Python and Chemistry

MOLE TO MOLE STOICHIOMETRY WITH PYTHON

Recall: Balanced Chemical Equation

A balanced chemical equation shows the quantitative relationships between each of the chemical species involved in a chemical reaction.

This means a balanced chemical equation can tell us the **ratio of the number of moles** of reactants to products taking part in a chemical reaction.

Therefore, a balanced chemical equation provides important information:

1. *Type* and *number* of atoms and molecules that **interact and how they arrange**
2. The **relative number of moles** of atoms and molecules that interact and form

Mole Ratio

Ex. Nitrogen gas and hydrogen gas react to form ammonia

$$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$$

The coefficients in the equation tell us that 1 mole of N_2 reacts with 3 moles of H_2, forming 2 moles of NH_3. This quantitative relationship can be written as a mole ratio:

$$1 \text{ mol } N_2 : 3 \text{ mol } H_2 : 2 \text{ mol } NH_3$$

We can also write the relationship between two chemical species, rather that the entire chemical reaction. The relationship between N_2 and H_2 has a mole ratio of:

$$1 \text{ mol } N_2 : 3 \text{ mol } H_2$$

Mole Ratio

$$1 \text{ mol } N_2 : 3 \text{ mol } H_2 : 2 \text{ mol } NH_3$$

Using this mole ratio, the amount of moles of H_2 needed to fully react with a certain amount of N_2 or create a certain amount of NH_3 can be calculated.

Mole ratios can be used to **convert between amounts of any two substances in a chemical reaction.**

Group Discussion: If we have 2 mol of N_2, how many mol of H_2 is required to fully react if we are using the following equation,

$$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$$

Mole Ratio

Group Discussion: If we have 2 mol of N_2, how many mol of H_2 is required to fully react if we are using the following equation,

$$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$$

Answer:

$$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$$

x2 x2 x2

$$= 2N_{2(g)} + 6H_{2(g)} \rightarrow 4NH_{3(g)}$$

Therefore, 6 mol of H_2 is required to fully react with 2 mol of N_2.

Think-Pair-Share

What does the balanced chemical equation tell us about moles and how can it be used by a chemist?

Think-Pair-Share

What does the balanced chemical equation tell us about moles and how can it be used by a chemist?

A balanced chemical equation can tell us the **ratio of the number of moles** of reactants to products taking part in a chemical reaction.

Mole ratios can be used to **convert between amounts of any two substances in a chemical reaction.**

Mole to Mole Stoichiometry

The following techniques can be used to predict the # of moles that will react or form in an equation:

1. Balance the equation (always).
2. Identify givens and required.
3. Use Mole Ratio equation

$$\#\ \text{mol given}\ \times \left(\frac{\text{balanced mol of required}}{\text{balanced mol of given}}\right) = \#\ \text{mol required}$$

<u>Practice Problem:</u> Using the following equation,

$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$, determine how many moles of H_2 would be needed to fully react with 3 mol of N_2?

Mole to Mole Stoichiometry

Practice Problem: Using the following equation,

$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$, determine how many moles of H_2 would be needed to fully react with 3 mol of N_2?

Answer:

1. Balanced Equation: $N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$
2. Given: 3 mol N_2 Required: H_2 mol
3. Solve with Mole Ratio Equation

