WHAT IS THE MOLE?

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SUMMARY: There is a great deal of confusion about the mole. The SI formulation of it is carefully presented and explained.

INTRODUCTION

There is a great deal of confusion among chemists about the mole. Surveys have shown that even many teachers do not have a proper understanding of it (Furió *et al*., 2002).

A common misconception is that the mole is a counting unit like a dozen or a gross. In SI, it is not: it is the unit of a physical quantity called "amount of substance" or "chemical amount" (McGlashan, 1977; Nelson, 1991; Gorin, 1994). Thus one can write

$$\text{number of eggs} = 2\ \text{doz} = 24$$

but not

$$\text{number of molecules} = 2\ \text{mol} = 12{\cdot}0\times10^{23}$$

One can only write

$$\text{number of molecules} = 12{\cdot}0\times10^{23}$$

or

$$\text{amount of substance} = 2\ \text{mol}$$

A second problem is that many chemists carry out stoicheiometric calculations differently from other calculations in science (Packer, 1988; DeToma, 1994). For example, instead of writing

$$\text{amount of substance} = 2\ \text{mol}$$

they write

$$\text{number of moles} = 2\ \text{mol}$$

This goes against the way other physical quantities are expressed (McGlashan, 1968).

Again, instead of writing

$$\text{amount of substance} = \frac{\text{mass}}{\text{molar mass}}$$

they write

$$\text{number of moles} = \frac{\text{mass}}{\text{RMM}} \quad (\text{RMM = relative molecular mass})$$

This is dimensionally incorrect (mass/RMM is a mass).

My aim in this paper is to try to remove some of this confusion. I shall first formulate the mole as implied in IUPAC's *Quantities, Units and Symbols in Physical Chemistry* (Mills *et al*., 1993). I shall then explain its meaning.

FORMULATION

Preliminaries

Chemists consider substances as being made up of atoms, molecules, radicals, ions, or formula units (*eg* NaCl for crystalline sodium chloride). IUPAC refer to these as "entities". I shall use the more specific term "chemical entity".

Chemists specify the mass (m) of a chemical entity in two ways: either (a) in unified atomic mass units, defined by

$$\mathrm{u} = m(^{12}\mathrm{C\ atom})/12 \tag{1a}$$

or (b) relative to the atomic mass constant, m_u:

$$m_\mathrm{r} = m/m_\mathrm{u}, \quad m_\mathrm{u} = m(^{12}\mathrm{C\ atom})/12 \tag{1b}$$

Thus, for example, they express the mass of a hydrogen atom (more precisely, the average mass of hydrogen atoms in a terrestrial sample of hydrogen) either as m(H atom) = 1·008 u or as m_r(H atom) = 1·008.

Chemical amount

Chemists measure the quantity of a substance by mass (m), volume (V), or what IUPAC call "amount of substance" or "chemical amount" (n). This is defined by the equation

$$n = N/L \tag{2}$$

where N is the number of chemical entities in the sample, and L is a constant, having the same value for all substances. The chemical entity should always be clearly specified (*eg* S or S_8 for α-sulfur).

Chemists use n to calculate the quantities of substances involved in reactions. Consider, for example, the reaction

$$a\mathrm{A} + b\mathrm{B} \rightarrow c\mathrm{C}$$

The number of entities B that react with N(A) of A is given by:

$$N(\mathrm{B})/N(\mathrm{A}) = b/a \tag{3}$$

Thus from equation (2)

$$n(\mathrm{B})/n(\mathrm{A}) = b/a \tag{4}$$

Similar equations relate n(C) to n(A) and n(C) to n(B). These equations can be combined to give

$$n(\mathrm{A})/a = n(\mathrm{B})/b = n(\mathrm{C})/c \qquad (5)$$

The unit of chemical amount is the mole. This is defined to be such that the chemical amount of ^{12}C atoms in exactly 12 grams of carbon-12 is one mole:

$$\mathrm{mol} = n(^{12}\mathrm{C}\text{ atoms in 12 g of carbon-12}) \qquad (6)$$

Quantities per chemical amount

Chemists frequently use quantities of the type

$$X_\mathrm{m} = X/n \qquad (7)$$

IUPAC call these "molar" quantities (though this breaks the rule that the name of a physical quantity should not imply a particular choice of unit: "chemical" would be better).

