

NAME

Atom

SYNOPSIS

use Atom;

DESCRIPTION

Atom class provides the following methods:

new, AddHydrogens, Copy, DeleteAtom, DeleteHydrogens, DoesAtomNeighborhoodMatch, GetAtomicInvariantValue, GetAtomicWeight, GetBondToAtom, GetBonds, GetBondsToHeavyAtoms, GetBondsToHydrogenAtoms, GetBondsToNonHydrogenAtoms, GetExactMass, GetExplicitHydrogens, GetFormalCharge, GetGroupNumber, GetHeavyAtomNeighbors, GetHeavyAtomNeighborsAtomInformation, GetHeavyAtomNeighborsBondformation, GetHighestCommonValence, GetHydrogenAtomNeighbors, GetImplicitHydrogens, GetImplicitValence, GetLargestBondOrder, GetLargestBondOrderToHeavyAtoms, GetLargestBondOrderToNonHydrogenAtoms, GetLargestRing, GetLowestCommonValence, GetMassNumber, GetNeighbors, GetNeighborsUsingAtomSpecification, GetNonHydrogenAtomNeighbors, GetNonHydrogenAtomNeighborsAtomInformation, GetNonHydrogenAtomNeighborsBondInformation, GetNonHydrogenNeighborOfHydrogenAtom, GetNumOfAromaticBondsToHeavyAtoms, GetNumOfAromaticBondsToNonHydrogenAtoms, GetNumOfBondTypesToHeavyAtoms, GetNumOfBondTypesToNonHydrogenAtoms, GetNumOfBonds, GetNumOfBondsToHeavyAtoms, GetNumOfBondsToHydrogenAtoms, GetNumOfBondsToNonHydrogenAtoms, GetNumOfDoubleBondsToHeavyAtoms, GetNumOfDoubleBondsToNonHydrogenAtoms, GetNumOfHeavyAtomNeighbors, GetNumOfHydrogenAtomNeighbors, GetNumOfMissingHydrogens, GetNumOfNeighbors, GetNumOfNonHydrogenAtomNeighbors, GetNumOfRings, GetNumOfRingsWithEvenSize, GetNumOfRingsWithOddSize, GetNumOfRingsWithSize, GetNumOfRingsWithSizeGreaterThanOrLessThan, GetNumOfRingsWithSizeLessThan, GetNumOfSigmaAndPiBondsToHeavyAtoms, GetNumOfSigmaAndPiBondsToNonHydrogenAtoms, GetNumOfSingleBondsToHeavyAtoms, GetNumOfSingleBondsToNonHydrogenAtoms, GetNumOfTripleBondsToHeavyAtoms, GetNumOfTripleBondsToNonHydrogenAtoms, GetPeriodNumber, GetRings, GetRingsWithEvenSize, GetRingsWithOddSize, GetRingsWithSize, GetRingsWithSizeGreaterThanOrLessThan, GetRingsWithSizeLessThan, GetSizeOfLargestRing, GetSizeOfSmallestRing, GetSmallestRing, GetSumOfBondOrders, GetSumOfBondOrdersToHeavyAtoms, GetSumOfBondOrdersToHydrogenAtoms, GetSumOfBondOrdersToNonHydrogenAtoms, GetValence, GetValenceElectrons, GetValenceFreeElectrons, GetX, GetXYZ, GetXYZVector, GetY, GetZ, IsAmideCarbon, IsAmideNitrogen, IsAromatic, IsBromine, IsCarbon, IsCarboxylCarbon, IsCarboxylOxygen, IsCarboxylateCarbon, IsCarboxylateOxygen, IsChlorine, IsFluorine, IsFunctionalClassType, IsGuanidiniumCarbon, IsGuanidiniumNitrogen, IsHBondAcceptor, IsHBondDonor, IsHalogen, IsHetroAtom, IsHydrogen, IsHydrogenBondAcceptor, IsHydrogenBondDonor, IsHydrophobic, IsInRing, IsInRingOfSize, IsIodine, IsIsotope, IsLipophilic, IsMetallic, IsNegativelyIonizable, IsNitrogen, IsNonCarbonOrHydrogen, IsNotInRing, IsOnlyInOneRing, IsOxygen, IsPhosphateOxygen, IsPhosphatePhosphorus, IsPhosphorus, IsPolarAtom, IsPolarHydrogen, IsPositivelyIonizable, IsSaturated, IsSilicon, IsStereoCenter, IsSulfur, IsSulphur, IsTopologicalPharmacophoreType, IsUnsaturated, SetAtomSymbol, SetAtomicNumber, SetMassNumber, SetStereoCenter, SetStereochemistry, SetX, SetXYZ, SetY, SetZ, StringifyAtom

Atom class is derived from ObjectProperty base class which provides methods not explicitly defined in Atom or ObjectProperty class 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>();
```

METHODS

new

```
$NewAtom = new Atom([%PropertyNameAndValues]);
```

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

```
ID = SequentialObjectID
Name = "Atom <SequentialObjectID>"
AtomSymbol = ""
AtomicNumber = 0
XYZ = ZeroVector
```

Except for *ID* property, all other default properties and other additional properties can be set during invocation of this method.

Examples:

```
$Atom = new Atom();
$CarbonAtom = new Atom(AtomSymbol' => 'C', 'XYZ' => (0.0, 1.0,
0.0));
$OxygenAtom = new Atom('AtomName' => 'Oxygen', AtomSymbol' => 'O',
'XYZ' => (1.0, 1.0, 1.0));
```

AddHydrogens

```
$NumOfHydrogensAdded = $Atom->AddHydrogens();
```

Adds hydrogens to an Atom present in a Molecule object and returns the number of added hydrogens. The current release of MayaChemTools doesn't assign hydrogen positions.

Copy

```
$AtomCopy = $Atom->Copy();
```

Copy *Atom* and its associated data using `Storable::dclone` and return a new *Atom* object.

DeleteAtom

```
$Atom->DeleteAtom();
```

Delete *Atom* from a molecule.

DoesAtomNeighborhoodMatch

