

## What is reduced mass?

The reduced mass  $\mu$  (kg) of a system of two bodies is determined as

$$\frac{1}{\mu} = \left( \frac{1}{m_A} + \frac{1}{m_B} \right)$$

where  $m_A$  and  $m_B$  are the masses (kg) of the bodies.

## Why is the reduced mass of a molecule needed in quantum mechanical calculations?

When we consider vibration or rotation of a molecule, using the reduced mass of the molecule assures us that we are viewing the motion (vibration or rotation) from a framework that is truly stationary. This is a key requirement for correct mathematical calculations in quantum mechanics because time is not a factor in the formulations. A stationary point does not change its position with time, though all other parts of the system (molecule) may.

## How is the reduced mass of a molecule determined?

The reduced mass of a monoatomic molecule (such as Ar) is just the mass of the atom. However, monoatomic molecules do not have vibrational or rotational modes, and therefore their reduced mass is not important for such calculations.

The reduced mass of a diatomic molecule (such as CO) is determined by the above formula using the masses of the respective atoms. A shortcut exists to calculate the reduced mass of such systems. Consider for a molecule that each mass ( $m_A$  or  $m_B$ ) is related to the molar mass of the respective atom by  $m_i = M'_i/N_o$ , where  $M'_i$  is the molar mass in units of kg/g mol and  $N_o$  is Avagadro's number ( $6.02214 \times 10^{23}$  particles/g mol). Since values of  $M_i$  are tabulated in g/g mol, an easier to use formulation is  $m_i = M_i(10^{-3})/N_o$ . Using this relationship, we find

$$\frac{1}{\mu} = \left( \frac{N_o}{10^{-3}} \right) \left( \frac{1}{M_A} + \frac{1}{M_B} \right) \quad \text{or} \quad \mu = A \left( \frac{1}{M_A} + \frac{1}{M_B} \right)^{-1} \quad (1)$$

The value  $A = 10^{-3}/N_o = 1.66054 \times 10^{-27}$  (kg g mol/particle or just kg) is typically reported as a constant called the atomic mass unit (amu or u).

For multi-atom molecules, the reduced mass is determined by replacing the two values of  $m_i$  with the total masses of the molecule to both sides of the bond in question. In other words, the multi-atom molecule is calculated as though it is a molecule with two atoms, where each atom is the part of the molecule on either side of the bond.

## Examples

Calculations for vibration of or rotation about the highlighted bond are being done.

carbon monoxide  $^{12}\text{C}-^{16}\text{O}$  :  $\mu = A/(1/12 + 1/16) = 1.1387 \times 10^{-26}$  kg

deuterated ammonia  $^1\text{H}_2^{14}\text{N}-^2\text{D}$  :  $\mu = A/(1/(2(1) + 14) + 1/2) = 2.952 \times 10^{-27}$  kg