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Values and change laws of atoms and ions radii

In the chemical technology industry many products are produced by aqueous-salt systems. In such systems the charged particles of mineral substances used as raw materials are in the form of ions and play a decisive role in the formation of the target products. Today research results in the theoretical chemistry show that there is no high level scientifically substantiated data on the radii of atoms that are the material basis of such ion particles. The atomic and ion radius values of chemical elements give rise to several values for a single element in known literary data. These data are different from each other. Within the periodic table per each atom and each ion about 30 scaling values are determined by the calculation or physico-chemical methods. According to the results obtained, the values have been found that are close to the known data and preserve their own numerical values within the periodic system. At this point two different equations are used to calculate radii of the atoms and ions of the elements. Version 1 is for elements in the periodic table moving from period to another, while the other is for elements in the 1st and 8th groups in each period of the periodic table. All chemical elements in the periodic table allow calculating the radius values of atoms and ions.

Keywords: ion, atom, radius, periodic system, particle, charge, electron, physical and chemical properties.

Introduction

In many areas of chemical technology the processes occurring in aqueous-salt systems are used. In this case the mineral substances used as primary raw materials in the process are the elementary charge particles, ions, and play a decisive role in the formation of target products. Nowadays the research results [1–5] in scientific chemistry have shown that there is no high level scientifically substantiated data on the radii of such ion particles and their material basis. In general within the Periodic Table of Chemical Elements of D. Mendeleev the data of radii determined by calculation and physico-chemical methods show about 30 scale values for each atom and each ion [6–11]. As examples we can include the research results on the radii of the ionic and atom particles [12] of Melvin-Hughes (MH), Goldschmidt (G), Poling (P), Ingold (In) and Boki (B) that are widely used in educational and scientific practice today (Table 1).

Table 1

Radii of atoms and ions

Elements	Radius of atom, $r_a \cdot 10$, nm				Ion charge	Radius of ion, $r_i \cdot 10$, nm				
	M.H	G	P	B		M.H	G	P	In	B
	2	3	4	5	6	7	8	9	10	11
Ag	1.445	1.44	1.53	1.44	+1	1.014	1.13	1.26	1.26	1.13
Al	1.432	1.43	1.26	1.43	+3	0.55	0.57	0.50	0.72	0.57
As	1.248	1.22	1.18	1.48	+5	–	0.46	–	0.71	(0.47)
Au	1.442	1.44	1.50	1.44	+1	–	1.37	–	1.37	(1.37)
B	(0.795)	0.91	0.89	0.91	+3	(0.20)	0.23	0.20	0.35	(0.20)
Ba	2.174	2.17	–	2.21	+2	1.395	1.34	1.35	1.53	1.38
Be	1.113	1.11	1.07	1.13	+2	0.314	0.35	0.31	0.44	0.34
Bi	1.548	1.55	1.46	1.82	+5	–	0.74	–	0.98	(0.74)
Br	1.1415	1.14	1.14	–	+7	–	–	–	0.62	(0.39)
C	0.771	0.77	0.77	0.77	+4	0.195	0.16	0.15	0.29	0.2
Ca	1.974	1.37	–	1.97	+2	1.051	0.99	0.99	0.99	1.04
Cd	1.490	1.48	1.48	1.56	+2	0.99	0.97	–	1.14	0.99
Cl	0.994	0.99	0.99	–	+7	–	–	–	0.49	(0.26)
Co	1.253	1.25	1.25	1.25	+3	0.65	0.63	–	–	0.64
Cr	1.249	1.25	1.25	1.27	+6	–	0.52	–	0.81	0.35
Cs	2.655	2.62	–	2.68	+1	1.678	1.67	1.69	1.69	1.65