```
$Status = $Atom->DoesAtomNeighborhoodMatch($CentralAtomSpec);
$Status = $Atom->DoesAtomNeighborhoodMatch($CentralAtomSpec,
                                           $NbrAtomSpecsRef);
$Status = $Atom->DoesAtomNeighborhoodMatch($CentralAtomSpec,
                                           $NbrAtomSpecsRef, $AllowedNbrBondSpecsRef);
$Status = $Atom->DoesAtomNeighborhoodMatch($CentralAtomSpec,
                                           $NbrAtomSpecsRef, $NbrBondSpecsRef,
                                           $AllowedNbrOfNbrAtomSpecsRef);
```

Returns 1 or 0 based on whether atom matches central atom and its neighborhood using specified atom and bonds specifications. Neighborhood atom and bond specifications are specified as array references containing neighbor atom and bond specifications.

Let:

```
AS = Atom symbol corresponding to element symbol, atomic number (#n)
    or any atom (A)

X<n> = Number of non-hydrogen atom neighbors or heavy atoms
      attached to atom
T<n> = Total number of atom neighbors including implicit and explicit
      hydrogens
BO<n> = Sum of bond orders to non-hydrogen atom neighbors or heavy
      atoms attached to atom
LBO<n> = Largest bond order of non-hydrogen atom neighbors or heavy
      atoms attached to atom
SB<n> = Number of single bonds to non-hydrogen atom neighbors or
      heavy atoms attached to atom
TSB<n> = Total number of single bonds to atom neighbors including implicit
      and explicit hydrogens
DB<n> = Number of double bonds to non-hydrogen atom neighbors or
      heavy atoms attached to atom
TB<n> = Number of triple bonds to non-hydrogen atom neighbors or
      heavy atoms attached to atom
AB<n> = Number of aromatic bonds to non-hydrogen atom neighbors or
      heavy atoms attached to atom
H<n> = Number of implicit and explicit hydrogens for atom
Ar = Aromatic annotation indicating whether atom is aromatic
RA or RA<n> = Ring atom annotation indicating whether atom
            is a ring
TR<n> = Total number of rings containing atom
FC<+n/-n> = Formal charge assigned to atom
MN<n> = Mass number indicating isotope other than most abundant isotope
SM<n> = Spin multiplicity of atom. Possible values: 1 (singlet),
      2 (doublet) or 3 (triplet)
```

Then, atom specification corresponds to:

```
AS.X<n>.T<n>.BO<n>.LBO<n>.<SB><n>.<TSB><n>.<DB><n>.<TB><n>.AB<n>.H<n>.Ar.
RA<n>.TR<n>FC<+n/-n>.MN<n>.SM<n>
```

Except for AS which is a required atomic invariant in atom specification, all other atomic invariants are optional. For an atom specification to match an atom, the values of all specified atomic invariants must match. Exclamation in front of atomic invariant can be used to negate its effect during the match.

For *FC* value matching, the following value operators are also supported:

- o `+` : Any positive value
- o `-` : Any negative value
- o `>` ValidNumber or `>=` ValidNumber
- o `<` ValidNumber or `<=` ValidNumber

A comma delimited atom specification string is used to match any one of the specified atom specification.

Notes:

- o During atom specification match to an atom, the first atomic invariant is always assumed to atom symbol.

Examples:

- o ('N', 'N', 'N')
- o ('N.FC0', 'N.FC0', 'N,N.FC+1.H1')
- o ('N.H2', 'N.H2', 'N.H1')
- o ('C,N', '!N', '!H')
- o ('C,N', 'N.Ar', 'N.R5')

Let:

```
-|1|s|Single = Single bond
=|2|d|Double = Double bond
#|3|t|Triple  = Triple bond
:|1.5|a|Ar|Aromatic = Aromatic bond
```

```
@|RB|Ring = Ring bond
~|*|Any = Any bond
```

Then, bond specification corresponds to:

```
-.:
=.@
Double.Aromatic
```

For a bond specification to match bond between two atoms, the values of all specified bond symbols must match. Exclamation in front of bond symbol can be used to negate its effect during the match.

A comma delimited bond specification string is used to match any one of the specified atom specification.

Notes:

- o During atom neighborhood match for central atom neighborhood atom and bond specifications, implicit or missing hydrogens are automatically checked for any matches to unmatched specifications.

Examples:

```
Aromatic carbon in a 5 membered ring:
$Atom->DoesAtomNeighborhoodMatch('C.Ar.RA5');
```

```
AcetylenicCarbon: $Atom->DoesAtomNeighborhoodMatch('C.T2.TB1'); or
$Atom->DoesAtomNeighborhoodMatch('C.T2.TB1',
['*', '*'], ['#', '-']);
```

```
GuadiniumCarbon: $Atom->DoesAtomNeighborhoodMatch('C.X3.BO4',
['N.FC0', 'N.FC0', 'N.FC0,N.FC+1'],
['-', '-', '='],
['C,H', 'C,H', 'C,H']);
```

```
AmideCarbon: $Atom->DoesAtomNeighborhoodMatch('C.X3.BO4,C.X2.BO3',
['C,H', 'O', 'N'],
['-', '=', '-'],
['C,H', 'C', 'C,H,N,O,S,P,F,Cl,Br,I']);
```

```
CarboxylCarbon: $Atom->DoesAtomNeighborhoodMatch('C.X3.BO4,C.X2.BO3',
['C,H', 'O', 'O.X1.FC0'],
['-', '=', '-'],
['C,H', 'C', 'C']);
```

```
CarboxylateCarbon: $Atom->DoesAtomNeighborhoodMatch('C.X3.BO4,C.X2.BO3',
['C,H', 'O', 'O.X1.FC-1'],
['-', '=', '-'],
['C,H', 'C', 'C']);
```

DeleteHydrogens

```
$NumOfHydrogensDeleted = $Atom->AddHydrogens();
```

Delete hydrogens from an Atom present in a Molecule object and returns the number of deleted hydrogens.

GetAtomicInvariantValue

```
$Value = $Atom->GetAtomicInvariantValue($AtomicInvariant);
```

Returns atomic invariant value for a specified *AtomicInvariant*. The current release of MayaChemTools supports following abbreviations and descriptive names for *AtomicInvariants*:

```
AS : Atom or element symbol
X  : NumOfNonHydrogenAtomNeighbors or NumOfHeavyAtomNeighbors
T  : TotalNumOfAtomNeighbors
BO : SumOfBondOrdersToNonHydrogenAtoms or SumOfBondOrdersToHeavyAtoms
LBO : LargestBondOrderToNonHydrogenAtoms or LargestBondOrderToHeavyAtoms
SB  : NumOfSingleBondsToNonHydrogenAtoms or NumOfSingleBondsToHeavyAtoms
TSB : TotalNumOfSingleBonds
DB  : NumOfDoubleBondsToNonHydrogenAtoms or NumOfDoubleBondsToHeavyAtoms
```

