

## Assignment 2

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<b>1 Hierarchical Index</b>	<b>1</b>
1.1 Class Hierarchy	1
<b>2 Class Index</b>	<b>3</b>
2.1 Class List	3
<b>3 File Index</b>	<b>5</b>
3.1 File List	5
<b>4 Class Documentation</b>	<b>7</b>
4.1 ChemEntity.ChemEntity Class Reference	7
4.1.1 Member Function Documentation	7
4.1.1.1 num_atoms()	7
4.2 CompoundT.CompoundT Class Reference	8
4.2.1 Detailed Description	8
4.2.2 Constructor & Destructor Documentation	8
4.2.2.1 __init__()	8
4.2.3 Member Function Documentation	9
4.2.3.1 constit_elems()	9
4.2.3.2 equals()	9
4.2.3.3 get_molec_set()	10
4.2.3.4 num_atoms()	10
4.3 ChemTypes.ElementT Class Reference	10
4.3.1 Detailed Description	13
4.4 ElmSet.ElmSet Class Reference	13
4.4.1 Detailed Description	13
4.5 Equality.Equality Class Reference	14
4.5.1 Detailed Description	14
4.5.2 Member Function Documentation	14
4.5.2.1 equals()	14
4.6 MolecSet.MolecSet Class Reference	15
4.6.1 Detailed Description	15
4.7 MoleculeT.MoleculeT Class Reference	15
4.7.1 Detailed Description	16
4.7.2 Constructor & Destructor Documentation	16
4.7.2.1 __init__()	16
4.7.3 Member Function Documentation	16
4.7.3.1 __eq__()	16
4.7.3.2 constit_elems()	17
4.7.3.3 equals()	17
4.7.3.4 get_elm()	18
4.7.3.5 get_num()	18
4.7.3.6 num_atoms()	18

4.8 ReactionT.ReactionT Class Reference	19
4.8.1 Detailed Description	19
4.8.2 Constructor & Destructor Documentation	19
4.8.2.1 <code>__init__()</code>	19
4.8.3 Member Function Documentation	20
4.8.3.1 <code>__elm_in_chem_eq__()</code>	20
4.8.3.2 <code>get_lhs()</code>	20
4.8.3.3 <code>get_lhs_coeff()</code>	20
4.8.3.4 <code>get_rhs()</code>	21
4.8.3.5 <code>get_rhs_coeff()</code>	21
4.9 Set.Set Class Reference	21
4.9.1 Detailed Description	22
4.9.2 Constructor & Destructor Documentation	22
4.9.2.1 <code>__init__()</code>	22
4.9.3 Member Function Documentation	22
4.9.3.1 <code>add()</code>	22
4.9.3.2 <code>equals()</code>	23
4.9.3.3 <code>member()</code>	23
4.9.3.4 <code>rm()</code>	24
4.9.3.5 <code>size()</code>	24
4.9.3.6 <code>to_seq()</code>	24
<b>5 File Documentation</b>	<b>25</b>
5.1 <code>src/ChemEntity.py</code> File Reference	25
5.1.1 Detailed Description	25
5.2 <code>src/ChemTypes.py</code> File Reference	25
5.2.1 Detailed Description	26
5.3 <code>src/CompoundT.py</code> File Reference	26
5.3.1 Detailed Description	26
5.4 <code>src/Equality.py</code> File Reference	26
5.4.1 Detailed Description	27
5.5 <code>src/MolecSet.py</code> File Reference	27
5.5.1 Detailed Description	27
5.6 <code>src/MoleculeT.py</code> File Reference	27
5.6.1 Detailed Description	27
5.7 <code>src/ReactionT.py</code> File Reference	28
5.7.1 Detailed Description	28
5.8 <code>src/Set.py</code> File Reference	28
5.8.1 Detailed Description	28
<b>Index</b>	<b>29</b>

