exciting input reference

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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 Ha = 2 Ry = 27.21138386(68) eV = $4.35926 \cdot 10^{-18}$ J

- Lengths are given in Bohr:

  1 a_{Bohr} = 0.52917720859(36) Å = $0.52917720859(36) \cdot 10^{-10}$ m

- Magnetic fields are given in units of

  1 a.u. = $\dfrac{e}{a_{\mathrm{Bohr}}^2}$ = 1717.2445320376 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, xsltpath

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

1.2   Attribute: xsltpath

Type:	anyURI
Default:	"http://xml.exciting-code.org"
Use:	optional
XPath:	/input/@xsltpath

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: symmetries (optional)
            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 (82.1)
Default: "1.0d-6"
Use: optional
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

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

with

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

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

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

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 (82.5)
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

Set to it to `"true"` if the crystal can be 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 (82.1)
Default: "10.0d0"
Use: optional
XPath: /input/structure/@vacuum

5 Element: symmetries

This element is used by the spacegroup tool to generate structures and supercells

Contains: lattice (1 times)
WyckoffPositions (optional)
XPath: /input/structure/symmetries

This element allows for specification of the following attributes:

HermannMauguinSymbol (required), HallSymbol, SchoenfliesSymbol, spaceGroupNumber

5.1 Attribute: HallSymbol

Type: string
Use: optional
XPath: /input/structure/symmetries/@HallSymbol

5.2 Attribute: HermannMauguinSymbol

Herman Mauguin symbol giving the spacegroup

Type: string
Use: required
XPath: /input/structure/symmetries/@HermannMauguinSymbol

5.3   Attribute: SchoenfliesSymbol

Type: string
Use: optional
 XPath: /input/structure/symmetries/@SchoenfliesSymbol

5.4   Attribute: spaceGroupNumber

Type: string
Use: optional
 XPath: /input/structure/symmetries/@spaceGroupNumber

6   Element: lattice

The lattice element defines lattice from a,b,c, and angles.

Type: no content
 XPath: /input/structure/symmetries/lattice

This element allows for specification of the following attributes:

> a (required), ab (required), ac (required), b (required), bc (required), c (required), ncell, scale, stretch

6.1   Attribute: a

Type: fortrandouble (82.1)
Use: required
 XPath: /input/structure/symmetries/lattice/@a

6.2   Attribute: ab

Type: fortrandouble (82.1)
Use: required
 XPath: /input/structure/symmetries/lattice/@ab

6.3   Attribute: ac

Type: fortrandouble (82.1)
Use: required
 XPath: /input/structure/symmetries/lattice/@ac

6.4   Attribute: b

Type: fortrandouble (82.1)
Use: required
 XPath: /input/structure/symmetries/lattice/@b

6.5 Attribute: bc

Type: fortrandouble (82.1)
Use: required
XPath: /input/structure/symmetries/lattice/@bc

6.6 Attribute: c

Type: fortrandouble (82.1)
Use: required
XPath: /input/structure/symmetries/lattice/@c

6.7 Attribute: ncell

Number of repeated cells in each direction.

Type: integertriple (82.6)
Default: "1 1 1"
Use: optional
XPath: /input/structure/symmetries/lattice/@ncell

6.8 Attribute: scale

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

Type: fortrandouble (82.1)
Default: "1"
Use: optional
XPath: /input/structure/symmetries/lattice/@scale

6.9 Attribute: stretch

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

Type: vect3d (82.4)
Default: "1.0d0 1.0d0 1.0d0 "
Use: optional
XPath: /input/structure/symmetries/lattice/@stretch

7 Element: WyckoffPositions

Contains: wspecies (zero or more)
XPath: /input/structure/symmetries/WyckoffPositions

8 Element: wspecies

Contains: wpos (zero or more)
XPath: /input/structure/symmetries/WyckoffPositions/wspecies

This element allows for specification of the following attributes:

speciesfile

8.1 Attribute: speciesfile

Type: string
Use: optional
XPath: /input/structure/symmetries/WyckoffPositions/wspecies/@speciesfile

