

Species file format reference

exciting developers team

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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 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**

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

4.2 Attribute: **kappa**

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

4.3 Attribute: **l**

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

4.4 Attribute: **n**

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

4.5 Attribute: **occ**

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**

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**

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**

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 basisfunctions for the calculation inside the MT are linear combinations of these and Ylm.

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**

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

8.2 Attribute: **searchE**

if true E0 is optimized to match boundary condtions

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