## Chapter 1

# Hierarchical Index

### 1.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

ReactionT.ReactionT . . . . .	19
ABC	
ChemEntity.ChemEntity . . . . .	7
CompoundT.CompoundT . . . . .	8
MoleculeT.MoleculeT . . . . .	15
Equality.Equality . . . . .	14
CompoundT.CompoundT . . . . .	8
MoleculeT.MoleculeT . . . . .	15
Set.Set . . . . .	21
ElmSet.ElmSet . . . . .	13
MolecSet.MolecSet . . . . .	15
Enum	
ChemTypes.ElementT . . . . .	10



## Chapter 2

# Class Index

### 2.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

<a href="#">ChemEntity.ChemEntity</a> . . . . .	7
<a href="#">CompoundT.CompoundT</a> Class that represents a Compound, inherits ChemEntity and Equality . . . . .	8
<a href="#">ChemTypes.ElementT</a> A data type to hold all elements in the periodic table . . . . .	10
<a href="#">ElmSet.ElmSet</a> Inherits from Set, just used for new name of Set . . . . .	13
<a href="#">Equality.Equality</a> An abstract class for comparing two objects . . . . .	14
<a href="#">MolecSet.MolecSet</a> Inherits from Set, just used for new name of Set . . . . .	15
<a href="#">MoleculeT.MoleculeT</a> Class that represents a molecule, inherits ChemEntity and Equality . . . . .	15
<a href="#">ReactionT.ReactionT</a> Class to simulate a reaction with balancing the equation . . . . .	19
<a href="#">Set.Set</a> Class that represents a <a href="#">Set</a> . . . . .	21





## Chapter 3

# File Index

### 3.1 File List

Here is a list of all documented files with brief descriptions:

src/ <a href="#">ChemEntity.py</a>	Abstract interface for methods about chemical entities . . . . .	25
src/ <a href="#">ChemTypes.py</a>	Definition of Element types . . . . .	25
src/ <a href="#">CompoundT.py</a>	Class for holding a MolecSet . . . . .	26
src/ <a href="#">Equality.py</a>	Used for comparing two objects @Date Feb 1, 2020 . . . . .	26
src/ <a href="#">MolecSet.py</a>	Class used to rename the Set, set of MoleculeT . . . . .	27
src/ <a href="#">MoleculeT.py</a>	Class for holding the Molecule which includes element and number of it . . . . .	27
src/ <a href="#">ReactionT.py</a>	Class that holds two compounds for the reactions . . . . .	28
src/ <a href="#">Set.py</a>	Class for Set building and applying methods to the Set . . . . .	28

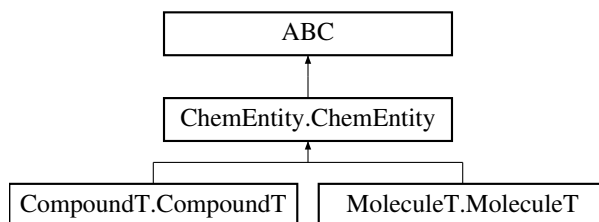


## Chapter 4

# Class Documentation

### 4.1 ChemEntity.ChemEntity Class Reference

Inheritance diagram for ChemEntity.ChemEntity:



#### Public Member Functions

- def `num_atoms` (self, element\_t)  
*An abstract method for counting number of atoms.*
- def `constit_elems` (self)

#### 4.1.1 Member Function Documentation

##### 4.1.1.1 num\_atoms()

```
def ChemEntity.ChemEntity.num_atoms (  
    self,  
    element_t )
```

An abstract method for counting number of atoms.

## Parameters

<i>element</i> ↔	
<i>_t</i>	

Reimplemented in [MoleculeT.MoleculeT](#), and [CompoundT.CompoundT](#).

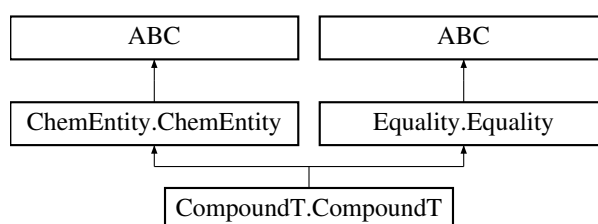
The documentation for this class was generated from the following file:

- [src/ChemEntity.py](#)

## 4.2 CompoundT.CompoundT Class Reference

Class that represents a Compound, inherits ChemEntity and Equality.

