



INSTITUTE OF THEORETICAL  
AND EXPERIMENTAL PHYSICS

ITEP - 7

V.M.Byakov, V.I.Kulakov, Y.B.Rumer,  
A.I.Fet

11110100

GROUP THEORETICAL CLASSIFICATION  
OF CHEMICAL ELEMENTS

M O S C O W 1 9 7 7

V.M.Byakov, V.I.Kulakov, Y.B.Rumer, A.I.Pet

GROUP THEORETICAL CLASSIFICATION  
OF CHEMICAL ELEMENTS

Moscow

1977

УДК 541.9

М-16

© ИТЭФ 1977

**В.М. Бяков, Ю.И. Кулков, Ю.Б. Румер, А.И. Фет**  
**Теоретико-групповая классификация хими-**  
**ческих элементов.**  
**Сопоставление со свойствами химических**  
**элементов.**

Работа поступила в ОНТИ 7/1-1977 г.

---

Подписано к печати 17/1-77г. Т-01612. Формат 70 x 108 1/16.  
Печ. л. 1,5. Тираж 295 экз. Заказ 7. Цена 8 коп. Индекс 3624.

---

## S U M M A R Y

The method of classification of chemical element, based on group symmetry principles, developed in pp. I, II, is compared with element properties. Elements are considered to be states of a single quantum system, the atomic structure being ignored. The number of basic states of this system (i.e. of elements) is, in principle, infinite. Elements thus treated as states of the system, break down into successively diminishing subsystems, big and small multiplets. Big multiplets are numbered by the quantum number  $\nu = 1, 2, \dots$ . Each  $\nu$ -multiplet breaks down, then, into  $2\nu - 1$  small multiplets, numbered by pairs of quantum numbers  $(\lambda, \ell_\lambda)$ , where  $\lambda = 0, 1, \dots, \nu - 1$  and  $\ell_\lambda = \lambda - 1/2, \lambda + 1/2$  for  $\lambda > 0$ , corr.  $\ell_\lambda = 1/2$  for  $\lambda = 0$ . Each element gets an "address" consisting of four quantum numbers  $(\nu, \lambda, \ell_\lambda, \kappa)$ , the last referring to its place within its  $(\lambda, \ell_\lambda)$ -multiplet. The atomic number is expressed in these quantum numbers as follows:

$$Z = \frac{1}{6} d(d^2 - 1) + \frac{(d+1)^2}{2} - \frac{1 - (-1)^d}{2} \cdot \frac{d+1}{2} - 4\lambda(\lambda+1) + \ell_\lambda(2\lambda+1) + \kappa - 1$$

where  $d = \nu + \lambda$ . If our quantum numbers are essential characteristics of elements, we may expect that each property of elements allowing of a quantitative measure is expressible in these numbers. Though the analytical form of this dependence is unknown, we may suppose it to be regular within small multiplets and changing leapwise between them. Regu-

lar dependence of properties of the "classical quantum numbers" is traced on several quantities considered below, as ionization potential, electronegativity, atomic volume, density, melting heat, magnetic susceptibility, and even rate constants of hydrated electrons. Thus, our theory, being a group classification, does not describe in detail any of element properties, but leads to a unified qualitative description of all of them simultaneously,

As will be seen, this is convincingly corroborated by experimental data. The general picture of element properties thus revealed could not be represented before, in the absence of a natural division of elements into multiplets. The idea now to do it adopted from the  $SU(3)$ - and  $SU(6)$ -symmetry. Especially useful are the  $(\lambda, L_2)$ -multiplets, first separated in [3]; these are to be regarded as a most essential feature distinguishing our classification from others available in the literature.

In particular, for actinoids our multiplets correspond, in general, to the subdivision of this family into two subfamilies proposed by Heyssinsky. The incomplete analogy of properties between lanthanoids and actinoids is also reflected by this classification; it implies that actinoids are to be considered not only analogues of the lanthanoids, but in some respects of transition elements too.

In the following, the theory developed in pp. I [1], II [2] (cf [3-5] for original physical treatment) is compared with the experiment.

Results of the classification procedure for chemical elements, as described at the end of p.I, are summarized in table II. This table differs from the conventional forms of the Mendeleev table by explicit consideration of the symmetry group governing regularities appearing in the system of elements. These are set into rooms of the table assigned to them, and thus are divided into big  $\nu$ -multiplets and small  $(\lambda, \ell_2)$ -multiplets, which establishes their addresses. Let us see now to what extent our classification is corroborated by the properties of elements.

