



Species file format reference

version lithium

July 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. Therefore 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.