9 Element: wpos

Type: no content
XPath: /input/structure/symmetries/WyckoffPositions/wspecies/wpos

This element allows for specification of the following attributes:

coord

9.1 Attribute: coord

Type: vect3d (82.4)
Use: optional
XPath: /input/structure/symmetries/WyckoffPositions/wspecies/wpos/@coord

10 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

10.1 Attribute: scale

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

Type: fortrandouble (82.1)
Default: "1.0d0"
Use: optional
XPath: /input/structure/crystal/@scale

10.2 Attribute: stretch

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

Type: vect3d (82.4)
Default: ”`1.0d0 1.0d0 1.0d0` ”
Use: optional
XPath: /input/structure/crystal/@stretch

11 Element: basevect

Defines one basis vector in Cartesian coordinates.

Type: vect3d (82.4)
XPath: /input/structure/crystal/basevect

12 Element: species

Defines the atomic species, i.e. the chemical element. The atomic 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), atomicNumber, chemicalSymbol, href, rmt

12.1 Attribute: atomicNumber

Optional attribute that may be used in visualization and by converters. It is not used in **exciting**

Type: integer
Use: optional
XPath: /input/structure/species/@atomicNumber

12.2 Attribute: chemicalSymbol

Optional attribute that may be used in visualization and by converters. It is ignored by **exciting**

Type: string
Default: ””
Use: optional
XPath: /input/structure/species/@chemicalSymbol

12.3   Attribute: href

Defines the address/URI of a species file provided in web. If this attribute is specified, all other attributes

Type:	anyURI
Default:	""
Use:	optional
XPath:	/input/structure/species/@href

12.4   Attribute: rmt

Defines the muffin-tin radius; this optional parameter allows to override species file or 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 (=region not belonging to any muffin-tin) is described by planewaves.

Type:	fortrandouble (82.1)
Default:	"-1.0d0"
Use:	optional
XPath:	/input/structure/species/@rmt

12.5   Attribute: speciesfile

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

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

13   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

13.1 Attribute: bfcmt

Muffin-tin external magnetic field in Cartesian coordinates.

Type:	vect3d (82.4)
Default:	"0.0d0 0.0d0 0.0d0"
Use:	optional
XPath:	/input/structure/species/atom/@bfcmt

13.2 Attribute: coord

Position in lattice coordinates.

Type:	vect3d (82.4)
Use:	required
XPath:	/input/structure/species/atom/@coord

13.3 Attribute: mommtfix

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

Type:	vect3d (82.4)
Default:	"0.0d0 0.0d0 0.0d0"
Use:	optional
XPath:	/input/structure/species/atom/@mommtfix

14 Element: LDAplusU

The LADplusU element is used to specify the I,J and U parameters of a 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

14.1 Attribute: J

Type:	fortrandouble (82.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/structure/species/LDAplusU/@J

14.2 Attribute: U

Type:	fortrandouble (82.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/structure/species/LDAplusU/@U

14.3 Attribute: l

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

15 Element: groundstate

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

Contains:	spin (optional)
	HartreeFock (optional)
	solver (optional)
	OEP (optional)
	RDMFT (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

15.1 Attribute: autokpt

Decides if the -point set is to be determined automatically from the total number of required -points given by nktot.

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

15.2 Attribute: beta0

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

Type:	fortrandouble (82.1)
Default:	"0.4d0"
Use:	optional
XPath:	/input/groundstate/@beta0

15.3 Attribute: betadec

Mixing parameter decrease. Used in linear mixing.

Type:	fortrandouble (82.1)
Default:	"0.6d0"
Use:	optional
XPath:	/input/groundstate/@betadec

15.4 Attribute: betainc

Mixing parameter increase. Used in linear mixing.

Type:	fortrandouble (82.1)
Default:	"1.1d0"
Use:	optional
XPath:	/input/groundstate/@betainc

15.5 Attribute: cfdamp

Damping coefficient for characteristic function.

Type:	fortrandouble (82.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/groundstate/@cfdamp

15.6 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 (82.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/groundstate/@chgexs

15.7 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 $(E_t + E_b)/2$. If either E_t or E_b cannot be found then the band energy is set to the default value.

