



Inorganic and Physics Chemistry Department

Fundamentals of quantitative calculations in pharmacy

Fundamentals of quantitative calculations in pharmacy. Calculations by chemical formulas

For specialty 226 Pharmacy, industrial pharmacy



1. Structural particles of matter: atom, molecule, ion.

2. The amount of substance.

3. Basic laws of chemistry, formulas and calculations.

4. Examples of solution of exercise.



Structural particles of matter

Chemistry is the science of the structure, properties, and transformations of substances.

Substance - a set of particles with the same properties.

Simple substances consist of one type of atoms.

- **C** graphite, consisting of atoms of C;
- H_2 hydrogen, the molecule consists of two atoms of H.
- P_4 phosphorus, the molecule consists of four atoms of P.
- Fe iron, consisting of Fe atoms.

Structural particles of matter

Structural particles of matter are atoms, molecules, ions.

Chemical formula – conditional record of the composition of a substance using the symbols of chemical elements and indices.

The index is the number of atoms of a given chemical element in the formulas of substances.



Complex substances consist of atoms of various chemical elements.

Valence is the ability of atoms of a chemical element to combine with a certain number of atoms of other elements to form chemical bonds. 4

Valence of atoms of some elements

Chemical element	Valence	Examples of compound formulas				
Constant valence						
H, Li, Na, K		H ₂ O, Na ₂ O				
O, Ca, Zn	II	CaO, ZnO				
Al	III	Al ₂ O ₃				
Variable valence						
Cu	l i ll	Cu ₂ O, CuO				
Fe, Co, Ni	II i III	FeO, Fe ₂ O ₃				
C, Sn, Pb	ll i IV	CO, CO ₂				
Р	III i V	PH ₃ , P ₂ O ₅				
Cr	II, III i IV	CrO, Cr ₂ O ₃ , CrO ₃				
S	II, IV i VI	H_2S, SO_2, SO_3				
As a rule, the maximum valence = Nº of the group in the						
Periodic Table ⁵						

PERIODIC TABLE OF THE ELEMENTS



Compilation of formulas for valence

1. H C 1. S 0 1. Fe²⁺(SO₄²⁻).

2. H_1Cl_1 2. S_2O_6 2. $Fe_2(SO_4)_2$

3. HCl 3. SO₃ 3. FeSO₄



Structural particles of matter

Chemical formulas of complex substances

- CO₂ carbon (IV) oxide one C atom and two O atoms;
- H₂SO₄ sulphuric acid two H atoms, one S atom and four O atoms;

- Fe(OH)₂ iron (II) hydroxide one Fe atom, two O atoms, two H atoms;
- CuSO₄ Copper (II) sulphate is one Cu atom, one S atom, and four O atoms.



Types of chemical formulas

Formula	Description	Examples
The simplest	the ratio of chemical elements	H₂O CH
Rational	groups of atoms characteristic of classes of chemical compounds	NaOH CH ₃ COOH K ₄ [Fe(CN) ₆] C ₂ H ₅ OH CH ₃ -CH ₂ -OH
Empirical formula	the simplest true	C_2H_6O C_2H_6O C_2H_5OH
Structural	relative position of atoms in a molecule by their of valence	
Electronic	schematic formation of common electronic pairs (chemical bonds)	H H H: C : C : O : H H H

Structural particles of matter

Coefficient - a number before the chemical formula, which indicates the number of atoms, molecules, a given substance or individual ions, atoms

- 20 two separate Oxygen atoms;
- $2O_2$ two molecules of Oxygen;
- 4K⁺ four Potassium cations;
- 2CuSO₄ two molecules of copper (II) sulphate

H₂SO₄: 2(H), 1(S), 4(O); (NH₄)₂C₂O₄: 2(N), 8(H), 2(C), 4(O). Ba(OH)₂: (Ba), 2(O), 2(H); 10

Atomic unit of mass is 1/12 of the mass of the Carbon isotope ¹²C 1.660·10⁻²⁷ kg.