Molar quantities are used extensively in thermodynamics, along with "partial" molar quantities. The latter relate to components of solutions, and are defined similarly (by $\partial X/\partial n_\mathrm{X}$ for component X).

Measuring chemical amount

Pure substances, (a) using atomic mass units

The chemical amount of a pure substance is usually determined from its mass. The number of chemical entities in a sample of the substance is given by

$$N = m_\mathrm{s}/m_\mathrm{x} \qquad (8)$$

where m_s is the mass of the sample and m_x is the mass of the entity (x = at, mol, etc.). Hence from equation (2)

$$n = m_\mathrm{s}/M \qquad (9)$$

where

$$M = Lm_\mathrm{x} \qquad (10a)$$

M is the molar mass of the substance [compare equation (9) with equation (7)] reckoned in terms of x.

Now the mole is defined to be such that $n(^{12}\mathrm{C}\text{ atoms}) = 1$ mol for m_s(carbon-12) = 12 g. Since $m_\mathrm{at}(^{12}\mathrm{C}) = 12$ u, equations (9) and (10a) give

$$L = 1\ \mathrm{g\ u^{-1}\ mol^{-1}} \qquad (11a)$$

Thus L in equation (10a) converts m in atomic mass units into M in g mol^{-1}.

Example: What is the chemical amount of H_2 in 1·000 g of hydrogen?
Answer: From $m(H_2)$ = 2·016 u, equations (10a) and (11a) give $M(H_2)$ = 2·016 u × 1 g u^{-1} mol^{-1} = 2·016 g mol^{-1}. Hence from equation (9), $n(H_2)$ = 1·000 g / 2·016 g mol^{-1} = 0·496 mol.

Pure substances, (b) using relative masses

If relative masses [equation (1b)] are used, equation (10a) becomes

$$M = Lm_u m_r = M^\circ m_r \qquad (10b)$$

Since $m_r(^{12}\text{C atom}) = 12$, the definition of the mole now gives

$$M^\circ = 1 \text{ g mol}^{-1} \qquad (11b)$$

Thus M° in equation (10b) converts relative mass into molar mass. IUPAC call this constant the "standard molar mass". (I prefer "molar mass constant".)

Answer to the above example: From $m_r(H_2)$ = 2·016, equations (10b) and (11b) give $M(H_2)$ = 2·016 × 1 g mol^{-1} = 2·016 g mol^{-1}. Hence $n(H_2)$ = 1·000 g / 2·016 g mol^{-1} = 0·496 mol as before.

Substances in solution

The chemical amount of a substance in solution can be calculated from its mass concentration (γ) and the volume (V) of the solution. Mass concentration is defined by

$$\gamma = m_s/V \qquad (12)$$

Hence from equations (9) and (12)

$$n = cV \qquad (13)$$

where

$$c = \gamma/M \qquad (14)$$

c is commonly called the "molarity" of the solution. IUPAC prefer the name "amount (or 'substance') concentration", an abbreviation for "amount-of-substance concentration". (A better name would be "chemical concentration", meaning "chemical-amount concentration".)

Gases

The chemical amount of a gas can be derived from Avogadro's principle: at low pressures, equal volumes of gases at the same temperature and pressure contain equal numbers of molecules. This means that, at a particular temperature (T) and low pressure (p, $p \to 0$), the volume of a gas per molecule

$$V_{mol} = V/N \qquad (15)$$

is the same for all gases. Now we know from the the gas laws

$$V \propto 1/p \quad (N, T \text{ const.}; p \to 0) \tag{16}$$

$$V \propto T \quad (N, p \text{ const.}; p \to 0) \tag{17}$$

that at $p \to 0$, V_{mol} is proportional to $1/p$ and T. It must therefore be given by

$$V_{\text{mol}} = kT/p \quad (p \to 0) \tag{18}$$

where k is a constant having the same value for all gases. Thus, from equations (15), (18), and (2),

$$pV = NkT = nLkT = nRT \quad (p \to 0) \tag{19}$$

The value of R can be obtained by measuring pV/nT for a gas and extrapolating this to $p = 0$. Equations (7) and (19) give

$$n = V/V_{\text{m}}, \quad V_{\text{m}} = RT/p \quad (p \to 0) \tag{20}$$

At higher pressures, these equations describe an ideal gas. They are, however, used as approximations for real gases. Thus

$$n \approx V/V_{\text{m}}^{\text{ideal}}, \quad V_{\text{m}}^{\text{ideal}} = RT/p \tag{21}$$

