



# Species file format reference

version lithium

August 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.