4.6 EMPIRICAL AND MOLECULAR FORMULAS

PRACTICE

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Understanding Concepts

1. Empirical means derived from observation and experimentation.
2. A molecular formula gives the number of each kind of atom or ion, as opposed to an empirical formula which gives the simplest numerical ratio of the component atoms and/or ions.
3. Different compounds can exist because the same number and kind of atoms are bonded together differently, like ethanol, CH_3CH_2OH, and dimethyl ether, CH_3OCH_3. These two different compounds have very different properties, but would have the same percentage composition.
4. Possible molecular formulas could be C_2H_6, C_3H_9, C_4H_{12}, or indeed, any compound with the general formula C_nH_{2n}, where n is any integer.
5. (a) NO_2
   (b) CO_2
   (c) CH_2O
   (d) C_3H_2Cl
6. Sodium chloride does not exist as molecules, but as a three-dimensional lattice of ions; so there is no such concept as a molecular formula for this, or any other, ionic compound. The same rule applies to network solid elements and compounds — the formulas we use are always the simplest ratio of component ions or atoms.

Try This Activity : Distinguish Between Empirical and Molecular Formulas

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Name	Empirical Formula	Molecular Formula
ethane	CH_3	C_2H_6
butane	C_2H_5	C_4H_{10}
hexane	C_3H_7	C_6H_{14}
ethene	CH_2	C_2H_4
butene	CH_2	C_4H_8
hexene	CH_2	C_6H_{12}

4.7 CALCULATING CHEMICAL FORMULAS

PRACTICE

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Understanding Concepts

1. Empirical formulas can be determined from mass percent information.
2. Molecular formulas can be determined if one also has molar mass information.
3. Assume a 100 g sample, for convenience.

$m_{K^+} = 28.9\ \text{g} \qquad M_{K^+} = 39.10\ \text{g/mol}$

$m_S = 23.7\ \text{g} \qquad M_S = 32.06\ \text{g/mol}$

$m_O = 47.4\ \text{g} \qquad M_O = 16.00\ \text{g/mol}$

$$n_{K^+} = 28.9\ \cancel{\text{g}} \times \frac{1\ \text{mol}}{39.10\ \cancel{\text{g}}}$$

$$n_{K^+} = 0.739\ \text{mol}$$

$$n_S = 23.7\ \cancel{g} \times \frac{1\ mol}{32.06\ \cancel{g}}$$

$$n_S = 0.739\ mol$$

$$n_O = 47.4\ \cancel{g} \times \frac{1\ mol}{16.00\ \cancel{g}}$$

$$n_O = 2.96\ mol$$

The mole ratio, K^+ : S : O, is 0.739 : 0.739 : 2.96.

Simplifying (dividing each value by the lowest), we obtain 1.00 : 1.00 : 4.01, or almost exactly 1 : 1 : 4, making the empirical formula $KSO_{4(s)}$.

4. (a) Assume a 100.0 g sample, for convenience.

m_C = 40.87 g $\quad$ M_C = 12.01 g/mol

m_H = 3.72 g $\quad$ M_H = 1.01 g/mol

m_N = 8.67 g $\quad$ M_N = 14.01 g/mol

m_O = 24.77 g $\quad$ M_O = 16.00 g/mol

m_{Cl} = 21.98 g $\quad$ M_{Cl} = 35.45 g/mol

$$n_C = 40.87\ \cancel{g} \times \frac{1\ mol}{12.01\ \cancel{g}}$$

$$n_C = 3.403\ mol$$

$$n_H = 3.72\ \cancel{g} \times \frac{1\ mol}{1.01\ \cancel{g}}$$

$$n_H = 3.68\ mol$$

$$n_N = 8.67\ \cancel{g} \times \frac{1\ mol}{14.01\ \cancel{g}}$$

$$n_N = 0.619\ mol$$

$$n_O = 24.77\ \cancel{g} \times \frac{1\ mol}{16.00\ \cancel{g}}$$

$$n_O = 1.548\ mol$$

$$n_{Cl} = 21.98\ \cancel{g} \times \frac{1\ mol}{35.45\ \cancel{g}}$$

$$n_{Cl} = 0.6200\ mol$$

The mole ratio, C:H:N:O:Cl, is 3.403 : 3.68 : 0.619 : 1.548 : 0.6200.

Simplifying (dividing each by 0.619), we obtain 5.50 : 5.95 : 1.00 : 2.50 : 1.00. This is obviously not an integral ratio, but two more of the values become integers upon doubling, which gives 11.0 : 11.9 : 2.00 : 5.00 : 2.00, or 11: 12 : 2 : 5 : 2, making the empirical formula for chloromycetin $C_{11}H_{12}N_2O_5Cl_{2(s)}$.