```

TB : NumOfTripleBondsToNonHydrogenAtoms or NumOfTripleBondsToHeavyAtoms
AB : NumOfAromaticBondsToNonHydrogenAtoms or NumOfAromaticBondsToHeavyAtoms
H : NumOfImplicitAndExplicitHydrogens
Ar : Aromatic
Str : Stereochemistry
RA : RingAtom
FC : FormalCharge
AN : AtomicNumber
AM : AtomicMass
MN : MassNumber
SM : SpinMultiplicity

```

GetAtomicWeight

```
$Value = $Atom->GetAtomicWeight();
```

Returns atomic weight of an *Atom* which corresponds to either explicitly set *AtomicWeight* atom property or atomic weight of the corresponding element in the periodic table available by *PeriodicTable* module.

GetBondToAtom

```
$Bond = $Atom->GetBondToAtom($OtherAtom);
```

Returns a *Bond* object corresponding to bond between *Atom* and *OtherAtom* in a molecule.

GetBonds

```
@Bonds = $Atom->GetBonds();
```

Returns an array of *Bond* objects corresponding to all bonds from *Atom* to other bonded atoms in a molecule.

GetBondsToHeavyAtoms

```
@Bonds = $Atom->GetBondsToHeavyAtoms();
```

Returns an array of *Bond* objects corresponding to bonds from *Atom* to other bonded non-hydrogen atoms in a molecule.

GetBondsToHydrogenAtoms

```
@Bonds = $Atom->GetBondsToHydrogenAtoms();
```

Returns an array of *Bond* objects corresponding to bonds from *Atom* to any other hydrogen atom in a molecule.

GetBondsToNonHydrogenAtoms

```
@Bonds = $Atom->GetBondsToNonHydrogenAtoms();
```

Returns an array of *Bond* objects corresponding to bonds from *Atom* to other bonded non-hydrogen atoms in a molecule.

GetExactMass

```
$ExactMass = $Atom->GetExactMass();
```

Returns exact mass of an *Atom* which correspond to one of these three values: explicitly set *ExactMass* property; mass of natural isotope for an explicitly set value of *MassNumber*; most abundant natural isotope mass for *Atom* with valid atomic number value available by *PeriodicTable* module.

GetExplicitHydrogens

```
$NumOfExplicitHydrogens = $Atom->GetExplicitHydrogens();
```

Returns number of hydrogens explicitly bonded to an *Atom* in a molecule.

GetFormalCharge

```
$FormalCharge = $Atom->GetFormalCharge();
```

Returns formal charge of an *Atom* in a molecule.

GetGroupNumber

```
$GroupNumber = $Atom->GetGroupNumber();
```

Returns group number of an *Atom* in a molecule with a valid atomic number.

GetHeavyAtomNeighbors

```
$NumOfHeavyAtoms = $Atom->GetHeavyAtomNeighbors();
@HeavyAtoms = $Atom->GetHeavyAtomNeighbors();
```

Return number of heavy atoms or an array of *Atom* objects corresponding to heavy atoms bonded to an *Atom* in a molecule.

GetHeavyAtomNeighborsAtomInformation

```
($NumOfAtomNeighbors, $AtomNeighborsRef,
 $NumOfAtomNeighborsType, $AtomNeighborsTypeMapRef) = $Atom->
  GetHeavyAtomNeighborsAtomInformation();
```

Returns atoms information for all non-hydrogen atoms attached to an *Atom* in a molecule.

The following values are returned:

- o Number of non-hydrogen atom neighbors
- o A reference to an array containing atom objects corresponding to non-hydrogen atom neighbors
- o Number of different types of non-hydrogen atom neighbors
- o A reference to a hash containing atom symbol as key with value corresponding to its count for non-hydrogen atom neighbors

GetHeavyAtomNeighborsBondformation

```
($NumOfBonds, $BondTypeCountMapRef,
 $AtomsBondTypesCountMapRef,
 $AtomsBondTypeAtomsMap) = $Atom->
  GetHeavyAtomNeighborsBondformation();
```

Returns bonds information for all non-hydrogen atoms attached to an *Atom* in a molecule.

The following values are returned:

- o Number of bonds to non-hydrogen atom neighbors
- o A reference to an array containing bond objects corresponding to non-hydrogen atom neighbors
- o A reference to a hash containing bond type as key with value corresponding to its count for non-hydrogen atom neighbors. Bond types are: Single, Double or Triple
- o A reference to a hash containing atom symbol as key pointing to bond type as second key with values corresponding to count of bond types for atom symbol for non-hydrogen atom neighbors
- o A reference to a hash containing atom symbol as key pointing to bond type as second key with values corresponding to atom objects array involved in corresponding bond type for atom symbol for non-hydrogen atom neighbors

GetHighestCommonValence

```
$HighestCommonValence = $Atom->GetHighestCommonValence();
```

Returns highest common valence of an *Atom* which corresponds to either explicitly set *HighestCommonValence* atom property or highest common valence of the corresponding element in the periodic table available by *PeriodicTable* module.

GetHydrogenAtomNeighbors

```
$NumOfHydrogenAtomNeighbors = $Atom->GetHydrogenAtomNeighbors();
@HydrogenAtomNeighbors = $Atom->GetHydrogenAtomNeighbors();
```

Return number of hydrogen atoms or an array of *Atom* objects corresponding to hydrogen atoms bonded to an *Atom* in a molecule.

GetImplicitHydrogens

```
$NumOfImplicitHydrogens = $Atom->GetImplicitHydrogens();
```

Returns number of implicit hydrogens for an *Atom* in a molecule. This value either corresponds to explicitly set *ImplicitHydrogens* atom property or calculated as the difference between the value of implicit valence and sum of bond orders to explicit non-hydrogen atoms.

GetImplicitValence