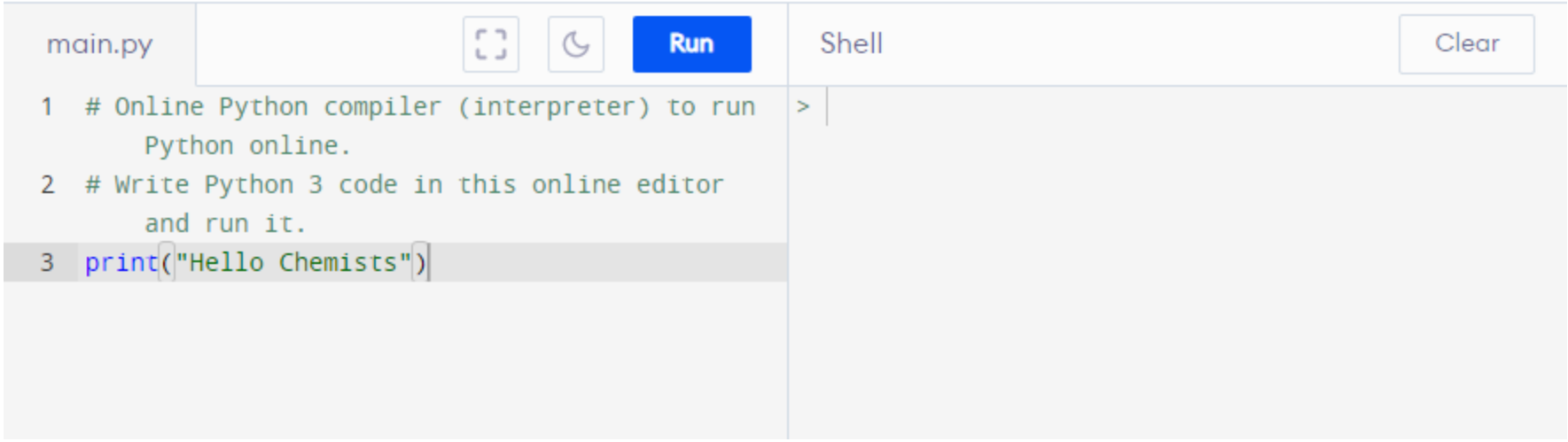
$$3 \text{ mol } N_2 \text{ x } \left(\frac{3 \text{ mol } H_2}{1 \text{ mol } N_2}\right) = 9 \text{ mol } H_2$$

Statement: Therefore, 9 mol of H_2 is required to fully react with 3 moles of N_2.

Intro to Python

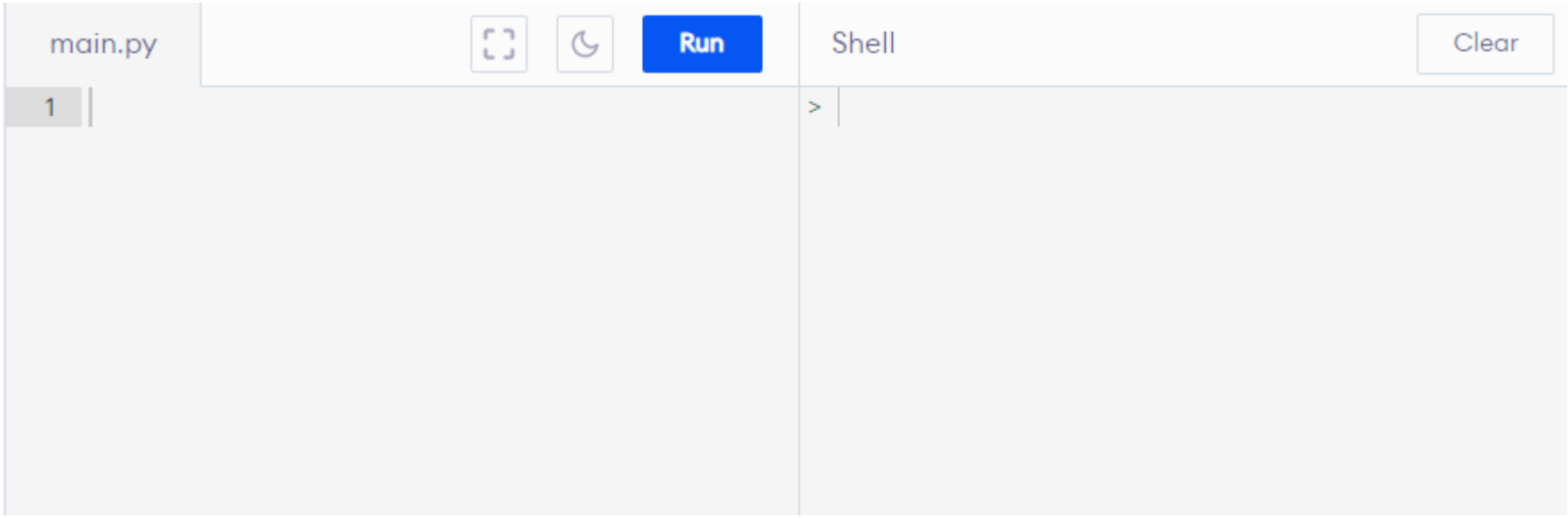
1. Begin by accessing your Code Editor, Compiler, or Interpreter.
    a. Programiz: Online Python Compiler https://www.programiz.com/python-programming/online-compiler/
    b. Replit: https://replit.com/
    c. Online Python: https://www.online-python.com/