(b) Assume a 100.0 g sample, for convenience.

m_C = 41.86 g $\quad$ M_C = 12.01 g/mol

m_H = 4.65 g $\quad$ M_H = 1.01 g/mol

m_N = 16.28 g $\quad$ M_N = 14.01 g/mol

m_O = 18.60 g $\quad$ M_O = 16.00 g/mol

m_S = 18.60 g $\quad$ M_S = 32.06 g/mol

$$n_C = 41.86\ \cancel{g} \times \frac{1\ \text{mol}}{12.01\ \cancel{g}}$$
$$n_C = 3.485\ \text{mol}$$
$$n_H = 4.65\ \cancel{g} \times \frac{1\ \text{mol}}{1.01\ \cancel{g}}$$
$$n_H = 4.60\ \text{mol}$$
$$n_N = 16.28\ \cancel{g} \times \frac{1\ \text{mol}}{14.01\ \cancel{g}}$$
$$n_N = 1.162\ \text{mol}$$
$$n_O = 18.60\ \cancel{g} \times \frac{1\ \text{mol}}{16.00\ \cancel{g}}$$
$$n_O = 1.163\ \text{mol}$$
$$n_S = 18.60\ \cancel{g} \times \frac{1\ \text{mol}}{32.06\ \cancel{g}}$$
$$n_S = 0.5802\ \text{mol}$$

The mole ratio, C:H:N:O:S, is 3.485 : 4.60 : 1.162 : 1.163 : 0.5802.

Simplifying, we obtain 6.007 : 7.93 : 2.003 : 2.005 : 1.000. This is obviously nearly an integral ratio, or 6 : 8 : 2 : 2 : 1, making the empirical formula for sulfanilamide $C_6H_8N_2O_2S_{(s)}$.

5. (a) Assume a 100 g sample, for convenience.

m_P = (100 – 43.6) g = 56.4 g M_P = 30.97 g/mol

m_O = 43.6 g M_O = 16.00 g/mol

$$n_P = 56.4\ \cancel{g} \times \frac{1\ \text{mol}}{30.97\ \cancel{g}}$$
$$n_P = 1.82\ \text{mol}$$
$$n_O = 43.6\ \cancel{g} \times \frac{1\ \text{mol}}{16.00\ \cancel{g}}$$
$$n_O = 2.73\ \text{mol}$$

The mole ratio, P : O is 1.82 : 2.73.

Simplifying (dividing each value by the lowest), we obtain 1.00 : 1.50, which, when doubled, is 2 : 3, making the empirical formula $P_2O_{3(s)}$.

(b) Assume a 100 g sample, for convenience.

m_P = (100 – 56.6) g = 43.4 g M_P = 30.97 g/mol

m_O = 56.6 g M_O = 16.00 g/mol

$$n_P = 43.4\ \cancel{g} \times \frac{1\ \text{mol}}{30.97\ \cancel{g}}$$
$$n_P = 1.40\ \text{mol}$$
$$n_O = 56.6\ \cancel{g} \times \frac{1\ \text{mol}}{16.00\ \cancel{g}}$$
$$n_O = 3.54\ \text{mol}$$

The mole ratio, P : O, is 1.40 : 3.54.

Simplifying (dividing each value by the lowest), we obtain 1.00 : 2.53, which, when doubled, is 2.00 : 5.06, or 2:5, making the empirical formula $P_2O_{5(s)}$.

6. Assume a 100.0 g sample, for convenience.

$m_C = (26.80 - 4.90)\text{ g} = 21.90\text{ g} \qquad M_C = 12.01\text{ g/mol}$

$m_H = 4.90\text{ g} \qquad M_H = 1.01\text{ g/mol}$

$$n_C = 21.90\ \cancel{\text{g}} \times \frac{1\text{ mol}}{12.01\ \cancel{\text{g}}}$$

$$n_C = 1.823\text{ mol}$$

$$n_H = 4.90\ \cancel{\text{g}} \times \frac{1\text{ mol}}{1.01\ \cancel{\text{g}}}$$

$$n_H = 4.85\text{ mol}$$

The mole ratio, C:H, is 1.823 : 4.85.
Simplifying, we obtain 1.000 : 2.66. This is obviously not an integral ratio, nor will doubling the ratio help. Multiplying the ratio through by three gives 3.000 : 7.98, or 3 : 8, making the empirical formula for propane $C_3H_{8(g)}$.