Type:	fortrandouble (82.1)
Default:	"0.0025d0"
Use:	optional
XPath:	/input/groundstate/@deband

15.8 Attribute: dlinengyfermi

Energy difference between linearisation and Fermi energy.

Type:	fortrandouble (82.1)
Default:	"-0.1d0"
Use:	optional
XPath:	/input/groundstate/@dlinengyfermi

15.9 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

15.10 Attribute: epsband

Energy tolerance for search of linearisation energies.

Type:	fortrandouble (82.1)
Default:	"1.0d-6"
Use:	optional
XPath:	/input/groundstate/@epsband

15.11 Attribute: epschg

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

Type: fortrandouble (82.1)
Default: "1.0d-3"
Use: optional
XPath: /input/groundstate/@epschg

15.12 Attribute: epsengy

Energy convergence tolerance.

Type: fortrandouble (82.1)
Default: "1.0d-4"
Use: optional
XPath: /input/groundstate/@epsengy

15.13 Attribute: epsforce

Convergence tolerance for the forces during the SCF run.

Type: fortrandouble (82.1)
Default: "5.0d-5"
Use: optional
XPath: /input/groundstate/@epsforce

15.14 Attribute: epsocc

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

Type: fortrandouble (82.1)
Default: "1.0d-8"
Use: optional
XPath: /input/groundstate/@epsocc

15.15 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 (82.1)
Default: "1.0d-6"
Use: optional
XPath: /input/groundstate/@epspot

15.16 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

15.17 Attribute: findlinentype

Select method to determine the linearisation energies.

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

15.18 Attribute: fracinr

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

Type:	fortrandouble (82.1)
Default:	"0.25d0"
Use:	optional
XPath:	/input/groundstate/@fracinr

15.19 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

15.20 Attribute: gmaxvr

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

Type:	fortrandouble (82.1)
Default:	"12.0d0"
Use:	optional
XPath:	/input/groundstate/@gmaxvr

15.21 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

15.22 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

15.23 Attribute: lmaxapw

Angular momentum cut-off for the APW functions.

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

15.24 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

15.25 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

15.26   Attribute: lmaxvr

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

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

15.27   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

15.28   Attribute: maxscl

Upper limit for te self-consistency loop.

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

15.29   Attribute: mixer

select the mixing (relaxation) scheme for SCF

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

15.30 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 -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

15.31 Attribute: ngridk

Number of k grid points along the basis vector directions.

Type:	integertriple (82.6)
Use:	required
XPath:	/input/groundstate/@ngridk

15.32 Attribute: nktot

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

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

15.33 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

15.34 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

15.35 Attribute: nprad

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

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

15.36 Attribute: npsden

oOrder of polynomial for pseudo-charge density.

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

15.37 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

15.38 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

15.39 Attribute: radkpt

Used for the automatic determination of the -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 (82.1)
Default:	”40.0d0”
Use:	optional
XPath:	/input/groundstate/@radkpt

15.40 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

15.41 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 $\mathbf{G}+\mathbf{k}$ vectors. Because each $\mathbf{G}+\mathbf{k}$ 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 (82.1)
Default:	”7.0d0”
Use:	optional
XPath:	/input/groundstate/@rgkmax

15.42 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

15.43   Attribute: swidth

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

Type:	fortrandouble (82.1)
Default:	"0.001d0"
Use:	optional
XPath:	/input/groundstate/@swidth

15.44   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

15.45   Attribute: tevecsv

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

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

15.46   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

15.47 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

15.48 Attribute: vkloff

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

Type:	vect3d (82.4)
Default:	"0.0d0 0.0d0 0.0d0"
Use:	optional
XPath:	/input/groundstate/@vkloff

15.49 Attribute: xctype

Type of exchange-correlation functional to be used

- No exchange-correlation funtional ($E_{\mathrm{xc}} \equiv 0$)

- 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

16 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`

16.1 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

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

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 (82.4)
Default:	”0.0d0 0.0d0 0.0d0 ”
Use:	optional
XPath:	/input/groundstate/spin/@bfieldc

16.2 Attribute: fixspin

Type:	choose from:
	`none`
	`total FSM`
	`localmt FSM`
	`both`
Default:	"none"
Use:	optional
XPath:	/input/groundstate/spin/@fixspin

16.3 Attribute: momfix

The desired total moment for a FSM calculation.

