Atomic Mass

The mass of an atom or a molecule is often called its **atomic mass**. Mass is a basic physical property of matter and stricIty speaking there is no difference between **mass** and **atomic mass**. Therefore the term 'atomic mass 'is really technobabble. The (atomic) mass is used to find the average mass of elements and molecules and to help solve stoichiometry problems.

Introduction

In chemistry, there are many different concepts of mass that are often used incoherently and are often ill defined. It is often assumed that **atomic mass** is the mass of an atom indicated in**unified atomic mass units (u)**. However, the book "Quantities, Units and Symbols in Physical Chemistry" published by the IUPAC clearly states:

Neither the name of the physical quantity, nor the symbol used to denote it, should imply a particular choice of unit.

The name "atomic mass" is a historical baggage and comes from the fact that chemistry was the first science that investigated the same physical objects on macroscopic and microscopic levels. In addition the situation is rendered more complicated by the isotopic distribution. On the macroscopic level, most mass measurements of pure substances refer to a mixture of isotopes. This means from a physical stand point, these mixtures are not pure. For example, the macroscopic mass of oxigen (O_2) does not correspond to the microscopic mass of O_2. The former usually implies a certain isotopic distribution, whereas the later usually refes to the most common isotope ($^{16}O_2$). Note that the former is now often referred to as the "molecular weight" or "atomic weight".

Mass Concepts in Chemistry

name in chemistry	physical meaning	symbol	units
atomic mass	mass on microscopic scale	m, m_a	Da, u, kg, g
molecular mass	mass of a molecule	m	Da, u, kg, g
isotopic mass	mass of a specific isotope		Da, u, kg, g
mass of entity	mass of a chemical formula	m, m_f	Da, u, kg, g
average mass	average mass of a isotopic distribution	m	Da, u, kg, g
molar mass	average mass per mol	$M = m/n$	kg/mol or g/mol
atomic weight	average mass of an element	$A_r = m / m_u$	unitless
molecular weight	average mass of a molecule	$M_r = m / m_u$	unitless
relative atomic mass	ratio of mass m and and the atomic mass constant m_u	$A_r = m / m_u$	unitless

Mass Concepts in Chemistry

name in chemistry	physical meaning	symbol	units
atomic mass constant	$m_u = m(^{12}C)/12$	m_u = 1 Da = 1 u	Da, u, kg, g
relative molecular mass	ratio of mass m of a molecule and and the atomic mass constant m_u	$M_r = m / m_u$	unitless
relative molar mass	?	?	?
mass number	nucleon number	A	nucleons, or unitless
integer mass	nucleon number * Da	m	Da, u
nominal mass	integer mass of molecule consisting of most abundant isotopes	m	Da, u
exact mass	mass of molecule calculated from the mass of its isotopes (in contrast of measured ba a mass spectrometer)		Da, u, kg, g
accurate mass	mass (not nomnal mass)		Da, u, kg, g

In the following the different concepts are explained.

Average Mass

Isotopes are atoms with the same atomic number, but different mass number. The larger mass size is due to the difference in the number of nuetrons that an atom contains. Although mass numbers are whole numbers, the actual masses of individual atoms are never whole numbers (except for carbon-12). This explains how Lithium can have an atomic mass of 6.941 Da. The atomic masses on the periodic table take these isotopes into account, weighing them based on their abundance in nature, therefore, more weight is given to the isotopes that occur most frequently in nature. Average mass of the element E is defined as:

$$m(E)=\sum_{n=1} m(I_n)\times p(I_n)$$

where $\sum$ represents a n-times summation over all isotopes I_n of element E, and p(I) represents the relative abundance of the isotope I.

