NAME

UFFAtomTypes

SYNOPSIS

use UFFAtomTypes;

use UFFAtomTypes qw(:all);

DESCRIPTION

UFFAtomTypes class provides the following methods:

new, AssignAtomTypes, GetAllPossibleUFFAtomTypes, GetAllPossibleUFFNonHydrogenAtomTypes, GetUFFAtomTypesData, StringifyUFFAtomTypes

The following functions are available:

GetAllPossibleUFFAtomTypes, GetAllPossibleUFFNonHydrogenAtomTypes, GetUFFAtomTypesData

UFFAtomTypes is derived from AtomTypes class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in UFFAtomTypes, 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 UFFAomTypes.csv distributed with MayaChemTools release contains all possible UFF [Ref 81-82] atom types.

Format of a Five-character mnemonic label used for UFF 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 or geometry: 1 - linear;
  2 - trigonal; R - resonant; 3 = tetrahedral; 4 - square planar;
  5 - trigonal bipyramidal; 6 - octahedral
o Fourth and fifth characters are used as indicators of alternate
  parameters: formal oxidation state, bridging hydrogens and so on.
```

Examples of UFF atom types:

```
C_3, C_2, C_R, N_3, N_R, O_3, O_2, and so on
```

METHODS

new

```
$NewUFFAtomTypes = new UFFAtomTypes(%NamesAndValues);
```

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

```
Molecule = ''
Type = 'UFF'
IgnoreHydrogens = 0
```

Examples:

```
$UFFAtomTypes = new UFFAtomTypes(
                            'Molecule' => $Molecule,
                            'IgnoreHydrogens' => 0);
```

AssignAtomTypes

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

Assigns UFF atom types to all the atoms in a molecule and returns *UFFAtomTypes*.

GetAllPossibleUFFAtomTypes

```
$AllAtomTypesDataRef = $UFFAtomTypes->
                       GetAllPossibleUFFAtomTypes();
$AllAtomTypesDataRef = UFFAtomTypes::
                       GetAllPossibleUFFAtomTypes();
```

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

GetAllPossibleUFFNonHydrogenAtomTypes

```
$AtomTypesDataRef = $UFFAtomTypes->
                    GetAllPossibleUFFNonHydrogenAtomTypes();
$AtomTypesDataRef = UFFAtomTypes::
```

```
GetAllPossibleUFFNonHydrogenAtomTypes();
```

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

GetUFFAtomTypesData

```
$AtomTypesDataMapRef = $UFFAtomTypes->GetUFFAtomTypesData();
$AtomTypesDataMapRef = UFFAtomTypes::GetUFFAtomTypesData();
```

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

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

StringifyUFFAtomTypes

```
$String = $UFFAtomTypes->StringifyUFFAtomTypes();
```

Returns a string containing information about *UFFAtomTypes* object.

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SEE ALSO

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

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