Applying Inquiry Skills

7. (a) **Experimental Design**

A sample of copper oxide will be reacted with carbon to burn away the oxygen and leave copper. The empirical formula of the oxide will be determined from the proportions of copper and oxygen in the oxide.

Procedure

1. Measure and record the mass of the empty crucible to 0.01 g.
2. Add the copper oxide sample to the crucible and measure and record the total mass to 0.01 g.
3. Add excess carbon to the crucible, and heat strongly until all the carbon has burned away, and only copper metal remains.
4. Allow the crucible and contents to cool, and measure and record the total mass to 0.01 g.

Evidence

mass of crucible	______ g
mass of crucible plus copper oxide	______ g
mass of crucible plus copper	______ g

Analysis

The masses of copper and oxygen in the sample are found by subtraction, if we assume the sample contained only copper and oxide ions. These masses are converted to moles, to allow determination of the mole ratio, and thus the formula.

(b) If the oxide is $Cu_2O_{(s)}$, then the evidence would show:

$m_{Cu^+} = 63.55\text{ u} \times 2 = 127.10\text{ u}$

$m_{O^{2-}} = 16.00\text{ u} \times 1 = 16.00\text{ u}$

$m_{Cu_2O_{(s)}} = 143.10\text{ u}$

$$\%\ Cu^+ = \frac{127.10\ \cancel{\text{u}}}{143.10\ \cancel{\text{u}}} \times 100\%$$

$$\%\ Cu^+ = 88.819\%$$

$$\%\ O^{2-} = \frac{16.00\ \cancel{\text{u}}}{143.10\ \cancel{\text{u}}} \times 100\%$$

$$\%\ O^{2-} = 11.18\%$$

The percentage composition of $Cu_2O_{(s)}$ is approximately 89% copper ions and 11% oxygen ions by mass. If the sample were this compound, the evidence would show these proportions.

PRACTICE

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Understanding Concepts

8. Assume one mole of compound, 58.1 g.

   mass % C = 62.0% $M_C = 12.01$ g/mol

   mass % H = 10.4% $M_H = 1.01$ g/mol

   mass % O = 27.5% $M_O = 16.00$ g/mol

   $$n_C = \frac{62.0}{100} \times 58.1\ \cancel{g} \times \frac{1\ mol}{12.01\ \cancel{g}}$$
   $$n_C = 3.00\ mol$$
   $$n_H = \frac{10.4}{100} \times 58.1\ \cancel{g} \times \frac{1\ mol}{1.01\ \cancel{g}}$$
   $$n_H = 5.98\ mol$$
   $$n_O = \frac{27.5}{100} \times 58.1\ \cancel{g} \times \frac{1\ mol}{16.00\ \cancel{g}}$$
   $$n_O = 0.999\ mol$$

   The integral mole ratio is 3 : 6 : 1, so the molecular formula is C_3H_6O.

9. Assume one mole of compound, 92.0 g.

   mass % N = 30.4% $M_N = 14.01$ g/mol

   mass % O = 69.6% $M_O = 16.00$ g/mol

   $$n_N = \frac{30.4}{100} \times 92.0\ \cancel{g} \times \frac{1\ mol}{14.01\ \cancel{g}}$$
   $$n_N = 2.00\ mol$$
   $$n_O = \frac{69.6}{100} \times 92.0\ \cancel{g} \times \frac{1\ mol}{16.00\ \cancel{g}}$$
   $$n_O = 4.00\ mol$$

   The integral mole ratio is 2 : 4, so the molecular formula is N_2O_4, and the name is dinitrogen tetraoxide.

Applying Inquiry Skills

10. (a) **Analysis**

    Assume one mole of compound, 180.2 g.

    mass % C = 40.0% $M_C = 12.01$ g/mol

    mass % H = 6.8% $M_H = 1.01$ g/mol

    mass % O = 53.2% $M_O = 16.00$ g/mol

    $$n_C = \frac{40.0}{100} \times 180.2\ \cancel{g} \times \frac{1\ mol}{12.01\ \cancel{g}}$$
    $$n_C = 6.00\ mol$$
    $$n_H = \frac{6.8}{100} \times 180.2\ \cancel{g} \times \frac{1\ mol}{1.01\ \cancel{g}}$$
    $$n_H = 12\ mol$$
    $$n_O = \frac{53.2}{100} \times 180.2\ \cancel{g} \times \frac{1\ mol}{16.00\ \cancel{g}}$$
    $$n_O = 5.99\ mol$$

    The integral mole ratio is 6 : 12 : 6, so the molecular formula of this carbohydrate is $C_6H_{12}O_6$.