At "standard" temperature and pressure (STP: 0 °C, 1 atm), $V_{\text{m}}^{\text{ideal}} = 22{\cdot}41 \text{ l mol}^{-1}$; at standard ambient temperature and pressure (SATP: 298.15 K, 1 bar) its value is $24{\cdot}79 \text{ l mol}^{-1}$ (Atkins & de Paula, 2002).

The five boxed equations derived above are used routinely in stoicheiometric calculations.

Substances in electrolysis

The chemical amount of a substance produced or consumed in electrolysis can be calculated from relations based on Faraday's laws. If these are formulated as I have described elsewhere (Nelson, 2002), they give, for the mass of a substance produced or consumed by the passage of a quantity of electricity, Q,

$$m_{\text{s}} \propto Qm_{\text{x}}/v \tag{22}$$

where m_{x} is the mass of the atom or radical composing the substance and v is its valency. From equations (8) and (2), this gives

$$N = Q/ev, \quad n = Q/Fv \tag{23}$$

where e and F are constants, related by $F = Le$. F is the Faraday constant, e the elementary charge.

The constant L

The formulation of the mole has been designed so that stoicheiometric calculations can be carried out without having to evaluate the constant L in equation (2).

An accurate value for L can be obtained from the density (ρ) of a crystal of silicon and the volume of the crystal per atom (V_{at}) as measured by X-ray crystallography:

$$V_m = M/\rho = LV_{at} \qquad (24)$$

This gives $L = 6{\cdot}0221\times10^{23}$ mol^{-1}. From this, u = m_u = (1 g mol^{-1})/L = 1.6605×10^{-24} g [equation (11a) or (10b) and (11b)]. L is called the Avogadro "constant". [This is distinct from the Avogadro "number", N_A = g/u = $6{\cdot}0221\times10^{23}$, a pure number (Nelson, 1991).]

EXPLANATION

What is chemical amount?

The above formulation raises a number of questions. The first is, what exactly is the physical quantity "chemical amount"?

A partial answer to this can be inferred from equation (2): chemical amount is the macroscopic measure of the amount of a substance that corresponds at an atomic level to the number of chemical entities the substance contains (Nelson, 1991). The mole is accordingly the amount of a substance that corresponds to a standard number of entities. (A mole of any substance contains the same number of entities, but it is difficult to formulate chemical amount from this.)

A more complete answer follows from equation (20). This indicates that, at a given temperature and low pressure, one mole samples of different substances in the gas phase, reckoned in terms of their gaseous molecules, all have the same volume. Moreover, this volume will vary with temperature and pressure in the same way. In these respects the samples are all identical – they constitute equal amounts of gas. Chemical amount can accordingly be identified as the amount of a substance *reckoned as a gas*.

[Any substance can in principle be reckoned as a gas. It is only necessary to imagine a gas comprising the specified entities as molecules. This can often be realized in practice. For example, the chemical amount of crystalline sodium chloride in terms of its formula unit can be measured by the volume of its vapour at temperatures at which this comprises NaCl molecules.]

Why use chemical amount?

A second question is, why introduce chemical amount? Why not simply use number of entities, and the Avogadro number (N_A) as a genuine counting unit (Nelson, 1991, 1994, 2002)?

The answer to this is historical. In the late 19th and early 20th century, some influential scientists doubted the existence of atoms and molecules (Knight, 1967). They accepted the laws of chemical combination, but preferred to carry out stoicheiometric calculations without

reference to these entities. It was one of these scientists, the physical chemist Wilhelm Ostwald, who coined the term "mole" (Ostwald, 1900). Although he later changed his views about the existence of atoms and molecules, his approach to stoicheiometry has persisted.

[Some authors state that chemists use the mole because this avoids having to count atoms and molecules. However, it is possible to use *N* without counting entities, as I have described elsewhere (Nelson, 1991).]

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