

Species file format 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 13, 2012

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 should 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 treated separately by numeric integration.

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 treated 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**

Occupation 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**

Specifies 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

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

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.