Python code can be written in a console like the one below.



Intro to Python

2. Erase everything in the console so it is blank.
3. The code program is executed from top to bottom.



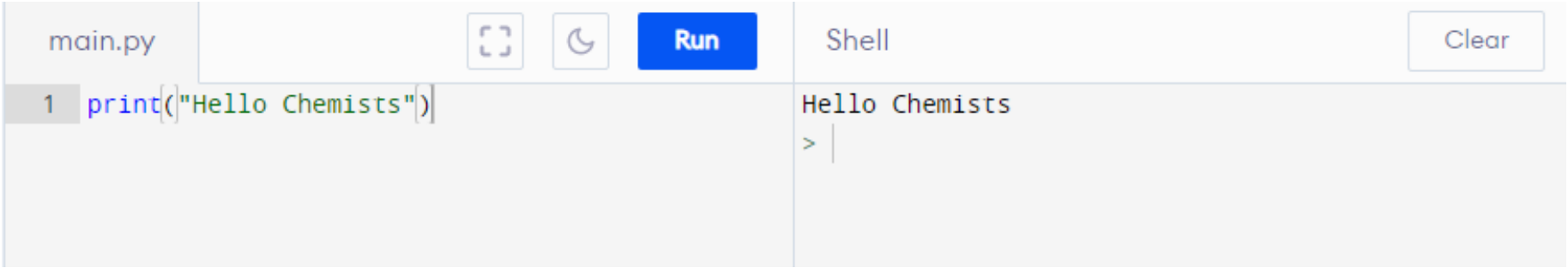
Intro to Python: Vocabulary

print: print() is one of the most basic Python functions as it allows us to display the result of the code we've written. The print() function literally prints (displays) the result to the screen.

Usually something is needed inside the bracket. If there is data text, single or double quotes surround the data text, also referred to as a string. A string is combining multiple pieces of text.

Let's try it:

1. Type in print("Hello Chemists")
2. Click Run



Intro to Python: Vocabulary

Variables: A variable is used to temporarily store data (text, numbers, etc.) in the memory of a computer. Ex. the price of a product or someone's name.

Creating a variable is called 'declaring the variable'. You name your variable and assign a value to it but there are some rules:

1. You can use letters, digits, and underscores (_) in a variable name.
2. Variable names are case sensitive: example, Example, and eXampLe are all different variables as far as Python is concerned.
3. You can't start a variable name with a digit.
4. You can't use a reserved word (i.e. def, if, else, False, True, None...) as a variable name. If you're not sure what words are reserved (i.e. Python uses them for certain functions), type help('keywords') into your shell.
5. You assign a value to a variable using the equals sign (=). First comes the variable name, then the equals sign, then the value:

```
favourite_subject = 'chemistry!'
age = 20
```

