element allows for specification of the following attributes:

intv, points

61.1 Attribute: intv

energy interval lower and upper limits.

Type:	vect2d (74.5)
Default:	"-0.5d0 0.5d0"
Use:	optional
XPath:	/input/xs/energywindow/@intv

61.2 Attribute: points

number of points to be sampled linearly inside the energy interval including the lower limit.

Type:	integer
Default:	"500"
Use:	optional
XPath:	/input/xs/energywindow/@points

Part II
Reused Elements

The following elements can occur more than once in the input file. There for they are listed separately.

62 Element: origin

Type:	no content
XPath:	/origin
Parent:	/plot2d/parallelogram
	/plot3d/box

This element allows for specification of the following attributes:

coord

62.1 Attribute: coord

Type:	vect3d (74.4)
Use:	optional
XPath:	/origin/@coord

63 Element: point

Type: no content
XPath: /point
Parent: /plot1d/path
/plot2d/parallelogram
/plot3d/box

This element allows for specification of the following attributes:

coord (required), label

63.1 Attribute: coord

Type: vect3d (74.4)
Use: required
XPath: /point/@coord

63.2 Attribute: label

Type: string
Default: ""
Use: optional
XPath: /point/@label

64 Element: plot1d

The element plot1d specifies sample points along a path. The coordinate space (lattice or cartesian)is chosen in the context of the parent.

Contains: path (1 times)
XPath: /plot1d
Parent: /input/phonons/phonondispplot
/input/properties/bandstructure
/input/properties/wfplot
/input/properties/chargedensityplot
/input/properties/exccplot
/input/properties/elfplot
/input/properties/gradmvecfield

65 Element: path

Contains: point (2 times or more)
XPath: /plot1d/path

This element allows for specification of the following attributes:

steps (required), outfileprefix

65.1 Attribute: outfileprefix

Type: string
Use: optional
XPath: /plot1d/path/@outfileprefix

65.2 Attribute: steps

Type: integer
Use: required
XPath: /plot1d/path/@steps

66 Element: plot2d

Defines a 2d plot domain.

Contains: parallelogram (1 times)
XPath: /plot2d
Parent: /input/properties/STM
/input/properties/wfplot
/input/properties/chargedensityplot
/input/properties/exccplot
/input/properties/elfplot
/input/properties/mvecfield
/input/properties/xcmvecfield
/input/properties/electricfield
/input/properties/gradmvecfield

67 Element: parallelogram

Contains: origin (1 times)
point (2 times)
XPath: /plot2d/parallelogram

This element allows for specification of the following attributes:

grid (required), outfileprefix

67.1 Attribute: grid

Type: integerpair (74.8)
Use: required
XPath: /plot2d/parallelogram/@grid

67.2 Attribute: outfileprefix

Type: string
Use: optional
XPath: /plot2d/parallelogram/@outfileprefix

68 Element: plot3d

Defines a 3d plot domain.

Contains: box (1 times)
XPath: /plot3d
Parent: /input/properties/wfplot
/input/properties/chargedensityplot
/input/properties/exccplot
/input/properties/elfplot
/input/properties/mvecfield
/input/properties/xcmvecfield
/input/properties/electricfield
/input/properties/gradmvecfield

69 Element: box

Contains: origin (1 times)
point (3 times)
XPath: /plot3d/box

This element allows for specification of the following attributes:

grid (required), outfileprefix

69.1 Attribute: grid

Type: integertriple (74.6)
Use: required
XPath: /plot3d/box/@grid

69.2 Attribute: outfileprefix

Type: string
Use: optional
XPath: /plot3d/box/@outfileprefix

70 Element: kstlist

The kstlist element is used in the LSJ and wavefunction plot element This is a user-defined list of **k**-point and state index pairs which are those used for plotting wavefunctions and writing **L**, **S** and **J** expectation values.

Contains: pointstatepair (1 times or more)
XPath: /kstlist
Parent: /input/properties/wfplot
/input/properties/LSJ
/input/properties/expiqr

71 Element: pointstatepair

The element `pointstatepair` defines a **k**-point and state index pair.

Type: integerpair (74.8)
XPath: /kstlist/pointstatepair

72 Element: qpointset

Contains: qpoint (1 times or more)
XPath: /qpointset
Parent: /input/phonons
/input/xs

73 Element: qpoint

a q-point is given in reciprocal space coordinates

Type: vect3d (74.4)
XPath: /qpointset/qpoint

74 Data Types

The Input definition uses derived data types. These are described here.

74.1 Type fortrandouble

The type `fortrandouble` allows to use the letters `"eEdDqQ"` for exponent operators. This alters in what precision the number is parsed.

74.2 Type vector

A vector is a space separated list of floating point numbers.
Example: `"1.3 2.3e4 3 90"`

74.3 Type integerlist

List of space separated integers.

74.4 Type vect3d

Three dimensional vector as three space separated floating point numbers.

74.5 Type vect2d

Three dimensional vector as three space separated floating point numbers.

74.6 Type integertriple

Space separated list of three integers.
Example: `"1 2 3"`

74.7 Type integerquadrupel

Space separated list of three integers.
Example: `"1 2 3 4"`

74.8 Type integerpair

Space separated list of two integers
Example: `"1 2"`