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.

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SEE ALSO

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

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