Assignment 2

Generated by Doxygen 1.8.13

Contents

1 Hierarchical Index **1**

1.1 Class Hierarchy 1

2 Class Index **3**

2.1 Class List 3

3 File Index **5**

3.1 File List 5

4 Class Documentation **7**

4.1 ChemEntity.ChemEntity Class Reference 7

4.1.1 Detailed Description 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() 9

4.2.3.4 num_atoms() 10

4.3 ChemTypes.ElementT Class Reference 10

4.3.1 Detailed Description 12

4.4 ElmSet.ElmSet Class Reference 13

4.4.1 Detailed Description 13

4.5 Equality.Equality Class Reference 13
4.5.1 Detailed Description 14
4.6 MolecSet.MolecSet Class Reference 14
4.6.1 Detailed Description 14
4.7 MoleculeT.MoleculeT Class Reference 14
4.7.1 Detailed Description 15
4.7.2 Constructor & Destructor Documentation 15
4.7.2.1 __init__() 15
4.7.3 Member Function Documentation 16
4.7.3.1 constit_elems() 16
4.7.3.2 equals() 16
4.7.3.3 get_elm() 16
4.7.3.4 get_num() 17
4.7.3.5 num_atoms() 17
4.8 ReactionT.ReactionT Class Reference 18
4.8.1 Detailed Description 18
4.8.2 Constructor & Destructor Documentation 18
4.8.2.1 __init__() 18
4.8.3 Member Function Documentation 19
4.8.3.1 get_lhs() 19
4.8.3.2 get_lhs_coeff() 19
4.8.3.3 get_rhs() 19
4.8.3.4 get_rhs_coeff() 20
4.9 Set.Set Class Reference 20
4.9.1 Detailed Description 21
4.9.2 Constructor & Destructor Documentation 21
4.9.2.1 __init__() 21
4.9.3 Member Function Documentation 21
4.9.3.1 add() 21
4.9.3.2 equals() 22
4.9.3.3 member() 22
4.9.3.4 rm() 22
4.9.3.5 size() 23

5 File Documentation **25**

5.1 src/ChemEntity.py File Reference 25

5.1.1 Detailed Description 25

5.2 src/ChemTypes.py File Reference 25

5.2.1 Detailed Description 26

5.3 src/CompoundT.py File Reference 26

5.3.1 Detailed Description 26

5.4 src/Equality.py File Reference 26

5.4.1 Detailed Description 27

5.5 src/MolecSet.py File Reference 27

5.5.1 Detailed Description 27

5.6 src/MoleculeT.py File Reference 27

5.6.1 Detailed Description 28

5.7 src/ReactionT.py File Reference 28

5.7.1 Detailed Description 29

5.7.2 Function Documentation 29

5.7.2.1 elm_in_chem_eq() 29

5.7.2.2 frac_into_int() 29

5.7.2.3 gcd() 30

5.7.2.4 gcd_of_list() 30

5.7.2.5 is_bal_elm() 30

5.7.2.6 is_balanced() 31

5.7.2.7 n_atoms() 31

5.7.2.8 pos() 32

5.7.2.9 result_into_coeff() 32

5.7.2.10 result_into_list() 33

5.8 src/Set.py File Reference 33

5.8.1 Detailed Description 33

Index **35**

Chapter 1

Hierarchical Index

1.1 Class Hierarchy

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

- ReactionT.ReactionT 18
- ABC
  - ChemEntity.ChemEntity 7
    - CompoundT.CompoundT 8
    - MoleculeT.MoleculeT 14
  - Equality.Equality 13
    - CompoundT.CompoundT 8
    - MoleculeT.MoleculeT 14
    - Set.Set 20
      - ElmSet.ElmSet 13
      - MolecSet.MolecSet 14
- Enum
  - ChemTypes.ElementT 10

Chapter 2

Class Index

2.1 Class List

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

ChemEntity.ChemEntity
An interface that has two functions: num_atoms and constit_elms . . . 7
CompoundT.CompoundT
An abstract data type that represents a compound . . . 8
ChemTypes.ElementT
Enumerated element type . . . 10
ElmSet.ElmSet
An abstract data type that inherit everything from Set but will be used particularly on type ElementT . . . 13
Equality.Equality
An interface that contains the syntax of a function . . . 13
MolecSet.MolecSet
An abstract data type that inherit everything from Set but will be used particularly on type MoleculeT . . . 14
MoleculeT.MoleculeT
An abstract data type that represents a molecule . . . 14
ReactionT.ReactionT
An abstract data type that represents a chemical reaction . . . 18
Set.Set
An generic abstract data type that represents a set . . . 20