Type:	vect3d (82.4)
Default:	"0.0d0 0.0d0 0.0d0"
Use:	optional
XPath:	/input/groundstate/spin/@momfix

16.4 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 (82.1)
Default:	"1.0d0"
Use:	optional
XPath:	/input/groundstate/spin/@reducebf

16.5 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

16.6 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

16.7 Attribute: taufsm

Type: fortrandouble (82.1)
Default: "0.01d0"
Use: optional
XPath: /input/groundstate/spin/@taufsm

16.8 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

$$\Psi_{\mathbf{k}}^{\mathbf{q}}(\mathbf{r}) = \begin{pmatrix} U_{\mathbf{k}}^{\mathbf{q}\uparrow}(\mathbf{r})e^{i(\mathbf{k}+\mathbf{q/2})\cdot\mathbf{r}} \\ U_{\mathbf{k}}^{\mathbf{q}\downarrow}(\mathbf{r})e^{i(\mathbf{k}-\mathbf{q/2})\cdot\mathbf{r}} \end{pmatrix} . \Psi_{\mathbf{k}}^{\mathbf{q}}(\mathbf{r}) = \begin{pmatrix} U_{\mathbf{k}}^{\mathbf{q}\uparrow}(\mathbf{r})e^{i(\mathbf{k}+\mathbf{q/2})\cdot\mathbf{r}} \\ U_{\mathbf{k}}^{\mathbf{q}\downarrow}(\mathbf{r})e^{i(\mathbf{k}-\mathbf{q/2})\cdot\mathbf{r}} \end{pmatrix} . \tag{5}$$

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

$$\mathbf{m}^{\mathbf{q}}(\mathbf{r}) = (m_x(\mathbf{r})\cos(\mathbf{q}\cdot\mathbf{r}), m_y(\mathbf{r})\sin(\mathbf{q}\cdot\mathbf{r}), m_z(\mathbf{r})), \mathbf{m}^{\mathbf{q}}(\mathbf{r}) = (m_x(\mathbf{r})\cos(\mathbf{q}\cdot\mathbf{r}), m_y(\mathbf{r})\sin(\mathbf{q}\cdot\mathbf{r}), m_z(\mathbf{r})), \tag{6}$$

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

Type: vect3d (82.4)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/groundstate/spin/@vqlss

17 Element: HartreeFock

If preset Hartree-Fock calculation is triggered.

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

This element allows for specification of the following attributes:

epsengy

17.1 Attribute: epsengy

Energy convergence tolerance.

Type: fortrandouble (82.1)
Default: "1.0d-4"
Use: optional
XPath: /input/groundstate/HartreeFock/@epsengy

18   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

18.1   Attribute: epsarpack

Tolerance parameter for the ARPACK shift invert solver

Type: fortrandouble (82.1)
Default: ”1.0d-8”
Use: optional
XPath: /input/groundstate/solver/@epsarpack

18.2   Attribute: evaltol

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

Type: fortrandouble (82.1)
Default: ”1.0d-8”
Use: optional
XPath: /input/groundstate/solver/@evaltol

18.3   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

18.4   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

19   Element: OEP

If present exact exchange calculation is triggered. (experimental)

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

This element allows for specification of the following attributes:

> maxitoep, tauoep

19.1   Attribute: maxitoep

Maximum number of iterations when solving the exact exchange integral equations.

Type: integer
Default: "120"
Use: optional
XPath: /input/groundstate/OEP/@maxitoep

19.2   Attribute: tauoep

The optimised effective potential is determined using an iterative method. [Phys. Rev. Lett. 98, 196405 (2007)]. At the first iteration the step length is set to tauoep(1). Dur- ing subsequent iterations, the step length is scaled by tauoep(2) or tauoep(3), when the residual is increasing or decreasing, respectively. See also maxitoep.

