

NAME

DREIDINGAtomTypes

SYNOPSIS

```
use AtomTypes::DREIDINGAtomTypes;

use AtomTypes::DREIDINGAtomTypes qw(:all);
```

DESCRIPTION

DREIDINGAtomTypes class provides the following methods:

new, AssignAtomTypes, GetAllPossibleDREIDINGAtomTypes, GetAllPossibleDREIDINGNonHydrogenAtomTypes, GetDREIDINGAtomTypesData, StringifyDREIDINGAtomTypes

The following functions are available:

GetAllPossibleDREIDINGAtomTypes, GetAllPossibleDREIDINGNonHydrogenAtomTypes, GetDREIDINGAtomTypesData

DREIDINGAtomTypes is derived from AtomTypes class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in DREIDINGAtomTypes, AtomTypes or ObjectProperty classes using Perl's AUTOLOAD functionality. These methods are generated on-the-fly for a specified object property:

```
Set<PropertyName>(<PropertyValue>);
$PropertyValue = Get<PropertyName>();
Delete<PropertyName>();
```

The data file DREIDINGAtomTypes.csv distributed with MayaChemTools release contains all possible DREIDING [Ref 88] atom types.

Format of a Five-character mnemonic label used for DREIDING atom types:

- o First two characters correspond to chemical symbol with an underscore as second character for elements with one character symbol
- o Third character describes hybridization: 1 - linear (sp); 2 - trigonal (sp²); 3 = tetrahedral (sp³); R - sp² involved in resonance situation
- o Fourth character used to indicate number of implicit hydrogens
- o Fourth and fifth characters are used as indicators of alternate parameters: formal oxidation state, bridging hydrogens and so on. The `_HB` type denotes a hydrogen atom capable of forming hydrogen bonds attached to (N, O, F). The `H_b` is the bridging hydrogen of diborane.

Examples of DREIDING atom types:

H_, C_3, C_R, C_2, N_3, N_R, O_3, O_R and so on

METHODS

new

```
$NewDREIDINGAtomTypes = new AtomTypes::DREIDINGAtomTypes(%NamesAndValues);
```

Using specified *DREIDINGAtomTypes* property names and values hash, new method creates a new object and returns a reference to newly created DREIDINGAtomTypes object. By default, the following properties are initialized:

```
Molecule = ''
Type = 'DREIDING'
IgnoreHydrogens = 0
```

Examples:

```
$DREIDINGAtomTypes = new AtomTypes::DREIDINGAtomTypes(
    'Molecule' => $Molecule,
    'IgnoreHydrogens' => 0);
```

AssignAtomTypes

```
$DREIDINGAtomTypes->AssignAtomTypes();
```

Assigns DREIDING atom types to all the atoms in a molecule and returns *DREIDINGAtomTypes*.

GetAllPossibleDREIDINGAtomTypes

```
$AllAtomTypesDataRef = $DREIDINGAtomTypes->
    GetAllPossibleDREIDINGAtomTypes();
$AllAtomTypesDataRef = AtomTypes::DREIDINGAtomTypes::
    GetAllPossibleDREIDINGAtomTypes();
```

Returns all possible DREIDING atom types corresponding to hydrogen and non-hydrogen atoms as an array reference.

GetAllPossibleDREIDINGNonHydrogenAtomTypes

```
$AtomTypesDataRef = $DREIDINGAtomTypes->
    GetAllPossibleDREIDINGNonHydrogenAtomTypes();
$AtomTypesDataRef = AtomTypes::DREIDINGAtomTypes::
    GetAllPossibleDREIDINGNonHydrogenAtomTypes();
```

Returns all possible DREIDING atom types corresponding to non-hydrogen atoms as an array reference.

GetDREIDINGAtomTypesData

```
$AtomTypesDataMapRef = $DREIDINGAtomTypes->GetDREIDINGAtomTypesData();
$AtomTypesDataMapRef = AtomTypes::DREIDINGAtomTypes::
    GetDREIDINGAtomTypesData();
```

Returns DREIDING atom types and associated data loaded from DREIDING data file as a reference to hash with the following hash data format:

```
@{$DREIDINGAtomTypesDataMap{AtomTypes}} - Array of all possible atom
    types for all atoms
@{$DREIDINGAtomTypesDataMap{NonHydrogenAtomTypes}} - Array of all
    possible atom types for non-hydrogen atoms
@{$DREIDINGAtomTypesDataMap->{ColLabels}} - Array of column labels
%{$DREIDINGAtomTypesDataMap->{DataCol<Num>}} - Hash keys pair:
    DataCol<Num>, AtomType
```

StringifyDREIDINGAtomTypes

```
$String = $DREIDINGAtomTypes->StringifyDREIDINGAtomTypes();
```

Returns a string containing information about *DREIDINGAtomTypes* object.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

AtomTypes.pm, AtomicInvariantsAtomTypes.pm, EStateAtomTypes.pm, FunctionalClassAtomTypes.pm, MMFF94AtomTypes.pm, SLogPAtomTypes.pm, SYBYLAtomTypes.pm, TPSAAAtomTypes.pm, UFFAtomTypes.pm

COPYRIGHT

Copyright (C) 2024 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.