Example

Find the average atomic mass of boron using the Table 1 below:

Mass and abundance of Boron isotopes

n	isotope I_n	mass m (Da)	isotopic abundance p
1	^{10}B	10.013	0.199
2	^{11}B	11.009	0.801

Solution: The average mass of Boron is:

$$m(B) = (10.013 \text{ Da})(.199) + (11.009 \text{ Da})(.801) = 1.99 \text{ Da} + 8.82 \text{ Da} = 10.81 \text{ Da}$$

Relative Mass

Traditionally it was common practice in chemistry to not use any units when indicating atomic masses (e.g. masses on microscopic scale). Even today you can overhear chemsitry jargon like "^{12}C has exactly mass 12". However, since mass is not a dimensionless quantity, it is clear that a mass indication in fact needs a unit. Since chemists are very sticky when it comes to jargon, many of them tried to rationalize why they don't need a unit instead of using a unit. The result is the concept of relative mass, which strictly speaking is not even a mass but a ratio of two masses. Rather than using a unit, these sticky chemists claim to indicate the ratio of the mass they want to indicate and the atomic mass constant m_u which is defined analoguous to the unit they want to avoid. Hence the relative atomic mass of the mass m is defined as:

$$A_r = m / m_u$$

It is now dimensionless and does not have any units. This trick is highly confusing and against the standards of modern metrology. Therefore we recommend not to use any "relative" mass.

Molecular Weight, Atomic Weight, Weight vs. Mass

In former times the concept of mass was not clearly distinguished by the concept of weight. In colloquial language this is still the case. Many people indicate their "weight" when they actually mean their mass. Mass is a fundamental property of objects, wehreas weight is a force. Weight is the force F exerted on a mass m by a gravitational field. The exact definition of the weight is controversial. Weight is an outdated concept and should no longer be used. The weight of a person is different on ground than on a plane. Stricly speaking, the weight even changes with your location on earth.

When talking about atoms and molecules, it is obvious that people address the mass of a molecule when they say "molecular weight". Unfortunately, many chemists prefer their outdated jargon over scientific rigour. There is not even an agreed definition of the term "molecular weight". However, the majority of the chemists agree that it means an average mass, and many think it is dimensionless. This would make "molecular weight" a synonym to "average relative mass".

Integer Mass

Since the proton and the neutron have simillar mass, and the electron has a very small mass compared to the former, most molecules have a mass that is close to an integer value when measured in daltons. Therefore it is quite common to only indicate the **integer mass** of molecules. Integer mass is only meaningful when using the unit dalton (or u).

Accurate Mass

Many mass spectrometers can detirmine the mass of molecules more accuratley than to the integer mass. These measurements are then called **accurate mass** of the molecule. The reason isotopes and hence molecules have atomic masses that are not integer masses is because of mass defect caused by binding energy in the nucleus.

Units

The atomic mass is usually measured in the units *unified atomic mass unit* (u), or dalton (Da). Both units are derived from the carbon-12 isotope, as 12 u is the exact atomic mass of that isotope. So 1 u is 1/12 of the mass of a carbon-12 isotope:

$$1 \text{ u} = 1 \text{ Da} = m(^{12}C)/12$$

It is expected that the somewhat clumbsy "*unified atomic mass unit*" will soon be replaced by the more modern dalton.

The first scientists to measure atomic mass were John Dalton (between 1803 and 1805) Jons Jacoband Berzelius (between 1808 and 1826). Early atomic mass theory was purposed by the English chemist William Prout in a series of published papers in 1815 and 1816. Known was Prout's Law, Prout propsed that the known elements all had atomic weights that were whole number multiples of the atomic mass of hydrogen. Berzelius discovered that this was not always true by showing that chlorine (Cl) had a mass of 35.45 which was not a whole number multiple of hydrogen's mass.

Note that some people use the atomic mass unit (amu). The amu had two definitions. It was defined differently by physicists and by chemists.

Physics: 1 amu = $m(^{16}O)/16$

Chemistry: 1 amu = $m(O)/16$

This means the chemists used Oxigen in the naturally occurring isotopic distribution as the reference. Since the isotopic distribution in nature can change, this definition is a moving target. Therefore both communities agreed to the compromise of using $m(^{12}C)/12$ as the new unit, and they called this unit "unified atomic mass unit" u. Hence, the amu is no longer in use and the people that still use it probably use it with the definition of the u in mind. Again we have a very confusing situation. This is why the use of the unit dalton (Da) is more and more recommended, whose definition is clear and whose name is not as clumbsy.

Historical note: Why did one compromise on $m(^{12}C)/12$ instead of the already established well defined $m(^{16}O)/16$? The reason are the sticky chemsists (see above) that refused to use units. All their papers and books were written without mass units. Therefore a change of unit was a desaster for those books: you could not tell wether the amu or the u was used. The sollution was to use $m(^{12}C)/12$ as the new unit which is very close to chemists amu = $m(O)/16$. The physicists could live with that because they usually used units in their publications, hence there was no ambigouity. Take-home message: do use units.

