Realising the mole

The mole, symbol mol, is the SI unit of amount of substance. It is defined in Chapter 2 of the SI Brochure (8th edition), Section 2.1.1.6, with the words:

1. The unit mole is the amount of substance which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12; its symbol is "mol".

2. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.

The mole may be realised by a variety of primary methods. Three examples are discussed below.

1. For a pure sample the amount of substance n in the sample may be measured by determining the mass m of the sample and dividing by the molar mass M using the relation:

$$n = m / M \tag{1}$$

If the mass m is expressed in gram, and the molar mass M in g/mol, then the amount of substance n is obtained in mol. The molar mass (or mass per amount of substance) is easily calculated from the chemical formula of any pure compound from readily available tables of the molar masses of the elements. The molar mass of an element of naturally occurring isotopic composition is obtained from the molecular weight (i.e. relative molecular mass) by multiplying by the unit g/mol. The molar masses of all the nuclides are known and tabulated with a relative standard uncertainty of 10^{-7} or less, and for many elements less than 10^{-8}. For a naturally occurring sample of an element it is generally necessary to calculate a weighted average over the isotopes using tables of relative abundance. Tabulated values of atomic weights are obtained in this way. This method of realising the mole is generally the most precise method available, because measuring the mass of a sample is a relatively simple and accurate procedure. The mole may easily be realised with a relative standard uncertainty of less than 1×10^{-6} by this method. However it is important to note that this procedure depends on having a pure sample of the material, which implies having a precise chemical analysis of the sample, and this will often be the limiting factor in an uncertainty evaluation.

2. For a pure gas the amount of substance may be determined from the equation of state for the gas in the form:

$$pV \ = \ nRT \left[1 + B(T) \left(\frac{n}{V} \right) + ... \right] \tag{2}$$

where p and V are the pressure and volume, T is the temperature, and R is the molar gas constant. The term involving the second virial coefficient $B(T)$, and possible higher terms involving the third virial coefficient, are small corrections. When expressed in terms of pressure these corrections may be written in the form:

$$pV = nRT\left[1 + B_p(T)\,p + \ldots\right] \tag{3}$$

where $B_p(T)$ is the second virial coefficient on a pressure basis. This shows that the correction terms may be eliminated by extrapolating to low pressure. For many purposes, at pressures below one atmosphere, the amount of substance may be calculated with sufficient accuracy from the ideal gas equation:

$$n = pV/RT \tag{4}$$

Virial coefficients expressed in SI units are tabulated for a number of simple gases. The molar gas constant R is known with a relative standard uncertainty of 1.7×10^{-6} (CODATA 2006) in the SI unit (Pa m^3 mol^{-1} K^{-1}), thus giving n in mol. The uncertainty in measurements of n made this way depend on the uncertainty in measuring p, V and T, and in correcting for gas imperfections. This method of realising the mole for a gas is also dependent on the use of a pure sample of the gas.

3. In chemical electrolysis, the amount of substance n liberated at an electrode is proportional to the charge Q passed through the system, and thus to the product of the electric current I multiplied by the time t for which it flows. The proportionality constant is the reciprocal of the charge number z of the ion that is liberated multiplied by the Faraday constant F, according to the formula:

$$n = Q/zF = It/zF \tag{5}$$

The Faraday constant F is known with a relative standard uncertainty of approximately 2.5×10^{-8} (CODATA 2006) in the SI unit (C/mol), thus giving n in mol.

The criteria used to determine whether a method has the potential to be primary are discussed in detail by Milton and Quinn [*Metrologia*, 2001, **38**, 289-296].

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