```
$ImplicitValence = $Atom->GetImplicitValence();
```

Returns implicit valence of an *Atom* in a molecule which corresponds to either explicitly set *ImplicitValence* atom property or calculated as described below.

For atoms with only one possible value of common valence available by *PeriodicTable* module, *ImplicitValence* corresponds to: $\text{CommonValence} + \text{FormalCharge} + \text{SpinMultiplicityCorrection}$.

For atoms with multiple values of common valence available by *PeriodicTable* module and formal charge, *ImplicitValence* corresponds to: $\text{HighestCommonValence} + \text{FormalCharge} + \text{SpinMultiplicityCorrection}$.

For atoms with multiple values of common valence available by *PeriodicTable* module and no formal charge, *ImplicitValence* corresponds to: First available valence higher than sum of bond orders to non-hydrogen atoms + $\text{SpinMultiplicityCorrection}$.

Notes:

For atoms with explicit assignment of *SpinMultiplicity* atom property values

- Singlet - two unpaired electrons corresponding to one spin state
- Doublet - free radical; an unpaired electron corresponding to two

```

        spin states
Triplet - two unpaired electrons corresponding to three spin states
        (divalent carbon atoms: carbenes)

```

SpinMultiplicityCorrection is calculated as follows:

```

Doublet: -1 (one valence electron not available for bonding)
Singlet: -2 (two valence electrons not available for bonding)
Triplet: -2 (two valence electrons not available for bonding)

```

GetLargestBondOrder

```
$LargestBO = $Atom->GetLargestBondOrder();
```

Returns largest bond order for an *Atom* among the bonds to other atoms in a molecule.

GetLargestBondOrderToHeavyAtoms

```
$LargestBO = $Atom->GetLargestBondOrderToHeavyAtoms();
```

Returns largest bond order for an *Atom* among the bonds to other heavy atoms in a molecule.

GetLargestBondOrderToNonHydrogenAtoms

```
$LargestBO = $Atom->GetLargestBondOrderToNonHydrogenAtoms();
```

Returns largest bond order for an *Atom* among the bonds to other non-hydrogen atoms in a molecule.

GetLargestRing

```
@RingAtoms = $Atom->GetLargestRing();
```

Returns an array of ring *Atom* objects corresponding to the largest ring containing *Atom* in a molecule.

GetLowestCommonValence

```
$LowestCommonValence = $Atom->GetLowestCommonValence();
```

Returns lowest common valence of an *Atom* which corresponds to either explicitly set *LowestCommonValence* atom property or highest common valence of the corresponding element in the periodic table available by PeriodicTable module.

GetMassNumber

```
$MassNumber = $Atom->GetMassNumber();
```

Returns atomic weight of an *Atom* which corresponds to either explicitly set *MassNumber* atom property or mass number of the most abundant natural isotope of the corresponding element in the periodic table available by PeriodicTable module.

GetNeighbors

```

$NumOfNeighbors = $Atom->GetNeighbors();
@Neighbors = $Atom->GetNeighbors();

```

Returns number of neighbor atoms or an array of *Atom* objects corresponding to all atoms bonded to an *Atom* in a molecule.

GetNeighborsUsingAtomSpecification

```

@AtomNeighbors = $Atom->GetNeighborsUsingAtomSpecification($AtomSpec);
$NumOfNeighbors = $Atom->GetNeighborsUsingAtomSpecification($AtomSpec);

@AtomNeighbors = $Atom->GetNeighborsUsingAtomSpecification($AtomSpec,
    @ExcludeNeighbors);

```

Returns number of neighbor atoms or an array of *Atom* objects matching atom specification corresponding to atom neighbors of an *Atom* in a molecule. Optionally, *Atom* neighbors can be excluded from the neighbors list using *ExcludeNeighbors*.

Notes:

- o AtomSpecification correspond to any valid AtomicInvariant based atomic specifications as supported by DoesAtomNeighborhoodMatch method
- o Multiple atom specifications can be used in a string delimited by comma

GetNonHydrogenAtomNeighbors

```

$NumOfNeighbors = $Atom->GetNonHydrogenAtomNeighbors();
@Neighbors = $Atom->GetNonHydrogenAtomNeighbors();

```

Returns number of non-hydrogen atoms or an array of *Atom* objects corresponding to non-hydrogen atoms bonded to an *Atom* in a molecule.

GetNonHydrogenAtomNeighborsAtomInformation

```
($NumOfAtomNeighbors, $AtomNeighborsRef,
 $NumOfAtomNeighborsType, $AtomNeighborsTypeMapRef) = $Atom->
  GetNonHydrogenAtomNeighborsAtomInformation();
```

Returns atoms information for all non-hydrogen atoms attached to an *Atom* in a molecule.

The following values are returned:

- o Number of non-hydrogen atom neighbors
- o A reference to an array containing atom objects corresponding to non-hydrogen atom neighbors
- o Number of different types of non-hydrogen atom neighbors
- o A reference to a hash containing atom symbol as key with value corresponding to its count for non-hydrogen atom neighbors

GetNonHydrogenAtomNeighborsBondInformation

```
($NumOfBonds, $BondTypeCountMapRef,
 $AtomsBondTypesCountMapRef,
 $AtomsBondTypeAtomsMap) = $Atom->
  GetNonHydrogenAtomNeighborsBondInformation();
```

Returns bonds information for all non-hydrogen atoms attached to an *Atom* in a molecule.

The following values are returned:

- o Number of bonds to non-hydrogen atom neighbors
- o A reference to an array containing bond objects corresponding to non-hydrogen atom neighbors
- o A reference to a hash containing bond type as key with value corresponding to its count for non-hydrogen atom neighbors. Bond types are: Single, Double or Triple
- o A reference to a hash containing atom symbol as key pointing to bond type as second key with values corresponding to count of bond types for atom symbol for non-hydrogen atom neighbors
- o A reference to a hash containing atom symbol as key pointing to bond type as second key with values corresponding to atom objects array involved in corresponding bond type for atom symbol for non-hydrogen atom neighbors

GetNonHydrogenNeighborOfHydrogenAtom

```
$Atom = $Atom->GetNonHydrogenNeighborOfHydrogenAtom();
```

Returns non-hydrogen or heavy atom neighbor of a hydrogen atom in a molecule..

GetNumOfAromaticBondsToHeavyAtoms

```
$NumOfBonds = $Atom->GetNumOfAromaticBondsToHeavyAtoms();
```

Returns number of aromatic bonds from an *Atom* to other non-hydrogen or heavy atoms in a molecule.

GetNumOfAromaticBondsToNonHydrogenAtoms