Relative atomic mass (Ar) - a value that shows how many times the mass of the atom of this element is greater than the atomic unit of mass:

$$A_r(H) = \frac{m(H)}{\frac{1}{12}m\binom{12}{6}} = \frac{1.674 \times 10^{-27} \text{kg}}{1.660 \times 10^{-27} \text{kg}} = 1.008$$

The values of A_r are given in the Periodic Table

Relative molecular weight (Mr) is a number that indicates how many times the mass of a molecule of a given substance is greater than 1/12 of the mass of a carbon atom. Numerically equal to the molar mass.

PERIODIC TABLE OF THE ELEMENTS



The relative molecular mass of a compound is the sum of the relative atomic masses of the elements that make up this compound, taking into account their number.

 $M_{r}(H_{3}PO_{4}) = 3A_{r}(H) + A_{r}(P) + 4A_{r}(O) =$ $= 3 \times 1 + 31 + 4 \times 16 = 98;$ $M_{r}[(Ca(OH)_{2}] = A_{r}(Ca) + 2A_{r}(O) + 2A_{r}(H) =$ $= 40 + 2 \times 16 + 2 \times 1 = 74;$ $M_{r}[(NH_{4})_{2}SO_{4}] = 2A_{r}(N) + 8A_{r}(H) + A_{r}(S) + 4A_{r}(O) =$ $= 2 \times 14 + 8 \times 1 + 32 + 4 \times 16 = 132;$ $M_{r}(K_{4}Fe(CN)_{6}) = 4A_{r}(K) + A_{r}(Fe) + 6A_{r}(C) + 6A_{r}(N) =$ $= 4 \times 39 + 56 + 6 \times 12 + 6 \times 14 = 368.$

Avogadro's number (6.02·10²³) - the number of atoms contained in 12 g of Carbon ¹²C, calculated by dividing 12 g by the mass of one carbon atom (1.993×10⁻²³ g):

$$N_A = \frac{12}{1.993 \times 10^{-23}} = 6.02 \times 10^{23} \frac{1}{\text{mol}} (\text{or mol}^{-1})$$

Quantity of matter - the ratio of the number of structural units of matter (atoms, molecules, etc.) to the Avogadro constant: $v = \frac{N}{N_A}$

 ν – amount of substance, mol;

N – the number of structural units of matter.

The amount of substance of the element in a certain amount of the substance of the compound:

 $v_{(element)} = n_{(element)} \cdot v_{(substance)}$ n – index in the chemical formula.

Mol (ν) – unit of substance: contains as many structural units as atoms contained in 12 g of Carbon ¹²C

1 mole of Hydrogen contains 6.02×10^{23} molecules H₂; 1 mol of hydrogen atoms contains 6.02×10^{23} atoms of H; 1 mol of water contains 6.02×10^{23} molecules of H₂O Molar mass (M) - mass of 1 mol of substance : $M = \frac{m}{v}$ Units of measurement - g/mol or kg /mol. 15 Mass percent of an element in a compound

the ratio of the mass of the element to the corresponding mass of the compound: m(F)

$$\omega(E) = \frac{m(E)}{m(compound)}$$

- ✓ the mass of the element and the compound must be in the same dimension (g or kg)
- \checkmark expressed in% or fractions of 1

Based on the compound formula:

$$\omega(E) = \frac{n(E) \cdot A_r(E)}{M_r(compound)}$$

Mass percent of an element in in the mixture

the mixture – a system consisting of two or more substances (components of a mixture).

Homogeneous the mixture - solution (gaseous, liquid or solid).

Heterogeneous - mechanical the mixture.

Any of the mixture can be divided into components by physical methods; the components of the mixture do not change the properties. Mass percent of an element in in the mixture

the ratio of the mass of the element to the corresponding mass of the mixture:

$$\omega(E) = \frac{m(E)}{m(mixture)}$$

 \checkmark expressed in% or fractions of 1

✓ the mass of the element and the mixture is denoted in same dimension (g or kg)

The law of constant composition states, (1808)

law of constant **composition** states that a given chemical compound always contains its component elements in fixed ratio (by mass) and does not depend on

its source and method of preparation.