Chapter 3

File Index

3.1 File List

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

src/ChemEntity.py
Module that implement the interface of two functions 25
src/ChemTypes.py
Definition of types used for representing chemistry elements 25
src/CompoundT.py
Module that implements a type of CompoundT 26
src/Equality.py
Module that implements an interface of a function equals 26
src/MolecSet.py
Module that implements a set of type MoleculeT 27
src/MoleculeT.py
Module that implements a type of MoleculeT 27
src/ReactionT.py
Module that implements a type of ReactionT 28
src/Set.py
Module that creates a generic set 33

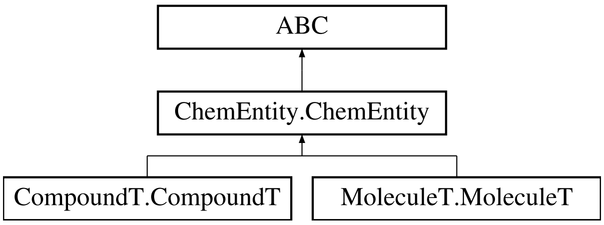
Chapter 4

Class Documentation

4.1 ChemEntity.ChemEntity Class Reference

An interface that has two functions: num_atoms and constit_elms.

Inheritance diagram for ChemEntity.ChemEntity:



Public Member Functions

- def num_atoms (self, element)

  Interface of function num_atoms.
- def constit_elems (self)

  Interface of function constit_elms.

4.1.1 Detailed Description

An interface that has two functions: num_atoms and constit_elms.

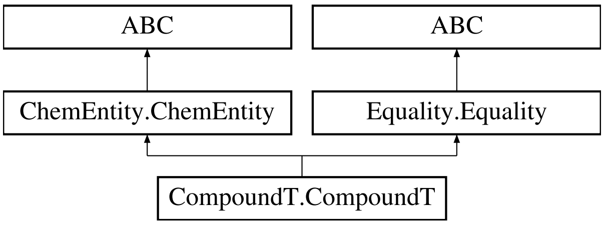
The documentation for this class was generated from the following file:

- src/ChemEntity.py

4.2 CompoundT.CompoundT Class Reference

An abstract data type that represents a compound.

Inheritance diagram for CompoundT.CompoundT:



Public Member Functions

- def __init__ (self, M)

  CompoundT constructor.
- def get_molec_set (self)

  The getter method of the class CompoundT.
- def num_atoms (self, e)

  Determine the number of the given element contained in the compound.
- def constit_elems (self)

  Determine the elements contained in the compound.
- def equals (self, D)

  Determine if the given compound is equal to this one.

Public Attributes

- **molec_set**

4.2.1 Detailed Description

An abstract data type that represents a compound.

4.2.2 Constructor & Destructor Documentation

4.2.2.1 __init__()

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

CompoundT constructor.

Construct a compound with a given set of molecules

Parameters

M	the given set of molecules

4.2.3 Member Function Documentation

4.2.3.1 constit_elems()

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

Determine the elements contained in the compound.

Returns

The set of elements contained in the compound

4.2.3.2 equals()

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

Determine if the given compound is equal to this one.

Parameters

D	the given compound

Returns

True if two compound contain the same set of molecules, false otherwise

4.2.3.3 get_molec_set()

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

The getter method of the class CompoundT.

Returns

The set of molecules contained in the compound

4.2.3.4 num_atoms()

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

Determine the number of the given element contained in the compound.

Parameters

e	the element that needs to be checked

Returns

The number of the given element contained in the compound

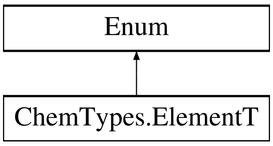
The documentation for this class was generated from the following file:

- src/CompoundT.py

4.3 ChemTypes.ElementT Class Reference

Enumerated element type.

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

Enumerated element type.

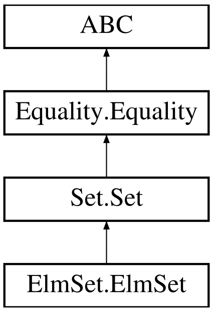
The documentation for this class was generated from the following file:

- src/ChemTypes.py

4.4 ElmSet.ElmSet Class Reference

An abstract data type that inherit everything from Set but will be used particularly on type ElementT.

