introduction

October 17, 2023

1 MolSSI Python Workshop

1.1 Allan Hancock College

october 6,2023

[1]:
```
3+7
```

[1]:
```
10
```

[2]:
```
deltaH = -541.5     #kj/mole
deltaS = 10.4       #kJ/(mole K)
temp = 298          #kelvin
deltaG = deltaH - temp*deltaS
```

[3]:
```
print(deltaG)
```

```
-3640.7000000000003
```

[4]:
```
print(deltaG,'kJ/mole')
```

```
-3640.7000000000003 kJ/mole
```

[6]:
```
print(F'the value of free energy is {deltaG} in kJ/mole.')
```

```
the value of free energy is -3640.7000000000003 in kJ/mole.
```

[7]:
```
deltaG*1000
print(deltaG)
```

```
-3640.7000000000003
```

[8]:
```
deltaG_joules = deltaG*1000
print(deltaG)
print(deltaG_joules)
```

```
-3640.7000000000003
-3640700.0000000005
```

1.2 Data Types

Whether your data is a number or a word and how it is stored.

[9]:
```
type(deltaG)
```

[9]:
```
float
```

[10]:
```
type(temp)
```

[10]:
```
int
```

[11]:
```
print(temp)
```

```
298
```

[12]:
```
# Recasting - changing the data type of a variable
temp = float(temp)
```

[13]:
```
print(temp)
```

```
298.0
```

[14]:
```
type(temp)
```

[14]:
```
float
```

Find the force of a 145 gram object where the acceleration is the acceleration due to gravitu 9.8 m/s^2.Write a neatly formatted print statemnt with your answer, in cluding units

[20]:
```
mass = 145/1000 #grams
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 list is a python data type where a variable has more than one value.

[21]:
```
energy_kcal = [-13.4, -2.7, 5.4, 42.1]
energy_length = len(energy_kcal)
```

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

```
4
```

[23]:
```
type(energy_length)
```

[23]:
```
int
```

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

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

[25]:
```
print(energy_kcal[0])  #counting start at zero
```

```
-13.4
```

[26]:
```
energy_kcal[1]
```

[26]:
```
-2.7
```

[27]:
```
energy_kJ = energy_kcal[0]*4.184
print(energy_kJ)
```

```
-56.0656
```

[28]:
```
# Taking s slice - making a new list that is a subject of another list
# new_list = old_list[start:end]
short_list = energy_kcal[0:2]
print(short_list)
```

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

[30]:
```
slice1 = energy_kcal[1:]
slice2 = energy_kcal[:3]
print(F'slice1 is {slice1}')
```

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

[31]:
```
print(F'slice2 is {slice2}')
```

```
slice2 is [-13.4, -2.7, 5.4]
```

[33]:
```
# A for Loop lets is do something to every element in a list
# for a variable in list name:
#     do things with variable

for number in energy_kcal:
    kJ = number*4.184
    print(kJ)
```

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

[34]:
```
print(kJ)
```

```
176.1464
```

[39]:
```
energy_kJ = []

for number in energy_kcal:
    kJ = number*4.184
    energy_kJ.append(kJ)

    print(energy_kJ)
```

```
  Input In [39]
    for number in energy_kcal:
    ^
IndentationError: unexpected indent
```

[40]:
```
print(energy_kJ)
```

```
-56.0656
```

[41]:
```
print(energy_kcal)
```

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

[44]:
```
negative_numebrs = []

for numbers in energy_kcal:
    if number<0:

        negtive_numbers.append(number)
print(negative_numbers)
```

```
---------------------------------------------------------------------------
NameError                                 Traceback (most recent call last)
Input In [44], in <module>
      4     if number<0:
      6         negtive_numbers.append(number)
----> 7 print(negative_numbers)

NameError: name 'negative_numbers' is not defined
```

[ ]:
```

```