Inheritance diagram for CompoundT.CompoundT:



### Public Member Functions

- `def __init__ (self, molec_set)`  
*Constructor to initialize the object with a MolecSet.*
- `def get_molec_set (self)`  
*Return the Compound which is a MolecSet.*
- `def num_atoms (self, element)`  
*Return the number of atoms in the MolecSet with the specified element.*
- `def constit_elems (self)`  
*Returns the ElmSet of the all the different ElementT in the compound.*
- `def equals (self, other_compound)`  
*Check if the two compounds are equal.*
- `def __eq__ (self, other)`

#### 4.2.1 Detailed Description

Class that represents a Compound, inherits ChemEntity and Equality.

#### 4.2.2 Constructor & Destructor Documentation

##### 4.2.2.1 \_\_init\_\_()

```
def CompoundT.CompoundT.__init__ (
    self,
    molec_set )
```

Constructor to initialize the object with a MolecSet.

## Parameters

<i>molec_set</i>	- MolecSet to be stored in a Compound
------------------	---------------------------------------

## 4.2.3 Member Function Documentation

### 4.2.3.1 constit\_elems()

```
def CompoundT.CompoundT.constit_elems (
    self )
```

Returns the ElmSet of the all the different ElementT in the compound.

Using get\_elm() function for MoleculeT to get the element

## Returns

ElmSet of all the ElementT

Reimplemented from [ChemEntity.ChemEntity](#).

### 4.2.3.2 equals()

```
def CompoundT.CompoundT.equals (
    self,
    other_compound )
```

Check if the two compounds are equal.

## Parameters

<i>other_compound</i>	- other compound to compare with
-----------------------	----------------------------------

## Returns

true if equal else false

Reimplemented from [Equality.Equality](#).

#### 4.2.3.3 get\_molec\_set()

```
def CompoundT.CompoundT.get_molec_set (
    self )
```

Return the Compound which is a MolecSet.

##### Returns

MolecSet

#### 4.2.3.4 num\_atoms()

```
def CompoundT.CompoundT.num_atoms (
    self,
    element )
```

Return the number of atoms in the MolecSet with the specified element.

Using functional programming functions, turn the MolecSet into a sequence to iterate over and find the number of atoms for each MolecSet with a specified element then sum up the list

##### Parameters

<i>element</i>	- ElementT
----------------	------------

##### Returns

the total number of atoms of element in the Compound

Reimplemented from [ChemEntity.ChemEntity](#).

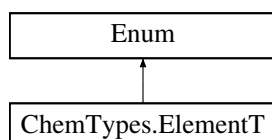
The documentation for this class was generated from the following file:

- [src/CompoundT.py](#)

## 4.3 ChemTypes.ElementT Class Reference

A data type to hold all elements in the periodic table.

Inheritance diagram for ChemTypes.ElementT:



## Static Public Attributes

- **H** = auto()
- **He** = auto()
- **Li** = auto()
- **Be** = auto()
- **B** = auto()
- **C** = auto()
- **N** = auto()
- **O** = auto()
- **F** = auto()
- **Ne** = auto()
- **Na** = auto()
- **Mg** = auto()
- **Al** = auto()
- **Si** = auto()
- **P** = auto()
- **S** = auto()
- **Cl** = auto()
- **Ar** = auto()
- **K** = auto()
- **Ca** = auto()
- **Sc** = auto()
- **Ti** = auto()
- **V** = auto()
- **Cr** = auto()
- **Mn** = auto()
- **Fe** = auto()
- **Co** = auto()
- **Ni** = auto()
- **Cu** = auto()
- **Zn** = auto()
- **Ga** = auto()
- **Ge** = auto()
- **As** = auto()
- **Se** = auto()
- **Br** = auto()
- **Kr** = auto()
- **Rb** = auto()
- **Sr** = auto()
- **Y** = auto()
- **Zr** = auto()
- **Nb** = auto()
- **Mo** = auto()
- **Tc** = auto()
- **Ru** = auto()
- **Rh** = auto()
- **Pd** = auto()
- **Ag** = auto()
- **Cd** = auto()
- **In** = auto()
- **Sn** = auto()
- **Sb** = auto()
- **Te** = auto()
- **I** = auto()