Inheritance diagram for ElmSet.ElmSet:



Additional Inherited Members

4.4.1 Detailed Description

An abstract data type that inherit everything from Set but will be used particularly on type ElementT.

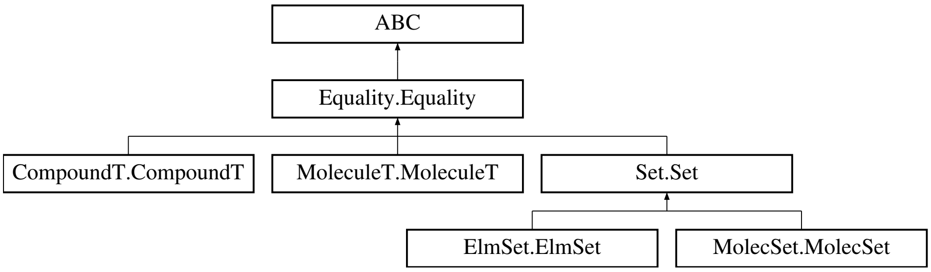
The documentation for this class was generated from the following file:

- src/ElmSet.py

4.5 Equality.Equality Class Reference

An interface that contains the syntax of a function.

Inheritance diagram for Equality.Equality:



Public Member Functions

- def equals (self, T)

  @ brief Interface of function equals

4.5.1 Detailed Description

An interface that contains the syntax of a function.

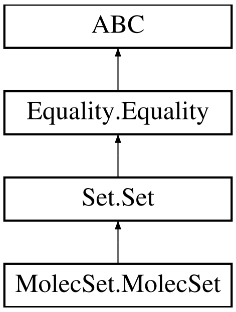
The documentation for this class was generated from the following file:

- src/Equality.py

4.6 MolecSet.MolecSet Class Reference

An abstract data type that inherit everything from Set but will be used particularly on type MoleculeT.

Inheritance diagram for MolecSet.MolecSet:



Additional Inherited Members

4.6.1 Detailed Description

An abstract data type that inherit everything from Set but will be used particularly on type MoleculeT.

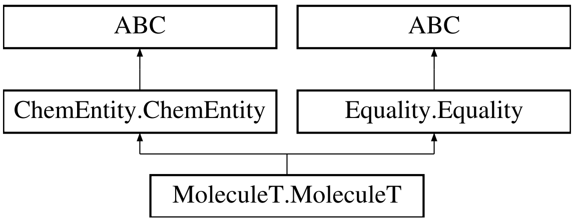
The documentation for this class was generated from the following file:

- src/MolecSet.py

4.7 MoleculeT.MoleculeT Class Reference

An abstract data type that represents a molecule.

Inheritance diagram for MoleculeT.MoleculeT:



Public Member Functions

- def __init__ (self, n, e)

  MoleculeT constructor.
- def get_num (self)

  The getter method of class MoleculeT.
- def get_elm (self)

  The getter method of class MoleculeT.
- def num_atoms (self, e)

  Determine the number of a given element in the molecule.
- def constit_elems (self)

  Determine the element contained in the molecule.
- def equals (self, m)

  Determine if two molecules are equal.

Public Attributes

- **num**
- **elm**

4.7.1 Detailed Description

An abstract data type that represents a molecule.

4.7.2 Constructor & Destructor Documentation

4.7.2.1 __init__()

```
def MoleculeT.MoleculeT.__init__ (
              self,
              n,
              e )
```

MoleculeT constructor.

Construct a molecule with a given element and the number of that element

Parameters

n	the number of the given element
e	the given element

4.7.3 Member Function Documentation

4.7.3.1 constit_elems()

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

Determine the element contained in the molecule.

Returns

A set of elements contained in the molecule

4.7.3.2 equals()

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

Determine if two molecules are equal.

Returns

True if two molecules contain the exact same elements and with the exact same numbers, false otherwise

4.7.3.3 get_elm()

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

The getter method of class MoleculeT.

Returns

The element contained in the molecule

4.7.3.4 get_num()

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

The getter method of class MoleculeT.

Returns

The number of elements contained in the molecule

4.7.3.5 num_atoms()

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

Determine the number of a given element in the molecule.

Parameters

e	The given element that needs to be checked

Returns

The number of that given element contained in the molecule; if that element is not in this molecule, return 0

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

- src/MoleculeT.py

4.8 ReactionT.ReactionT Class Reference

An abstract data type that represents a chemical reaction.