Obtaining CO₂:

 $CaCO_3 = CO_2 + CaO$ $2HCI + Na_2CO_3 = CO_2 + 2NaCI + H_2O$ $CH_4 + 2O_2 = CO_2 + 2H_2O$ $2CO + O_2 = 2CO_2$ Always composed CO₂ 36.6% C and 63.4% O
It is valid only for molecular compounds - daltonides.

Daltonides are substances of constant composition - simple formulas with integer indices : H₂SO₄, HCl, CO₂.



The law of multiple proportions(1803)

Law of multiple proportions, statement that when two elements combine with each other to form more than one compound, the mass of one element that combine with a fixed

mass of the other are in a ratio of small whole numbers

The composition of nitrogen oxides (as a percent by mass):								
Formula	N ₂ O	NO	N ₂ O ₃	NO ₂	N_2O_5			
N, %	63.7	46.7	36.8	30.4	25.9			
O, %	36.3	53.3	63.2	69.6	74.1			
Ratio O/N	0.57	1.14	1.71	2.28	2.85			
Valence N	1	2	3	4	4			

 $CaCl_2 \cdot H_2O$, $CaCl_2 \cdot 2H_2O$, $CaCl_2 \cdot 4H_2O$, $CaCl_2 \cdot 6H_2O$ water masses are rated to as water masses are rated to as 1:2:4:6 Avogadro's law and its consequences (1811)

the same volumes of gases under the same conditions contain the same number of molecules

The first consequence:

1 mole of any gas under the same conditions will occupy the same volume - the molar volume V_m :

$$V_{\rm m} = \frac{M}{\rho} = \frac{V}{\nu} \qquad [V_{\rm m}] = \frac{L}{mol}$$

Under normal conditions Vm = 22.4 L/mol (or m³/mol)

Normal conditions – T = 273 K (0 °C) p = 101.3 kPa (1 atm. or 760 millimeters of mercury).

The second consequence :

the ratio of the masses of the same volumes of different gases under the same conditions is the density of one gas by another:

$$D = \frac{m}{m_1} = \frac{M}{M_1}, therefore$$
$$D(Xgas/MH_2) = \frac{M_{gas}}{2} \qquad D(Xgas/air) = \frac{M_{gas}}{29}$$

For conditions other than normal

Clapeyron-Mendeleev's law

combined gas law Boyle-Marriott and Gay-Lussac

$$pV = \frac{m}{M}RT$$

where: p -

pressure, Pa;

V - volume, m³;

14.02.2022

 $\begin{array}{ll} & \prod\limits_{m = 1}^{p_0 V_0} = \frac{pV}{T} \\ m = mass, kg; & \prod\limits_{T_0}^{T_0} = \frac{pV}{T} \\ M = molar mass, kg/mol; \\ R = universal gas table, 8.314 J \cdot mol^{-1} \cdot K^{-1}; \\ T = temperature, K. \end{array}$

The volume fraction of the component in the gas mixture:

$$v_{(component)} = \frac{V_{(component)}}{V_{(mixture)}}$$

- the volumes of the components and mixtures are denoted in the same dimension (L or mL)
- \checkmark expressed in % or fractions of 1

The average molar mass of the gas mixture(M): $\overline{M} = \sum M_i \phi_i = M_1 \phi_1 + M_2 \phi_2 + \dots + M_n \phi_n$ M_1, M_2, M_n – molar masses of gases; ϕ_1, ϕ_2, ϕ_n – volume fractions of gases; n – number of components. Average molar mass of $air(\overline{M})$

1) Oxigen (21%) and Nitrogen (79%):

$$M_{air} = M_{O_2} \phi_{O_2} + M_{N_2} \phi_{N_2}$$

 $\overline{M}_{air} = 32 \times 0.21 + 28 \times 0.79 = 28.82 \approx 29 \frac{g}{mol}$