Intro to Python: Vocabulary

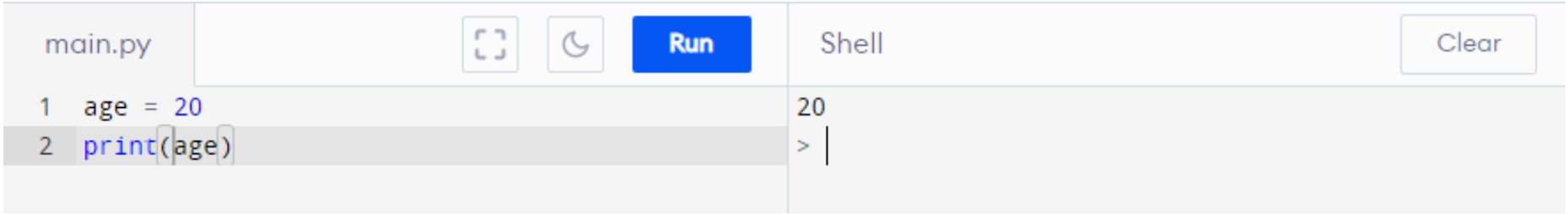
Variable Examples:

age = 20

Let's try to display (print) the age variable:

1. Type in: age = 20
2. Type in: print(age)
3. Click Run

Notice we are not adding in the quotations "" because we want to print the value of the age variable. If we included the quotations, print("age") , we would see the text age displayed.



Intro to Python: Vocabulary

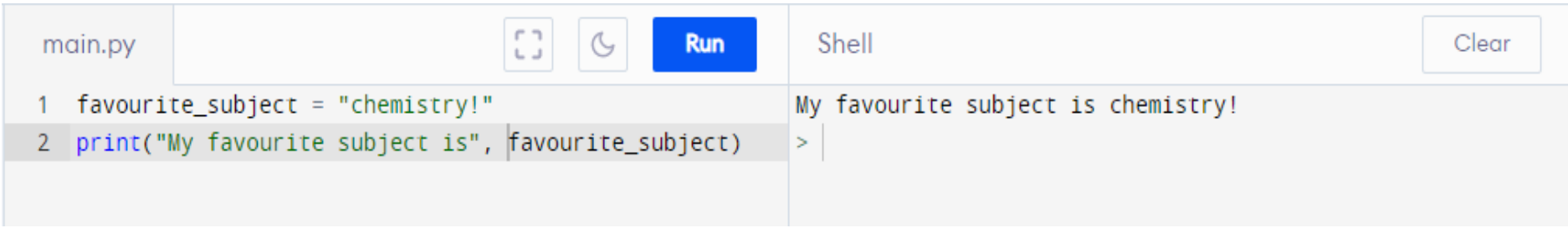
Variable Examples:

favourite_subject = 'chemistry!'

You can print both a string (multiple pieces of text) and a variable by including the string in quotations following by a comma and the variable name

Let's try to display (print) the favourite_subject variable:

