SCI-CONF.COM.UA

MODERN SCIENCE: PROBLEMS AND INNOVATIONS

ABSTRACTS OF VII INTERNATIONAL SCIENTIFIC AND PRACTICAL CONFERENCE
SEPTEMBER 20-22, 2020

STOCKHOLM
2020

MODERN SCIENCE: PROBLEMS AND INNOVATIONS

Abstracts of VII International Scientific and Practical Conference

Stockholm, Sweden

20-22 September 2020

Stockholm, Sweden

2020

UDC 001.1

The 7th International scientific and practical conference "Modern science: problems and innovations" (September 20-22, 2020) SSPG Publish, Stockholm, Sweden. 2020. 485 p.

ISBN 978-91-87224-07-2

The recommended citation for this publication is:
Ivanov I. Analysis of the phaunistic composition of Ukraine // Modern science: problems and innovations. Abstracts of the 7th International scientific and practical conference. SSPG Publish. Stockholm, Sweden. 2020. Pp. 21-27. URL: https://sci-conf.com.ua/vii-mezhdunarodnaya-nauchno-prakticheskaya-konferentsiya-modern-science-problems-and-innovations-20-22-sentyabrya-2020-goda-stokgolm-shvetsiya-arhiv/.

Editor
Komarytskyy M.L.
Ph.D. in Economics, Associate Professor

Collection of scientific articles published is the scientific and practical publication, which contains scientific articles of students, graduate students, Candidates and Doctors of Sciences, research workers and practitioners from Europe, Ukraine, Russia and from neighbouring coutries and beyond. The articles contain the study, reflecting the processes and changes in the structure of modern science. The collection of scientific articles is for students, postgraduate students, doctoral candidates, teachers, researchers, practitioners and people interested in the trends of modern science development.

e-mail: sweden@sci-conf.com.ua

homepage: ***https://sci-conf.com.ua***

CHEMICAL SCIENCES

TECHNICAL SCIENCES

CHEMICAL SCIENCES

CALCULATION OF DENSITY AND MOLAR VOLUME OF COMPOUNDS THROW THE AVERAGE MOLAR VOLUMES OF CHEMICAL ELEMENTS

Kozub Pavlo Anatolijovuch
Candidate of Technical Science, Associate Professor
Kharkiv National University of Radio Electronics
Kozub Svitlana Mukolaivna
Candidate of Technical Science, Associate Professor
Kharkiv National Medical University
Kharkiv, Ukraine

Introductions. Mass, volume and the presence of indivisible particles - atoms are the main concepts for determining matter in modern chemistry, which leads to the formulation of the main principle - the law of conservation of mass.

Therefore, all stoichiometric calculations in chemistry are based on the principle of additivity of atomic masses and independence of compound mass from its structure. This allows calculations by chemical formula, regardless of its phase state, composition, or conditions of its production.

The logical development of this approach should be the assumption of the invariance of the volume of atoms in the formation of chemical compounds. But so far this approach is almost undeveloped.

The basis of the modern approach to the calculation of the spatial characteristics of compounds is the modeling of their structure on the basis of various theoretical models, the structure of bonds between atoms, and, most importantly, the definition of molecules as separate independent objects.

As a result, today, different types of radii are used for both individual atoms and functional groups, various corrections are made to the effect of charge, relative position, etc .. But a general and simple algorithm for calculating the density or molar volume, the most necessary from the point of view of practical use of characteristics, still does not exist. So far, the only achievement of modern chemistry in this matter is still the law of constant molar volume of gas.

Aim. To solve this problem the simple condensed matter model, which requires a minimum information about the compound but best describes the already known experimental data of the density of the compounds in the condensed state is required.

Materials and methods. The basic principle of this model is the position that the shape and volume of atoms are independent of each other. The second principle is the position that the total volume depends on the relative position of the atoms.

According to this provision, in the case of a random relative position of atoms in a substance (amorphous, vitreous, liquid), the volume of a mixture of atoms will be the sum of the volumes of individual atoms arranged like soft spherical objects occupying all possible interatomic space, and thus their total volume will consist of the volumes of each of the atoms.

