Section 6: Moles, Molecular Formulae and Stoichiometric Calculations

We began with a circular dilemma: we could determine molecular formulae provided that we knew atomic masses, but that we could only determine atomic masses from a knowledge of molecular formulae. Since we now have a method for determining all atomic masses, we have resolved this dilemma and we can determine the molecular formula for any compound for which we have percent composition by mass.

As a simple example, we consider a compound which is found to be 40.0% carbon, 53.3% oxygen, and 6.7% hydrogen by mass. Recall from the Law of Definite Proportions that these mass ratios are independent of the sample, so we can take any convenient sample to do our analysis. Assuming that we have 100.0g of the compound, we must have 40.0g of carbon, 53.3g of oxygen, and 6.7g of hydrogen. If we could count or otherwise determine the number of atoms of each element represented by these masses, we would have the molecular formula. However, this would not only be extremely difficult to do but also unnecessary.

From our determination of atomic masses, we can note that 1 atom of carbon has a mass which is 12.0 times the mass of a hydrogen atom. Therefore, the mass of N

atoms of carbon is also 12.0 times the mass of N atoms of hydrogen atoms, no matter what N is. If we consider this carefully, we discover that 12.0g of carbon contains exactly the same number of atoms as does 1.0g of hydrogen. Similarly, we note that 1 atom of oxygen has a mass which is 16.012.0 times the mass of a carbon atom. Therefore, the mass of N atoms of oxygen is 16.012.0 times the mass of N

atoms of carbon. Again, we can conclude that 16.0g of oxygen contains exactly the same number of atoms as 12.0g of carbon, which in turn is the same number of atoms as 1.0g of hydrogen. Without knowing (or necessarily even caring) what the number is, we can say that it is the same number for all three elements.

For convenience, then, we define the number of atoms in 12.0g of carbon to be 1 mole of atoms. Note that 1 mole is a specific number of particles, just like 1 dozen is a specific number, independent of what objects we are counting. The advantage to defining the mole in this way is that it is easy to determine the number of moles of a substance we have, and knowing the number of moles is equivalent to counting the number of atoms (or molecules) in a sample. For example, 24.0g of carbon contains 2.0 moles of atoms, 30.0g of carbon contains 2.5 moles of atoms, and in general, x

grams of carbon contains x12.0 moles of atoms. Also, we recall that 16.0g of oxygen contains exactly as many atoms as does 12.0g of carbon, and therefore 16.0g of oxygen contains exactly 1.0 mole of oxygen atoms. Thus, 32.0g of oxygen contains 2.0 moles of oxygen atoms, 40.0g of oxygen contains 2.5 moles, and x grams of oxygen contains x16.0 moles of oxygen atoms. Even more generally, then, if we have m grams of an element whose atomic mass is M, the number of moles of atoms, n

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n=mM

Now we can determine the relative numbers of atoms of carbon, oxygen, and hydrogen in our unknown compound above. In a 100.0g sample, we have 40.0g of carbon, 53.3g of oxygen, and 6.7g of hydrogen. The number of moles of atoms in each element is thus

nC==40.0g12.0gmol3.33moles

nO==53.3g16.0gmol3.33moles

nH==6.7g1.0gmol6.67moles

We note that the numbers of moles of atoms of the elements are in the simple ratio nC:nO:nH=1:1:2

. Since the number of particles in 1 mole is the same for all elements, then it must also be true that the number of atoms of the elements are in the simple ratio 1 : 1 : 2. Therefore, the molecular formula of the compound must be COH2

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Or is it? On further reflection, we must realize that the simple ratio 1 : 1 : 2 need not represent the exact numbers of atoms of each type in a molecule of the compound, since it is indeed only a ratio. Thus the molecular formula could just as easily be C2O2H4

or C3O3H6. Since the formula COH2 is based on empirical mass ratio data, we refer to this as the empirical formula of the compound. To determine the molecular formula, we need to determine the relative mass of a molecule of the compound, i.e. the molecular mass. One way to do so is based on the Law of Combining Volumes, Avogadro's Hypothesis, and the Ideal Gas Law. To illustrate, however, if we were to find that the relative mass of one molecule of the compound is 60.0, we could conclude that the molecular formula is C2O2H4.