Comparing the arrangement of elements in table II with that in the classical Mendeleev table, it is readily seen that every line corresponding to fixed values of  $\lambda$ ,  $\ell_2$ ,  $\nu$  contains elements with similar chemical properties, the so called homologues. Together they correspond to one of the subgroups known from the common forms of the Mendeleev table. However, in our table these subgroups are arranged otherwise, which will be seen to make sense. Multiplets with  $\lambda = 0$  or  $\lambda = 1$  include elements contained in the principal "a" subgroups of the classical table; multiplets with  $\lambda = 2$  or  $\lambda = 3$  include those from the collateral subgroup ("b" subgroups). Each Mendeleevian period consists of one ( $\lambda = 0$ ) multiplet with  $\nu + \lambda$  equal to the number of the period, and of ( $\lambda > 0$ ) multiplets (if present) with  $\nu + \lambda$  exceeding the period number by one.

Note that in the table II hydrogen and helium are included, correspondingly, into subgroups of alkali metals and alkaline-earths metals, but not into these of halogens and rare gases, as accepted in most modern tables. Then, in contrast to the subgroup (IIIb), Sc - Y - La - Ac, of the classical Mendeleev table, according to table II immediate chemical analogues of Sc and Y are Lu and Lr, and not La and Ac. Therefore, the first and the second groups of rare-earths metals begin corr. with lanthanum and actinium, and not with cerium and thorium, whereas lutetium and laurentium fall out of these families <sup>\*)</sup>. Then, classical tables have no place for lanthanoids and actinoids, so that these families are carried out of the table and figure as supplements. Our table II, on the contrary, contains these elements on equal terms. Furthermore, our classification according to numbers  $\lambda$ ,  $\mu$  accounts for the analogy in properties of corresponding lanthanoids and actinoids, Sm - Pu, Eu - Am, Gd - Cm, ..., discovered by Seaborg. Division of elements into metals and non-metals, not altogether unambiguous but implanted in chemistry, is traced more clearly in table II: metallic and metalloid properties alternate when  $\lambda$  increases. Elements with  $\lambda = 0$  or  $\lambda = 2$  are typical metals (with the exception of He and H). Multiplets with  $\lambda = 1$ , on the contrary, include basically elements with non-metal properties (excepted Al, Ga, In, Tl, and possibly, Sn, Pb, Bi).

---

<sup>\*)</sup> Lu, by most of its physical and chemical properties, ranks with Sc and Y, rather than with La. Attaching Lu to rare earths is found incorrect from the point of view of electronic shells analysis, as emphasized e.g. by L.Landau and E.Lifshitz [6].

The quantum mechanical explanation of periodicity in properties of elements, as given by Bohr, is known to be intimately related to the theory of the hydrogen atom. Our approach reveals the same analogy with the excited states of the hydrogen atom. The reason of this is that the hydrogen atom (in its excited states) and the system of chemical elements are both objects possessing  $SO(4,2)$  symmetry.

Just as in electronic states of the hydrogen atom degeneracy means coincidence of their energies, "degeneracy" in the system of chemical elements may be understood as coincidence of their physico-chemical properties. Accordingly, approximate degeneracy with respect to a chemical quantum number is to be interpreted as proximity of element properties. Thus, elements with possible affinity in their properties are known a priori (which is an advantage of the group theoretical approach). However, group theory has generally little to say on the extent of this affinity.

If the property we are interested in can be expressed quantitatively, it is natural to suppose there is an Hermitian operator expressing it by means of its eigenvalues. This operator is to act on the space of system states, i.e. on the space of our "chemical system", specific states of which are atoms of different elements. But, in the present theory, this space appears as the space of a certain irreducible unitary representation of the conformal group  $SO(4,2)$  (cf. p.II). Therefore, it is plausible that the operator accounting for the property considered is to be expressed in the Lie algebra operators of the  $SO(4,2)$  group like those involved in the mass formulas of unitary sym-

incidentally, the Casimir operators of the symmetry group. The exact form of the operator is, of course, unknown (cf. p.I, where similar considerations are developed in application to the atomic number). However, we are lead thus to a possible analogy between different systems described by one and the same symmetry group. The Casimir operators for such systems being constructed from the same Lie algebra, it is to be expected that resulting operators have spectra similar in their basic features. One can trace this analogy quantitatively comparing our chemical system with another system described by the same representation of the  $SO(4,2)$  group, the hydrogen atom.