In the presence of features in the form of atoms, their groups with a smaller volume (molecules, crystal lattices), or a larger volume (densely packed crystals) due to the denser arrangement of atoms or with the presence of space between atoms (layered structures, molecular crystals, cellular structures) may be formed. The average molar volume of such compounds will naturally differ from the molar volume of the liquid or amorphous state.

Results and discussion. Analysis of the available experimental data has shown that, indeed, the main parameter that determines the molar volume is the chemical composition of the substance. The experimental values of the molar volume of the compound depending on temperature, pressure, phase state, polymorphic modification is differed on average by 10% (although for some classes of compounds reaches 300%), which allows to calculate the molar volume and density of the compound for condensed state by chemical formula with this accuracy even without determining its structural features.

Thus, for the case when the average volume of a substance in the condensed state does not depend on specific conditions (ie the structure of the substance and its composition), it can be represented by the sum of the average volumes of each of atoms and depends only on the number of atoms in the substance.

$$V_c = \sum n_i \cdot V_i$$

were,

V_c – average molar volume of compound, cm^3/mol;

n_i – the number of i-element atoms in the compound;

V_i – average molar volume of i-element, cm^3/mol.

In this case the average density can be obtained as the ratio of the average molar mass to the average molar volume

$$d_c = \frac{M_c}{V_c}$$

$$M_c = \sum n_i \cdot M_i$$

were,

d_c – density of compound, cm^3/g;

M_c – molar mass of compound, g/mol;

n_i – the number of i-element atoms in compound;

M_i – molar (atomic) mass of the i-element, g/mol.

For calculations of the average molar volumes of the elements, experimental data of the density of 1233 compounds were used, the number of compounds for individual elements reached 55, for some unexplored elements only 3 compounds were taken. Some compounds were represented by several polymorphic modifications, and different phases (solid and liquid).

An additional test of the reliability of the obtained values was the presence of their regular changes depending on the period and group of elements in the periodic table.

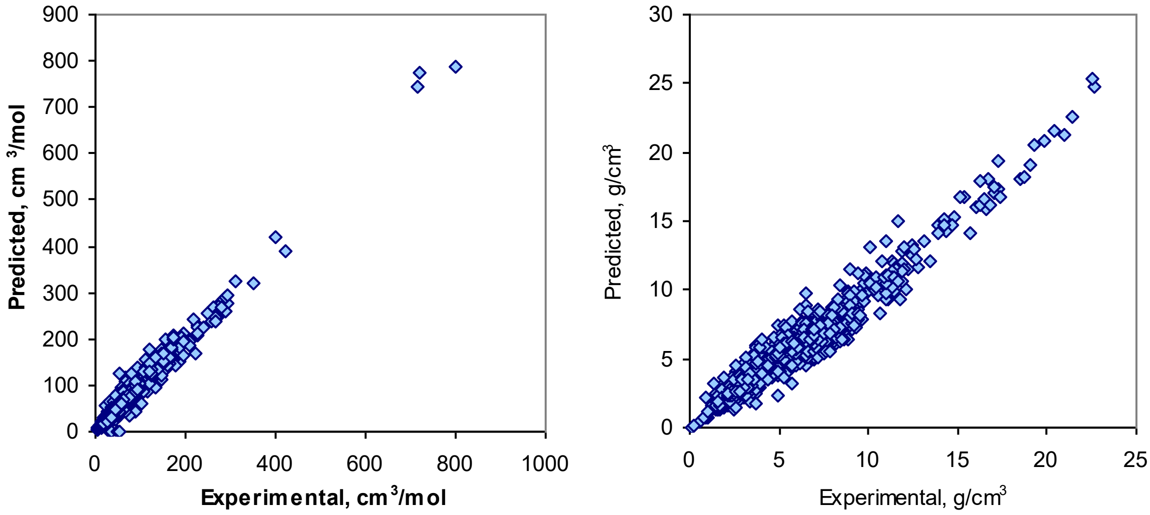

Fig.1 Results of calculations of molar volume and density

Thus, these studies allow us to obtain the average volumes of elements (Table 1), which with an average error of up to 11.9% allow to calculate the molar volume and with an average error of up to 11.5% the density of the compound in the condensed phase only by chemical formula (Fig.1).

As expected, several groups of compounds that had systematic deviations from the general dependence were identified in the calculations, but all of them can be explained by the peculiarities of their structure.