```
$NumOfBonds = $Atom->GetNumOfAromaticBondsToNonHydrogenAtoms();
```

Returns number of aromatic bonds from an *Atom* to other non-hydrogen or heavy atoms in a molecule.

GetNumOfBonds

```
$NumOfBonds = $Atom->GetNumOfBonds();
```

Returns number of bonds from an *Atom* to other atoms in a molecule.

GetNumOfBondsToHeavyAtoms

```
$NumOfBondsToHeavyAtoms = $Atom->GetNumOfBondsToHeavyAtoms();
```

Returns number of bonds from an *Atom* to other heavy atoms in a molecule.

GetNumOfBondsToHydrogenAtoms

```
$NumOfBonds = $Atom->GetNumOfBondsToHydrogenAtoms();
```

Returns number of bonds from an *Atom* to other hydrogen atoms in a molecule.

GetNumOfBondsToNonHydrogenAtoms

```
$NumOfBonds = $Atom->GetNumOfBondsToNonHydrogenAtoms();
```

Returns number of bonds from an *Atom* to other non-hydrogen atoms in a molecule.

GetNumOfBondTypesToHeavyAtoms

```
($NumOfSingleBonds, $NumOfDoubleBonds,
 $NumOfTripleBonds, $NumOfAromaticBonds) = $Atom->
  GetNumOfBondTypesToHeavyAtoms($CountAromaticBonds);
```

Get number of single, double, triple, and aromatic bonds from an *Atom* to all other non-hydrogen atoms in a molecule. Value of *CountAromaticBonds* parameter controls whether number of aromatic bonds is returned; default is not to count aromatic bonds. During counting of aromatic bonds, the bond marked aromatic is not included in the count of other bond types.

GetNumOfBondTypesToNonHydrogenAtoms

```
($NumOfSingleBonds, $NumOfDoubleBonds,
 $NumOfTripleBonds, $NumOfAromaticBonds) = $Atom->
  GetNumOfBondTypesToNonHydrogenAtoms($CountAromaticBonds);
```

Get number of single, double, triple, and aromatic bonds from an *Atom* to all other non-hydrogen atoms in a molecule. Value of *CountAromaticBonds* parameter controls whether number of aromatic bonds is returned; default is not to count aromatic bonds. During counting of aromatic bonds, the bond marked aromatic is not included in the count of other bond types.

GetNumOfDoubleBondsToHeavyAtoms

```
$NumOfDoubleBonds = $Atom->GetNumOfDoubleBondsToHeavyAtoms();
```

Returns number of double bonds from an *Atom* to other heavy atoms or non-hydrogen atoms in a molecule.

GetNumOfDoubleBondsToNonHydrogenAtoms

```
$NumOfDoubleBonds = $Atom->GetNumOfDoubleBondsToNonHydrogenAtoms();
```

Returns number of double bonds from an *Atom* to other heavy atoms or non-hydrogen atoms in a molecule.

GetNumOfHeavyAtomNeighbors

```
$NumOfNeighbors = $Atom->GetNumOfHeavyAtomNeighbors();
```

Returns number heavy atom neighbors for an *Atom* in a molecule.

GetNumOfHydrogenAtomNeighbors

```
$NumOfNeighbors = $Atom->GetNumOfHydrogenAtomNeighbors();
```

Returns number hydrogens atom neighbors for an *Atom* in a molecule.

GetNumOfMissingHydrogens

```
$NumOfMissingHydrogens = $Atom->GetNumOfMissingHydrogens();
```

Returns number of missing hydrogens for an *Atom* in a molecule corresponding to the difference between number of implicit and explicit hydrogens.

GetNumOfNeighbors

```
$NumOfNeighbors = $Atom->GetNumOfNeighbors();
```

Returns number atom neighbors for an *Atom* in a molecule.

GetNumOfNonHydrogenAtomNeighbors

```
$NumNeighbors = $This->GetNumOfNonHydrogenAtomNeighbors();
```

Returns number non-hydrogens atom neighbors for an *Atom* in a molecule.

GetNumOfRings

```
$NumOfRings = $Atom->GetNumOfRings();
```

Returns number of rings containing *Atom* in a molecule.

GetNumOfRingsWithEvenSize

```
$NumOfRings = $Atom->GetNumOfRingsWithEvenSize();
```

Returns number of rings with even size containing *Atom* in a molecule.

GetNumOfRingsWithOddSize

```
$NumOfRings = $Atom->GetNumOfRingsWithOddSize();
```

Returns number of rings with odd size containing *Atom* in a molecule.

GetNumOfRingsWithSize

```
$NumOfRings = $Atom->GetNumOfRingsWithSize($RingSize);
```

Returns number of rings with specific *RingSize* containing *Atom* in a molecule.

GetNumOfRingsWithSizeGreaterThan

```
$NumOfRings = $Atom->GetNumOfRingsWithSizeGreaterThan($RingSize);
```

Returns number of rings with size greater than specific *RingSize* containing *Atom* in a molecule.

GetNumOfRingsWithSizeLessThan

```
$NumOfRings = $Atom->GetNumOfRingsWithSizeLessThan($RingSize);
```

Returns number of rings with size less than specific *RingSize* containing *Atom* in a molecule.

GetNumOfSigmaAndPiBondsToHeavyAtoms

```
($NumOfSigmaBonds, $NumOfPiBonds) = $Atom->
    GetNumOfSigmaAndPiBondsToHeavyAtoms();
```

Get number of sigma and pi bonds from an *Atom* to all other non-hydrogen atoms in a molecule.

Sigma and pi bonds are counted using the following methodology: a single bond correspond to one sigma bond; a double bond contributes one to sigma bond count and one to pi bond count; a triple bond contributes one to sigma bond count and two to pi bond count.

GetNumOfSigmaAndPiBondsToNonHydrogenAtoms

```
($NumOfSigmaBonds, $NumOfPiBonds) = $Atom->
    GetNumOfSigmaAndPiBondsToNonHydrogenAtoms();
```

Get number of sigma and pi bonds from an *Atom* to all other non-hydrogen atoms in a molecule.

Sigma and pi bonds are counted using the following methodology: a single bond correspond to one sigma bond; a double bond contributes one to sigma bond count and one to pi bond count; a triple bond contributes one to sigma bond count and two to pi bond count.

GetNumOfSingleBondsToNonHydrogenAtoms