- **Xe** = auto()
- **Cs** = auto()
- **Ba** = auto()
- **La** = auto()
- **Ce** = auto()
- **Pr** = auto()
- **Nd** = auto()
- **Pm** = auto()
- **Sm** = auto()
- **Eu** = auto()
- **Gd** = auto()
- **Tb** = auto()
- **Dy** = auto()
- **Ho** = auto()
- **Er** = auto()
- **Tm** = auto()
- **Yb** = auto()
- **Lu** = auto()
- **Hf** = auto()
- **Ta** = auto()
- **W** = auto()
- **Re** = auto()
- **Os** = auto()
- **Ir** = auto()
- **Pt** = auto()
- **Au** = auto()
- **Hg** = auto()
- **Tl** = auto()
- **Pb** = auto()
- **Bi** = auto()
- **Po** = auto()
- **At** = auto()
- **Rn** = auto()
- **Fr** = auto()
- **Ra** = auto()
- **Ac** = auto()
- **Th** = auto()
- **Pa** = auto()
- **U** = auto()
- **Np** = auto()
- **Pu** = auto()
- **Am** = auto()
- **Cm** = auto()
- **Bk** = auto()
- **Cf** = auto()
- **Es** = auto()
- **Fm** = auto()
- **Md** = auto()
- **No** = auto()
- **Lr** = auto()
- **Rf** = auto()
- **Db** = auto()
- **Sg** = auto()
- **Bh** = auto()
- **Hs** = auto()



- **Mt** = auto()
- **Ds** = auto()
- **Rg** = auto()
- **Cn** = auto()
- **Nh** = auto()
- **Fl** = auto()
- **Mc** = auto()
- **Lv** = auto()
- **Ts** = auto()
- **Og** = auto()

### 4.3.1 Detailed Description

A data type to hold all elements in the periodic table.

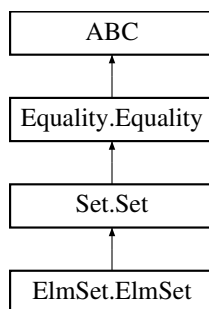
The documentation for this class was generated from the following file:

- [src/ChemTypes.py](#)

## 4.4 ElmSet.ElmSet Class Reference

Inherits from Set, just used for new name of Set.

Inheritance diagram for ElmSet.ElmSet:



### Additional Inherited Members

#### 4.4.1 Detailed Description

Inherits from Set, just used for new name of Set.

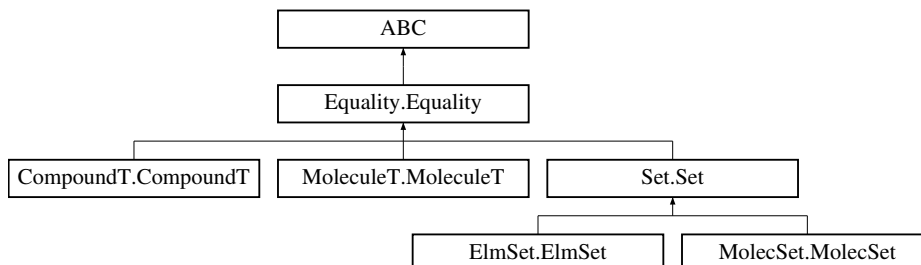
The documentation for this class was generated from the following file:

- [src/ElmSet.py](#)

## 4.5 Equality.Equality Class Reference

An abstract class for comparing two objects.

Inheritance diagram for Equality.Equality:



### Public Member Functions

- `def equals (self, other)`  
*Abstract method for checking if two objects are equal.*

#### 4.5.1 Detailed Description

An abstract class for comparing two objects.

#### 4.5.2 Member Function Documentation

##### 4.5.2.1 equals()

```
def Equality.Equality.equals (  
    self,  
    other )
```

Abstract method for checking if two objects are equal.

