

Atomic and molecular structure

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The **Atomic mass unit (amu)** is the 12th part of the mass of C_6^{12} atom.
Thus the mass of C_6^{12} atom = 12 amu

- Neutron mass = 1,00897 amu
- Proton mass = 1,00758 amu
- Electron mass = 0,00055 amu
- Mass of hydrogen atom = 1,00758amu + 0,00055 amu = 1.00813 amu

One mole of atoms of every element is the quantity of substance containing exactly the same number of atoms of 12 g of pure C_6^{12} .

This number is the **Avogadro number** $N_A = 6,0221415 \cdot 10^{23}$ (according to CODATA of 2002). Thus:

$$\text{mass of 1 mole of atoms} = N_A \cdot \text{mass of 1 atom} = N_A \cdot 12 \text{ amu} = 12 \text{ g}$$

$$1 \text{ g} = N_A \text{ amu}$$

$$1 \text{ amu} = \frac{1}{N_A} \text{ g} = \frac{1}{6,022 \cdot 10^{23}} \text{ g}$$

The quantity of material containing $6,022 \cdot 10^{23}$ atoms is called gram-atom.

The quantity of material containing $6,022 \cdot 10^{23}$ molecules is called gram-moles.

The Avogadro's number $N_A = 6,0221415 \cdot 10^{23}$ is the number of molecules contained in equal volumes of ideal gases at the same temperature and pressure.

$$6,022 \cdot 10^{23} \frac{\text{number of molecules}}{\text{gram.mol (g}_{mol})} \text{ or } \frac{\text{number of atoms}}{\text{gram.atom (g}_{at})}$$

The molar volume is the volume of a gas containing "1 mole" i.e. a mass measured in gram numerically equal to its molecular mass. At the standard conditions:

$$1,013 \cdot 10^5 \text{ Pa and } 273 \text{ K} = 0^\circ \text{C} - \text{this volume, for an ideal gas is } 22,4 \text{ dm}^3.$$

Example 1 *The natural proportions referring to the different isotopes of Silicon Si are:*

Isotopes	Proportions	Mass of Nucleus
Si ²⁸	92,21/100	27,977
Si ²⁹	4,70/100	28,976
Si ³⁰	3,09/100	29,974

Find the atomic mass of Silicon.

$$A = \frac{9221 \cdot 27.977 + 4.70 \cdot 28.976 + 3.09 \cdot 29.974}{100} = 28.08566$$

Example 2 The natural Carbon consists of 2 isotopes: C^{12} and C^{13} , whose masses are: 12,00000 and 13,0034. What is the percentage of the two isotopes in a sample of Carbon having atomic mass of 12,01112?

Let's be: $x =$ the percentage of C^{13} $100 - x =$ the percentage of C^{12}

$$1201112 = \frac{12.00000 \cdot (100 - x) + 13.0034 \cdot x}{100}$$

From the equation we find: $x = 1.109/100$ C^{13} $100 - x = 98.891/100$ C^{12}

Example 3 Before 1961 a physical scale of the atomic masses was adopted, based on 16,00000 for the O^{16} atom. In our actual scale the nucleus mass of O^{16} is 15,9949.

What would have been in the old scale (chemical scale) the physical atomic mass of C^{12} ?

The mass ratios of whatever nuclei are constant with respect to any reference system; therefore we can write:

$$\left[\frac{\text{mass of } C^{12}}{\text{mass of } O^{16}} \right]_{\text{old scale}} = \left[\frac{\text{mass of } C^{12}}{\text{mass of } O^{16}} \right]_{\text{new scale}} = \frac{12.00000}{15.9949}$$

$$(M \text{ of } C^{12})_{\text{old scale}} = 12.0000 \cdot \frac{160000}{15.9949} = 12.0038 \quad (1)$$

Example 4 From 10 g of we have obtained 3.6111 g of Calcium. Since the atomic mass of Chlorine is 35.453 g / g_{at} what is the atomic mass of Calcium?

We can write the proportion

$$\frac{\text{Mass of } C_aCl_2}{m_{C_a} + 2 \cdot m_{cl}} = \frac{\text{Mass of } C_a}{m_{C_a}} = \frac{\text{Mass of } Cl_2}{2 \cdot m_{cl}}$$

Mass of $C_aCl_2 = 10.0000$ g

Mass of C_a in $C_aCl_2 = 3.6111$ g

Mass of Cl in $C_aCl_2 = (10.0000 - 3.6111) = 6.388$ g

$$n_{Cl} = \frac{6.388 \text{ g}}{35.453 \text{ g} / g_{at}} = 0.1802 g_{at}$$

From the formula C_aCl_2 we note that:

$$n_{C_a} = \frac{1}{2}n_{Cl} = \frac{1}{2}0.1802 = 0.0901 g_{at}$$

The atomic mass of Calcium is:

$$M_{C_a} = \frac{3.6111}{0.0901} = 40.078 \text{ g} / g_{at}$$

Example 5 1. How many gram-atoms are contained in: a) 15 g of Hydrogen, b) 15 g of Deuterium.

2. How many moles of Hydrogen are contained in 10 g of H_2 ?

3. How many atoms are contained in 1 g of Deuterium?

atomic mass of $H^1 = 1.008142$ amu. Therefore 1 g_{at} of $H^1 = 1.008142$ g of H^1

atomic mass of $H^2 = 2.014735$ amu. Therefore 1 g_{at} of $H^2 = 2.014735$ g of H^2

1.

$$\frac{\text{mass of hydrogen}}{\text{atomic mass of hydrogen}} = \frac{15 \text{ g}}{1.008142 \text{ g/g}_{at}} = 14.8789 \text{ g}_{at} \text{ of } H^1$$

$$\frac{\text{mass of deuterium}}{\text{atomic mass of deuterium}} = \frac{15 \text{ g}}{2.014735 \text{ g/g}_{at}} = 14.8789 \text{ g}_{at} \text{ of } H^1$$

2. molecular mass of hydrogen $H_2 = 2 \cdot \text{atomic mass of } H = 2.016284 \text{ g/g}_{at}$

$$\text{moles of } H_2 = \frac{10 \text{ g of } H}{\text{molecular mass of } H_2} = \frac{10 \text{ g}}{2.01628 \text{ g/g}_{at}} = 0.49596 \text{ g}_{at}$$

$$\text{atoms of } H^2 = 0.49596 \text{ g}_{at} \cdot 6.022 \cdot 10^{23} \text{ atoms/g}_{at} = 2.9867 \cdot 10^{23} \text{ atoms of } H^2$$