Type: vect3d (82.4)
Default: "1.0d0 0.2d0 1.5d0"
Use: optional
XPath: /input/groundstate/OEP/@tauoep

20   Element: RDMFT

If present Reduced Density Matrix Funcional Theory calculation is triggered

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

This element allows for specification of the following attributes:

> maxitc, maxitn, rdmalpha, rdmmaxscl, rdmtemp, rdmxctype, taurdmc, taurdmn

20.1 Attribute: maxitc

maximum number of iteration for natural orbital optimization.

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

20.2 Attribute: maxitn

maximum number of iteration for occupation number optimization.

Type: integer
Default: "250"
Use: optional
XPath: /input/groundstate/RDMFT/@maxitn

20.3 Attribute: rdmalpha

exponent for the functional.

Type: fortrandouble (82.1)
Default: "0.7d0"
Use: optional
XPath: /input/groundstate/RDMFT/@rdmalpha

20.4 Attribute: rdmmaxscl

maximum number of self-consistent loops.

Type: integer
Default: "1"
Use: optional
XPath: /input/groundstate/RDMFT/@rdmmaxscl

20.5 Attribute: rdmtemp

temperature.

Type: fortrandouble (82.1)
Default: "0.0d0"
Use: optional
XPath: /input/groundstate/RDMFT/@rdmtemp

20.6 Attribute: rdmxctype

XC functional.

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

20.7 Attribute: taurdmc

Step size for natural orbital coefficients.

Type:	fortrandouble (82.1)
Default:	"0.5d0"
Use:	optional
XPath:	/input/groundstate/RDMFT/@taurdmc

20.8 Attribute: taurdmn

step size for occupation numbers.

Type:	fortrandouble (82.1)
Default:	"1.0d0"
Use:	optional
XPath:	/input/groundstate/RDMFT/@taurdmn

21 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

21.1 Attribute: state

Selects the file format of the STATE file.

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

22 Element: libxc

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

This element allows for specification of the following attributes:

correlation, exchange, xc

22.1 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

22.2 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

22.3 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

23 Element: structureoptimization

The structure optimization element triggers if present a geometry relaxation.

Type: no content
XPath: /input/structureoptimization

This element allows for specification of the following attributes:

epsforce, resume, tau0atm

23.1 Attribute: epsforce

Convergence tolerance for the forces during a structural optimization run.

Type: fortrandouble (82.1)
Default: "5.0d-5"
Use: optional
XPath: /input/structureoptimization/@epsforce

23.2 Attribute: resume

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

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

23.3 Attribute: tau0atm

The step size to be used for structural optimization

The position of atom α is updated on step m of a structural optimization run using

$$\mathbf{r}_\alpha^{m+1} = \mathbf{r}_\alpha^m + \tau_\alpha^m \left(\mathbf{F}_\alpha^m + \mathbf{F}_\alpha^{m-1} \right), \mathbf{r}_\alpha^{m+1} = \mathbf{r}_\alpha^m + \tau_\alpha^m \left(\mathbf{F}_\alpha^m + \mathbf{F}_\alpha^{m-1} \right), \quad (7)$$

where τ_α is set to `tau0atm` for $m = 0$, and incremented by the same amount if the atom is moving in the same direction between steps. If the direction changes then τ_α is reset to `tau0atm`.

Type: fortrandouble (82.1)
Default: "0.2d0"
Use: optional
XPath: /input/structureoptimization/@tau0atm

24 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

25 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

25.1 Attribute: character

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

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

25.2   Attribute: scissor

Value to shift bandgap.

Type: fortrandouble (82.1)
Default: ”0.0d0”
Use: optional
XPath: /input/properties/bandstructure/@scissor

26   Element: STM

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

27   Element: wfplot

Wavefunction plot.

