



ON ENERGY PRINCIPLES OF STRUCTURAL INTERACTIONS

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The notion of spatial-energy parameter (*P*-parameter) is introduced based on the modified Lagrangian equation for relative motion of two interacting material points, which is a complex characteristic of important atomic values. Wave properties of *P*-parameter are found, its wave equation having a formal analogy with the equation of Ψ -function is given. In the systems in which the interactions proceed along the potential gradient (positive performance) the resulting potential energy is found based on the principle of adding reciprocals of the corresponding energies of subsystems. Some correlations of *P*-parameter values with Lagrangian and Hamiltonian functions are obtained.

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exceeds the total of their covalent radii, “superexchange” processes of overlapping cation orbitals take place through the anion between them.

In this work similar equilibrium-exchange processes are evaluated through the notion of spatial-energy parameter, *P*-parameter.

Introduction

To obtain the dependence between energy parameters of free atoms and degree of structural interactions in simple and complex systems is one of strategic tasks in physical chemistry. Classical physics and quantum mechanics widely use Coulomb interactions and their varieties for this.

Thus in Van der Waals theory,¹ orientation and charge-dipole interactions are referred to electron-conformation interactions in bio-systems, and as a particular case in exchange-resonance transfer of energy. But biological and many cluster systems are electroneutral in structural basis. And non-Coulomb equilibrium-exchange spatial-energy interactions, i.e. non-charge electrostatic processes, are mainly important for them.

The structural interactions of summed electron densities of valence orbitals of corresponding conformation centers, processes of equilibrium flow of electron densities, take place due to overlapping of their wave functions.

Heisenberg and Dirac² proposed the exchange Hamiltonian derived assumption on direct overlapping of wave functions of interacting centers as $\bar{H} = -I_0 S_1 S_2$. where \bar{H} is spin operator of isotropic exchange interaction for pair of atoms, I_0 is the exchange constant, S_1 and S_2 are the overlapping integrals of wave functions.

In this model electrostatic interactions are modelled by effective exchange Hamiltonian acting in the space of spin functions.

In particular, such approach is applied to the analysis of structural interactions in cluster systems. It is demonstrated in Anderson's works³ that in compounds of transition elements when the distance between paramagnetic ions considerably

Results and discussion

On two principles of adding energy characteristics of interactions

The analysis of kinetics of various physical and chemical processes shows that in many cases the reciprocals of velocities, kinetic or energy characteristics of the corresponding interactions are added.

Some examples: ambipolar diffusion, resulting velocity of topochemical reaction, change in the light velocity during the transition from vacuum into the given medium, effective permeability of bio-membranes.

In particular, such supposition is confirmed by the formula of electron transport possibility (W_∞) due to the overlapping of wave functions 1 and 2 (in steady state) during electron-conformation interactions:

$$W_\infty = \frac{1}{2} \frac{W_1 W_2}{W_1 + W_2} \quad (1)$$

Eqn. (1) is used when evaluating the characteristics of diffusion processes followed by non-radiating transport of electrons in proteins.¹

From classical mechanics it is known that the relative motion of two particles with the interaction energy $U(r)$ takes place as the motion of material point with the reduced mass μ in the field of central force $U(r)$, and general translational motion as a free motion of material point with the mass (Eqns. 2 and 3). Such things take place in quantum mechanics as well.⁴

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \quad (2)$$

$$m = m_1 + m_2 \quad (3)$$

The task of two-particle interactions taking place along the bond line was solved in the times of Newton and Lagrange (Eqn. 4).

$$E = \frac{m_1 v_1^2}{2} + \frac{m_2 v_2^2}{2} + U(\bar{r}_2 - \bar{r}_1) \quad (4)$$

where E is the total energy of the system, first and second elements are the kinetic energies of the particles, third element is the potential energy between particles 1 and 2, vectors \bar{r}_2 and \bar{r}_1 characterize the distance between the particles in final and initial states.

For dynamic thermodynamic systems the first commencement of thermodynamics is as follows.

$$\delta E = d\left(U + \frac{mv^2}{2}\right) \pm \delta A m \quad (5)$$

where δE is amount of energy transferred to the system, element $d[U + (mv^2/2)]$ characterizes the changes in internal and kinetic energies of the system, $+\delta A$ is the work performed by the system and $-\delta A$ is worked performed with the system.