```
$NumOfSingleBonds = $Atom->GetNumOfSingleBondsToNonHydrogenAtoms();
```

Returns number of single bonds from an *Atom* to other heavy atoms or non-hydrogen atoms in a molecule.

GetNumOfSingleBondsToHeavyAtoms

```
$NumOfSingleBonds = $Atom->GetNumOfSingleBondsToHeavyAtoms();
```

Returns number of single bonds from an *Atom* to other heavy atoms or non-hydrogen atoms in a molecule.

GetNumOfTripleBondsToNonHydrogenAtoms

```
$NumOfTripleBonds = $Atom->GetNumOfTripleBondsToNonHydrogenAtoms();
```

Returns number of triple bonds from an *Atom* to other heavy atoms or non-hydrogen atoms in a molecule.

GetNumOfTripleBondsToHeavyAtoms

```
$NumOfTripleBonds = $Atom->GetNumOfTripleBondsToHeavyAtoms();
```

Returns number of triple bonds from an *Atom* to other heavy atoms or non-hydrogen atoms in a molecule.

GetPeriodNumber

```
$PeriodNumber = $Atom->GetPeriodNumber();
```

Returns periodic table period number for an *Atom* in a molecule with a valid atomic number .

GetRings

```
@Rings = $Aotm->GetRings();
```

Returns an array of references to arrays containing ring atoms corresponding to all rings containing *Atom* in a molecule.

GetRingsWithEvenSize

```
@Rings = $Aotm->GetRingsWithEvenSize();
```

Returns an array of references to arrays containing ring atoms corresponding to all rings with even size containing *Atom* in a molecule.

GetRingsWithOddSize

```
@Rings = $Aotm->GetRingsWithOddSize();
```

Returns an array of references to arrays containing ring atoms corresponding to all rings with odd size containing *Atom* in a molecule.

GetRingsWithSize

```
@Rings = $Aotm->GetRingsWithSize($RingSize);
```

Returns an array of references to arrays containing ring atoms corresponding to all rings with specific *RingSize* containing *Atom* in a molecule.

GetRingsWithSizeGreaterThan

```
@Rings = $Atom->GetRingsWithSizeGreaterThan($RingSize);
```

Returns an array of references to arrays containing ring atoms corresponding to all rings with size greater than specific *RingSize* containing *Atom* in a molecule.

GetRingsWithSizeLessThan

```
@Rings = $Atom->GetRingsWithSizeLessThan($RingSize);
```

Returns an array of references to arrays containing ring atoms corresponding to all rings with size less than specific *RingSize* containing *Atom* in a molecule.

GetSizeOfLargestRing

```
$Size = $Atom->GetSizeOfLargestRing();
```

Returns size of the largest ring containing *Atom* in a molecule.

GetSizeOfSmallestRing

```
$Size = $Atom->GetSizeOfSmallestRing();
```

Returns size of the smallest ring containing *Atom* in a molecule.

GetSmallestRing

```
@RingAtoms = $Atom->GetSmallestRing();
```

Returns an array of ring *Atom* objects corresponding to the largest ring containing *Atom* in a molecule.

GetSumOfBondOrders

```
$SumBondOrders = $Atom->GetSumOfBondOrders();
```

Returns sum of bond orders corresponding to all atoms bonded to an *Atom* in a molecule.

GetSumOfBondOrdersToHeavyAtoms

```
$SumBondOrders = $Atom->GetSumOfBondOrdersToHeavyAtoms();
```

Returns sum of bond orders corresponding to all heavy atoms bonded to an *Atom* in a molecule.

GetSumOfBondOrdersToHydrogenAtoms

```
$SumBondOrders = $Atom->GetSumOfBondOrdersToHydrogenAtoms();
```

Returns sum of bond orders corresponding to all hydrogen atoms bonded to an *Atom* in a molecule.

GetSumOfBondOrdersToNonHydrogenAtoms

```
$SumBondOrders = $Atom->GetSumOfBondOrdersToNonHydrogenAtoms();
```

Returns sum of bond orders corresponding to all non-hydrogen atoms bonded to an *Atom* in a molecule.

GetValence

```
$Valence = $Atom->GetValence();
```

Returns valence of an *Atom* in a molecule. Valence corresponds to number of electrons used by an atom in bonding:

```
Valence = ValenceElectrons - ValenceFreeElectrons = BondingElectrons
```

Single, double and triple bonds with bond orders of 1, 2, and 3 correspond to contribution of 1, 2, and 3 bonding electrons. So:

```
Valence = SumOfBondOrders + FormalCharge
```

where positive and negative values of *FormalCharge* increase and decrease the number of bonding electrons, respectively.

Notes:

- . For neutral molecules, valence and sum of bond orders are equal.
- . For molecules containing only single bonds, *SumOfBondOrders* and *NumOfBonds* are equal.

GetValenceElectrons

```
$ValenceElectrons = $Atom->GetValenceElectrons();
```

Returns valence electrons for an *Atom* which corresponds to either explicitly set *ValenceElectrons* atom property or valence electrons for the corresponding element in the periodic table available by *PeriodicTable* module.

GetValenceFreeElectrons

```
$ValenceFreeElectrons = $Atom->GetValenceFreeElectrons();
```

Returns valence free electrons for an *Atom* in a molecule. It corresponds to:

ValenceElectrons - SumOfBondOrders - FormalCharge

Examples:

```
NH3: ValenceFreeElectrons = 5 - 3 - 0 = 2
NH4+: ValenceFreeElectrons = 5 - 4 - 1 = 0
C(=O)O- : ValenceFreeElectrons on O- = 6 - 1 + 1 = 6
C(=O)O- : ValenceFreeElectrons on =O = 6 - 2 - 0 = 4
```

GetX

```
$X = $Atom->GetX();
```

Returns value of X-coordinate for an *Atom*.

GetXYZ

```
@XYZ = $Atom->GetXYZ();
$XYZRef = $Atom->GetXYZ();
```

Returns an array or a reference to an array containing values for *Atom* coordinates.

GetXYZVector

```
$XYZVector = $Atom->GetXYZVector();
```

Returns a *Vector* object containing values for *Atom* coordinates

GetY