Another note: Both, the u and the Da are not SI units. However, they are recognized by the SI.

Molar Mass

The molar mass is the mass of one mole of substance, whether the substance is an element or a compound. A mole of substance is equal to Avogadro's number or 6.023x10^23 atoms. The molar mass is indicated in the units g/mol or kg/mol. When using the unit g/mol, the numerical value of the molar mass of a molecule is the same as its average mass in dalton:

- Average mass of C: 12.011 Da
- Molar mass of C: 12.011 g/mol

This allows for a smooth transition from the microscopic world, where mass is measured in dalton, to the macroscopic world where mass is measured in kg.

Example

What is the molar mass of phenol, C_6H_5OH?

Average mass m = 6 * 12.011 Da + 6 * 1.008 Da + 1 * 15.999 Da = 94.113 Da

Molar mass = 94.113 g/mol = 0.094113 kg/mo

Measuring Masses in the Atomic Scale

Masses of atoms and molecules are measured by a mass spectrometer. Mass Spectrometry is a technology to measure the mass-to-charge ratio m/Q of ions. This implies that all molecules and atoms to be measured must first be ionized. After this, the ions are then seperated in a mass analyzer according to their mass-to-charge ratio. The charge of the measured ion can then usually be figured out because it is a multiple of the elementary charge. Then the ion's mass can be deduced. The average masses indicated in the Periodic Table are then calculated using the isotopic abundances, as explained above.

Note that the masses of all isotopes have been measured with very high accuracy. Therefore it is much simpler and more accurate to calculate the mass of a molecule as a sum of its isotopes than measuring it with a commercial mass spectrometer.

Note that the same is not true on the nucleon scale. The mass of an isotope cannot be calculated accurately as the sum of its particles (table below) since this would ignore the mass defect caused by the binding energy of the nucleons, which is significant.

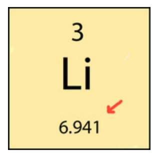
Table 2 - Mass of three sub-atomic particles

Particle	SI (kg)	Atomic (Da)	Mass Number A
Proton	1.6726×10^{-27}	1.0073	1
Neutron	1.6749×10^{-27}	1.0087	1
Electron	9.1094×10^{-31}	0.00054858	0

As one can see in Table 2, the mass of an electron is relatively small so that it only contributes less than 1/1000 to the overall mass of the atom.

Where to Find Atomic Mass

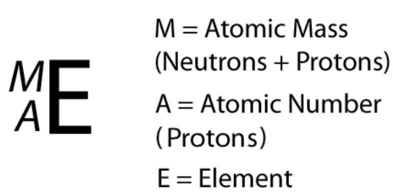
The atomic mass found on the Periodic Table (below the element's name) is the average atomic mass. For example, for Lithium:



The red arrow indicates the atomic mass of Lithium. As shown in Table 2 above and mathematically explained later, the masses of a protons and neutrons are about 1u. This, however, does not explain why Lithium has an atomic mass of 6.941 Da were we would expect 6 Da. You can notice this for all elements on the Periodic Table. The atomic mass for Lithium is actually the average atomic mass based on its Isotopes. We will go into further details on this on the next section.

One particularly useful way of writing an isotope is as follows:

$^{A}_{Z}E$



E = Element

A = Mass Number

Z = Atomic number = Proton Number

N = A - Z = Number of Neutron Number

Applications

Applications Include:

1. Average Molecular Mass
2. Stoichiometry

*Please Note: One particularly important relationship is illustrated by the fact that an atomic mass unit is equal to 1.66 * 10^{-24} g. This is the reciprocal of Avogadro's constant, but this is no mere coincidence:

\displaytype**Atomic Mass (g)1g×1mol6.022×10^{23}=Mass (g)1atom**

Because a Mol can also be expressed as gram x atoms,

1u = M_u(molar mass unit)/N_A(Avogadro's Number)=1g/mol/N_A

N_A known as Avoagrado's Number or Constant is equal to 6.023x10^23 atoms.

Atomic mass is particularly vital when dealing with Stoichiometry.

Source: http://chemwiki.ucdavis.edu/Physical_Chemistry/Atomic_Theory/Atomic_Mass