Basic formulas for calculations $n_A: n_B: \ldots: n_Z = \nu_A: \nu_B: \ldots: \nu_Z$ $v_{(\text{element})} = n_{(\text{element})} \cdot v_{(\text{compound})}$ $\nu = \frac{m}{M}$ $\frac{N}{N_A} = \frac{m}{M} = \frac{V}{V_m}$ $v = \frac{N}{N_A}$ $v = \frac{v}{V_m}$ $\omega(E) = \frac{n(E) \cdot A_r(E)}{M_r(\text{compound})}$ $\omega(E) = \frac{m(E)}{m(mixture)}$ $\varphi_{\text{(volume fraction of component)}} = \frac{V_{\text{(component)}}}{V_{\text{(mixture)}}}$ \overline{M} average molar mass = $\sum M_i \phi_i = M_1 \phi_1 + M_2 \phi_2 + \dots + M_n \phi_n$

1. For water mass of 9 g, calculate : a) amount of substance;
 b) the number of molecules; c) volume.
 Given: Solution:

 $\frac{m(H_2O) = 9 r}{\nu(H_2O) - ?}$ $\frac{N(H_2O) - ?}{N(H_2O) - ?}$ $\frac{m(H_2O) = \frac{m(H_2O)}{M(H_2O)} = \frac{9 g}{18 g/mol} = 0.5 mol$ $N(H_2O) = \nu(H_2O) \cdot N_A = 0.5 mol \times 6.02 \cdot 10^{23} = 3.01 \times 10^{23} (molecules)$ $V(H_2O) = \nu(H_2O) \cdot V_m = 0.5 mol \times 22.4 L/mol = 0.5 mol \times 22.4 L/$

= 11.2 L

Answer: a) 0.5 mol; b) 3.01×10^{23} (molecules); c) 11.2 L.

2. Calculate the amount of calcium orthophosphate containing 1.6 mol of Oxygen.

Given :

v(O) = 1.6 mol $v(Ca_3(PO_4)_2) - ?$ Solution:

 ν (element) = n(element) $\cdot \nu$ (compound)

 ν (compound) = $\frac{\nu$ (element)}{n(element)}

$$v(Ca_3(PO_4)_2) = \frac{v(0)}{n(0)} = \frac{1.6 \text{ mol}}{8} = 0.2 \text{ mol}$$

Answer : 0.2 mol.

3.Determine the formula of the compound containing 0.14 g of Iron and 0.06 g of Oxygen.

Given: Solution: m(Fe) = 0.14 g m(O) = 0.06 g $v(Fe) = \frac{m(Fe)}{M(Fe)} = \frac{0.14 \text{ g}}{56 \text{ mol}} = 0.0025 \text{ mol}$ $Fe_xO_v - ?$ $\nu(0) = \frac{m(0)}{M(0)} = \frac{0.06 \text{ g}}{16 \text{ mol}} = 0.00375 \text{ mol}$ n(Fe): n(0) = v(Fe): v(0)n(Fe): n(0) = 0.0025 : 0.00375n(Fe): n(0) = 1: 1.5 = ratio 2: 3

Answer : Fe_2O_3 .

 At roasting 2.66 g of unknown substance A gave 784 mL of carbon (IV) oxide and 1568 mL of sulphur (IV) oxide.
 Determine the gross formula of substance A.

Given : Solution: m(A) = 2.66 g $\nu(C) = \nu(CO_2)$ $V(CO_2) = 784 \text{ mL}$ $\frac{V(CO_2) - 784 \text{ mL}}{V(SO_2) = 1568 \text{ mL}} \quad v(CO_2) = \frac{V(CO_2)}{V_m} = \frac{0.784 \text{ L}}{22.4 \text{ L/mol}} =$ $C_x S_v O_z - ?$ = 0.035 mol; $m(C) = v(C) \cdot M(C) = 0.035 \text{ mol} \cdot 12 \text{ g/mol} = 0.42 \text{ g}.$ $v(S) = v(SO_2); v(SO_2) = 0.07 \text{ mol}; m(S) = 2.24 \text{ g}.$ m(C) + m(S) = 0.42 g + 2.24 g = 2.66 g.0 is absent (z = 0) n(C): n(S) = v(C): v(S) = 0.035: 0.07 = 1:2Answer : CS_2 29