```
$Y = $Atom->GetY();
```

Returns value of Y-coordinate for an *Atom*.

GetZ

```
$Z = $Atom->GetZ();
```

Returns value of Z-coordinate for an *Atom*.

IsAmideCarbon

```
$Status = $Atom->IsAmideCarbon();
```

Returns 1 or 0 based on whether it's amide carbon *Atom*.

An amide group is defined as:

```
R-C(=O)-N(-R')-R''
```

where:

- o R = Hydrogen or groups of atoms attached through carbon
- o R' = Hydrogens or groups of atoms attached through carbon or hetro atoms
- o R'' = Hydrogens or groups of atoms attached through carbon or hetro atoms

IsAmideNitrogen

```
$Status = $Atom->IsAmideNitrogen();
```

Returns 1 or 0 based on whether it's amide nitrogen *Atom*.

IsAromatic

```
$Status = $Atom->IsAromatic();
```

Returns 1 or 0 based on whether it's an aromatic *Atom*.

IsBromine

```
$Status = $Atom->IsBromine();
```

Returns 1 or 0 based on whether it's a bromine *Atom*.

IsCarbon

```
$Status = $Atom->IsCarbon();
```

Returns 1 or 0 based on whether it's a carbon *Atom*.

IsCarboxylCarbon

```
$Status = $Atom->IsCarboxylCarbon();
```

Returns 1 or 0 based on whether it's a carboxyl carbon atom in carboxyl group: R-C(=O)-OH.

IsCarboxylOxygen

```
$Status = $Atom->IsCarboxylOxygen();
```

Returns 1 or 0 based on whether it's a carboxyl oxygen atom in carboxyl group: R-C(=O)-OH.

IsCarboxylateCarbon

```
$Status = $Atom->IsCarboxylateCarbon();
```

Returns 1 or 0 based on whether it's a carboxylate carbon atom in carboxyl group: R-C(=O)-O-.

IsCarboxylateOxygen

```
$Status = $Atom->IsCarboxylateOxygen();
```

Returns 1 or 0 based on whether it's a carboxylate oxygen atom in carboxyl group: R-C(=O)-O-.

IsChlorine

```
$Status = $Atom->IsChlorine();
```

Returns 1 or 0 based on whether it's a chlorine *Atom*.

IsFluorine

```
$Status = $Atom->IsFluorine();
```

Returns 1 or 0 based on whether it's a fluorine *Atom*.

IsFunctionalClassType

```
$Status = $Atom->IsFunctionalClassType($Type);
```

Returns 1 or 0 based on whether it's a specified functional class *Type*.

The current release of MayaChemTools supports following abbreviations and descriptive names for *FunctionalClassType*:

```
HBD: HydrogenBondDonor
HBA: HydrogenBondAcceptor
PI : PositivelyIonizable
NI : NegativelyIonizable
Ar : Aromatic
Hal : Halogen
H : Hydrophobic
RA : RingAtom
CA : ChainAtom
```

The following definitions are used to determine functional class types: [Ref 60-61, Ref 65-66]:

```
HydrogenBondDonor: NH, NH2, OH
HydrogenBondAcceptor: N[!H], O
PositivelyIonizable: +, NH2
NegativelyIonizable: -, C(=O)OH, S(=O)OH, P(=O)OH
```

IsGuadiniumCarbon

```
$Status = $Atom->IsGuadiniumCarbon();
```

Returns 1 or 0 based on whether it's a guadinium carbon in guadinium group by checking its neighbors for a nitrogen in guadinium group.

IsGuadiniumNitrogen

```
$Status = $Atom->IsGuadiniumNitrogen();
```

Returns 1 or 0 based on whether it's a guadinium nitrogen in guadinium group.

A guadinium group is defined as:

```
R2N-C(=NR)-(NR2) or R2N-C(=NR2+)-(NR2)
```

where:

- o R = Hydrogens or group of atoms attached through carbon
- o Only one of the three nitrogens has a double bond to carbon and has optional formal charge allowing it to be neutral or charged state

IsHBondAcceptor

```
$Status = $Atom->IsHBondAcceptor();
$Status = $Atom->IsHBondAcceptor($HydrogenBondsType);
```

Returns 1 or 0 based on whether it's a hydrogen bond acceptor *Atom*.

IsHBondDonor

```
$Status = $Atom->IsHBondDonor();
```

```
$Status = $Atom->IsHBondDonor($HydrogenBondsType);
```

Returns 1 or 0 based on whether it's a hydrogen bond donor *Atom*.

IsHydrogenBondAcceptor

```
$Status = $Atom->IsHydrogenBondAcceptor();
$Status = $Atom->IsHydrogenBondAcceptor($HydrogenBondsType);
```

Returns 1 or 0 based on whether it's a hydrogen bond acceptor *Atom*.

IsHydrogenBondDonor

```
$Status = $Atom->IsHydrogenBondDonor();
$Status = $Atom->IsHydrogenBondDonor($HydrogenBondsType);
```

Returns 1 or 0 based on whether it's a hydrogen bond donor *Atom*.

The current release of MayaChemTools supports identification of two types of hydrogen bond donor and acceptor atoms with these names:

```
HBondsType1 or HydrogenBondsType1
HBondsType2 or HydrogenBondsType2
```

The names of these hydrogen bond types are rather arbitrary. However, their definitions have specific meaning and are as follows:

```
HydrogenBondsType1 [ Ref 60-61, Ref 65-66 ]:
```

```
Donor: NH, NH2, OH - Any N and O with available H
Acceptor: N[!H], O - Any N without available H and any O
```

```
HydrogenBondsType2 [ Ref 91 ]:
```

```
Donor: NH, NH2, OH - N and O with available H
Acceptor: N, O - And N and O
```

By default, *HydrogenBondsType1* is used to calculate number hydrogen bond donor and acceptor atoms. *HydrogenBondsType2* corresponds to RuleOf5 definition of hydrogen bond donors and acceptors.

IsHalogen

```
$Status = $Atom->IsHalogen();
```

Returns 1 or 0 based on whether it's a halogen *Atom*.

IsHetroAtom

```
$Status = $Atom->IsHetroAtom();
```

Returns 0 or 1 based on whether it's a hetro *Atom*. Following atoms are considered hetro atoms: N, O, F, P, S, Cl, Br, I

IsHydrogen