As the work value numerically equals the change in the potential energy, it is apparent that

$$\delta A = -\Delta U \quad (6)$$

and

$$-\delta A = +\Delta U \quad (7)$$

It is probable that not only in thermodynamic but in many other processes in the dynamics of moving particles interaction not only the value of potential energy is critical, but changes in it are as well. Therefore, similar to the equation (4), the following equations should be applicable to two-particle interactions.

$$\delta E = d\left(\frac{m_1 v_1^2}{2} + \frac{m_2 v_2^2}{2}\right) \pm \Delta U \quad (8)$$

where

$$U = U_2 - U_1 \quad (9)$$

where U_1 and U_2 are the potential energies of the system in final and initial states.

At the same time, the total energy (E) and kinetic energy ($mv^2/2$) can be calculated from their zero value, then only the last element is modified in Eqn. (4).

The character of the change in the potential energy value ΔU was analyzed by its sign for various potential fields and the results are given in Table 1. From the table it is seen that the values $-\Delta U$ and accordingly $+\delta A$ (positive work) correspond to the interactions taking place along the potential gradient, and $+\Delta U$ and $-\delta A$ (negative work) occur during the interactions against the potential gradient.

The solution of two-particle task of the interaction of two material points with masses m_1 and m_2 , obtained under the condition of the absence of external forces, corresponds to the interactions flowing along the gradient, the positive work is performed by the system (similar to the attraction process in the gravitation field).

The solution of this equation via the reduced mass (μ) is the Lagrange equation for the relative motion of the isolated system of two interacting material points with masses m_1 and m_2 , which are related to x in the following way:

$$\mu \cdot x'' = -\frac{\partial U}{\partial x} \quad (10)$$

Here U is the mutual potential energy of material points, μ is the reduced mass. At the same time, $x'' = a$ (feature of the system acceleration). For elementary portions of the interactions Δx can be taken as follows:

$$\frac{\partial U}{\partial x} \approx \frac{\Delta U}{\Delta x}$$

That is $\mu a \Delta x = \Delta U$, therefore

$$\frac{1}{1/(a\Delta x)} \frac{1}{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)} \approx -\Delta U,$$

$$\frac{1}{1/(m_1 a \Delta x) + 1/(m_2 a \Delta x)} \approx -\Delta U$$

or

$$\frac{1}{\Delta U} \approx \frac{1}{\Delta U_1} + \frac{1}{\Delta U_2} \quad (11)$$

where ΔU_1 and ΔU_2 are the potential energies of material points on the elementary portion of interactions and ΔU is the resulting (mutual) potential energy of this interactions.

Table 1. Direction of the interaction processes .

No.	Systems	Potential field	Process	U	Relations of parameters		Sign of		Process direction
							ΔU	δA	
1	opposite electrical charges	electrostatic	attraction	$-k \frac{q_1 q_2}{r}$	$r_2 < r_1$	$U_2 > U_1$	-	+	along the gradient
			repulsion	$-k \frac{q_1 q_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	+	-	against the gradient
2	similar electrical charges	electrostatic	attraction	$k \frac{q_1 q_2}{r}$	$r_2 < r_1$	$U_2 > U_1$	+	-	against the gradient
			repulsion	$k \frac{q_1 q_2}{r}$	$r_2 > r_1$	$U_2 > U_1$	-	+	along the gradient
3	elementary masses (m_1, m_2)	gravitational	attraction	$-\gamma \frac{m_1 m_2}{r}$	$r_2 < r_1$	$U_2 > U_1$	-	+	along the gradient
			repulsion	$-\gamma \frac{m_1 m_2}{r}$	$r_2 > r_1$	$U_2 > U_1$	+	-	against the gradient
4	spring deformation	elastic forces	compression	$k \frac{\Delta x^2}{2}$	$x_2 < x_1$	$U_2 > U_1$	+	-	against the gradient
			extension	$k \frac{\Delta x^2}{2}$	$x_2 > x_1$	$U_2 > U_1$	+	-	against the gradient
5	photoeffect	electrostatic	repulsion	$k \frac{q_1 q_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	-	+	along the gradient

Thus:

1. In the systems in which the interactions proceed along the potential gradient (positive performance) the resulting potential energy is found based on the principle of adding reciprocals of the corresponding energies of subsystems.⁵ Similarly, the reduced mass for the relative motion of two-particle system is calculated.