Public Member Functions

- def __init__ (self, l, r)

  The constructor of the ReactionT.
- def get_lhs (self)

  The getter method of class ReactionT.
- def get_rhs (self)

  The getter method of class ReactionT.
- def get_lhs_coeff (self)

  The getter method of class ReactionT.
- def get_rhs_coeff (self)

  The getter method of class ReactionT.

Public Attributes

- **coeffL**
- **coeffR**
- **lhs**
- **rhs**

4.8.1 Detailed Description

An abstract data type that represents a chemical reaction.

4.8.2 Constructor & Destructor Documentation

4.8.2.1 __init__()

```
def ReactionT.ReactionT.__init__ (
              self,
              l,
              r )
```

The constructor of the ReactionT.

Parameters

l	the sequence of compoundT that represents the compounds on the left side of the chemical equation
r	the sequence of compoundT that represents the compounds on the righr side of the chemical equation

4.8.3 Member Function Documentation

4.8.3.1 get_lhs()

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

The getter method of class ReactionT.

Returns

The list of compounds on the left side of the equation

4.8.3.2 get_lhs_coeff()

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

The getter method of class ReactionT.

Returns

The list of coefficients on the left side of the equation

4.8.3.3 get_rhs()

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

The getter method of class ReactionT.

Returns

The list of compounds on the rignt side of the equation

4.8.3.4 get_rhs_coeff()

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

The getter method of class ReactionT.

Returns

The list of coefficients on the right side of the equation

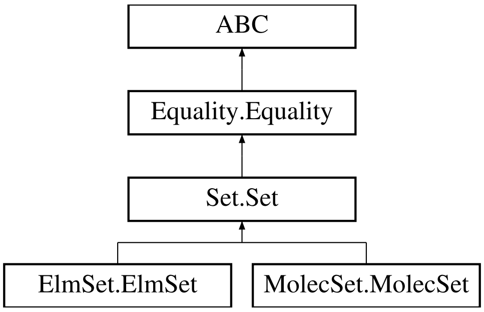
The documentation for this class was generated from the following file:

- src/ReactionT.py

4.9 Set.Set Class Reference

An generic abstract data type that represents a set.

Inheritance diagram for Set.Set:



Public Member Functions

- def __init__ (self, ss)

  Set constructor.
- def add (self, e)

  A function that adds an element into the Set.
- def rm (self, e)

  A function that removes an element from the Set.
- def member (self, e)

  A function that checks if the given element is in the Set.
- def size (self)

  A function that determines how many elements in the Set.
- def equals (self, R)

  A function that determines if the current Set object is equal to the given Set object.
- def to_seq (self)

  A function that turns the current Set into a sequence return A set that is turned from Set.

Public Attributes

- **s**

4.9.1 Detailed Description

An generic abstract data type that represents a set.

4.9.2 Constructor & Destructor Documentation

4.9.2.1 __init__()

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

Set constructor.

Put the elements of the input set or sequence into a new Set

Parameters

ss	a sequence or a set of elements of some type

4.9.3 Member Function Documentation

4.9.3.1 add()

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

A function that adds an element into the Set.

Parameters

e	an input element

4.9.3.2 equals()

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

A function that determines if the current Set object is equal to the given Set object.

Parameters

R	the given Set

Returns

True if two Sets are in the same size and contains the same elements, false otherwise

4.9.3.3 member()

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

A function that checks if the given element is in the Set.

Parameters

e	an input element

Returns

True if the given element is in the Set, false otherwise

4.9.3.4 rm()

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

A function that removes an element from the Set.

Raise ValueError if the element is not in the Set

Parameters

e	an input element

4.9.3.5 size()

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

A function that determines how many elements in the Set.

Returns

The number of elements in the Set

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

Module that implement the interface of two functions.

Classes

- class ChemEntity.ChemEntity

  An interface that has two functions: num_atoms and constit_elms.

5.1.1 Detailed Description

Module that implement the interface of two functions.

Author

Senni Tan

Date

Feb 6,2020

5.2 src/ChemTypes.py File Reference

Definition of types used for representing chemistry elements.

Classes

- class ChemTypes.ElementT

  Enumerated element type.

5.2.1 Detailed Description

Definition of types used for representing chemistry elements.

Author

Senni Tan

Date

Feb 6, 2020

5.3 src/CompoundT.py File Reference

Module that implements a type of CompoundT.

Classes

- class CompoundT.CompoundT

  An abstract data type that represents a compound.

5.3.1 Detailed Description

Module that implements a type of CompoundT.