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

28   Element: dos

If present a DOS calculation is started.
  DOS and optics plots require integrals of the kind

$$g(\omega_i) = \frac{\Omega}{(2\pi)^3} \int_{\mathrm{BZ}} f(\mathbf{k})\delta(\omega_i - e(\mathbf{k}))d\mathbf{k}.g(\omega_i) = \frac{\Omega}{(2\pi)^3} \int_{\mathrm{BZ}} f(\mathbf{k})\delta(\omega_i - e(\mathbf{k}))d\mathbf{k}. \tag{8}$$

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

28.1 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

28.2 Attribute: ngrdos

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

28.3 Attribute: nsmdos

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

28.4 Attribute: nwdos

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

28.5 Attribute: scissor

Type:	fortrandouble (82.1)
Default:	”`0.0d0`”
Use:	optional
XPath:	/input/properties/dos/@scissor

28.6 Attribute: sqados

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

Type: vect3d (82.4)
Default: "0.0d0 0.0d0 1.0d0"
Use: optional
XPath: /input/properties/dos/@sqados

28.7   Attribute: winddos

Frequency/energy window for the DOS or optics plot.

Type: vect2d (82.5)
Default: "-0.5d0 0.5d0"
Use: optional
XPath: /input/properties/dos/@winddos

29   Element: LSJ

Output L, S and J expectation values.

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

30   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

30.1   Attribute: deltaem

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

Type: fortrandouble (82.1)
Default: "0.025d0"
Use: optional
XPath: /input/properties/masstensor/@deltaem

30.2 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

30.3 Attribute: vklem

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

Type: vect3d (82.4)
Default: ”0.0d0 0.0d0 0.0d0”
Use: optional
XPath: /input/properties/masstensor/@vklem

31 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

31.1 Attribute: plotgradient

Calculate and plot the module of the density gradient

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

32 Element: exccplot

Exchange-correlation and Coulomb potential plots.

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

33 Element: elfplot

Electron localization function (ELF).

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

34 Element: mvecfield

Plot of magnetization vector field.

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

35 Element: xcmvecfield

Plot of exchange-correlation magnetic vector field.

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

36 Element: electricfield

Writes the electric field to file.

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

37 Element: gradmvecfield

Plot of he gradient of the magnetic vector field.

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

38 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

38.1 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

38.2 Attribute: separate

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

39 Element: EFG

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

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

40 Element: mossbauer

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

41 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

41.1 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

42 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

42.1 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

42.2 Attribute: scissor

Type:	fortrandouble (82.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/properties/dielectric/@scissor

42.3 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

43 Element: optcomp

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

Type:	integertriple (82.6)
Default:	"1 1 1"
XPath:	/input/properties/dielectric/optcomp

44 Element: moke

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

45 Element: expiqr

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

46 Element: elnes

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

This element allows for specification of the following attributes:

vecql

46.1 Attribute: vecql

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

Type:	vect3d (82.4)
Default:	"0.0d0 0.0d0 0.0d0"
Use:	optional
XPath:	/input/properties/elnes/@vecql

47 Element: eliashberg

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

This element allows for specification of the following attributes:

mustar

47.1 Attribute: mustar

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

Type:	fortrandouble (82.1)
Default:	”0.15d0”
Use:	optional
XPath:	/input/properties/eliashberg/@mustar

48 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

48.1 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 (82.1)
Default:	”0.03d0”
Use:	optional
XPath:	/input/phonons/@deltaph

48.2 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

48.3 Attribute: ngridq

Number of q grid points along the basis vector directions.

Type:	integertriple (82.6)
Use:	required
XPath:	/input/phonons/@ngridq

48.4 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

48.5 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

49 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

49.1 Attribute: ngrdos

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

49.2 Attribute: nsmdos

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

49.3 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

49.4 Attribute: nwdos

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

50 Element: phonondispplot

Phonon dispersion plot.

Contains:	plot1d
XPath:	/input/phonons/phonondispplot

51 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

52 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

52.1 Attribute: ngridq

q-point grid for interpolation.

Type:	integertriple (82.6)
Use:	required
XPath:	/input/phonons/interpolate/@ngridq

52.2 Attribute: vqloff

The q-point offset vector in lattice coordinates.