$$\frac{1}{q^2/r_i} + \frac{1}{W_i n_i} = \frac{1}{P_E} \quad (12)$$

or

2. In the systems in which the interactions proceed against the potential gradient (negative performance) the algebraic addition of their masses as well as the corresponding energies of subsystems is performed (by an analogy with Hamiltonian).

$$\frac{1}{P_0} = \frac{1}{q^2} + \frac{1}{(Wrn)_i} \quad (13)$$

Spatial-energy parameter (P -parameter)

From the equation (11) it is seen that the resulting energy characteristic of the system of two material points interaction is found based on the principle of adding reciprocals of initial energies of interacting subsystems.

Electron with the mass m moving near the proton with the mass M is equivalent to the particle with the mass

$$\mu = mM/(m + M)^6.$$

Therefore, when modifying the equation (11), we can assume that the energy of atom valence orbitals (responsible for interatomic interactions) can be calculated⁵ by the principle of adding reciprocals of some initial energy components based on the following equations.

where W_i is the electron orbital energy,⁷ r_i is the orbital radius of i orbital,⁸ $q=Z^*/n^*$,⁹ n_i is the number of electrons of the given orbital, Z^* and n^* is the effective nuclear charge and effective main quantum number, r is the bond dimensional characteristics.

P_0 was called a spatial-energy parameter (SEP), and P_E is the effective P -parameter (effective SEP). Effective SEP has a physical sense of some averaged energy of valence electrons in the atom and is measured in energy units, electron-volts (eV).

The values of P_0 -parameter are the tabulated constants for the electrons of the given atom orbital.

For dimensionality SEP can be written down as follows:

$$[P_E] = [q^2] = [E] \cdot [r] = [h] \cdot [v] = \frac{\text{kg} \cdot \text{m}^3}{\text{s}^2} = \text{J} \cdot \text{m} \quad (15)$$

where $[E]$, $[h]$ and $[v]$ are the dimensions of energy, Planck constant and velocity, respectively. Thus P -parameter corresponds to a processes going along the potential gradient.

The introduction of P -parameter should be considered as further development of quasi-classical notions using quantum-mechanical data on atom structure to obtain the criteria of energy conditions of phase-formation. At the same time, for the systems of similarly charged (e.g. – orbitals in the given atom), homogeneous systems the principle of algebraic addition of such parameters is preserved:

$$\sum P_E = \sum (P_0/r_i) \quad (16)$$

$$\sum P_E = \frac{\sum P_0}{r} \quad (17)$$

or

$$\sum P_0 = P'_0 + P''_0 + P'''_0 + \dots \quad (18)$$

$$r \sum P_E = \sum P_0 \quad (19)$$

Here P -parameters are summed on all atom valence orbitals. To calculate the values of P_E -parameter at the given distance from the nucleus, depending on the bond type, either atomic radius (R) or ionic radius (r_i) can be used instead of r .

Regarding the reliability of such approach, the calculations demonstrated that the values of P_E -parameters are numerically equal (within 2 %) to the total energy of valence electrons (U) by the atom statistic model. Using the known correlation between the electron density (β) and interatomic potential by the atom statistic model,¹⁰ we can obtain the direct dependence of P_E -parameter on the electron density at the distance r_i from the nucleus.

The rationality of such approach is confirmed by the calculation of electron density using wave functions of Clementi and its comparison with the value of electron density calculated via the value of P_E -parameter.

Wave equation of P -parameter

To characterize atom spatial-energy properties two types of P -parameters are introduced. The relation between them is a simple one, $P_E = P_0/R$, where R is an atom-dimensional characteristic. Taking into account additional quantum characteristics of sublevels in the atom, this equation can be written down in coordinate x as follows: $\Delta P_E = \Delta P_0/\Delta x$ or $\partial P_E = \partial P_0/\partial x$, where the value ΔP equals the difference between P_0 -parameter of i^{th} orbital and PCD–countdown parameter (parameter of main state at the given set of quantum numbers).

According to the established rule⁵ of adding P -parameters of similarly charged or homogeneous systems for two orbitals in the given atom with different quantum characteristics and according to the energy conservation rule we have:

$$\Delta P''_E - \Delta P'_E = P_{E,\lambda} \quad (20)$$

where $P_{E,\lambda}$ – spatial-energy parameter of quantum transition.