##### Parameters

<i>other</i>	Object to compare against
--------------	---------------------------

##### Returns

true is equal else false

Reimplemented in [Set.Set](#), [MoleculeT.MoleculeT](#), and [CompoundT.CompoundT](#).

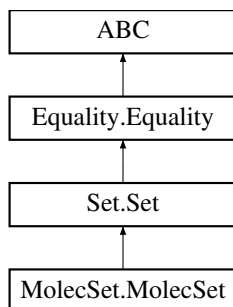
The documentation for this class was generated from the following file:

- [src/Equality.py](#)

## 4.6 MolecSet.MolecSet Class Reference

Inherits from Set, just used for new name of Set.

Inheritance diagram for MolecSet.MolecSet:



### Additional Inherited Members

#### 4.6.1 Detailed Description

Inherits from Set, just used for new name of Set.

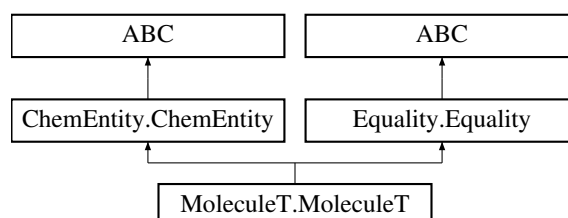
The documentation for this class was generated from the following file:

- [src/MolecSet.py](#)

## 4.7 MoleculeT.MoleculeT Class Reference

Class that represents a molecule, inherits ChemEntity and Equality.

Inheritance diagram for MoleculeT.MoleculeT:



## Public Member Functions

- def `__init__` (self, num, elm)  
*Constructor that initializes a Molecule with element and number of those element.*
- def `get_num` (self)  
*Get the number of atoms in the molecule.*
- def `get_elm` (self)  
*Get the element.*
- def `num_atoms` (self, element)  
*Return the number of atom in the Molecule.*
- def `constit_elems` (self)  
*Return the element in a ElmSet.*
- def `equals` (self, other\_m)  
*Check if the other [MoleculeT](#) is the same as current object.*
- def `__eq__` (self, other)  
*The default equals for Python.*
- def `__hash__` (self)

### 4.7.1 Detailed Description

Class that represents a molecule, inherits ChemEntity and Equality.

### 4.7.2 Constructor & Destructor Documentation

#### 4.7.2.1 `__init__()`

```
def MoleculeT.MoleculeT.__init__ (  
    self,  
    num,  
    elm )
```

Constructor that initializes a Molecule with element and number of those element.

Parameters

<code>num</code>	- number of element in that molecule, elm - ElementT
------------------	--

### 4.7.3 Member Function Documentation

#### 4.7.3.1 `__eq__()`

```
def MoleculeT.MoleculeT.__eq__ (  
    self,
```

*other* )

The default equals for Python.

But we don't want that we want to use our equals method

#### Parameters

<i>Other</i>	- <a href="#">MoleculeT</a>
--------------	-----------------------------

#### Returns

the result of our equals method

#### 4.7.3.2 `constit_elems()`

```
def MoleculeT.MoleculeT.constit_elems (
    self )
```

Return the element in a ElmSet.

#### Returns

ElmSet of the element

Reimplemented from [ChemEntity.ChemEntity](#).

#### 4.7.3.3 `equals()`

```
def MoleculeT.MoleculeT.equals (
    self,
    other_m )
```

Check if the other [MoleculeT](#) is the same as current object.

Checking by if it is the same ElementT and same number of atoms

#### Parameters

<i>other</i> ↔ <i>_m</i>	- <a href="#">MoleculeT</a> to compare with
-----------------------------	---

#### Returns

True if the same else False

Reimplemented from [Equality.Equality](#).

#### 4.7.3.4 get\_elm()

```
def MoleculeT.MoleculeT.get_elm (
    self )
```

Get the element.

##### Returns

ElementT of element

#### 4.7.3.5 get\_num()

```
def MoleculeT.MoleculeT.get_num (
    self )
```

Get the number of atoms in the molecule.

