Assignment 3

Problem 1

Write a Python code in a `Jupyter notebook` to compute the value of the following two-dimensional functions for $x = 3.0$ and $y = 4.0$. *Note* that variables are case-sensitive, and lowercase variable names are generally preferred.
Hint: Import the `numpy` library in your `Jupyter notebook`. You will need to use `numpy` functions such as: `exp()`, `sqrt()`, `sin()`, and `pi`.

(a) $F(x,y) = yA\exp\left[-\frac{(x-x_0)^2}{2\sigma_x^2}\right]$ where $A = 1.5,\ x_0 = 0.5,\ \sigma_x = 3.0.$

(b) $g(x,y) = \frac{\sqrt{x+y}}{\sqrt{x}+\sqrt{y}}$

(c) $f(x,y) = \exp\left(\frac{-\sin(\pi x)}{(x+y)^2+xy^6}\right)$

(d) $G(x,y) = \log_{10}(x) + \ln(y)$

Problem 2

Create a Python code in a `Jupyter notebook` to calculate the mean molar mass of dry air based on the composition and masses reported in the following table:

Molecule	**Molar Mass (g·mol^{-1})**	**Composition (%)**
N_2	28.013	78.084
O_2	31.999	20.946
Ar	39.948	0.9290
CO_2	44.010	0.041

The mean molar mass of dry air is given by the weighted average:

$$< M >_{\text{air}} = \sum_i x_i M_i$$

where x_i is the fractional composition and M_i is the molar mass of the ith component.

Problem 3

In a `Jupyter notebook`, create a Python code to write an `XYZ` file for a water molecule with the following atomic Cartesian coordinates using Python lists (or dictionaries) and simple loops.

Atom	x (bohr)	y (bohr)	z (bohr)
O	0.00000000	0.00000000	0.00000000
H	1.80941647	0.00000000	0.00000000
H	-0.45334744	1.75170319	0.00000000

Use an **if**-statement to handle units: If the units are bohr, convert all coordinates to ångström. Otherwise (for any other value), assume the numbers are already in ångström. Write the XYZ file `water.xyz` with the standard format:

1. First line: number of atoms.

2. Second line: a short comment, e.g. `H2O coordinates in Å`.

3. Then one line per atom: `symbol x y z` with 6 decimals.

Hint: Below is an example of Python code to write to a text file. *Note* that `\n` is used to break a line.

```
with open('example.txt', 'w') as f:
    f.write('This is an example, line 1' + '\n')
    f.write('This is an example, line 2' + '\n')
```

Problem 4

Using the Cartesian coordinates of the atoms of a water molecule from the previous problem, compute:

(a) The distance (in bohr) between the oxygen atom and each hydrogen atom.

(b) The H–O–H bond angle (in degrees).

Hints:

1. The distance between two points in Cartesian coordinates, $\mathbf{r}_1 = (x_1, y_1, z_1)$ and $\mathbf{r}_2 = (x_2, y_2, z_2)$, is given by:
$$d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}$$

2. To compute the bond angle, define two vectors $\mathbf{a}$ and $\mathbf{b}$ along the O–H bonds, both pointing away from the oxygen atom:
$$\mathbf{a} = \mathbf{r}_{\mathrm{H1}} - \mathbf{r}_{\mathrm{O}}, \qquad \mathbf{b} = \mathbf{r}_{\mathrm{H2}} - \mathbf{r}_{\mathrm{O}}$$
The bond angle θ can then be obtained from the dot product:
$$\cos(\theta) = \frac{\mathbf{a} \cdot \mathbf{b}}{|\mathbf{a}|\,|\mathbf{b}|}$$
where $|\mathbf{a}| = \sqrt{a_x^2 + a_y^2 + a_z^2}$ is the norm (or magnitude) of vector $\mathbf{a}$.

3. In the calculations, you can use the `np.dot`, `np.linalg.norm`, and `np.arccos` functions.