Author

Senni Tan

Date

Feb 8, 2020

5.4 src/Equality.py File Reference

Module that implements an interface of a function equals.

Classes

- class Equality.Equality

  An interface that contains the syntax of a function.

5.4.1 Detailed Description

Module that implements an interface of a function equals.

Author

Senni Tan

Date

Feb 6, 2020

5.5 src/MolecSet.py File Reference

Module that implements a set of type MoleculeT.

Classes

- class MolecSet.MolecSet

  An abstract data type that inherit everything from Set but will be used particularly on type MoleculeT.

5.5.1 Detailed Description

Module that implements a set of type MoleculeT.

Author

Senni Tan

Date

Feb 8, 2020

5.6 src/MoleculeT.py File Reference

Module that implements a type of MoleculeT.

Classes

- class MoleculeT.MoleculeT

  An abstract data type that represents a molecule.

5.6.1 Detailed Description

Module that implements a type of MoleculeT.

Author

Senni Tan

Date

Feb 8, 2020

5.7 src/ReactionT.py File Reference

Module that implements a type of ReactionT.

Classes

- class ReactionT.ReactionT

  An abstract data type that represents a chemical reaction.

Functions

- def ReactionT.pos (s)

  A local function that determines if every element in a set is positive.
- def ReactionT.n_atoms (C, c, e)

  A local function that determines the number of atom 'e' in a given chemical reaction.
- def ReactionT.elm_in_chem_eq (C)

  A local function that determines the elements in the chemical equation.
- def ReactionT.is_bal_elm (L, R, cL, cR, e)

  A local function that determines if the given element is balanced in the given chemical equation with the given coefficients.
- def ReactionT.is_balanced (L, R, cL, cR)

  A local function that determines if the given chemical equation is balanced with the given compounds and coefficients.
- def ReactionT.result_into_list (r)

  A local function that turns the result into a list.
- def ReactionT.result_into_coeff (result, sym)

  A local function that turns the result into a list of number.
- def ReactionT.gcd (a, b)

  A local function that determine the greatest common factor of two numbers.
- def ReactionT.gcd_of_list (a)

  A local function that determine the greatest common factor of a list of numbers.
- def ReactionT.factorial_100 ()

  A local function that determine the factorial of 100 number of factorial of 100.
- def ReactionT.frac_into_int (r)

  A local function that turns a list of numbers that represents the coefficients by fractions into representing by integers.

5.7.1 Detailed Description

Module that implements a type of ReactionT.

Author

Senni Tan

Date

Feb 8, 2020

5.7.2 Function Documentation

5.7.2.1 elm_in_chem_eq()

```
def ReactionT.elm_in_chem_eq (
              C )
```

A local function that determines the elements in the chemical equation.

Parameters

C	the given sequence of compounds which represents a chemical reactiona

Returns

The set of elements in the chemical equation

5.7.2.2 frac_into_int()

```
def ReactionT.frac_into_int (
              r )
```

A local function that turns a list of numbers that represents the coefficients by fractions into representing by integers.

Parameters

r	the given list of numbers

Returns

The list of numbers that represents the coefficients by integer

5.7.2.3 gcd()

```
def ReactionT.gcd (
              a,
              b )
```

A local function that determine the greatest common factor of two numbers.

Parameters

a	one of the two given numbers
b	one of the two given numbers

Returns

the greatest common factor of two given numbers

5.7.2.4 gcd_of_list()

```
def ReactionT.gcd_of_list (
              a )
```

A local function that determine the greatest common factor of a list of numbers.

Parameters

a	the given list of numbers

Returns

the greatest common factor of all numbers in the list

5.7.2.5 is_bal_elm()

```
def ReactionT.is_bal_elm (
              L,
              R,
              cL,
              cR,
              e )
```

A local function that determines if the given element is balanced in the given chemical equation with the given coefficients.

Parameters

L	sequence of CompoundT that represents the compounds of left side of the chemical equation
R	sequence of Compound that represents the compounds of right side of the chemical equation
cL	sequence of number that represents the coefficients of the left side of the chemical equation
cR	sequence of number that represents the coefficients of the left side of the chemical equation
e	the given element

Returns

True if the given elements is balanced in the given chemical equaiton, false otherwise

5.7.2.6 is_balanced()

```
def ReactionT.is_balanced (
              L,
              R,
              cL,
              cR )
```

A local function that determines if the given chemical equation is balanced with the given compounds and coefficients.

