Task1 - Working with functions

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1. Write a simple computer program that consists of a single function that takes as input the equilibrium concentration of the reactants of the following reaction, $2NO_2 <-> N_2O_4$ and gives as output the K_{eq} (with the correct units) of the following reaction. Test the function with the following equilibrium concentrations: $[NO_2] = 2; [N_2O_4] = 3$

```
def equilibrium_constant(NO2, N2O4):
    '''Calculates the equilibrium constant of the reaction 2NO2 <-> N2O4
    Parameters:
    NO2 (int): Concentration of NO2 in Mol
    N2O4 (int): Concentration of N2O4 in Mol

    Returns:
    k_eq (float): Equilibrium constant of the reaction
    units (str): Units of the equilibrium constant
    '''
    k_eq = N2O4 / (NO2**2)
    units = "M^-1"
    return k_eq, units

NO2 = 2
N2O4 = 3

k_eq, units = equilibrium_constant(NO2, N2O4)
print(f'The equilibrium constant is {k_eq} {units}')
```

```
The equilibrium constant is 0.75 M^-1
```

2. Modify the previous function to calculate the K_eq with the correct units for the following reaction: $Na_2CO_3 + CaCl_2 <-> CaCO_3 + 2NaCl$ with equilibrium concentrations: $[Na_2CO_3] = 2; [CaCl_2] = 0.5; [CaCO_3] = 2; [NaCl] = 1.2$

```python
def equilibrium_constant2(reactives, products):
    '''Calculate equilibrium constant of a reaction
    Parameters:
    reactives (list): List with the concentration of reactives of the reaction
    products (list): List with the concentration of products of the reaction

    Returns:
    k_eq (float): Equilibrium constant of the reaction
    units (str): Units of the equilibrium
    '''
    k_eq = products[0] * products[1]**2 / (reactives[0] * reactives[1])
    units = "M^1"
    return k_eq, units

reactives= [2, 0.5]
products = [2, 1.2]

k_eq, units = equilibrium_constant2(reactives, products)
print(f'The equilibrium constant is {k_eq} {units}')
```

```
The equilibrium constant is 2.88 M^1
```

3. Write a general function for this.

```python
def equilibrium_constant_general(reactives, products):
    '''Calculate equilibrium constant of a reaction
    Parameters:
    reactives (dict): Dictionary with the reactives of the reaction
        and their stoichiometry
    products (dict): Dictionary with the products of the reaction
        and their stoichiometry

    Returns:
    k_eq (float): Equilibrium constant of the reaction
    units (str): Units of the equilibrium
    '''
    k_eq = 1.0  # Initialize equilibrium constant
    units = ""

    for species, (concentration, coeff) in products.items():
        k_eq *= concentration ** coeff
```

```
    for species, (concentration, coeff) in reactives.items():
        k_eq /= concentration ** coeff

    # Assuming concentration units are in mol/L
    reactant_order = sum(coeff for _, coeff in reactives.values())
    product_order = sum(coeff for _, coeff in products.values())
    net_order = product_order - reactant_order

    if net_order > 0:
        units = f"(mol/L)^{net_order}"
    elif net_order < 0:
        units = f"(L/mol)^{-net_order}"
    else:
        units = "dimensionless"

    return k_eq, units


reactives = {"Na2CO3": (2, 1), "CaCl2": (0.5, 1)}
products = {"CaCo3": (2, 1), "NaCl": (1.2, 2)}

k_eq, units = equilibrium_constant_general(reactives, products)
print(f"Equilibrium constant: {k_eq} {units}")
```

```
Equilibrium constant: 2.88 (mol/L)^1
```