##### Returns

the number of atoms of the element

#### 4.7.3.6 num\_atoms()

```
def MoleculeT.MoleculeT.num_atoms (
    self,
    element )
```

Return the number of atom in the Molecule.

If the inputted element is the same as the [MoleculeT](#) then return the number of atoms else 0

##### Parameters

<i>element</i>	- ElementT to get
----------------	-------------------

##### Returns

Number of atoms or 0

Reimplemented from [ChemEntity.ChemEntity](#).

The documentation for this class was generated from the following file:

- [src/MoleculeT.py](#)

## 4.8 ReactionT.ReactionT Class Reference

Class to simulate a reaction with balancing the equation.

### Public Member Functions

- `def __init__(self, left_compound, right_compound)`  
*Constructor for [ReactionT](#) which balances before storing it.*
- `def get_lhs(self)`  
*Return the left hand side of [ReactionT](#).*
- `def get_rhs(self)`  
*Return the right hand side of [ReactionT](#).*
- `def get_lhs_coeff(self)`  
*Return the coeffs for the left side.*
- `def get_rhs_coeff(self)`  
*Return the coeffs for the right side.*
- `def __elm_in_chem_eq__(self, c)`  
*Return the [ElementT](#) in the compound.*
- `def __calc_coeffs__(self, left_compound, right_compound)`
- `def __n_atoms__(self, comp, c, element)`
- `def __is_bal_elm__(self, left_comp, right_comp, left_coef, right_coef, element)`
- `def __is_balanced__(self, left_comp, right_comp, left_coef, right_coef)`

### 4.8.1 Detailed Description

Class to simulate a reaction with balancing the equation.

### 4.8.2 Constructor & Destructor Documentation

#### 4.8.2.1 \_\_init\_\_()

```
def ReactionT.ReactionT.__init__(  
    self,  
    left_compound,  
    right_compound )
```

Constructor for [ReactionT](#) which balances before storing it.

Uses local functions to calculate the coeffs, then check if it is balanced else throw Value Error The reason I dont check for positive coeffs is because I make them positive in the calculation of coeffs

## Parameters

<i>left_compound</i>	- CompoundT right_compound - CompoundT
----------------------	--

## 4.8.3 Member Function Documentation

### 4.8.3.1 `__elm_in_chem_eq__()`

```
def ReactionT.ReactionT.__elm_in_chem_eq__ (
    self,
    c )
```

Return the ElementT in the compound.

## Returns

ElmSet of elements

### 4.8.3.2 `get_lhs()`

```
def ReactionT.ReactionT.get_lhs (
    self )
```

Return the left hand side of [ReactionT](#).

## Returns

the left side CompoundT

### 4.8.3.3 `get_lhs_coeff()`

```
def ReactionT.ReactionT.get_lhs_coeff (
    self )
```

Return the coeffs for the left side.

## Returns

list of coeffs



#### 4.8.3.4 get\_rhs()

```
def ReactionT.ReactionT.get_rhs (
    self )
```

Return the right hand side of [ReactionT](#).

##### Returns

the right side CompoundT

#### 4.8.3.5 get\_rhs\_coeff()

```
def ReactionT.ReactionT.get_rhs_coeff (
    self )
```

Return the coeffs for the right side.

##### Returns

list of coeffs

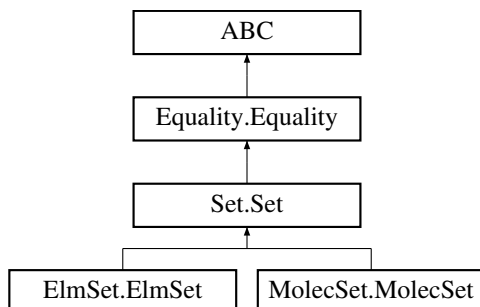
The documentation for this class was generated from the following file:

- [src/ReactionT.py](#)

## 4.9 Set.Set Class Reference

Class that represents a [Set](#).