$$\omega(H) = 3.03\%$$

 $\omega(S) = 96.97\%$
M_c(B) = 66

 $H_x S_v - ?$

$$n(E) = \frac{\omega(E) \cdot M_r(compound)}{A_r(E)}$$

 $\omega(E) = \frac{n(E) \cdot A_r(E)}{M (compound)}$

n(H) =
$$\frac{0.0303 \cdot 66}{1}$$
 = 2 n(S) = $\frac{0.9679 \cdot 66}{32}$ = 2
x = 2; y = 2

Answer : H_2S_2

 6. Calculate the mass of Carbon contained in 4.4 g of carbon (IV) oxide.

Given :
 $m(CO_2) = 4.4 \text{ g}$ Solution: $M_r(CO_2) = 44$ $\omega(C) = \frac{n(C) \cdot A_r(C)}{M_r(CO_2)}$ $\omega(C) = \frac{m(C)}{m(CO_2)}$ m(C) - ? $\frac{n(C) \cdot A_r(C)}{M_r(CO_2)} = \frac{m(C)}{m(CO_2)}$

m(C) =
$$\frac{n(C) \cdot A_r(C) \cdot m(CO_2)}{M_r(CO_2)} = \frac{1 \times 12 \times 4.4 \text{ g}}{44} = 1.2 \text{ g}$$

Answer : 1.2 g

 At roasting crystal hydrate composition Na₂SO₃·xH₂O, its mass decreased by 50%. Set the formula of the crystal hydrate.

Given : Solution: $\omega(H_2O) = 50\%$ $\omega(H_2 0) = \frac{n(H_2 0) \cdot M_r(H_2 0)}{M_r(Na_2 S 0_2 \cdot x H_2 0)}$ $Na_2SO_3 \cdot xH_2O - ?$ $M_r(Na_2SO_3 \cdot xH_2O) = \frac{n(H_2O) \cdot M_r(H_2O)}{\omega(H_2O)}$ $M_r(Na_2SO_3 \cdot xH_2O) = 2 \cdot 23 + 32 + 3 \cdot 16 + x \cdot 18 = 126 + 18x$ $126 + 18x = \frac{x \cdot 18}{0.5}$ x = 7

Anser: $Na_2SO_3 \cdot 7H_2O$

8. The sample of table salt (the main component of NaCl) contains 60% Chlorine. Calculate the mass percent of impurities in the salt.

Given :Solution: $\omega(Cl) = 60\%$ Let's admit m(sample) = 100 g $\omega(impurities) - ?$ $\nu(Cl) = \frac{m(Cl)}{A_r(Cl)} = \frac{60 g}{35.5 g/mol} = 1.7 mol$ $\nu(Na) = \nu(Cl) = 1.7 mol$

$$\begin{split} m(\text{Na}) &= \nu(\text{Na}) \cdot \text{A}_{r}(\text{Na}) &= 1.7 \text{ mol} \cdot 23 \text{ g/mol} &= 39.1 \text{ g} \\ m(\text{NaCl}) &= m(\text{Na}) + m(\text{Cl}) = 39.1 \text{ g} + 60 \text{ g} = 99.1 \text{ g} \\ m(\text{sample}) &= m(\text{NaCl}) + m(\text{impurities}) \\ m(\text{impurities}) &= m(\text{sample}) - m(\text{NaCl}) = 100 \text{ g} - 99.1 \text{ g} = 0.9 \text{ g} \\ \omega(\text{impurities}) &= \frac{m(\text{impurities})}{m(\text{sample})} = \frac{0.9 \text{ g}}{100 \text{ g}} = 0.009 \end{split}$$

Answer: 0.009 or 0,9%



Thank
 you for

attention!