Continuation of Table 1

1	2	3	4	5	6	7	8	9	10	11
Cu	1.278	1.27	1.35	1.28	+2	0.47	0.72	–	0.96	0.80
F	0.709	0.64	0.64	–	+7	–	–	–	0.10	–
Fe	1.241	1.26	–	1.26	+3	0.67	0.64	–	–	0.07
H	0.3707	0.36	0.30	0.46	–1	–	1.53	–	2.08	1.36
Hg	1.503	1.50	1.48	1.60	+2	0.66	1.10	–	1.25	1.12
I	1.333	2.20	1.28	–	+7	–	0.50	–	0.77	(0.50)
K	2.272	2.36	–	2.36	+1	1.341	1.33	1.33	1.33	1.33
La	1.870	1.86	–	1.87	+3	1.14	1.14	1.15	1.39	1.04
Li	1.520	1.55	1.34	1.55	+1	0.758	0.68	0.60	0.60	0.68

Results and discussions

As can be seen from Table 1, there are large quantitative differences that can not be ignored for any element in their atomic and ionic radius values. The research findings show the results of recent research aimed at eliminating such shortcomings. The research has revealed that some of the latest scientific findings about the definite patterns of traction and drainage and the atomic structure, which arise between charged particles, have been used [13–17]. At this point two different equations are used to calculate the atoms and ions of the elements. For elements in version 1 (1–3) elements according to their formula that move from period to period in the periodic table. They are lithium, sodium, potassium, rubidium, cesium, and francium.

$$\frac{Zne^2}{4\pi\epsilon_0(R_{atom\ of\ previous\ element} + X)^2} = \frac{K \cdot m \cdot v^2}{(R_{atom\ of\ previous\ element} + X)}. \quad (1)$$

From the 1st formula we find X .

$$X = \frac{Zne^2 - K4\pi\epsilon_0 m v^2 \cdot R_{atom\ of\ previous\ element}}{K4\pi\epsilon_0 m v^2}. \quad (2)$$

Next, we find the atomic or ion radius of the element as follows:

$$R_{atom} = R_{atom\ of\ previous\ element} + X. \quad (3)$$

In version 2 (4–6) formulas are for the elements of 1 and 8 groups in each period in the Periodic Table. The laws are known that by an increase in the line number the atoms and ions radius of elements is decreased. Therefore, we deduce X from the radius of the element and ion radius of the element, and we formulate the formula as follows.

$$\frac{Zne^2}{4\pi\epsilon_0(R_{atom\ of\ previous\ element} - X)^2} = \frac{K \cdot m \cdot v^2}{(R_{atom\ of\ previous\ element} - X)}. \quad (4)$$

From the 4th formula we find X .

$$X = \frac{K4\pi\epsilon_0 m v^2 R_{atom\ of\ previous\ element} - Zne^2}{K4\pi\epsilon_0 m v^2}, \quad (5)$$

here ϵ_0 — dielectric permeability of vacuum, F/m; e — electron charge, C; m — electron mass, kg; z — number of protons; R — distance between the charged particles, Å; v — velocity of rotating electrons in radius orbitals, m/sec.; K — constant value determining by the arrangement of elements electrons in the cells.

Next, we find the atomic or ion radius of the element as follows:

$$R_{atom} = R_{atom\ of\ previous\ element} - X. \quad (6)$$

The new calculation results obtained for the elements described in Table 1 above are relative to the data given in Table 2, Figure 1.2.