As expected, several groups of compounds that had systematic deviations from the general dependence were identified in the calculations, but all of them can be explained by the peculiarities of their structure.

Thus, active metals, inert and diatomic gases, coordination compounds had larger molar volumes, with patterns that will be determined in future studies.

The addition of new compounds to the calculations did not increase the calculation error and statistically significant changes in the values of the average volumes of the elements, which indicates the reliability of the obtained data.

Table 1

Average molar volumes of elements, cm3 / mol

H	4.1	Sc	7.9	Nb	8.8	Pm	12.6	Tl	12.5	Md	14.8
He	7.4	Ti	6.5	Mo	8.6	Sm	13.1	Pb	17.2	No	16.0
Li	5.4	V	5.8	Tc	9.3	Eu	13.7	Bi	20.4	Lr	10.0
Be	4.5	Cr	5.8	Ru	8.1	Gd	14.4	Po	24.5	Rf	8.4
B	4.4	Mn	6.8	Rh	7.8	Tb	17.3	At	30.0	Db	7.6
C	5.7	Fe	5.5	Pd	8.3	Dy	16.0	Rn	36.9	Sg	8.0
N	5.9	Co	4.6	Ag	11.3	Ho	15.8	Fr	30.0	Bh	8.6
O	6.7	Ni	4.8	Cd	13.0	Er	15.5	Ra	25.0	Hs	7.5
F	8.2	Cu	7.9	In	11.5	Tm	15.3	Ac	17.3	Mt	7.5
Ne	13.3	Zn	9.4	Sn	15.5	Yb	16.3	Th	15.4	Ds	8.5
Na	10.9	Ga	9.2	Sb	19.1	Lu	10.4	Pa	13.8	Rg	17.5
Mg	7.8	Ge	11.5	Te	23.0	Hf	8.8	U	12.4	Cn	20.0
Al	7.4	As	14.1	I	27.5	Ta	7.7	Np	11.0	Nh	14.0
Si	8.7	Se	17.4	Xe	31.0	W	8.1	Pu	11.7	Fl	20.0
P	10.3	Br	21.1	Cs	27.2	Re	8.7	Am	12.4	Mc	25.0
S	12.3	Kr	25.1	Ba	22.0	Os	7.7	Cm	13.2	Lv	30.0
Cl	14.9	Rb	21.3	La	19.4	Ir	7.6	Bk	16.2	Ts	36.0
Ar	19.2	Sr	16.6	Ce	17.4	Pt	8.6	Cf	15.0	Og	42.8
K	17.8	Y	11.4	Pr	15.6	Au	14.5	Es	14.9		
Ca	14.5	Zr	9.8	Nd	14.1	Hg	16.4	Fm	14.8		

Conclusions. Thus, the use of average molar volumes of elements makes it easy to determine not only the mass characteristics of compounds, but also such important characteristics as density and molar volume only by a chemical formula with an average error of 12%. And taking into account the structural features of the compounds, this error can be significantly reduced.

REFERENCES

1. W. L. Bragg. The arrangement of atoms in crystals.Lond. Edinb. Dubl. Phil.Mag., 40(236):169–189, 1920.

2. Mack, E., The Spacing of Non-Polar Molecules in Crys-tal Lattices: The Atomic Domain of Hydrogen, J. Am.Chem. Soc., 1932, vol. 54, no. 6, pp. 2141–2165.

3. Pauling, L., The Nature of the Chemical Bond, Ithaca:Cornell Univ., 1960, 3rd ed.

4. Bondi, A., Van der Waals Volumes and Radii, J. Phys.Chem., 1964, vol. 68, no. 3, pp. 441–451

5. Waber JT, Cromer DT. Orbital radii of atoms and ions. J Chem Phys 1965; 42: 4116-23.

6. Ghosh DC, Biswas R. Theoretical calculation of absolute radii of atoms and ions. part 1. the atomic radii. Int J Mol Sci 2002; 3: 87-113.

7. P. Ganguly, “Atomic sizes and atomic properties,” J. Phys. B At. Mol. Opt. Phys., vol. 41, no. 10, p. 105002, May 2008

8. A. Houari, “Hall determination of atomic radii,” Inst. Phys., vol. 43, pp. 519–521, 2008.