What is the mole?

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Abstract The mole is a difficult concept. Surveys have shown that even many teachers do not have a proper understanding of it. To help to meet this problem, the SI/IUPAC formulation of the mole is carefully presented and explained. New SI proposals are also briefly discussed.

Keywords Amount of substance · Chemical amount · Mole · Number of entities · Avogadro constant · Avogadro number · Stoicheiometry

Introduction

The mole is a difficult concept. 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" (McGlashan 1977; Nelson 1991). Thus, one can write

number of
$$eggs = 2 doz = 24$$

but not

number of molecules =
$$2 \text{ mol} = 12.0 \times 10^{23}$$

One can only write

number of molecules =
$$12.0 \times 10^{23}$$

or

amount of substance $= 2 \mod 2$

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A second problem is that many chemists carry out stoicheiometric¹ calculations differently from other calculations in science (Packer 1988; DeToma 1994). For example, instead of writing

amount of substance $= 2 \mod 2$

they write

number of moles
$$= 2 \mod 1$$

This goes against the way other physical quantities are expressed (McGlashan 1968: 4). Again, instead of writing

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

they write

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

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

My aim in this paper is to explain the mole, and to help instructors to teach it more correctly. I shall first formulate the concept as implied in IUPAC's "Quantities, Units and Symbols in Physical Chemistry" which is based on SI (Cohen et al. 2007). I shall then explain its meaning. I also briefly discuss new SI proposals concerning the mole.

Formulation

Preliminaries

Chemists consider substances as being made up of atoms, molecules, radicals, ions, or formula units (e.g. 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 (symbol u) or daltons (Da), defined by

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

or (b) relative to the atomic mass constant, $m_{\rm u}$:²

$$m_{\rm r} = m/m_{\rm u}, \quad m_{\rm u} = m(^{12}{\rm C \ atom})/12$$
 (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 Da or as $m_r(H \text{ atom}) = 1.008$. Relative mass corresponds to what many chemists call "atomic or molecular weight".

¹ From Greek stoicheion, element. Often spelt "stoichiometric".

² IUPAC denote the relative mass of an atom by A_r and of a molecule by M_r .

Chemical amount

Chemists measure the amount 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

$$n = KN \tag{2}$$

where *N* is the number of chemical entities in the sample, and *K* is a constant, having the same value for all substances. The chemical entity should always be clearly specified (e.g. S or S₈ for α -sulfur). The full specification of *n* is *n*(substance: entity), but *n*(entity) usually suffices. "Amount of substance" is the SI name; "chemical amount" was suggested by Gorin (1982).

From Eq. 2, the constant K is the chemical amount per entity (n/N). As we shall see, a more convenient quantity is its reciprocal (L), the number of entities per chemical amount (N/n). In terms of this, Eq. 2 is

$$n = N/L \tag{3}$$

I discuss the constant L further below.

Chemists use chemical amount to calculate the amounts of substances involved in chemical reactions (hence the name). Consider, for example, the reaction

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

The number of entities B that react with N(A) of A is given by:³

$$N(\mathbf{B})/N(\mathbf{A}) = b/a \tag{4}$$

Thus from Eq. 2 or 3

$$n(\mathbf{B})/n(\mathbf{A}) = b/a \tag{5}$$

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

$$n(\mathbf{A})/a = n(\mathbf{B})/b = n(\mathbf{C})/c \tag{6*}$$

The asterisk indicates that this is a key equation.

The unit of chemical amount is the mole. This is defined in SI to be such that the chemical amount of carbon-12, reckoned in terms of atoms, in a sample having a mass of exactly 12 grams, is one mole:

$$mol = n(12 \text{ g of carbon}-12 : {}^{12}C \text{ atoms})$$

A new definition is currently being considered as discussed below.

Quantities per chemical amount

Chemists frequently use quantities of the type

$$X_{\rm m} = X/n \tag{7}$$

³ This is most easily seen by considering a simple example, e.g. $2H_2 + O_2 \rightarrow 2H_2O$. In this reaction, the number of H_2 molecules reacting is equal to twice the number of O_2 molecules reacting, as given by Eq. 4.

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, with subscript c).

Quantities of this kind are used extensively in thermodynamics, along with "partial" molar quantities. The latter relate to multicomponent systems, and are defined similarly (by $\partial X/\partial n_X$ for quantity X and component X).

Measuring chemical amount

Pure substances, (a) using daltons

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

$$N = m_{\rm s}/m_{\bullet} \tag{8}$$

where m_s is the mass of the sample and m_{\bullet} is the mass of the entity (the dot denoting a particle).⁴ Hence from Eq. 3

$$n = m_{\rm s}/M \tag{9*}$$

where

$$M = Lm_{\bullet} \tag{10a}$$

M is the molar mass of the substance (compare Eq. 9 with Eq. 7) reckoned in terms of the specified entity.