Inheritance diagram for Set.Set:



## Public Member Functions

- def `__init__` (self, sequence)  
*Constructor that initializes the object with set.*
- def `add` (self, element)  
*Add an element to the set.*
- def `rm` (self, element)  
*Remove a specified from the set.*
- def `member` (self, element)  
*Checks if the element is in the set.*
- def `size` (self)  
*Returns the size of the set.*
- def `equals` (self, other\_set)  
*Checks if the two sets are the same.*
- def `to_seq` (self)  
*Convert the set into a list for it to be iterable.*

### 4.9.1 Detailed Description

Class that represents a [Set](#).

### 4.9.2 Constructor & Destructor Documentation

#### 4.9.2.1 `__init__()`

```
def Set.Set.__init__ (
    self,
    sequence )
```

Constructor that initializes the object with set.

Takes in a sequence and converts it into set and holds it in the state variable

#### Parameters

<code>sequence</code>	- Takes in a sequence (list)
-----------------------	------------------------------

### 4.9.3 Member Function Documentation

#### 4.9.3.1 `add()`

```
def Set.Set.add (
    self,
```

```
element )
```

Add an element to the set.

Uses the add function of set object to add the element

#### Parameters

<i>Element</i>	to add
----------------	--------

### 4.9.3.2 equals()

```
def Set.Set.equals (
    self,
    other_set )
```

Checks if the two sets are the same.

First check if the two sets are the same then check if all the elements occur in the other set

#### Parameters

<i>other_set</i>	- <a href="#">Set</a> to check with
------------------	-------------------------------------

#### Returns

True if the same else false

Reimplemented from [Equality.Equality](#).

### 4.9.3.3 member()

```
def Set.Set.member (
    self,
    element )
```

Checks if the element is in the set.

#### Parameters

<i>Element</i>	to check
----------------	----------

#### Returns

True if in the set else false

#### 4.9.3.4 rm()

```
def Set.Set.rm (
    self,
    element )
```

Remove a specified from the set.

Uses the remove function from the [Set](#) Object

##### Parameters

<i>Specified</i>	Element
------------------	---------

##### Exceptions

<i>ValueError</i>	if element not in set
-------------------	-----------------------

#### 4.9.3.5 size()

```
def Set.Set.size (
    self )
```

Returns the size of the set.

Using len function

##### Returns

the size of the set as an integer

#### 4.9.3.6 to\_seq()

```
def Set.Set.to_seq (
    self )
```

Convert the set into a list for it to be iterable.

##### Returns

List of the sets

The documentation for this class was generated from the following file:

- src/[Set.py](#)

## Chapter 5

# File Documentation

### 5.1 src/ChemEntity.py File Reference

Abstract interface for methods about chemical entities.

#### Classes

- class [ChemEntity.ChemEntity](#)

#### 5.1.1 Detailed Description

Abstract interface for methods about chemical entities.

#### Author

Dhruv Bhavsar

#### Date

Feb 1, 2020

### 5.2 src/ChemTypes.py File Reference

Definition of Element types.

#### Classes

- class [ChemTypes.ElementT](#)  
*A data type to hold all elements in the periodic table.*

### 5.2.1 Detailed Description

Definition of Element types.

Author

Dhruv Bhavsar

Date

Feb 1, 2020

## 5.3 src/CompoundT.py File Reference

Class for holding a MolecSet.

### Classes

- class [CompoundT.CompoundT](#)

*Class that represents a Compound, inherits ChemEntity and Equality.*

### 5.3.1 Detailed Description

Class for holding a MolecSet.

Author

Dhruv Bhavsar

Date

Feb 3, 2020

## 5.4 src/Equality.py File Reference

Used for comparing two objects @Date Feb 1, 2020.

### Classes

- class [Equality.Equality](#)

*An abstract class for comparing two objects.*

### 5.4.1 Detailed Description

Used for comparing two objects @Date Feb 1, 2020.

Author

Dhruv Bhavsar

## 5.5 src/MolecSet.py File Reference

Class used to rename the Set, set of MoleculeT.

