NAME

SYBYLAtomTypes

SYNOPSIS

use AtomTypes::SYBYLAtomTypes;

use AtomTypes::SYBYLAtomTypes qw(:all);

DESCRIPTION

SYBYLAtomTypes class provides the following methods:

new, AssignAtomTypes, GetAllPossibleSYBYLAtomTypes, GetAllPossibleSYBYLNonHydrogenAtomTypes, GetSYBYLAtomTypesData, StringifySYBYLAtomTypes

The following functions are available:

GetAllPossibleSYBYLAtomTypes, GetAllPossibleSYBYLNonHydrogenAtomTypes, GetSYBYLAtomTypesData

SYBYLAtomTypes is derived from AtomTypes class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in SYBYLAtomTypes, 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 SYBYLAomTypes.csv distributed with MayaChemTools release contains all possible Triops SYBYL [Ref 79-80] atom types.

Examples of SYBYL atom types:

```
C.3,C.2, C.ar, N.3, N.2, N.ar and so on
```

METHODS

new

```
$NewSYBYLAtomTypes = new AtomTypes::SYBYLAtomTypes(%NamesAndValues);
```

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

```
Molecule = ''
Type = 'SYBYL'
IgnoreHydrogens = 0
```

Examples:

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

AssignAtomTypes

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

Assigns SYBYL atom types to all the atoms in a molecule and returns *SYBYLAtomTypes*.

GetAllPossibleSYBYLAtomTypes

```
$AllAtomTypesDataRef = $SYBYLAtomTypes->
                       GetAllPossibleSYBYLAtomTypes();
$AllAtomTypesDataRef = AtomTypes::SYBYLAtomTypes::
                       GetAllPossibleSYBYLAtomTypes();
```

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

GetAllPossibleSYBYLNonHydrogenAtomTypes

```
$AtomTypesDataRef = $SYBYLAtomTypes->
                    GetAllPossibleSYBYLNonHydrogenAtomTypes();
$AtomTypesDataRef = AtomTypes::SYBYLAtomTypes::
                    GetAllPossibleSYBYLNonHydrogenAtomTypes();
```

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

GetSYBYLAtomTypesData

```
$AtomTypesDataMapRef = $SYBYLAtomTypes->GetSYBYLAtomTypesData();
$AtomTypesDataMapRef = AtomTypes::SYBYLAtomTypes::GetSYBYLAtomTypesData();
```

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

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

StringifySYBYLAtomTypes

```
$String = $SYBYLAtomTypes->StringifySYBYLAtomTypes();
```

Returns a string containing information about *SYBYLAtomTypes* object.

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SEE ALSO

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

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