Mean Molecular Mass

Derivation of μ

For an ideal gas composed of different atomic species, the equation of state can be written in the form

$$P = nkT, \tag{1}$$

where P is the gas pressure, T the temperature, k Boltzman's constant, and n the particle number density, i.e. the number of particles (of all species combined) per unit volume. If $\langle m \rangle$ represents the average mass per particle, we can write equation (1) as

$$\begin{aligned} P &= \frac{n\langle m\rangle}{\langle m\rangle} kT \\ &= \frac{\rho}{\langle m\rangle} kT, \end{aligned} \tag{2}$$

with ρ the total density of the gas mixture. In astronomy it is customary to express the mean mass per particle in terms of the atomic mass unit (amu), which, for our purposes, we declare to be the proton mass, m_p. We define a quantity μ, named "mean molecular mass," as

$$\mu = \langle m\rangle / m_p. \tag{3}$$

Defined this way, μ is numerically equal to the *average number of amu's per particle*. For example, suppose that the gas mixture consists of hydrogen only, and all of the hydrogen atoms are neutral. Then the mean mass per particle in amu's would be 1, making $\mu = 1$. If all the hydrogen is fully inonized, then the mass of one hydrogen atom (1 amu) would be shared by *two* particles (the H nucleus and the free electron), and the mean mass per particle would now be 1 amu per 2 particles, or $\mu = 0.5$. Similarly, for a pure He gas, with all He atoms fully ionized, the mass of one He atom (4 amu) would be shared by three particles (the He nucleus and two free electrons), or $\mu = 4/3 = 1.33$. In terms of μ, the equation of state (1) becomes

$$P = \frac{\rho}{\mu m_p} kT. \tag{4}$$

How to calculate μ for a gas that consists of a mixture of different atomic species? First, let us introduce a quantity that indicates the *fraction by mass*, X_j, of each atomic species j present in the mixture:

$$X_j = \frac{m_j}{m} = \frac{\rho_j}{\rho}. \tag{5}$$

Clearly, we can write

$$\sum_{j=1}^{100+} X_j = 1. \tag{6}$$

The density ρ_j of the species j part of the gas mixture can be written as

$$\rho_j = n_j m_j = n_j A_j m_p. \tag{7}$$

Solving for n_j, and using equation (5), we get

$$\begin{aligned} n_j &= \frac{\rho_j}{A_j m_p} \\ &= \frac{\rho}{m_p}\frac{X_j}{A_j}. \end{aligned} \tag{8}$$

For a gas where all species are fully ionized, each atom of species j contributes $j+1$ particles to the mixture (one nucleus and j electrons). Hence we can write:

$$\langle m \rangle = \frac{\sum_{j=1}^{100+} n_j m_j}{\sum_{j=1}^{100+} n_j (j+1)} \tag{9a}$$

$$= \frac{\sum_{j=1}^{100+} n_j A_j m_p}{\sum_{j=1}^{100+} n_j (j+1)} \tag{9b}$$

$$= \frac{m_p \sum_{j=1}^{100+} n_j A_j}{\sum_{j=1}^{100+} n_j (j+1)}, \tag{9c}$$

which leads to

$$\mu = \frac{\langle m \rangle}{m_p} = \frac{\sum_{j=1}^{100+} n_j A_j}{\sum_{j=1}^{100+} n_j (j+1)} \tag{10a}$$

$$= \frac{\sum_{j=1}^{100+} (\frac{\rho}{m_p}\frac{X_j}{A_j}) A_j}{\sum_{j=1}^{100+} (\frac{\rho}{m_p}\frac{X_j}{A_j})(j+1)} \tag{10b}$$

$$= \frac{\sum_{j=1}^{100+} X_j}{\sum_{j=1}^{100+} \frac{X_j}{A_j}(j+1)} \tag{10c}$$

$$= \frac{1}{\sum_{j=1}^{100+} (j+1)\frac{X_j}{A_j}}. \tag{10d}$$

Let us now take our definitions of the X_j's a step further. For hydrogen ($j = 1$), we declare $X_1 \equiv X$. For helium ($j = 2$), we set $X_2 \equiv Y$. All other chemical elements ($j \geq 3$) we lump together and define