Taking for the dimensional characteristic of the interaction $\Delta\lambda = \Delta x$, we have:

$$\frac{\Delta P''_0}{\Delta\lambda} - \frac{\Delta P'_0}{\Delta\lambda} = \frac{P_0}{\Delta\lambda}$$

or

$$\frac{\Delta P'_0}{\Delta\lambda} - \frac{\Delta P''_0}{\Delta\lambda} = \frac{P_{0,\lambda}}{\Delta\lambda} \quad (21)$$

Let us again divide both sides by $\Delta\lambda$ term

$$\left(\frac{\Delta P'_0}{\Delta\lambda} - \frac{\Delta P''_0}{\Delta\lambda} \right) / \Delta\lambda = - \frac{P_0}{\Delta\lambda^2} \quad (22)$$

where

$$\left(\frac{\Delta P'_0}{\Delta\lambda} - \frac{\Delta P''_0}{\Delta\lambda} \right) / \Delta\lambda \sim \frac{d^2 P_0}{d\lambda^2}$$

i.e.,

$$\frac{d^2 P_0}{d\lambda^2} + \frac{P_0}{\Delta\lambda^2} \approx 0 \quad (23)$$

Taking into account only those interactions when $2\pi\Delta x = \Delta\lambda$ (closed oscillator), we have the following equation:

$$\frac{d^2 P_0}{4\pi^2 \Delta\lambda^2} + \frac{P_0}{\Delta\lambda^2} = 0$$

or

$$\frac{d^2 P_0}{dx^2} + 4\pi^2 \frac{P_0}{\Delta\lambda^2} \approx 0 \quad (24)$$

Since

$$\Delta\lambda = \frac{h}{mv}$$

then

$$\frac{d^2 P_0}{dx^2} + 4\pi^2 \frac{P_0}{h^2} m^2 v^2 \approx 0 \quad (25)$$

or

$$\frac{d^2 P_0}{dx^2} + \frac{8\pi^2 m}{h^2} P_0 E_k = 0 \quad (26)$$

where $E_k = mv^2/2$ is the electron kinetic energy.

Schrodinger equation for the stationary state in coordinate x is as follows (Eqn. 27).

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} \psi E_k = 0 \quad (27)$$

Comparing these two equations it can be seen that the P_0 -parameter numerically correlates with the value of ψ -function, $P_0 \approx \psi$, and is generally proportional to it, $P_0 \sim \psi$. Taking into account the broad practical opportunities of applying the P -parameter methodology, we can consider this criterion as the materialized analog of ψ -function.

Since the P_0 -parameters like ψ -functions have wave properties, the superposition principles should be fulfilled for them, defining the linear character of the equations of adding and changing P -parameter.

Analog comparisons of Lagrange and Hamilton functions with spatial-energy parameter

Lagrange (L) and Hamilton (H) functions are the main provisions of analytical mechanics. Lagrange function is the difference between kinetic (T) and potential (U) energies of the system:

$$L = T - U \quad (28)$$

For uniform functions of the second degree Hamilton function can be considered as the sum of potential and kinetic energies, i.e. as the total mechanical energy of the system:

$$H = T + U \quad (29)$$

From these equations and in accordance with energy conservation law we can visualize eqns. (30) and (31).

$$H + L = 2T \quad (30)$$

$$H - L = 2U \quad (31)$$

Let us try to assess the movement of an isolated system of a free atom as a relative movement of its two subsystems, nucleus and orbital.

The structure of atom is formed of oppositely charged masses of nucleus and electrons. In this system, the energy characteristics of subsystems are the orbital energy of electrons (W_i) and effective energy of atom nucleus taking screening effects into account.

In a free atom, its electrons move in Coulomb field of nucleus charge. The effective nucleus charge characterizing the potential energy of such subsystem taking screening effects into account equals q^2/r_i , where $q = Z^*/n^*$.

Here Z^* and n^* are effective nucleus charge and effective main quantum number, respectively, r_i is the orbital radius. It can be presumed that orbital energy of electrons during their motion in Coulomb field of atom nucleus is mainly defined by the value of kinetic energy of such motion.

