

# Tools for chemical calculations

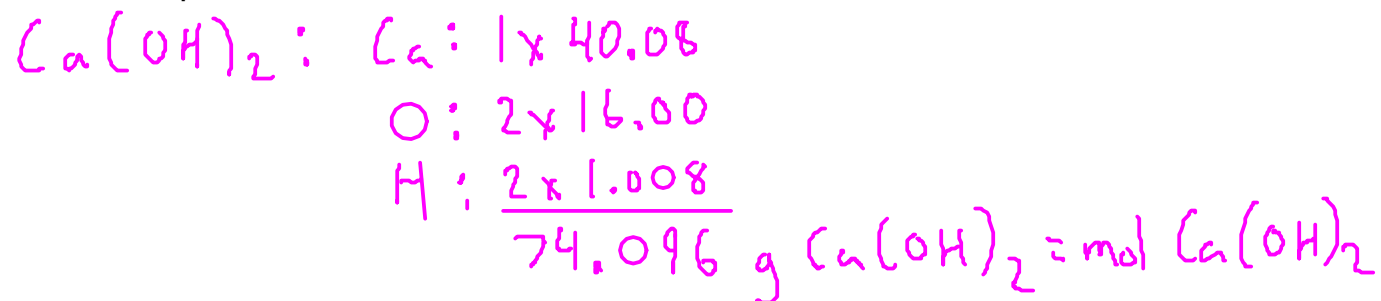
To relate ...	... and ...	..., use ...	
MASS	MOLES	FORMULA WEIGHT	Chapter 3
MOLES OF SUBSTANCE	MOLES OF DIFFERENT SUBSTANCE	BALANCED CHEMICAL EQUATION	
VOLUME OF SOLUTION	MOLES	MOLAR CONCENTRATION	Chapter 4
VOLUME OF GAS	MOLES	IDEAL GAS EQUATION	Chapter 5
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MOST chemical calculations follow this pattern:

- 1) Convert AMOUNT of given substance (mass, volume, etc.) to MOLES
- 2) Convert MOLES given substance to MOLES desired substance
- 3) Convert MOLES desired substance to AMOUNT

## FORMULA WEIGHT

To calculate the formula weight of a compound, add up the atomic weights of all atoms in the compound:



Use the formula weight as a conversion factor to relate mass and moles. The formula weight is the number of grams of a compound equivalent to one mole of the compound.

How many moles of calcium hydroxide are there in 36.0 grams calcium hydroxide?

$$36.0 \text{ g Ca(OH)}_2 \times \frac{\text{mol Ca(OH)}_2}{74.096 \text{ g Ca(OH)}_2} = 0.486 \text{ mol Ca(OH)}_2$$

How many grams of calcium hydroxide should be weighed to have 1.75 moles calcium hydroxide?

$$1.75 \text{ mol Ca(OH)}_2 \times \frac{74.096 \text{ g Ca(OH)}_2}{\text{mol Ca(OH)}_2} = 130 \text{ g Ca(OH)}_2$$

## BALANCED CHEMICAL EQUATION

Use a balanced chemical equation to relate moles of one substance to moles of a different substance.



The coefficients of the equation relate moles of one substance to moles of another. If a substance has no written coefficient, assume one mole. You can relate one reactant to another reactant, one reactant to one product, or one product to another product. In other words, ANY two substances in the chemical equation can be related.



How many moles of sodium chloride can be produced from 0.750 moles of chlorine gas?

$$0.750 \text{ mol Cl}_2 \times \frac{2 \text{ mol NaCl}}{\text{mol Cl}_2} = \boxed{1.50 \text{ mol NaCl}}$$

## MOLAR CONCENTRATION

Use a solution's molar concentration to relate volume in liters to moles. The molar concentration is equal to the number of moles in one liter of a solution.

3.00 M HCl means that 3.00 mol HCl = L

Sometimes, you will need to convert a solution's volume from milliliters to liters before using molar concentration, since most solution volumes in the lab are in milliliters.

How many moles of HCl are present in 45.0 mL of 3.00 M HCl?

$$\text{mL} = 10^{-3} \text{L}$$

$$45.0 \text{ mL} \times \frac{10^{-3} \text{L}}{\text{mL}} \times \frac{3.00 \text{ mol HCl}}{\text{L}} = 0.135 \text{ mol HCl}$$

How many mL of 3.00 M HCl are needed to have 0.656 moles of HCl?

$$\text{mL} = 10^{-3} \text{L}$$

$$0.656 \text{ mol HCl} \times \frac{\text{L}}{3.00 \text{ mol HCl}} \times \frac{\text{mL}}{10^{-3} \text{L}} = 219 \text{ mL of 3.00 M HCl}$$

## IDEAL GAS EQUATION

Use the ideal gas equation to relate gas conditions to moles. Usually, the amount of gas will be given in volume units (liters). You can also relate moles of gas to gas properties like volume.

$$PV = nRT$$

Rearrange the ideal gas equation to solve for the value you're trying to calculate.

$$n = \frac{PV}{RT} \quad V = \frac{nRT}{P}$$

To use the ideal gas equation, units for P, V, and T must match the units of the ideal gas constant, R.

How many moles of oxygen gas are there in 12.3 L at 25.0 C and 0.950 atm?

$$P = 0.950 \text{ atm} \quad V = 12.3 \text{ L} \quad R = 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \quad T = 25.0^\circ\text{C} = 298.2 \text{ K}$$

$$n = \frac{(0.950 \text{ atm})(12.3 \text{ L})}{(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}})(298.2 \text{ K})} = \boxed{0.478 \text{ mol O}_2}$$

What volume does 0.0125 moles of oxygen gas occupy at 25.0 C and 0.950 atm?

$$n = 0.0125 \text{ mol O}_2 \quad R = 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \quad T = 25.0^\circ\text{C} = 298.2 \text{ K} \quad P = 0.950 \text{ atm}$$

$$V = \frac{(0.0125 \text{ mol O}_2)(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}})(298.2 \text{ K})}{(0.950 \text{ atm})} = \boxed{0.322 \text{ L O}_2 \text{ at } 25.0^\circ\text{C}, 0.950 \text{ atm}}$$

## BALANCED THERMOCHEMICAL EQUATION

Use a balanced thermochemical equation to relate the enthalpy change (or heat at constant pressure ) to moles of a substance.



Treat the enthalpy/heat as if it is just another product of the reaction.

$$4 \text{ mol NH}_3 = -906 \text{ kJ}$$

How many moles of ammonia must be burned to release 1550 kJ of heat at constant pressure?

$$-1550 \text{ kJ} \times \frac{4 \text{ mol NH}_3}{-906 \text{ kJ}} = \boxed{6.84 \text{ mol NH}_3}$$

This sign is negative because the reaction is releasing (in other words, losing) the heat.

What is the enthalpy change for the combustion of 0.250 moles of ammonia gas?

$$0.250 \text{ mol NH}_3 \times \frac{-906 \text{ kJ}}{4 \text{ mol NH}_3} = \boxed{-56.6 \text{ kJ}}$$

Signs in thermodynamics:

+: system gains energy, endothermic

-: system loses energy, exothermic