PRACTICE

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Understanding Concepts

11. Natural source products usually contain traces of many other substances, and will normally vary somewhat in composition.

Making Connections

12. Vitamin D is produced naturally beneath the human skin surface by reaction of the body to exposure to sunlight. It is classed as an essential substance (a vitamin) because a lack of it causes a wide variety of deficiency diseases, the most notable of which is rickets. Rickets is characterized by a softening of the bones, causing limbs to grow bent, especially in children; and by a whole host of other symptoms. In fact, vitamin D is a steroid hormone that affects a great number of bodily functions.

    In 1921 Sir Edward Mellanby reported that dogs raised in the absence of sunlight could be kept healthy with a proper diet and that cod-liver oil contained some trace substance that prevented rickets. Cod-liver oil became a common tonic for people for the next several decades. Vitamin D (which actually has several forms) has since been synthesized, and is commonly available without prescription in tablet form in pharmacies. One of vitamin D's many aspects is that it aids bones to use calcium, so patients who take calcium supplements usually take vitamin D as well. Adding vitamin D to milk automatically ensures that the calcium in the milk is more useful and that small children receive an adequate amount of the vitamin itself.

    GO TO www.science.nelson.com, Chemistry 11, Teacher Centre.

Explore an Issue Debate: Are Natural Vitamins Better for Your Health?

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GO TO www.science.nelson.com, Chemistry 11, Teacher Centre.

PRACTICE

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Understanding Concepts

13. A mass spectrometer can provide data that allows the determination of the molar mass of a substance.
14. Since CH would be 13.02 g/mol, and the molar mass is known to be 26 g/mol, the molecular formula must be $C_2H_2(g)$.
15. Assume one mole of the compound ethane, 30.1 g.

    mass % C = 79.8% $M_C = 12.01$ g/mol

    mass % H = 20.2% $M_H = 1.01$ g/mol

    $$n_C = \frac{79.8}{100} \times 30.1\ \cancel{g} \times \frac{1\ \text{mol}}{12.01\ \cancel{g}}$$
    $$n_C = 2.00\ \text{mol}$$
    $$n_H = \frac{20.2}{100} \times 30.1\ \cancel{g} \times \frac{1\ \text{mol}}{1.01\ \cancel{g}}$$
    $$n_H = 6.02\ \text{mol}$$

    The integral mole ratio is 2 : 6, so the molecular formula of ethane from this evidence is $C_2H_{6(g)}$.

Applying Inquiry Skills

16. **Experimental Design**

    A sample of compound will be strongly heated to cause it to decompose to $CaO_{(s)}$ and $CO_{2(g)}$. The proportions of these two constituents will be determined from mass measurements.

Procedure

1. Measure and record the mass of the empty crucible to 0.01 g.
2. Add the compound sample to the crucible and measure and record the total mass to 0.01 g.
3. Heat strongly until all the sample has decomposed, and only $CaO_{(s)}$ remains.
4. Allow the crucible and contents to cool, and measure and record the total mass to 0.01 g.

Evidence

mass of crucible	______ g
mass of crucible plus compound	______ g
mass of crucible plus calcium oxide	______ g

Analysis

The masses of CaO and CO_2 in the sample are found by subtraction, if we assume the sample contained only these two constituents. These masses are converted to moles, to allow determination of the mole ratio, and thus the proportions.

Reflecting

17. The compound can be analyzed with a combustion analyzer and with a mass spectrometer to provide evidence to use in calculating its molecular formula.

SECTIONS 4.6 – 4.7 QUESTIONS

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Understanding Concepts

1. An empirical formula gives the simplest integral ratio of its constituent atoms, while a molecular formula also gives the correct actual number of atoms.
2. To calculate a molecular formula, the molar mass is needed.
3. To determine the empirical formula of a compound from the percentage composition, find the mass of each element in 100 g of the compound, using percentage composition; then find the amount in moles of each element by using the molar mass of the element; and then find the lowest integral ratio of atoms to determine the empirical formula.
4. The empirical formulas are, respectively:
   C_5H_4
   C_2H_6O
   NH_2
   O
   C_5H_7
   $C_6H_8N_2O_2S$
5. Ionic compounds do not exist as molecules, but as three-dimensional lattices of ions; so there is no such concept as a molecular formula for an ionic compound. The formulas we use are always the simplest ratio of component ions.
6. Assume a 100.00 g sample, for percentage conversion convenience.