Radii of atoms and ions

Elements	Atom radius, $r_a \cdot 10, \text{ nm}$						Ion charge	Ion radius $r_i \cdot 10, \text{ nm}$						
	M.H	G	P	B	Average literary	Calculation		M.H	G	P	In	B	Average literary	Calculation
Al	1.432	1.43	1.26	1.43	1.388	1.383	3	0.55	0.57	0.5	0.72	0.57	0.582	0.575
As	1.248	1.22	1.18	1.48	1.282	1.256	5	–	0.46	–	0.71	0.47	0.546	0.482
Au	1.442	1.44	1.5	1.44	1.455	1.503	1	–	1.37	–	1.37	1.37	1.37	1.377
B	0.795	0.91	0.89	0.91	0.876	0.888	3	0.2	0.23	0.2	0.35	0.2	0.236	0.333
Ba	2.174	2.17	–	2.21	2.184	2.171	2	1.395	1.34	1.35	1.53	1.38	1.399	1.357
Be	1.113	1.11	1.07	1.13	1.105	1.063	2	0.314	0.35	0.31	0.44	0.34	0.350	0.472
Bi	1.548	1.55	1.46	1.82	1.594	1.453	5	–	0.74	–	0.98	0.74	0.82	0.681
Br	1.141	1.14	1.14	–	1.140	1.166	7	–	–	–	0.62	0.39	0.505	0.383
C	0.771	0.77	0.77	0.77	0.770	0.799	4	0.195	0.16	0.15	0.29	0.2	0.199	0.213
Ca	1.974	1.37	–	1.97	1.771	1.777	2	1.051	0.99	0.99	0.99	1.04	1.012	1.119
Cd	1.49	1.48	1.48	1.56	1.502	1.505	2	0.99	0.97	–	1.14	0.99	1.022	1.989
Cl	0.994	0.99	0.99	–	0.991	1.007	7	–	–	–	0.49	0.26	0.375	0.372
Co	1.253	1.25	1.25	1.25	1.250	1.251	3	0.65	0.63	–	–	0.64	0.64	0.333
Cr	1.249	1.25	1.25	1.27	1.254	1.278	6	–	0.52	–	0.81	0.35	0.56	0.514
Cs	2.655	2.62	–	2.68	2.651	2.665	1	1.678	1.67	1.69	1.69	1.65	1.675	1.675
Cu	1.278	1.27	1.35	1.28	1.294	1.405	2	0.47	0.72	–	0.96	0.8	0.737	0.985
F	0.709	0.64	0.64	–	0.663	0.684	7	–	–	–	0.1	–	0.1	0.099
Fe	1.241	1.26	–	1.26	1.253	1.259	3	0.67	0.64	–	–	0.07	0.439	0.404
Hg	1.503	1.5	1.48	1.6	1.520	1.488	2	0.66	1.1	–	1.25	1.12	1.032	1.097
I	1.333	2.2	1.28	–	1.203	1.283	7	–	0.5	–	0.77	0.5	0.59	0.426

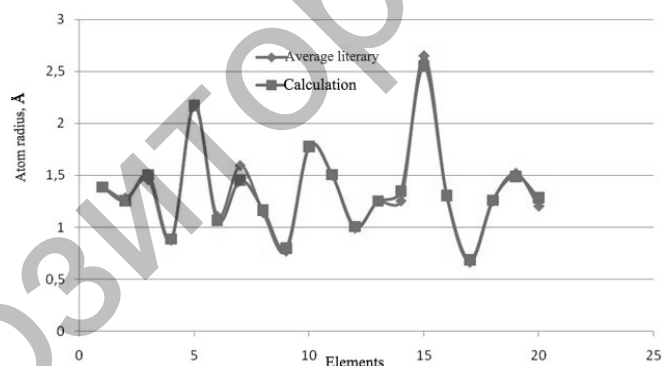


Figure 1. The laws of changes in average literary and calculation values of atomic radii

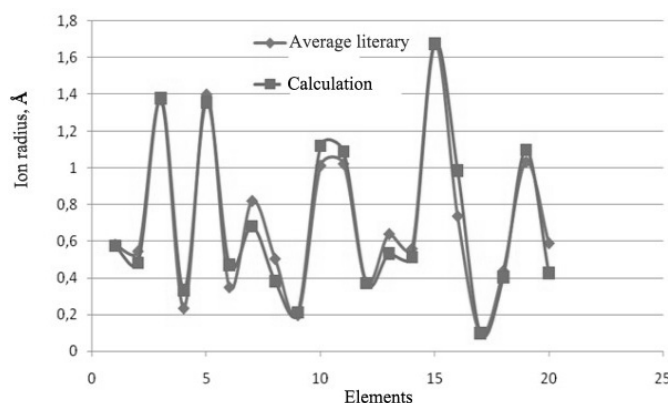


Figure 2. The laws of changes in average literary and calculation values of ion radii

Conclusions

As shown in Table 2 and Figures 1, 2, the results of the study were close to the known data, and the values of the latter were changed within the periodic system, but their numerical values were obtained. In order to verify their superior sequence and authenticity, calculations were made using the atomic and ion radii of any element in the periodic system group before and after of that element, upper and under the certain periods, under certain elements. At the same time, in all four different calculations, the same values of the atom and ion radii of the element under consideration were obtained. This result can be a proof of the novelty of the findings, as well as the high scientific value and significance of it.

