Species file format reference

exciting carbon

December 2015

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)
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 (10.1)
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 (10.1)
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 (10.1)
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 (10.1)
Use: required
XPath: /spdb/sp/muffinTin/@rinf

3.4 Attribute: rmin

The radius where radial mesh begins.

Type: fortrandouble (10.1)
Use: required
XPath: /spdb/sp/muffinTin/@rmin

4 Element: basis

Definion of the APW basis.

Contains: default (1 times)
custom (zero or more)
lo (zero or more)
XPath: /spdb/sp/basis

5 Element: default

Global definition of APW functions (valid for all L $\leq$ lmaxapw).

Contains: wf (zero or more)
XPath: /spdb/sp/basis/default

This element allows for specification of the following attributes:

searchE, trialEnergy, type

5.1 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
Default: "true"
Use: optional
XPath: /spdb/sp/basis/default/@searchE

5.2 Attribute: trialEnergy

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

Type: fortrandouble (10.1)
Default: "0.15d0"
Use: optional
XPath: /spdb/sp/basis/default/@trialEnergy

5.3 Attribute: type

Augmentation type (LAPW or APW+lo). Default lapw.

Type: string
Default: "lapw"
Use: optional
XPath: /spdb/sp/basis/default/@type

6 Element: custom

Custom definition of APW for a given L.

Contains: wf (zero or more)
XPath: /spdb/sp/basis/custom

This element allows for specification of the following attributes:

l (required), searchE, trialEnergy, type

6.1 Attribute: l

Specifies the azimuthal quantum number for which the custom definition of APW function applies.

Type: integer
Use: required
XPath: /spdb/sp/basis/custom/@l

6.2 Attribute: searchE

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

$$\psi(R_{MT}) = 0. \tag{2}$$

Type: boolean

Default: "true"
Use: optional
XPath: /spdb/sp/basis/custom/@searchE

6.3 Attribute: trialEnergy

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

Type: fortrandouble (10.1)
Default: "0.15d0"
Use: optional
XPath: /spdb/sp/basis/custom/@trialEnergy

6.4 Attribute: type

Augmentation type (LAPW or APW+lo). Default apw+lo.

Type: string
Default: "apw+lo"
Use: optional
XPath: /spdb/sp/basis/custom/@type

7 Element: lo

Definition of the local orbitals (LO). Note that the local orbitals corresponding to the APW+lo basis type are included automatically and need not to be specified here.

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

This element allows for specification of the following attributes:

l (required), wfproj

7.1 Attribute: l

Azimuthal quantum number for which the local orbital is defined.

Type: integer
Use: required
XPath: /spdb/sp/basis/lo/@l

7.2 Attribute: wfproj

Use this local orbital for projection while constructing Wannier functions.

Type: boolean
Default: "false"
Use: optional
XPath: /spdb/sp/basis/lo/@wfproj

8 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)

8.1 Attribute: core

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

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

8.2 Attribute: kappa

Relativistic quantum number.

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

8.3 Attribute: l

Azimuthal quantum number.

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

8.4 Attribute: n

Principal quantum number.

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

8.5 Attribute: occ

Ocuppation number.

Type:	fortrandouble (10.1)
Use:	required
XPath:	/spdb/sp/atomicState/@occ

Part II
Reused Elements

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

9 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/custom /spdb/sp/basis/lo /spdb/sp/basis/default

This element allows for specification of the following attributes:

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

9.1 Attribute: matchingOrder

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

Type:	integer

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

9.2 Attribute: searchE

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

$$\psi(R_{MT}) = 0. \tag{3}$$

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

9.3 Attribute: trialEnergy

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

Type: fortrandouble (10.1)
Use: required
XPath: `./wf/@trialEnergy`

10 Data Types

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

10.1 Type fortrandouble

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