Now the mole is defined to be such that, for a sample of carbon-12, $n(^{12}\text{C} \text{ atoms}) = 1 \text{ mol when } m_{\text{s}}(\text{carbon-12}) = 12 \text{ g}$. Since $m_{\bullet}(^{12}\text{C} \text{ atom}) = 12 \text{ Da}$, Eqs. 9 and 10a give

$$L = 1 \text{ g } \text{Da}^{-1} \text{mol}^{-1} \tag{11a}$$

Thus, L in Eq. 10a converts m_{\bullet} in daltons into M in g mol⁻¹.

Example: What is the chemical amount of hydrogen, reckoned in terms of H_2 molecules, in 1.000 g of the gas?

Answer: From $m_{\bullet}(H_2) = 2.016$ Da, Eqs. 10a and 11a give $M(H_2) = 2.016$ Da \times 1 g Da⁻¹ mol⁻¹ = 2.016 g mol⁻¹. Hence from Eq. 9, $n(H_2) = 1.000$ g/2.016 g mol⁻¹ = 0.496 mol.

Pure substances, (b) using relative masses

If relative masses (Eq. 1b) are used, Eq. 10a becomes

$$M = Lm_{\rm u}m_{\rm r} = M_{\rm u}m_{\rm r} \tag{10b}$$

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

⁴ IUPAC denote the mass of an atom by m_a and of a molecule or formula unit by m_f .

$$M_{\rm u} = 1 \text{ g mol}^{-1} \tag{11b}$$

Thus, M_u in Eq. 10b converts relative mass into molar mass. IUPAC call this constant the "molar mass constant".

Answer to the above example: From $m_r(H_2) = 2.016$, Eqs. 10b and 11b give $M(H_2) = 2.016 \times 1 \text{ g mol}^{-1} = 2.016 \text{ g mol}^{-1}$. Hence $n(H_2) = 1.000 \text{ g/}2.016 \text{ g mol}^{-1} = 0.496$ - 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

$$\gamma = m_{\rm s}/V \tag{12}$$

Hence from Eqs. 9 and 12

$$n = cV \tag{13*}$$

where

$$c = n/V = \gamma/M \tag{14*}$$

The quantity *c* is commonly called the "molarity" of the solution. IUPAC prefer the name "amount (or 'substance') concentration", an abbreviation for "amount-of-substance concentration". Other measures of concentration are "mole fraction" ($x = n/n_{total}$) and "molality" ($b = n/m_{solvent}$). (Better names for these quantities would be: *c*, "chemical concentration"; *x*, "chemical fraction"; *b*, "specific [chemical] 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 ($p, p \rightarrow 0$), the volume of a gas per molecule

$$V_{\rm mol} = V/N \tag{15}$$

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

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

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

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

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

where k is a constant having the same value for all gases. Thus, from Eqs. 15, 18, and 3,

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

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

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

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

$$n \approx V/V_{\rm m}^{\rm ideal}, \quad V_{\rm m}^{\rm ideal} = RT/p$$
 (21*)

At "standard" temperature and pressure (STP: 0 °C, 1 atm), $V_m^{\text{ideal}} = 22.41 \text{ l mol}^{-1}$; at standard ambient temperature and pressure (SATP: 298.15 K, 1 bar), its value is 24.79 l mol⁻¹ (Atkins and de Paula 2002).

The five equations marked with an asterisk 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,

$$m_{\rm s} \propto Q m_{\bullet} / v$$
 (22)

where m_{\bullet} is the mass of the atom or radical composing the substance and v is its valency. From Eqs. 8 and 3, 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 constant *L* in Eq. 3 has the dimensions (chemical amount)⁻¹, and is therefore properly called the Avogadro "constant", as distinct from the Avogadro "number" (N_{Avo}), which is a pure number (Nelson 1991). These are related by

$$L = N_{\rm Avo} \, \rm{mol}^{-1} \tag{24}$$

From the definition of the mole, N_{Avo} is equal to the number of ¹²C atoms in exactly 12 g of carbon-12. From Eq. 11a and 24, it is also equal to the number of daltons in a gram (g/ Da). IUPAC confusingly use N_A as an alternative symbol for the constant, despite N being their symbol for number.

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:

$$V_{\rm m} = M/\rho = LV_{\rm at} \tag{25}$$

This gives $L = 6.0221406(2) \times 10^{23} \text{ mol}^{-1}$ (Becker and Bettin 2011; Yang et al. 2012). From this, Da = $m_{\rm u} = g/N_{\rm Avo} = 1.6605391(1) \times 10^{-24}$ g.

The formulation of the mole has been designed so that stoicheiometric calculations can be carried out without having to evaluate Da, m_u , or L. This is no longer true of new SI proposals discussed below.

Explanation

What is chemical amount?

The above formulation raises a number of questions. The first is, what exactly is the physical quantity "amount of substance" or "chemical amount"? Milton and Mills (2009) define it as "a quantity that measures the size of an ensemble of entities", but as the size of an ensemble is measured by the number of members, this does not differentiate n from N.

A partial answer to the question can be inferred from Eq. 2: chemical amount is "the macroscopic measure of the amount of a substance that corresponds at an atomic level to the number of specified chemical entities the substance contains" (Nelson 1991). The mole is likewise the chemical amount "corresponding to" a standard number of entities. The distinction between *n* and *N* is thus that the former relates to substances as they are in bulk (e.g. water as a colourless liquid boiling at 100 °C) and the latter to what they are at an atomic level (e.g. an assembly of H₂O molecules).

