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

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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