### Classes

- class [MolecSet.MolecSet](#)  
*Inherits from Set, just used for new name of Set.*

### 5.5.1 Detailed Description

Class used to rename the Set, set of MoleculeT.

Author

Dhruv Bhavsar

Date

Feb 3, 2020

## 5.6 src/MoleculeT.py File Reference

Class for holding the Molecule which includes element and number of it.

### Classes

- class [MoleculeT.MoleculeT](#)  
*Class that represents a molecule, inherits ChemEntity and Equality.*

### 5.6.1 Detailed Description

Class for holding the Molecule which includes element and number of it.

Author

Dhruv Bhavsar

Date

Feb 3, 2020

## 5.7 src/ReactionT.py File Reference

Class that holds two compounds for the reactions.

### Classes

- class [ReactionT.ReactionT](#)

*Class to simulate a reaction with balancing the equation.*

### 5.7.1 Detailed Description

Class that holds two compounds for the reactions.

#### Author

Dhruv Bhavsar

#### Date

Feb 3, 2020

## 5.8 src/Set.py File Reference

Class for Set building and applying methods to the Set.

### Classes

- class [Set.Set](#)

*Class that represents a [Set](#).*

### 5.8.1 Detailed Description

Class for Set building and applying methods to the Set.

#### Author

Dhruv Bhavsar

#### Date

Feb 2, 2020



# Index

`__elm_in_chem_eq__`  
    ReactionT.ReactionT, 20

`__eq__`  
    MoleculeT.MoleculeT, 16

`__init__`  
    CompoundT.CompoundT, 8  
    MoleculeT.MoleculeT, 16  
    ReactionT.ReactionT, 19  
    Set.Set, 22

add  
    Set.Set, 22

ChemEntity.ChemEntity, 7  
    num\_atoms, 7

ChemTypes.ElementT, 10

CompoundT.CompoundT, 8  
    \_\_init\_\_, 8  
    constit\_elems, 9  
    equals, 9  
    get\_molec\_set, 9  
    num\_atoms, 10

constit\_elems  
    CompoundT.CompoundT, 9  
    MoleculeT.MoleculeT, 17

ElmSet.ElmSet, 13

Equality.Equality, 14  
    equals, 14

equals  
    CompoundT.CompoundT, 9  
    Equality.Equality, 14  
    MoleculeT.MoleculeT, 17  
    Set.Set, 23

get\_elm  
    MoleculeT.MoleculeT, 18

get\_lhs  
    ReactionT.ReactionT, 20

get\_lhs\_coeff  
    ReactionT.ReactionT, 20

get\_molec\_set  
    CompoundT.CompoundT, 9

get\_num  
    MoleculeT.MoleculeT, 18

get\_rhs  
    ReactionT.ReactionT, 20

get\_rhs\_coeff  
    ReactionT.ReactionT, 21

member

Set.Set, 23

MolecSet.MolecSet, 15

MoleculeT.MoleculeT, 15  
    \_\_eq\_\_, 16  
    \_\_init\_\_, 16  
    constit\_elems, 17  
    equals, 17  
    get\_elm, 18  
    get\_num, 18  
    num\_atoms, 18

num\_atoms  
    ChemEntity.ChemEntity, 7  
    CompoundT.CompoundT, 10  
    MoleculeT.MoleculeT, 18

ReactionT.ReactionT, 19  
    \_\_elm\_in\_chem\_eq\_\_, 20  
    \_\_init\_\_, 19  
    get\_lhs, 20  
    get\_lhs\_coeff, 20  
    get\_rhs, 20  
    get\_rhs\_coeff, 21

rm  
    Set.Set, 23

Set.Set, 21  
    \_\_init\_\_, 22  
    add, 22  
    equals, 23  
    member, 23  
    rm, 23  
    size, 24  
    to\_seq, 24

size  
    Set.Set, 24

src/ChemEntity.py, 25

src/ChemTypes.py, 25

src/CompoundT.py, 26

src/Equality.py, 26

src/MolecSet.py, 27

src/MoleculeT.py, 27

src/ReactionT.py, 28

src/Set.py, 28

to\_seq  
    Set.Set, 24