```
$Status = $Atom->IsHydrogen();
```

Returns 1 or 0 based on whether it's a hydrogen *Atom*.

IsHydrophobic

```
$Status = $Atom->IsHydrophobic();
```

Returns 1 or 0 based on whether it's a hydrophobic *Atom*.

IsInRing

```
$Status = $Atom->IsInRing();
```

Returns 1 or 0 based on whether *Atom* is present in a ring.

IsInRingOfSize

```
$Status = $Atom->IsInRingOfSize($Size);
```

Returns 1 or 0 based on whether *Atom* is present in a ring of specific *Size*.

IsIodine

```
$Status = $Atom->IsIodine();
```

Returns 1 or 0 based on whether it's an iodine *Atom*.

IsIsotope

```
$Status = $Atom->IsIsotope();
```

Returns 1 or 0 based on whether it's an isotope *Atom*.

IsLipophilic

```
$Status = $Atom->IsLipophilic();
```

Returns 1 or 0 based on whether it's a lipophilic *Atom*.

IsMetallic

```
$Status = $Atom->IsMetallic();
```

Returns 1 or 0 based on whether it's a metallic *Atom*.

IsNegativelyIonizable

```
$Status = $Atom->IsNegativelyIonizable();
```

Returns 1 or 0 based on whether it's a negatively ionizable atom *Atom*.

IsNitrogen

```
$Status = $Atom->IsNitrogen();
```

Returns 1 or 0 based on whether it's a nitrogen *Atom*.

IsNonCarbonOrHydrogen

```
$Status = $Atom->IsNonCarbonOrHydrogen();
```

Returns 1 or 0 based on whether it's not a carbon or hydrogen *Atom*.

IsNotInRing

```
$Status = $Atom->IsNotInRing();
```

Returns 1 or 0 based on whether *Atom* is not present in a ring.

IsOnlyInOneRing

```
$Status = $Atom->IsOnlyInOneRing();
```

Returns 1 or 0 based on whether *Atom* is only present in one ring.

IsOxygen

```
$Status = $Atom->IsOxygen();
```

Returns 0 or 1 based on whether it's an oxygen *Atom*.

IsPhosphorus

```
$Status = $Atom->IsPhosphorus();
```

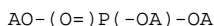
Returns 0 or 1 based on whether it's a phosphorus *Atom*.

IsPhosphateOxygen

```
$Status = $Atom->IsPhosphateOxygen();
```

Returns 1 or 0 based on whether it's a phosphate oxygen in phosphate group.

A phosphate group is defined as:



Where:

A - Any group of atoms including hydrogens

IsPhosphatePhosphorus

```
$Status = $Atom->IsPhosphatePhosphorus();
```

Returns 1 or 0 based on whether it's a phosphate phosphorus in phosphate group.

IsPolarAtom

```
$Status = $Atom->IsPolarAtom();
```

Returns 0 or 1 based on whether it's a polar *Atom*. Following atoms are considered polar atoms: N, O, P, S.

IsPolarHydrogen

```
$Status = $Atom->IsPolarHydrogen();
```

Returns 0 or 1 based on whether it's a hydrogen *Atom* bonded to a polar atom.

IsPositivelyIonizable

```
$Status = $Atom->IsPositivelyIonizable();
```

Returns 1 or 0 based on whether it's a positively ionizable *Atom*.

IsSaturated

```
$Status = $Atom->IsSaturated();
```

Returns 1 or 0 based on whether it's a saturated *Atom*. An atom attached to other atoms with only single bonds is considered a saturated atom.

IsStereoCenter

```
$Status = $Atom->IsStereoCenter();
```

Returns 0 or 1 based on whether it's marked as a stereo center *Atom* by explicit setting of *StereoCenter* atom property to value of 1.

IsSilicon

```
$Status = $Atom->IsSilicon();
```

Returns 0 or 1 based on whether it's a silicon *Atom*.

IsSulfur

```
$Status = $Atom->IsSulfur();
```

Returns 0 or 1 based on whether it's a sulfur *Atom*.

IsSulphur

```
$Status = $Atom->IsSulphur();
```

Returns 0 or 1 based on whether it's a sulfur *Atom*.

IsUnsaturated

```
$Status = $Atom->IsUnsaturated();
```

Returns 1 or 0 based on whether it's an unsaturated *Atom*. An atom attached to other atoms with at least one non-single bond is considered an unsaturated atom.

IsTopologicalPharmacophoreType

```
$Status = $Atom->IsTopologicalPharmacophoreType();
```

Returns 1 or 0 based on whether it's any of the supported topological pharmacophore *Atom* type. See *IsFunctionalClassType* for a list of supported types.

SetAtomSymbol

```
$Atom->SetAtomSymbol($AtomicSymbol);
```

Sets atom symbol for *Atom* and returns *Atom* object. The appropriate atomic number is also set automatically.

SetAtomicNumber

```
$Atom->SetAtomicNumber($AtomicNumber);
```

Sets atomic number for *Atom* and returns *Atom* object. The appropriate atom symbol is also set automatically.

SetMassNumber

```
$Atom->SetMassNumber($MassNumber);
```

Sets mass number for *Atom* and returns *Atom* object.

SetStereoCenter

```
$Atom->SetStereoCenter($StereoCenter);
```

Sets stereo center for *Atom* and returns *Atom* object.

SetStereochemistry

```
$Atom->SetStereochemistry($Stereochemistry);
```

Sets stereo chemistry for *Atom* and returns *Atom* object.

SetX

```
$Atom->SetX($Value);
```

Sets X-coordinate value for *Atom* and returns *Atom* object.

SetXYZ

```
$Atom->SetXYZ(@XYZValues);
```

```
$Atom->SetXYZ($XYZValuesRef);  
$Atom->SetXYZ($XYZVector);
```

Sets *Atom* coordinates using an array, reference to an array or a *Vector* object and returns *Atom* object.

SetY

```
$Atom->SetY($Value);
```

Sets Y-coordinate value for *Atom* and returns *Atom* object.

SetZ

```
$Atom->SetZ($Value);
```

Sets Z-coordinate value for *Atom* and returns *Atom* object.

StringifyAtom

```
$AtomString = $Atom->StringifyAtom();
```

Returns a string containing information about *Atom* object.

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SEE ALSO

Bond.pm, Molecule.pm, MoleculeFileIO.pm

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