1. Type in: favourite_subject = 'chemistry!'
2. Type in: print("My favourite subject is",favourite_subject)
3. Click Run

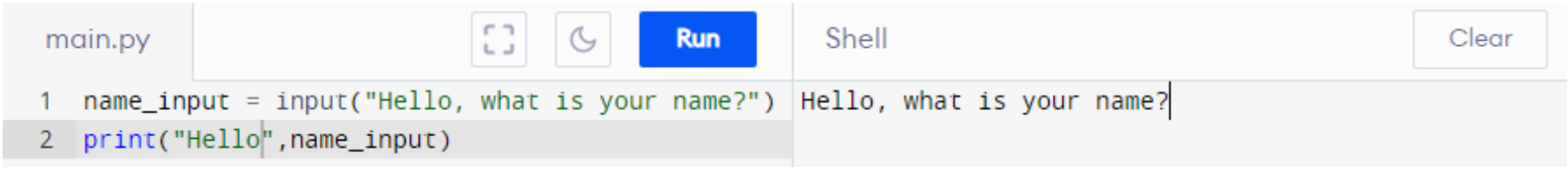


Intro to Python: Vocabulary

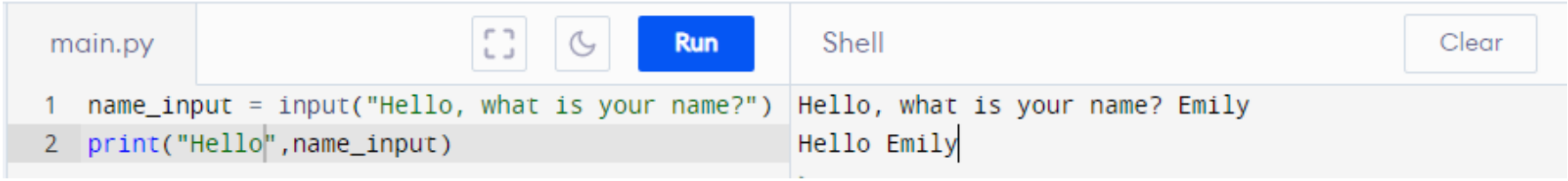
input: input() is a function that allows us to get input from the user by showing a prompt. Examples include someone's name or their favourite number.

Let's try it:

1. Type in: name_input = input("Hello, what is your name?")
2. Type in print("Hello", name_input)
3. Click Run



1. The user would then type their name and press the enter key.



Intro to Python: Vocabulary

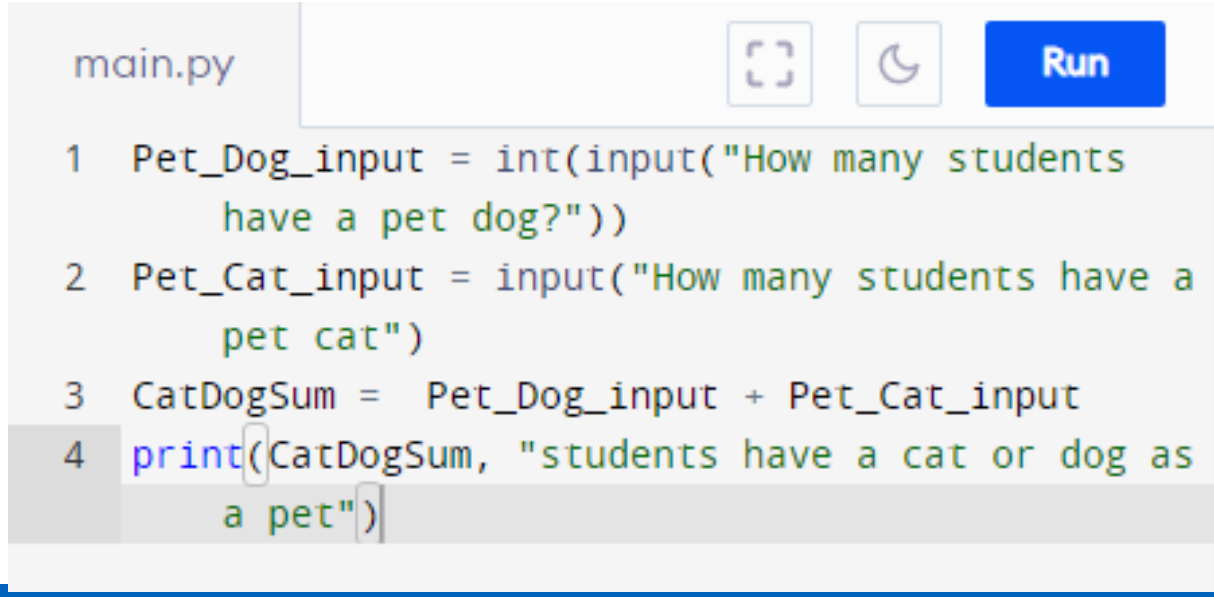
integer: int() is a whole number that is positive or negative (ex. 10)

float: a float() is a positive or negative number than contains a decimal (ex. 10.1)

String: a str() a combination of multiple pieces of text

Let's try a calculation with integers.

1. Type in the following
2. Click Run.
3. Complete the inputs by answering the questions.



Class Discussion:

What happened?

Can we solve this?

Intro to Python

Class Discussion:

What happened? A Bug! This means something is wrong with our code. The program will try to help you by displaying an error.