A more complete answer follows from Eq. 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 vapour 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 mainly NaCl molecules. In principle, therefore, stoicheiometry can be conducted entirely at a macroscopic level, with (1) *n* defined to be proportional to $pV/T(p \rightarrow 0)$ for a gas, (2) the mole defined to be equal to *n* for a specific amount of gas (e.g. 2 g of hydrogen), and (3) empirical coefficients in Eq. 6. The mole determines the value of the proportionality constant in (1) (1/*R*).

Why use chemical amount?

A second question is, why introduce chemical amount? Why not simply use number of entities, and the Avogadro number ($N_{Avo} = g/Da$) as a genuine counting unit (called, say, an "avogadro" or "avo", symbol Av)? This can be done without requiring the value of N_{Avo} (Nelson 1991):

Example: How many molecules are there in 1.000 g of hydrogen?

Answer: From $m_{\bullet}(H_2) = 2.016$ Da, $N(H_2) = 1.000$ g/2.016 Da = 0.496 g/Da = 0.496 Av. This corresponds to $n(H_2) = 0.496$ mol in the example above.

One could alternatively use the relative number of entities ($N_r = N/N_{Avo}$) corresponding to relative mass ($m_r = m/m_u$, Eq. 1b).

The reason for using chemical amount is largely 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 (compare my treatment in the last section). It was one of these scientists, the physical chemist Wilhelm Ostwald, who coined the term "mole" (Ger. *Mol*), the Latin *moles* meaning a large mass as opposed to

molecula, a small one (Ostwald 1893: 119; OED). Although he later changed his views about the existence of atoms and molecules, his approach to stoicheiometry has persisted.

Mills and Milton (2009) give other reasons for using *n* instead of *N*, but these overlook the fact that (1) *N* can be used without counting entities as in the example above, and (2) chemists are mainly interested in the amounts of substances taking part in reactions, which are determined at the atomic level (Eq. 4) not bulk. The use of *n*, however, is well established.⁵

Note that changing to *N* would involve replacing the constants *R* and *F* by *k* and *e* (Eqs. 19 and 23), "molar" quantities (*X/n*) by "per-entity" ones (*X/N*), amount concentrations (*n/V* etc.) by entity concentrations (*N/V* etc.), and differentials (d*n*) by finite increments (δN). Changing to N_r would involve similar modifications.

New SI proposals

The General Conference on Weights and Measures (CGPM) is currently proposing that the mole be redefined such that the Avogadro constant has a fixed value in mol⁻¹ (N^* mol⁻¹) (CGPM-24 2011: Resolution 1; cf. Mills et al. 2011; Milton 2011). The effect of this change on the above treatment is that *L* in Eq. 11a is no longer equal to exactly 1 g Da⁻¹ mol⁻¹ and M_u in Eq. 11b to exactly 1 g mol⁻¹. The exactness can be recovered by redefining the kilogram such that the mass of N^* carbon-12 atoms is exactly 12 g, but CGPM currently proposes to redefine the unit of mass by fixing the value of Planck's constant. The CGPM proposals are not supported by everyone (see, e.g., Jeannin 2010; Leonard 2010; Wheatley 2011; Price 2011; Pavese 2011; Hill 2011; Censullo et al. 2011; Miller et al. 2011), and may not ultimately be accepted. They assume that the equations linking the kilogram to Planck's constant are final, whereas they can only ever be provisional (Nelson 2011). If the proposals are accepted, the easiest way of incorporating them is to substitute the fixed value of *L* and experimental value of m_u in $M_u = Lm_u$ (Eq. 10b) to give an experimental value for M_u (cf. Taylor 2009).

Summary of suggested improvements to SI/IUPAC scheme

(I have added this section at the suggestion of a reviewer.)

- Call n "chemical amount" and define it as "the macroscopic measure of the amount of a substance that corresponds at an atomic level to the number of specified chemical entities the substance contains" (sections "Chemical amount" and "What is chemical amount?").
- Likewise define the mole as "the chemical amount of a substance that corresponds to the same number of specified entities as there are atoms in exactly 12 grams of carbon-12".
- 3. Rename "molar" quantities (X/n) "chemical" ones (section "Quantities per chemical amount").
- 4. Call *c* "chemical concentration", *x* "chemical fraction", and *b* "specific [chemical] concentration" (section "Substances in solution").

⁵ At the 2011 meeting of the IUPAC Commission on Isotopic Abundances and Atomic Weights (CIAAW), the Commission proposed that "amount of substance" be renamed "number of entities" and the mole be defined as a number. This confounds the two schemes.

- 5. Symbolize the Avogadro constant (N/n) by L not N_A (section "The constant L").
- 6. Consider changing to a scheme based on N or N_r (section "Why use chemical amount?").
- Redefine the kilogram as the mass of a specified number of ¹²C atoms (section "New SI proposals").

In suggestions 1-4, "chemical" could be abbreviated to "chemo", e.g. "chemoamount".

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