Package 'PeriodicTable'

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Type Package

Title Periodic Table of the Elements

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Encoding UTF-8

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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

RoxygenNote 5.0.1

Depends R (>= 3.3.1)

NeedsCompilation no

Repository CRAN

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R topics documented:

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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 symb) 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"))
```

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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 convertion 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.

rvdw 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 numerci 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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