Thus, it is assumed that $T \sim W$ and $U \sim q^2/r_i$. In such an approach the total of the values W and q^2/r_i are analogous to Hamilton function (H) i.e.,

$$W + q^2/r_i \sim H \quad (32)$$

An analogous comparison of P -parameter with Lagrange function can be carried out when investigating Lagrange equation for relative motion of isolated system of two interacting material points with masses m_1 and m_2 in coordinate x . The principle of adding reciprocals of energy values models their algebraic difference by Hamiltonian. If it is presumed that $P_E \sim L$, then Eqn. (30) becomes Eqn. (33).

$$\left(W + \frac{q^2}{r_i} \right) + P_E \approx 2W \quad (33)$$

Using the values of electron bond energy as the orbital electron energy, we calculated the values of P_E -parameters of free atoms (Table 2) by equations (12-14). When calculating the values of effective P_E -parameter, mainly the atom radius values by Belov-Bokiy or covalent radii (for non-metals) were applied as dimensional characteristics of atom (R).

At the same time, the average values of total energy, valence orbitals dividing their values by a number of valence electrons considered (N):

$$\left(\frac{q^2}{r_i} + W \right) \frac{1}{N} + P_E \approx 2W \quad (34)$$

This energy in terms of one valence electron is the analogue of Hamilton function, H .

In free atoms of Ia and IIa groups of periodic system, s -orbital is the only valence orbital, and that was considered via the introduction of the coefficient, $K = n/n^*$ where n is the main quantum number, n^* is the effective main quantum number, by the eqn. (35)

$$\left(\frac{q^2}{r_i} + W \right) \frac{1}{KN} + P_E \approx 2W \quad (35)$$

Table 2. Comparison of some basic energy atomic characteristics.

Element	Valence electrons	W (eV)	r_i (Å)	q^2 (eVÅ)	P_0 (eVÅ)	R (Å)	$P_E=P_0/R$ (eV)	N	B^*	2W (eV)
Li	2s ¹	5.3416	1.586-2	5.8892	3.475	1.55	2.2419	1	9.440	10.683
Be	2s ²	8.4157	1.040	13.159	7.512	1.13	6.6478	2	17.182	16.831
B	2p ¹	8.4315	0.776	21.105	4.9945	0.91	5.4885	3	17.365	16.863
	2s ²	13.462	0.769	23.890	11.092	0.91	12.189	3	27.032	26.924
C	2p ²	11.792	0.596	35.395	10.061	0.86	11.699/2	4	23.645	23.584
	2s ²	19.201	0.620	37.240	14.524	0.77	18.862	4	38.824	38.402
N	2p ³	15.445	0.4875	52.912	15.830	0.71	22.296/3	5	32.228	30.890
	2s ²	25.724	0.521	53.283	17.833	0.71	19.788/3	5	31.392	51.448
O	2p ¹	17.195	0.4135	71.383	6.4663	0.66	9.7979/4	6	34.087	34.390
	2s ²	33.859	0.450	72.620	21.466	0.66	32.524	6	65.064	67.718
F	2p ¹	19.864	0.3595	93.625	6.6350	0.64	10.367/5	7	42.115	39.728
	2s ²	42.792	0.396	94.641	24.961	0.64	39.002	7	79.257	85.584
Na	3s ¹	4.9552	1.713-2	10.058	4.6034	1.89	2.4357	1	10.327	9.9104
Mg	3s ¹	6.8859	1.279	17.501	5.8588	1.60	3.6618	2	13.946	13.772
Al	3p ¹	5.713	1.312	26.443	5.840	1.43	4.084	3	12.707	11.426
	3s ²	10.706	1.044	27.119	12.253	1.43	8.5685	3	20.796	21.412
Si	3p ¹	8.0848	1.068	29.377	6.6732	1.17	5.7036	4	14.600	16.170
	3s ²	14.690	0.904	38.462	15.711	1.17	13.428	4	17.737	29.380
P	3p ³	10.659	0.9175	38.199	16.594	1.30	12.765/3	3	21.686	21.318
	3s ¹	18.951	0.803	50.922	11.716	1.10	10.651	3	38.106	37.902
S	3p ¹	11.901	0.808	48.108	8.0143	1.04	7.7061	4	25.566	23.802
	3p ²	11.901	0.808	48.108	13.740	1.04	13.215/2	4	24.468	23.802
	3p ⁴	11.904	0.808	48.108	21.375	1.04	20.553/4	4	22.998	23.808

$$*B = \left(\frac{q^2}{r_i} + W \right) \frac{1}{KN} + P_E$$

Thus in Ia and IIa subgroups of short periods, $K = 1$ and then $K = 4/3.7$; $5/4$ and $6/4.2$ for 4th, 5th, and 6th periods of the system only for these subgroups. For all other cases $K = 1$. Besides, for the elements only of 1a group of periodic system, the value $2r_i$ (i.e. the orbital radius of i -orbital) was used as a dimensional characteristic in the first component of Eqn. 35.

