
# spacegroup input reference

**exciting** carbon

December 2015

## About this Document

# Part I
# Input Elements

## 1 Element: symmetries

The symmetries file format used by the **spacegroup** tool to generate structures and supercells as defined by lattice from the knowledge of Wyckoff positions and the space group. The space group is specified by the attribute HermannMauguinSymbol. The root element is symmetries.

**Contains:** title (1 times)
lattice (1 times)
WyckoffPositions (optional)
**XPath:** /symmetries

This element allows for specification of the following attributes:

HermannMauguinSymbol (required)

### 1.1 Attribute: HermannMauguinSymbol

The Herman Mauguin symbol specifies the spacegroup of the structure. **The table of all the symbols** (http://exciting-code.org/hermann-mauguin-symbol) lists all possible inputs.

**Type:** string
**Use:** required
**XPath:** /symmetries/@HermannMauguinSymbol

## 2 Element: title

**Type:** string
**XPath:** /symmetries/title

## 3 Element: lattice

The lattice element defines lattice from a,b,c, and angles.

**Type:** no content
**XPath:** /symmetries/lattice

This element allows for specification of the following attributes:

a (required), ab (required), ac (required), b (required), bc (required), c (required), epslat, ncell, primcell, scale, speciespath, stretch

## 3.1 Attribute: a

**Type:** fortrandouble (7.1)
**Use:** required
**Unit:** Bohr
**XPath:** /symmetries/lattice/@a

## 3.2 Attribute: ab

Angle between lattice vector a and b in degrees.

**Type:** fortrandouble (7.1)
**Use:** required
**Unit:** Degree
**XPath:** /symmetries/lattice/@ab

## 3.3 Attribute: ac

Angle between lattice vector a and c in degrees.

**Type:** fortrandouble (7.1)
**Use:** required
**Unit:** Degree
**XPath:** /symmetries/lattice/@ac

## 3.4 Attribute: b

**Type:** fortrandouble (7.1)
**Use:** required
**Unit:** Bohr
**XPath:** /symmetries/lattice/@b

## 3.5 Attribute: bc

Angle between lattice vector b and c in degrees.

**Type:** fortrandouble (7.1)
**Use:** required
**Unit:** Degree
**XPath:** /symmetries/lattice/@bc

### 3.6 Attribute: c

**Type:** fortrandouble (7.1)
**Use:** required
**Unit:** Bohr
**XPath:** /symmetries/lattice/@c

### 3.7 Attribute: epslat

**Type:** fortrandouble (7.1)
**Default:** "1.0d-6"
**Use:** optional
**XPath:** /symmetries/lattice/@epslat

### 3.8 Attribute: ncell

Number of repeated cells in each direction.

**Type:** integertriple (7.8)
**Default:** "1 1 1"
**Use:** optional
**XPath:** /symmetries/lattice/@ncell

### 3.9 Attribute: primcell

**Type:** boolean
**Default:** "false"
**Use:** optional
**XPath:** /symmetries/lattice/@primcell

### 3.10 Attribute: scale

Scales all the lattice vectors by the same factor. This is useful for varying the volume.

**Type:** fortrandouble (7.1)
**Default:** "1"
**Use:** optional
**XPath:** /symmetries/lattice/@scale

### 3.11 Attribute: speciespath

**Type:** string
**Default:** "http://xml.exciting-code.org/species/"

**Use:** optional
**XPath:** /symmetries/lattice/@speciespath

### 3.12 Attribute: stretch

Allows for an individual scaling of each lattice vector separately. "1 1 1" means no scaling.

**Type:** vect3d (7.6)
**Default:** "1.0d0 1.0d0 1.0d0 "
**Use:** optional
**XPath:** /symmetries/lattice/@stretch

## 4 Element: WyckoffPositions

**Contains:** wspecies (zero or more)
**XPath:** /symmetries/WyckoffPositions

## 5 Element: wspecies

**Contains:** wpos (zero or more)
**XPath:** /symmetries/WyckoffPositions/wspecies

This element allows for specification of the following attributes:

speciesfile

### 5.1 Attribute: speciesfile

**Type:** string
**Use:** optional
**XPath:** /symmetries/WyckoffPositions/wspecies/@speciesfile

## 6 Element: wpos

**Type:** no content
**XPath:** /symmetries/WyckoffPositions/wspecies/wpos

This element allows for specification of the following attributes:

coord

### 6.1 Attribute: coord

**Type:** vect3d (7.6)
**Use:** optional
**XPath:** /symmetries/WyckoffPositions/wspecies/wpos/@coord

# Part II
# Reused Elements

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

## 7 Data Types

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

### 7.1 Type fortrandouble

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

### 7.2 Type booleanlist

List of space separated booleans.

### 7.3 Type booleantriple

Space separated list of three booleans.
Example: `"true false true"`

### 7.4 Type vector

A vector is a space separated list of floating point numbers.
Example: `"1.3 2.3e4 3 90"`

### 7.5 Type integerlist

List of space separated integers.

### 7.6 Type vect3d

Three dimensional vector as three space separated floating point numbers.

### 7.7 Type vect2d

Two dimensional vector as two space separated floating point numbers.

### 7.8 Type integertriple

Space separated list of three integers.
Example: `"1 2 3"`

### 7.9 Type integerquadrupel

Space separated list of three integers.
Example: `"1 2 3 4"`

### 7.10 Type integerpair

Space separated list of two integers
Example: `"1 2"`