Species file format reference

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About this Document

This document describes the file format for the species definitions.

Part I
Input Elements

1 Element: spdb

Species-database element contains the species element sp

Contains: sp
XPath: /spdb

2 Element: sp

A species is an atom type definition containing all information to construct the basis functions.

Contains: muffinTin (1 times)
atomicState (1 times or more)
basis (1 times)
lorb (zero or more)
XPath: /spdb/sp

This element allows for specification of the following attributes:

chemicalSymbol (required), mass (required), z (required), name

2.1 Attribute: chemicalSymbol

Chemical Symbol.

Type: ID
Use: required
XPath: /spdb/sp/@chemicalSymbol

2.2 Attribute: mass

Mass in m_e.

Type: fortrandouble (9.1)
Use: required
XPath: /spdb/sp/@mass

2.3 Attribute: name

Optional element name.

Type: string
Use: optional
XPath: /spdb/sp/@name

2.4 Attribute: z

Atomic number.

Type: fortrandouble (9.1)
Use: required
XPath: /spdb/sp/@z

3 Element: muffinTin

This element gives the size of the muffin tin radius and the resolution of the radial functions.

Type: no content
XPath: /spdb/sp/muffinTin

This element allows for specification of the following attributes:

radialmeshPoints (required), radius (required), rinf (required), rmin (required)

3.1 Attribute: radialmeshPoints

Number of data points for radial atomic functions.

Type: integer
Use: required
XPath: /spdb/sp/muffinTin/@radialmeshPoints

3.2 Attribute: radius

The radius of the muffin tin sphere.

Type: fortrandouble (9.1)
Use: required
XPath: /spdb/sp/muffinTin/@radius

3.3 Attribute: rinf

Radius from which the influence on the potential is regarded to be negligible.

Type: fortrandouble (9.1)
Use: required
XPath: /spdb/sp/muffinTin/@rinf

3.4 Attribute: rmin

The radius where radial mesh begins.

Type: fortrandouble (9.1)
Use: required
XPath: /spdb/sp/muffinTin/@rmin

4 Element: atomicState

The atomicState element lists the atomic states that schould be used to approximate the wavefunction in the sphere. They can be marked as core or none core electrons by the core attribute. Core electrons are threated separately by numeric itegration.

Type: no content
XPath: /spdb/sp/atomicState

This element allows for specification of the following attributes:

core (required), kappa (required), l (required), n (required), occ (required)

4.1 Attribute: core

If true, state is threated as core state in the calculation.

Type: boolean
Use: required
XPath: /spdb/sp/atomicState/@core

4.2 Attribute: kappa

Relativistic quantum number.

Type: integer
Use: required
XPath: /spdb/sp/atomicState/@kappa

4.3 Attribute: l

Azimuthal quantum number.

Type: integer
Use: required
XPath: /spdb/sp/atomicState/@l

4.4 Attribute: n

Principal quantum number.

Type: integer
Use: required
XPath: /spdb/sp/atomicState/@n

4.5 Attribute: occ

Ocuppation number.

Type: fortrandouble (9.1)
Use: required
XPath: /spdb/sp/atomicState/@occ

5 Element: basis

Defines APW basis.

Contains: wf (1 times or more)
exception (zero or more)
XPath: /spdb/sp/basis

This element allows for specification of the following attributes:

order (required)

5.1 Attribute: order

Type: integer
Use: required
XPath: /spdb/sp/basis/@order

6 Element: exception

This element allows for defining exceptions to the APW basis functions.

Contains: wf (1 times or more)
XPath: /spdb/sp/basis/exception

This element allows for specification of the following attributes:

l

6.1 Attribute: l

Spezifies the azimuthal quantum number for which the exception applies.

Type: integer
Use: optional
XPath: /spdb/sp/basis/exception/@l

7 Element: lorb

Local orbital (APW+lo or LAPW+lo).

Contains: wf (1 times or more)
XPath: /spdb/sp/lorb

This element allows for specification of the following attributes:

l (required)

7.1 Attribute: l

Azimuthal quantum number for which the local orbital is defined.

Type: integer
Use: required
XPath: /spdb/sp/lorb/@l

Part II
Reused Elements

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

8 Element: wf

Defines the radial part of an atomic wavefunction. This functions used to construct a lapw orbital. The actual basis functions for the calculation inside the MT are linear combinations of these and Y_{lm}.

Type: no content
XPath: ./wf
Parent: /spdb/sp/basis
/spdb/sp/basis/exception
/spdb/sp/lorb

This element allows for specification of the following attributes:

matchingOrder (required), searchE (required), trialEnergy (required)

8.1 Attribute: matchingOrder

Gives the order of the derivative that must be matched to the plain wave.

Type: integer
Use: required
XPath: `./wf/@matchingOrder`

8.2 Attribute: searchE

If `true` the energy of the radial wave function, E_0 is optimized to match the boundary condition

$$\psi(R_{MT}) = 0. \tag{1}$$

Type: boolean
Use: required
XPath: `./wf/@searchE`

8.3 Attribute: trialEnergy

Energy level of the radial wave function (initial condition for numerical radial Schrodinger equation)

Type: fortrandouble (9.1)
Use: required
XPath: `./wf/@trialEnergy`

9 Data Types

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

9.1 Type fortrandouble

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