m_C = 40.00 g $\qquad M_C$ = 12.01 g/mol

m_H = 6.71 g $\qquad M_H$ = 1.01 g/mol

m_O = (100.00 – 40.00 – 6.71) g = 53.29 g $\qquad M_O$ = 16.00 g/mol

$$n_C = 40.00\ \cancel{g} \times \frac{1\ \text{mol}}{12.01\ \cancel{g}}$$

$$n_C = 3.331\ \text{mol}$$

$$n_H = 6.71\ \cancel{g} \times \frac{1\ \text{mol}}{1.01\ \cancel{g}}$$

$$n_H = 6.64\ \text{mol}$$

$$n_O = 53.29\ \cancel{g} \times \frac{1\ \text{mol}}{16.00\ \cancel{g}}$$

$$n_O = 3.331\ \text{mol}$$

The mole ratio, C : H : O, is 3.331 : 6.64 : 3.331.

Simplifying (dividing each value by the lowest), we obtain a ratio of 1.000 : 1.99 : 1.000, or almost exactly 1 : 2 : 1, making the empirical formula for the lactic acid CH_2O.

(b) Given a molar mass for lactic acid of 90 g/mol, and a molar mass for CH_2O (the empirical formula) of 30.03 g/mol, the molecular formula must be triple the empirical ratio, or $C_3H_6O_3$.

Applying Inquiry Skills

7. (a) **Procedure**

   1. Use a centigram balance to measure the masses of a penny and of a quarter, to 0.01 g.
   2. Use a decigram balance to measure the total masses of the pennies and of the quarters, to 0.1 g.
   3. Divide the total mass of the pennies by the mass of one penny to calculate the number of pennies.
   4. Divide the total mass of the quarters by the mass of one quarter to calculate the number of quarters.
   5. Express the numbers of the two types of coins as a ratio.

   (b) A parallel procedure a scientist might use:

   1. Use a reference to find the molar masses of each kind of atom in the compound, to 0.01 g/mol.
   2. Use a combustion analyzer to measure the total masses of each kind of atom in the compound, to 0.01 g.
   3. Divide the total mass of each type of atom by the molar mass, to calculate the amount of atoms.
   4. Express the numbers of the different types of atoms as a simplest integral ratio.

CHAPTER 4 REVIEW

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Understanding Concepts

1. Every compound has a specific proportion of constituent substances. This led scientists to the concept of specific kinds of atoms for each element, and to comparing their combining masses to obtain a relative scale of masses of atoms.
2. The relative atomic mass would be (exactly) 24 u.
3. A hydrogen atom would be 18/12 of its current mass, or 1.5×1.01 u, or 1.52 u.
4. Relative atomic masses cannot be assigned correctly unless the combining ratio is correctly known; so the correct molecular formula is necessary.
5. Elements consist of atoms with identical numbers of protons and electrons. The nuclei of atoms of elements, however, may vary in numbers of neutrons, which has negligible effect on chemical properties, but does change the atom's mass significantly. For nearly every element there are several of these *isotopes*, and the average mass of atoms of such an element is a value that depends on the mass of these isotopes and also their proportion in nature. The classic example is chlorine, where roughly 3/4 of any sample will consist of chlorine-35 atoms (molar mass 35.00 g/mol), and roughly 1/4 of the sample will be chlorine-37 atoms (molar mass 37.00 g/mol). The molar mass of chlorine, then, is the *average* molar mass of all the chlorine atoms in a sample, which works out to 35.45 g/mol.
6. For silicon, with significant amounts of three isotopes, and if we assume the molar mass of isotopes is the same as the mass number, to two decimals (which is approximately valid, although the last digit is uncertain ...)

$$M = [(0.9221 \times 28.00) + (0.0470 \times 29.00) + (0.0309 \times 30.00)] \text{ g/mol}$$

$$M = 28.11 \text{ g/mol} \qquad \text{(The actual value is 28.09 g/mol.)}$$

7. (a) 12 u exactly (by definition)
   (b) 12 g exactly (by definition)
   (c) Avogadro's constant is (by definition) the number of entities in exactly 12 g of pure carbon-12. This number is used to define the mole, which is the (numerical) amount of any substance that is this number of entities (atoms, ions, molecules, or formula units).
   (d) The symbol *M* represents the quantity, molar mass, in g/mol units.
8. (a) Formula: $CaCO_{3(s)}$

$$M = [(40.08) + (12.01) + (16.00 \times 3)]$$

$$M = 100.09 \text{ g/mol}$$