

CHAPTER 7 : APPROXIMATIONS

Approximation has a bad name - it has tended to become associated with sloppy observation and careless calculation. This is most unfortunate for the ability to approximate is really very useful - but even more useful is the ability to judge when it is reasonable to approximate and to what extent. To be hung up on extreme and unnecessary 'accuracy' is to waste time and effort and in the world of industry and commerce, that also means wasting money.

In a sense all answers are approximate. Associated with every observation there is necessarily some degree of error; what is important is the extent of that error. The purpose of this section is, however, not to deal explicitly with inherent errors but to discuss the value of an approximate answer. To know roughly the sizes of atoms, their mass, how many you happen to be dealing with in an experiment, to have some idea of their concentration, or the pressure they may exert, to have a feeling for bond strengths, all these notions will give you confidence when thinking about chemistry.

Some numbers are best learnt. For example you should remember that:

Number of atoms in one mole is *ca.* 6×10^{23} (*ca.* means "about" or "around")
 Mass proton or neutron $\sim 2000 \times$ mass of electron
 Atomic diameters $\sim 1 - 3 \text{ \AA}$ ($1 \text{ \AA} = 10^{-10} \text{ m}$)
 Speed of light is *ca.* $3 \times 10^8 \text{ m s}^{-1}$

.... but after that many others can be derived from a few basic facts.

It is also useful to know a few common equivalents

e.g. 1 electron volt (1 eV) $\sim 8000 \text{ cm}^{-1} \sim 100 \text{ kJ mol}^{-1}$

.... since a knowledge of these relationships will enable you to relate ionisation energies (in eV), to vibrational data (generally given in units of cm^{-1}) and to bond strengths (usually specified in kJ mol^{-1}).

Here are some examples of how to estimate approximate values for other items.

The Approximate Masses of a Proton and an Electron.

The relative atomic mass of hydrogen is 1. The hydrogen atom contains one proton and one electron, and the mass of the electron is about $(1/2000)^{\text{th}}$ of the proton. Thus the mass of the proton is, near enough, the mass of the hydrogen atom. From the definition of a mole:

1 mole of hydrogen atoms has a mass of 1 g or 10^{-3} kg.

Therefore 6×10^{23} protons have a mass of 10^{-3} kg

\Rightarrow 1 proton has a mass of *ca.* $\frac{10^{-3}}{6 \times 10^{23}} = \frac{1}{6} \times 10^{-26} \text{ kg}$

i.e. Mass of proton $\sim 1.67 \times 10^{-27} \text{ kg}$

The mass of the electron about $(1/2000)^{\text{th}}$ of that of the proton.

$$\Rightarrow 1 \text{ electron has a mass of ca. } \frac{1.67 \times 10^{-27}}{2000} \text{ kg}$$

i.e. Mass of electron $\sim 8 \times 10^{-31}$ kg

Note that the point of these calculations is not to derive accurate masses for the proton or the electron but to show how these masses can be estimated from very little basic information.

Sizes of Atoms - How Big is an Atom ?

The size of an argon atom can be estimated from the density of crystalline argon (1.772 g cm^{-3}) and its molar mass ($M = 39.95 \text{ g mol}^{-1}$).

$$\text{Density} = \frac{\text{mass}}{\text{volume}} = \frac{\text{mass per atom}}{\text{volume per atom}} = \frac{(M/N_A)}{V}$$

where V is the volume occupied by one atom.

If we use d to denote the density then,

$$V = \frac{(M/N_A)}{d}$$

If each atom is assumed to occupy a cube of side a (a rather crude approximation, but one that will still generate a sufficiently good answer to our question)

$$a^3 = V = \frac{(M/N_A)}{d}$$

To find a raise each side to the power $1/3$ (see section on *Indices*)

$$a = (a^3)^{1/3} = \left(\frac{M/N_A}{d} \right)^{1/3}$$

$$\begin{aligned} \text{Substituting } M &= 39.95 \text{ g mol}^{-1} \\ N_A &= 6.022 \times 10^{23} \text{ mol}^{-1} \\ d &= 1.772 \text{ g cm}^{-3} = 1.772 \times 10^6 \text{ g m}^{-3} \end{aligned}$$

$$\Rightarrow a = \left(\frac{39.95 \text{ g mol}^{-1} / 6.022 \times 10^{23} \text{ mol}^{-1}}{1.772 \times 10^6 \text{ g m}^{-3}} \right)^{1/3} = 3.345 \times 10^{-10} \text{ m}$$

$$\Rightarrow a = 3.345 \text{ \AA} \quad (\text{since } 1 \text{ \AA} = 10^{-10} \text{ m})$$

Thus atomic dimensions are of the order of Ångstroms and are traditionally expressed in those units. The nearest SI units are:

$$\begin{aligned} 1 \text{ nanometre} &= 1 \text{ nm} = 10^{-9} \text{ m} = 10 \text{ \AA} \\ 1 \text{ picometre} &= 1 \text{ pm} = 10^{-12} \text{ m} = 10^{-2} \text{ \AA} \end{aligned}$$

$$\Rightarrow \text{Approximate diameter of an Ar atom, } a = 3.345 \text{ \AA} = 0.3345 \text{ nm} = 334.5 \text{ pm}$$