Taking into account the remarks pointed out for the initial equation, the values of both the components of Eqn. (35) for 65 elements were calculated and compared. Some results are given in Table 2. The analysis of the data given in Table 2 reveals that the proximity of the values investigated is mostly within 5 %. Thus there is a certain analogy of equations (30) and (35), and the value of P_E -parameter can be considered as the analog of Lagrange function and value

$$\left(\frac{q^2}{r_i} + W \right) \frac{1}{KN}$$

as an analog of Hamilton function.¹¹

Structural exchange spatial-energy interactions

In the process of solid solution formation and other structural equilibrium-exchange interactions, the single electron density should be set in the points of atom-component contact. This process is accompanied by the redistribution of electron density between the valence areas of both particles and transition of the part of electrons from some external spheres into the neighbouring ones. Apparently, frame atom electrons do not take part in such exchange.

Obviously, when electron densities in free atom-components are similar, the transfer processes between boundary atoms of particles are minimal and this will be favorable for the formation of a new structure. Thus the evaluation of the degree of structural interactions in many cases means the comparative assessment of the electron density of valence electrons in free atoms (on averaged orbitals) participating in the process, which can be correlated with the help of P -parameter model.

The less the difference ($P'_o/r'_i - P''_o/r''_i$), more favorable is the formation of a new structure or solid solution from the energy point.

In this regard, the maximum total solubility, evaluated via the coefficient of structural interaction, α , is determined by the condition of minimum value of α , which represents the relative difference of effective energies of external orbitals of interacting subsystems:

$$\alpha = \frac{P'_o/r'_i - P''_o/r''_i}{(P'_o/r'_i + P''_o/r''_i)/2} 100 \% \quad (36)$$

$$\alpha = \frac{P'_C - P''_C}{P'_C + P''_C} 200 \% \quad (37)$$

where P_C – structural parameter is found by equation:

$$\frac{1}{P_C} = \frac{1}{N_1 P'_E} + \frac{1}{N_2 P''_E} + \dots \quad (38)$$

here N_1 and N_2 are the number of homogeneous atoms in subsystems.

The isomorphism degree and mutual solubility are evaluated in many (over one thousand) simple and complex systems (including nanosystems). The calculation results are in compliance with theoretical and experimental data.

Conclusions

1. The introduced spatial-energy parameter (P -parameter) can be considered as materialized analog of ψ -function.
2. The application of such methodology allows modelling of physical-chemical processes based on energy characteristics of a free atom.

References

- ¹Rubin, A. B., *Biophysics*, 1, *Theoretical biophysics*, Vysshaya shkola, Moscow, **1987**, 319.
- ²Dirac, P. A., *Quantum Mechanics*, Oxford University Press, London, **1935**.
- ³Anderson, P. W., *Magnetism*, Vol.1, Academic Press, New York, **1963**, 25.
- ⁴Blokhintsev, D. I., *Basics of quantum mechanics*, Vysshaya shkola, Moscow, **1961**, 512.
- ⁵Korablev, G. A., *Spatial-Energy Principles of Complex Structures Formation*, Brill Academic Publishers and VSP, Netherlands, **2005**, 426.
- ⁶Eyring, G., Walter, J., Kimball G., *Quantum chemistry*, M., F. L., **1948**, 528.
- ⁷Fischer, C. F., *Atomic Data*, **1972**, 4, 301-399.
- ⁸Waber, J. T., Cromer, D. T., *J. Chem. Phys.*, **1965**, 42(12), 4116-4123.
- ⁹Clementi, E., Raimondi, D. L., *J. Chem. Phys.*, **1963**, 38(11), 2686-2689.
- ¹⁰Gombash, P., *Statistic theory of an atom and its applications*, M.: I.L., 1951, 398.
- ¹¹Korablev, G. A., Kodolov, V. I., Lipanov, A. M., *Chem. Phys. Mesoscopy*, **2004**, 6(1), 5-18.

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