Can we solve this? Yes we can! How?

main.py

Run

```
1  Pet_Dog_input = int(input("How many students
       have a pet dog?"))
2  Pet_Cat_input = input("How many students have a
       pet cat")
3  CatDogSum =  Pet_Dog_input + Pet_Cat_input
4  print(CatDogSum, "students have a cat or dog as
       a pet")
```

We forgot the int()

Intro to Python: Bug

Class Discussion:

What happened?

A Bug! This means something is wrong with our code. The program will try to help you by displaying an error.

main.py | Run | Shell | Clear

```
1  Pet_Dog_input = int(input("How many students
       have a pet dog?"))
2  Pet_Cat_input = input("How many students have a
       pet cat")
3  CatDogSum =  Pet_Dog_input + Pet_Cat_input
4  print(CatDogSum, "students have a cat or dog as
       a pet")
```

```
How many students have a pet dog?5
How many students have a pet cat4
Traceback (most recent call last):
  File "<string>", line 3, in <module>
TypeError: unsupported operand type(s) for +: 'int'
    and 'str'
>
```

This error is telling us we are trying to add together an integer and a string, which represents text. We cannot calculate numbers with a string.

Intro to Python: Bug

Let's try fix the bug and code a calculation with integers.

1. Type in the following
2. Click Run.
3. Complete the inputs by answering the questions and pressing the Enter key.

main.py | Run | Shell | Clear

```
1  Pet_Dog_input = int(input("How many students
       have a pet dog?"))
2  Pet_Cat_input = int(input("How many students
       have a pet cat"))
3  CatDogSum =  Pet_Dog_input + Pet_Cat_input
4  print(CatDogSum, "students have a cat or dog as
       a pet")
```

```
How many students have a pet dog?5
How many students have a pet cat4
9 students have a cat or dog as a pet
>
```

Intro to Python: Code Calculator

integer: int() is a whole number that is positive or negative (ex. 10)

float: a float() is a positive or negative number than contains a decimal (ex. 10.1)

String: a str() a combination of multiple pieces of text

Task 1: Try to create code that completes a calculation with integers and floats.

Intro to Python: Code Calculator

Task 1: Try to create code that completes a calculation with integers and floats.

See Example Code:

main.py

Run

```
1  Candy_Have = float(10.80)
2  Group_Input = int(input("How many people are in
       a group? Choose a number between 1 and 5."
       ))
3  CandyDivide =  Candy_Have/Group_Input
4  print("Each person in the group will have",
       CandyDivide, "pieces of candy")
```

Shell

Clear

```
How many people are in a group? Choose a number
    between 1 and 5.3
Each person in the group will have 3.6 pieces of
    candy
>
```

Intro to Python: Mole Ratio Code

Task 2: Try to create code that completes a **mole ratio calculation** with integers and floats.

Intro to Python: Mole Ratio Code

Task 2: Try to create code that completes a **mole ratio calculation** with integers and floats.

See Example Code:

main.py

Run

```
1  Mol_Given_Input = float(input("How many moles do you
       have or will create?"))
2  Required_Balanced_Mol_Input = int(input("What is the
       coefficient, representing the mole ratio, of the
       required atom/molecule in the balanced equation? "
       ))
3  Given_Balanced_Mol_Input = int(input("What is the
       coefficient, representing the mole ratio, of the
       given atom/molecule in the balanced equation? "))
4  Mol_Required_Input =  Mol_Given_Input
       *(Required_Balanced_Mol_Input
       /Given_Balanced_Mol_Input)
5  print("Therefore", Mol_Required_Input, "mol will be
       required or produced.")
```

Shell

Clear

```
How many moles do you have or will create?2.5
What is the coefficient, representing the mole ratio, of
    the required atom/molecule in the balanced equation? 3
What is the coefficient, representing the mole ratio, of
    the given atom/molecule in the balanced equation? 1
Therefore 7.5 mol will be required or produced.
>
```