

Package ‘PeriodicTable’

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Type Package

Title Periodic Table of the Elements

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Description Provides a dataset containing properties for chemical elements.
Helper functions are also provided to access some atomic properties.

License GPL

LazyData FALSE

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Depends R (>= 3.3.1)

NeedsCompilation no

Repository CRAN

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atomNames

Atom names/types

Description

This data set provides various atom names/types and there associated atomic symbols which are used for atom recognition.

Usage

```
atomNames
```

Format

A data frame with the following columns.

atmname a character vector. Atom names/types.

symb a character vector. Atomic symbols.

Examples

```
data(atomNames)
atomNames
```

atomProperties

Atomic Properties

Description

Determine atomic properties from atomic symbols, atomic numbers or atom names.

Usage

```
mass(x)
```

```
rcov(x)
```

```
rvdw(x)
```

```
atomColor(x)
```

Arguments

x an R object for which to get atomic properties.

Details

The functions documented here allow to get atomic properties, such as atomic masses (`mass`), covalent radii (`rcov`), Van der Waals radii (`rvdw`) and atom colors (`atomColor`), from atomic symbols, atomic numbers or atom names.

The methods for atomic number (integer or numeric values) and atom names (character strings) first convert the values into atomic symbols (see [symp](#)) and then match them with the [periodicTable](#) dataset to determine the properties.

Value

Return a vector containing atomic properties.

See Also

[periodicTable](#), [atomRecognition](#), [match](#)

Examples

```
# Display all chemical element properties
data(periodicTable)
periodicTable
```

```
# From atomic symbols
mass(c("C", "O", "H"))
rcov(c("C", "O", "H"))
rvdw(c("C", "O", "H"))
atomColor(c("C", "O", "H"))
```

```
# From atomic numbers
mass(c(6, 8, 1))
rcov(c(6, 8, 1))
rvdw(c(6, 8, 1))
atomColor(c(6, 8, 1))
```

```
# From atom names
mass(c("CA", "OD", "H"))
rcov(c("CA", "OD", "H"))
rvdw(c("CA", "OD", "H"))
atomColor(c("CA", "OD", "H"))
```

atomRecognition

Atom Recognition

Description

Determine atomic symbols from atom names or atomic numbers.

Usage

```
symb(x, na.as.dummy = FALSE)
```

```
areSymb(x, na.action = FALSE)
```

```
isSymb(x, na.action = FALSE)
```

Arguments

x	an R object for which to determine atomic symbols or to be tested.
na.as.dummy	a logical value. Whether to consider NA values as dummy atoms or not.
na.action	a logical value or NA. NA values will be set to this value.

Details

In some files, atom names/types are specified instead of atomic symbols. It is then useful to convert atom names/types into atomic symbols. The `symb` function allow to perform this conversion by using the [atomNames](#) and [periodicTable](#) data sets.

Atom recognition from character vector is performed as follow:

- Remove numbers from character strings.
- Search for matching atom types in [atomNames](#) dataset.
- Truncate to first character and translate to upper case.
- Search for matching atomic symbols in [periodicTable](#) dataset.
- Unrecognized atoms are considered as dummy atoms ("Xx").

Function `symb` can also convert atomic numbers into atomic symbols. Atomic numbers are first checked to be whole numbers and then searched into the [periodicTable](#) dataset to determine atomic symbols.

Function `areSymb` can be used to check if the values in a vector are atomic symbols.

Function `isSymb` can be used to check if all the values in a vector are atomic symbols.

Value

`symb` returns a character vector containing atomic symbols. `areSymb` returns a logical vector. `isSymb` returns TRUE if x contains only atomic symbols or FALSE otherwise.

See Also

[atomNames](#), [periodicTable](#), [atomProperties](#), [match](#)

Examples

```
# Display atomNames
data(atomNames)
atomNames

# Get atomic symbols from atom names
```

```
symb(c("CA", "CB", "N", "NZ", "OXT"))  
  
# Get atomic symbols from atomic numbers  
symb(1:4)
```

periodicTable

Periodic Table of the Elements

Description

A dataset containing chemical element properties.

Usage

```
periodicTable
```

Format

A data.frame with the following columns:

numb an integer vector. Atomic numbers.
symb a character vector. Atomic symbols.
name a character vector. Name of chemical elements.
mass a numeric vector. Atomic masses.
rcov a numeric vector. Covalent radii.
rwdw a numeric vector. Van der Waals radii.
rion a numeric vector. Ionic radii.
red, green, blue numeric vectors. rgb colors.
period an integer vector. Element periods.
group an integer vector. Element groups
type a character vector. Element types.
phase a character vector. Most stable crystal.
crystal a character vector. Type of crystalline phases.
Eneg a numeric vector. Electronegativity.
IP a numeric vector. First ionization potential.
density a numeric vector. Densities.
melting a numeric vector. Melting points.
boiling a numeric vector. Boiling points.
isotopes an integer vector. Number of isotopes.
discoverer a character vector. Discoverer names.
year an integer vector. Discovery dates.

C a numeric vector. Heat capacities.

config a character vector. Electronic configurations

row an integer vector. Display rows.

col an integer vector. Display columns.

Source

<http://www.data-explorer.com/content/data/periodic-table-of-elements-csv.zip>

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