$$Z \equiv \sum_{j \geq 3} X_j, \tag{11}$$

Equation (6) then becomes

$$X + Y + Z = 1, \tag{12}$$

or

$$Z = 1 - X - Y. \tag{13}$$

Taking the reciprocal of equation (15), and introducing the quantities X, Y and Z, gives

$$\frac{1}{\mu} = \sum_{j=1}^{100+} (1+j)\frac{X_j}{A_j} \tag{14a}$$

$$= 2X + \frac{3Y}{4} + \sum_{j=3}^{100+} \frac{1+j}{A_j} X_j \tag{14b}$$

$$\cong 2X + \frac{3Y}{4} + \langle \frac{1+j}{A_j} \rangle \sum_{j=3}^{100+} X_j \tag{14c}$$

$$\cong 2X + \frac{3Y}{4} + \frac{1}{2}\sum_{j=3}^{100+} X_j \tag{14d}$$

$$\cong 2X + \frac{3Y}{4} + \frac{1}{2}Z. \tag{14e}$$

In here we have replaced the ratio $\frac{1+j}{A_j}$ in each of the terms by the average value for this ratio, $\langle\frac{j+1}{A_j}\rangle$, which has a value of approximately 1/2. After some minor algebra and eliminating Z via equation (13), we find the final formula for the mean molecular mass of a fully ionized gas mixture:

$$\mu = \frac{4}{6X + Y + 2}. \tag{15}$$

Note that this equation gives an approximate value for μ. For an exact value, we would need to know the abundances of all atomic species individually.

The following table summarizes the various quantities introduced in the above derivation.

Name	Notation	Unit
Atomic species	j	...
Atomic mass number	A_j	...
Number density of species j	n_j	m^{-3}
Mass density of species j	ρ_j	$\mathrm{kg\,m}^{-3}$
Total mass density	ρ	$\mathrm{kg\,m}^{-3}$
Total species j mass	m_j	kg
Total mass	m	kg
Mean mass per particle	$\langle m\rangle$	kg
Mean molecular mass	$\mu = \langle m\rangle/m_p$	...
Species j mass fraction	$X_j = m_j/m = \rho_j/\rho$	...
Fraction of H by mass	$X\ (= X_1)$	...
Fraction of He by mass	$Y\ (= X_2)$	...
Fraction of "metals" by mass	$Z\ (= \sum_{j\geq 3} X_j)$	...

Exercise

Calculate *and interpret* the mean molecular mass of a completely ionized gas under the following circumstances: (a) all hydrogen; (b) all helium; (c) all heavy elements (i.e. no H and no He). Which of these three values is *exactly* given by the approximate equation (15)?

Free Electron Number Density

For a fully ionized gas the number density of free electrons, n_e, can be written as

$$n_e = \sum_{j=1}^{100+} j n_j, \tag{16}$$

since each atom of species j contributes j free electrons to the mixture. Further evaluating equation (16) gives

$$\begin{aligned}
n_e &= \sum_{j=1}^{100+} j(\frac{\rho}{m_p}\frac{X_j}{A_j}) && \text{(17a)}\\
&= \frac{\rho}{m_p}\sum_{j=1}^{100+} j\frac{X_j}{A_j} && \text{(17b)}\\
&= \frac{\rho}{m_p}\left(X + \frac{1}{2}Y + \langle\frac{j}{A_j}\rangle \sum_{j=3}^{100+} X_j\right) && \text{(17c)}\\
&= \frac{\rho}{m_p}\left(X + \frac{1}{2}Y + \frac{1}{2}Z\right) && \text{(17d)}\\
&= \frac{1}{2}\frac{\rho}{m_p}(X+1). && \text{(17e)}
\end{aligned}$$

It is also common to use a quantity called the *mean molecular mass per electron*, μ_e, which is numerically equal to the average number of amu's per free electron in the gas. Convince yourself that

$$n_e = \frac{\rho}{m_p}\frac{1}{\mu_e}, \tag{18}$$

and hence,

$$\mu_e = \frac{2}{1+X}. \tag{19}$$