Introduction

October 16, 2023

1 MolSSI Python Workshop

1.1 Allan Hancock College

October 6, 2023

```python
[3]: 3+6
```

```
[3]: 9
```

```python
[8]: deltaH = -541.5     #k3/mole
     deltaS = 10.4       #k3/(mole k)
     temp = 298          #Kelvin
     deltaG = deltaH - temp*deltaS
```

```python
[9]: print(deltaG)
```

```
-3640.7000000000003
```

```python
[10]: print(deltaG, 'kj/mole')
```

```
-3640.7000000000003 kj/mole
```

```python
[16]: print(F'The value of free energy is {deltaG:.3f} in k3/mole.')
```

```
The value of free energy is -3640.700 in k3/mole.
```

```python
[14]: deltaG*1000
      print(deltaG)
```

```
-3640.7000000000003
```

```python
[18]: deltaG_joules = deltaG*1000
      print(deltaG)
      print(deltaG_joules)
```

```
-3640.7000000000003
-3640700.0000000005
```

1.2 Data types

Weather your data is a number or a word and how it is stored

```
[19]: type(deltaG)
```

```
[19]: float
```

```
[21]: type(temp)
```

```
[21]: int
```

```
[22]: print(temp)
```

```
298
```

```
[23]: # Recasting - changing the data type of a variable
      temp = float(temp)
```

```
[24]: print(temp)
```

```
298.0
```

```
[25]: type(temp)
```

```
[25]: float
```

Find the force of a 145 gram object where the accleration is the accleration due to gravity due to gravity 9.8 m/s^2. Write a neatly formatted print statment with your answer, including units.

```
[26]: mass = 145/1000 #kilograms
      accel = 9.8 #m/s^2
      force = mass*accel
      print(F'The force is {force} N.')
```

```
The force is 1.421 N.
```

1.3 Lists

A python data type where a variable has more than one variable.

```
[27]: energy_kcal = [-13.4, -2.7, 5.4, 42.1]
      energy_length = len(energy_kcal)
```

```
[28]: print(energy_length)
```

```
4
```

```
[29]: print(energy_kcal)
```

```
[-13.4, -2.7, 5.4, 42.1]
```

[31]:
```python
print(energy_kcal[0]) #counting starts at 0
```

```
-13.4
```

[32]:
```python
print(energy_kcal[1])
```

```
-2.7
```

[33]:
```python
energy_k3 = energy_kcal[0]*4,184
```

[34]:
```python
print(energy_k3)
```

```
(-53.6, 184)
```

[35]:
```python
# Taking a slice - making a new list is a subset of another lists
#new_list = old_lists[start:end]
short_list = energy_kcal[0:2]
print(short_list)
```

```
[-13.4, -2.7]
```

[39]:
```python
slice1 = energy_kcal[1:]
slice2 = energy_kcal[:3]
print(F' slice1 is {slice1}')
```

```
 slice1 is [-2.7, 5.4, 42.1]
```

[40]:
```python
print(F' slice1 is {slice1}')
```

```
 slice1 is [-2.7, 5.4, 42.1]
```

[45]:
```python
# A for Loop lets us do something to every element in a list
# for variable in List_name:
#     do things with variable
for number in energy_kcal:
        k3 = number*4.184
        print(k3)
```

```
-56.0656
-11.296800000000001
22.593600000000002
176.1464
```

[46]:
```python
print(k3)
```

```
176.1464
```

```
[52]: energy_k3 = []

      for number in energy_kcal:
          K3 = number*4.184
          energy_k3.append(k3)


      print(energy_k3)
```

```
[176.1464, 176.1464, 176.1464, 176.1464]
```

```
[53]: print(energy_kcal)
```

```
[-13.4, -2.7, 5.4, 42.1]
```

```
[ ]: negative_numbers = []
     for number in energy_kcal:
         if number<0:
             negative_numbers.append(number)

                print(negative_numbers)
```

```
[ ]:
```