Parameters

L	sequence of CompoundT that represents the compounds of left side of the chemical equation
R	sequence of Compound that represents the compounds of right side of the chemical equation
cL	sequence of number that represents the coefficients of the left side of the chemical equation
cR	sequence of number that represents the coefficients of the left side of the chemical equation

Returns

True if the given chemical equation is balanced, false otherwise

5.7.2.7 n_atoms()

```
def ReactionT.n_atoms (
              C,
              c,
              e )
```

A local function that determines the number of atom 'e' in a given chemical reaction.

Parameters

C	the given sequence of compounds which represents a chemical reaction
c	the given set of coefficients
e	the given element that needs to be checked

Returns

The number of atoms of element 'e' in the reaction

5.7.2.8 pos()

```
def ReactionT.pos (
              s )
```

A local function that determines if every element in a set is positive.

Parameters

s	the given set that needs to be checked

Returns

True if all elements are positive, false otherwise

5.7.2.9 result_into_coeff()

```
def ReactionT.result_into_coeff (
              result,
              sym )
```

A local function that turns the result into a list of number.

The linsolve function of the sympy library is used in this program to solve a matrix. The default result will be a relation between symbols and the result needs to be turned into numbers

Parameters

result	the list of the result

Returns

The list of the result turned into numbers

5.7.2.10 result_into_list()

```
def ReactionT.result_into_list (
              r )
```

A local function that turns the result into a list.

The linsolve function of the sympy library is used in this program to solve a matrix. The default result will be a tuple and the result needs to be turned in a list

Parameters

r	the tuple of the result

Returns

The list of the result

5.8 src/Set.py File Reference

Module that creates a generic set.

Classes

- class Set.Set

  An generic abstract data type that represents a set.

5.8.1 Detailed Description

Module that creates a generic set.

Author

Senni Tan

Date

Feb 6, 2020

Index

__init__
  CompoundT::CompoundT, 8
  MoleculeT::MoleculeT, 15
  ReactionT::ReactionT, 18
  Set::Set, 21

add
  Set::Set, 21

ChemEntity.ChemEntity, 7
ChemTypes.ElementT, 10
CompoundT.CompoundT, 8
CompoundT::CompoundT
  __init__, 8
  constit_elems, 9
  equals, 9
  get_molec_set, 9
  num_atoms, 9
constit_elems
  CompoundT::CompoundT, 9
  MoleculeT::MoleculeT, 16

elm_in_chem_eq
  ReactionT.py, 29
ElmSet.ElmSet, 13
Equality.Equality, 13
equals
  CompoundT::CompoundT, 9
  MoleculeT::MoleculeT, 16
  Set::Set, 21

frac_into_int
  ReactionT.py, 29

gcd
  ReactionT.py, 30
gcd_of_list
  ReactionT.py, 30
get_elm
  MoleculeT::MoleculeT, 16
get_lhs
  ReactionT::ReactionT, 19
get_lhs_coeff
  ReactionT::ReactionT, 19
get_molec_set
  CompoundT::CompoundT, 9
get_num
  MoleculeT::MoleculeT, 16
get_rhs
  ReactionT::ReactionT, 19
get_rhs_coeff
  ReactionT::ReactionT, 19

is_bal_elm
  ReactionT.py, 30
is_balanced
  ReactionT.py, 31

member
  Set::Set, 22
MolecSet.MolecSet, 14
MoleculeT.MoleculeT, 14
MoleculeT::MoleculeT
  __init__, 15
  constit_elems, 16
  equals, 16
  get_elm, 16
  get_num, 16
  num_atoms, 17

n_atoms
  ReactionT.py, 31
num_atoms
  CompoundT::CompoundT, 9
  MoleculeT::MoleculeT, 17

pos
  ReactionT.py, 32

ReactionT.py
  elm_in_chem_eq, 29
  frac_into_int, 29
  gcd, 30
  gcd_of_list, 30
  is_bal_elm, 30
  is_balanced, 31
  n_atoms, 31
  pos, 32
  result_into_coeff, 32
  result_into_list, 32
ReactionT.ReactionT, 18
ReactionT::ReactionT
  __init__, 18
  get_lhs, 19
  get_lhs_coeff, 19
  get_rhs, 19
  get_rhs_coeff, 19
result_into_coeff
  ReactionT.py, 32
result_into_list
  ReactionT.py, 32
rm

Set::Set, 22

Set.Set, 20
Set::Set
__init__, 21
add, 21
equals, 21
member, 22
rm, 22
size, 23
size
Set::Set, 23
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, 33