Thus, the results of the research can be considered as a new solution for calculating the high values of ion particles and their radicals' radii, which are their material basis in the field of chemistry. The methodology used in the work allow calculation of the radius values of atoms and ions all the chemical elements in the periodic system of D. Mendeleev.

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Атомдар мен иондардың радиустары мәндері мен өзгеру заңдылықтары

Химиялық технология салаларында сулы-тұзды жүйелер арқылы көптеген өнімдер өндірілуде. Мұндай жүйелерде шикізаттар ретінде пайдаланылатын минералды заттардың зарядтық бөлшектері иондар түрінде болып, керекті өнімдерді қалыптастыруда шешуші рол атқарады. Ғылыми-ілімдік химия саласында қазіргі кезде қолжеткен нәтижелерді талдау нәтижесі көрсеткендей, осындай иондық бөлшектердің және олардың материалдық негізі болып табылатын атомдардың радиустары туралы шынайылылығы жоғары, толықтама ғылыми дәйектелген мәліметтер жоқ. Химиялық элементтердің атомы мен ионы радиустары мәндері белгілі әдеби мағлұматтарда бір элемент үшін бірнеше мән береді. Олар бір-бірінен өте алшақты мәндер. Химиялық элементтердің периодтық жүйесі кестесі шеңберінде радиустары есептік немесе сан алуан физика-химиялық жолдармен анықталған

мәліметтерде әр атом әр ион үшін 30 жуық шкалалық мәндер келтіріледі. Ізденіс нәтижелері бойынша белгілі мәліметтерге жақын және де соңғылардың периодтық жүйе шеңберінде өзгеру заңдылықтарын сақтайтын, бірақ өзіндік сандық нәтижелері бар мәндер алынды. Осы кезде элементтердің атомдары мен иондары радиустарын есептеуде екі түрлі тәңдеулер қолданылады. 1-ші нұсқа элементтер периодтық жүйеде периодтан периодқа көшкендегі элементтер үшін, ал екіншісі периодтық жүйедегі әр периодтағы 1-ші және 8-ші топтағы элементтер үшін. Жұмыста қолданылған әдістеме Д. Менделеевтің периодтық жүйесіндегі барлық химиялық элементтердің атомдары және иондары радиустарының мәндерін есептеп анықтауға мүмкіндік береді.

Кілт сөздер: ион, атом, радиус, периодтық жүйе, бөлшектер, зарядтар, электрон, физика-химиялық қасиеті.

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Значения и закономерности изменения радиусов атомов и ионов

В отраслях химической промышленности многие продукты производятся с помощью водно-солевых систем. В таких системах заряженные частицы минеральных веществ, используемых в качестве сырья, находятся в форме ионов и играют решающую роль в формировании целевых продуктов. Результаты текущих исследований в области теоретической химии показали, что не существует высокоуровневых научно обоснованных данных о радиусах ионов и атомов. Атомные и ионные радиусы химических элементов имеют несколько значений для одного элемента по некоторым литературным данным. В данных о радиусах химических элементов периодической таблицы, определяемых физико-химическим и расчетным методом, каждый атом и ион имеют около 30 значений. По результатам исследования значения были близки к известным данным. Для вычисления радиусов атомов и ионов элементов используются два разных уравнения. Версия 1 предназначена для элементов в периодической таблице, перемещающихся из периода в период, а другая — для элементов 1-й и 8-й групп в каждом периоде периодической таблицы. Методология, используемая в работе, дает возможность рассчитать атомные и ионные радиусы всех химических элементов в периодической системе Д.И. Менделеева.

Ключевые слова: ион, атом, радиус, периодическая система, частицы, заряд, электрон, физико-химические свойства.

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