Type:	vect3d (82.4)
Default:	"0.0d0 0.0d0 0.0d0"
Use:	optional
XPath:	/input/phonons/interpolate/@vqloff

52.3 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

53 Element: parts

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

54 Element: dopart

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

This element allows for specification of the following attributes:

id (required)

54.1 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

55 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

55.1 Attribute: broad

Lorentzian broadening for all spectra

Type:	fortrandouble (82.1)
Default:	"0.01d0"
Use:	optional
XPath:	/input/xs/@broad

55.2 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

55.3 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

55.4 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

55.5 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 (82.1)
Default:	”`1.0d10`”
Use:	optional
XPath:	/input/xs/@emaxdf

55.6 Attribute: epsdfde

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

Type:	fortrandouble (82.1)
Default:	”`1.0d-8`”
Use:	optional
XPath:	/input/xs/@epsdfde

55.7 Attribute: fastemat

If set to `"true"`, a fast method to calculate APW-lo, lo-APW and lo-lo parts of the $\mathbf{q}$-dependent matrix elements in the muffin-tin is used.

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

55.8 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

55.9 Attribute: gqmax

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

Type: fortrandouble (82.1)
Default: ”`0.0d0`”
Use: optional
XPath: /input/xs/@gqmax

55.10 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

55.11 Attribute: lmaxapw

Angular momentum cut-off for the APW functions.

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

55.12 Attribute: lmaxapwwf

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

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

55.13 Attribute: lmaxemat

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

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

55.14 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

55.15 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

55.16 Attribute: ngridk

k-point grid sizes.

Type: integertriple (82.6)
Default: "1 1 1"
Use: optional
XPath: /input/xs/@ngridk

55.17 Attribute: ngridq

q-point grid sizes.

Type:	integertriple (82.6)
Default:	”1 1 1”
Use:	optional
XPath:	/input/xs/@ngridq

55.18 Attribute: nosym

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

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

55.19 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

55.20 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

55.21 Attribute: rgkmax

Smallest muffin-tin radius times gkmax.

Type:	fortrandouble (82.1)
Default:	”7.0d0”
Use:	optional
XPath:	/input/xs/@rgkmax

55.22 Attribute: scissor

Scissors correction to correct the conduction band energies.

Type: fortrandouble (82.1)
Default: "0.0d0"
Use: optional
XPath: /input/xs/@scissor

55.23 Attribute: swidth

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

Type: fortrandouble (82.1)
Default: "0.001d0"
Use: optional
XPath: /input/xs/@swidth

55.24 Attribute: tappinfo

"true" to append info to output file.

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

55.25 Attribute: tevout

"true" if energy outputs are in eV.

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

55.26 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 (82.4)
Default: "0.0d0 0.0d0 0.0d0 "
Use: optional
XPath: /input/xs/@vkloff

55.27 Attribute: xstype

Should TDDFT be used or BSE.

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

56 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

56.1 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

56.2 Attribute: alphalrc

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

Type:	fortrandouble (82.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/xs/tddft/@alphalrc

56.3 Attribute: alphalrcdyn

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

Type:	fortrandouble (82.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/xs/tddft/@alphalrcdyn

56.4 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

56.5 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

56.6 Attribute: betalrcdyn

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

Type:	fortrandouble (82.1)
Use:	optional
XPath:	/input/xs/tddft/@betalrcdyn

56.7 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

56.8 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 (82.1)
Default:	"1.0d-5"
Use:	optional
XPath:	/input/xs/tddft/@fxcbsesplit

56.9 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

56.10 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

56.11 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

56.12 Attribute: lindhard

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

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

56.13 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

56.14 Attribute: mdfqtype

Treatment of macroscopic dielectric function for $\mathbf{Q}$-point outside of Brillouin zone. A value of 0 uses the full $\mathbf{Q}$ 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

56.15 Attribute: nwacont

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

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

56.16 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

56.17 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

57 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

57.1 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

57.2 Attribute: nempty

Number of empty states.

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

57.3 Attribute: ngridk

k-point grid sizes for screening.

Type: integertriple (82.6)
Default: "0 0 0"
Use: optional
XPath: /input/xs/screening/@ngridk

57.4 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

57.5 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

57.6 Attribute: rgkmax

The smallest muffin-tin radius times gkmax for screening.

Type:	fortrandouble (82.1)
Default:	”0.0d0”
Use:	optional
XPath:	/input/xs/screening/@rgkmax

57.7 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

57.8 Attribute: vkloff

k-point offset for screening.

Type:	vect3d (82.4)
Default:	”-1.0d0 -1.0d0 -1.0d0”
Use:	optional
XPath:	/input/xs/screening/@vkloff

58 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

58.1   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

58.2   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

58.3   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

58.4   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

58.5 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

58.6 Attribute: nexcitmax

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

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

58.7 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

58.8 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

58.9 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 (82.7)
Default: ”0 0 0 0”
Use: optional
XPath: /input/xs/BSE/@nstlbse

58.10 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 (82.7)
Default:	"0 0 0 0"
Use:	optional
XPath:	/input/xs/BSE/@nstlbsemat

58.11 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

58.12 Attribute: rgkmax

Smallest muffin-tin radius times gkmax.

Type:	fortrandouble (82.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/xs/BSE/@rgkmax

58.13 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

58.14 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

58.15 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

58.16 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

58.17 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

58.18 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

58.19 Attribute: vkloff

k-point offset for BSE.

Type:	vect3d (82.4)
Default:	”-1.0d0 -1.0d0 -1.0d0”
Use:	optional
XPath:	/input/xs/BSE/@vkloff

59   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

60   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

61   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

61.1 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

61.2 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

61.3 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

61.4 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

62 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

63 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

63.1 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

63.2 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

63.3 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

63.4 Attribute: statestype

Select for initial or final state range.

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

63.5 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

64 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

65 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

65.1 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

65.2   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

65.3   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

65.4   Attribute: statestype

Select for initial or final state list.

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

66   Element: tetra

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

This element allows for specification of the following attributes:

cw1k, kordexc, qweights, tetradf, tetraocc

66.1 Attribute: cw1k

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

66.2 Attribute: kordexc

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

66.3 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

66.4 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

66.5 Attribute: tetraocc

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

67 Element: plan

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

68   Element: doonly

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

This element allows for specification of the following attributes:

      task (required)

68.1 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

69 Element: energywindow

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

This element allows for specification of the following attributes:

`intv`, `points`

69.1   Attribute: intv

energy interval lower and upper limits.

Type:	vect2d (82.5)
Default:	”-0.5d0 0.5d0”
Use:	optional
XPath:	/input/xs/energywindow/@intv

69.2   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.

70   Element: origin

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

This element allows for specification of the following attributes:

`coord`

70.1   Attribute: coord

Type:	vect3d (82.4)
Use:	optional
XPath:	./origin/@coord

71   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

71.1   Attribute: coord

Type: vect3d (82.4)
Use: required
XPath: ./point/@coord

71.2   Attribute: label

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

72   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

73   Element: path

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

This element allows for specification of the following attributes:

> steps (required), outfileprefix

73.1 Attribute: outfileprefix

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

73.2 Attribute: steps

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

74 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

75 Element: parallelogram

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

This element allows for specification of the following attributes:

grid (required), outfileprefix

75.1 Attribute: grid

Type: integerpair (82.8)
Use: required
XPath: ./plot2d/parallelogram/@grid

75.2   Attribute: outfileprefix

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

76   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

77   Element: box

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

This element allows for specification of the following attributes:

        grid (required), outfileprefix

77.1   Attribute: grid

Type: integertriple (82.6)
Use: required
XPath: ./plot3d/box/@grid

77.2   Attribute: outfileprefix

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

78 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

79 Element: pointstatepair

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

Type:	integerpair (82.8)
XPath:	./kstlist/pointstatepair

80 Element: qpointset

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

81 Element: qpoint

a q-point is given in reciprocal space coordinates

Type:	vect3d (82.4)
XPath:	./qpointset/qpoint

82 Data Types

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

82.1 Type fortrandouble

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

82.2 Type vector

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

82.3 Type integerlist

List of space separated integers.

82.4 Type vect3d

Three dimensional vector as three space separated floating point numbers.

82.5 Type vect2d

Three dimensional vector as three space separated floating point numbers.

82.6 Type integertriple

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

82.7 Type integerquadrupel

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

82.8 Type integerpair

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