In the hydrogen atom (with degeneracy removed) energy differences between levels corresponding to various  $j$  decrease when  $l$  increases within a spectral multiplet, i.e. for a fixed value of  $n$ . In the same way, differences between properties of elements within a  $(\nu, \lambda)$ -multiplet diminish as  $\lambda$  increases. If for  $\lambda = 1$  properties of elements numbered by different  $\lambda, \mu$  are rather distinct from each other, then, for  $\lambda = 2$ , this distinction is considerably effaced. Therefore, comparison between neighbouring elements within a multiplet makes sense, properties of which are found to be very similar, as for Zr, Nb, Mo or Hf, Ta and W. This analogy within a multiplet may even dominate over that within the underlying group. Proximity of properties revealed by some elements with  $\lambda = 2$  (Fe - Co - Ni, Ru - Rh - Pd, Os - Ir - Pt) is expressed by the classificial table placing them into a common subgroup (VIIIb) in triads. For  $\lambda = 3$  chemical properties of elements

(lanthanoids, corr. actinoids) are getting so near that each of these families is allotted a single square of the table. It is of interest in this connection that grouping of elements into "houses", i.e. ( $\nu$ ,  $\lambda$ )-multiplets, for  $\lambda = 2$  and 3 corresponds rather closely to families of geochemically allied elements: those of iron ( $22 \leq Z \leq 30$ ), of molybdenum ( $42 \leq Z \leq 46$ ), of rhenium ( $73 \leq Z \leq 78$ ), of lanthanum ( $54 \leq Z \leq 71$ ) and uranium ( $Z \geq 89$ ).

Then, rapprochement of properties is observed between elements of corresponding positron ( $\lambda$ ,  $l_\lambda$ ,  $\kappa$  fixed) in neighbouring  $\nu$ -multiplets when  $\nu$  increases. This becomes particularly apparent in multiplets with  $\lambda = 0$  or  $\lambda = 1$ . Thus, difference between lithium and matrium (and corr. between beryllium and magnesium) is relatively greater than between any other neighbouring alkali (or alkaline-earths) metals. Just, so, in the subgroup of elements O - S - Se - Te those with the nearest properties are S - Se - Te.

What are our grounds to expect that our classification is an adequate description of element properties? Of course, the very general approach of "group classification" is incapable of a detailed explanation of any specific property of the elements; in return, it gives some information on all properties together. Take, indeed, a certain property of elements allowing of a quantitative measure  $Q$ . Then, if our quantum numbers are really essential characteristics of elements (even if not immediately observable), it may be expected that  $Q$  is expressible in these characteristics:

$$Q = Q(\nu, \lambda, l_\lambda, \partial e).$$

We do not know this expression, but some qualitative results may be inferred and verified. Let us fix the quantum numbers  $\nu, \lambda, l_\lambda$  :  $\nu = \nu_1, \lambda = \lambda_1, l_\lambda = l_{\lambda_1}$  and change  $\partial e$  ; then the dependence of the property  $Q$  on  $\partial e$  (on the "room" within a "storey") is given by the function

$$Q_1(\partial e) = Q(\nu_1, \lambda_1, l_{\lambda_1}, \partial e).$$

Similarly, for another storey ( $\nu = \nu_2, \lambda = \lambda_2, l_\lambda = l_{\lambda_2}$ ), thus differing from the former by one of the quantum numbers  $\nu, \lambda, l_\lambda$  at least, we must have another, different dependence:

$$Q_2(\partial e) = Q(\nu_2, \lambda_2, l_{\lambda_2}, \partial e).$$

Indeed, it may be expected that the law according to which  $Q$  depends on  $\partial e$  undergoes a pronounced change on shifting from one storey to another (even within the same "house"); this is expressed by strong jumps of corresponding graphs between storeys. Meanwhile, within each of the small multiplets ("storeys") a regular alteration of chemical properties is to be observed.

Comparing observed properties of elements making a multiplet we find them regularly depending on  $\partial e, l_\lambda$ , and the form of this dependence similar for analogous multiplets (i.e. having the same  $\lambda$  )<sup>\*)</sup>. For a given  $\nu + \lambda$

\*) In analogous small multiplets ( $\lambda, l_\lambda = \text{idem}$ ) physico-chemical characteristics of elements are changing alike (see figs. 1-3).

physico-chemical characteristics of elements assume, as a rule, their extremal values on the bounds of "houses". Moreover, local extrema are observed within "houses" on passage to another  $l_{\lambda}$  (cf. fig. 1-7); meanwhile, alteration of element properties within a  $(\lambda, l_{\lambda})$  - multiplet is always regular. Further, there is another feature similar to that observed in atoms or nuclei, where energy differences between  $l - 1/2$  and  $l + 1/2$  states are increasing with  $l$ . In exactly the same way, we see that in the system of elements physico-chemical properties of "storeys" differ inessentially for  $l_{\lambda} = 3/2$  and  $l_{\lambda} = 5/2$ , i.e. within  $(\lambda = 2)$  "houses" (cf. fig. 4a); whereas for  $l_{\lambda} = 5/2$  and  $l_{\lambda} = 7/2$ , within  $(\lambda = 3)$  "houses", these differences are strongly pronounced (cf. figs. 4b and 5,6,7b).

Regularities discussed above are verified for ionization potentials, oxidation degrees, melting heats (fig. 1-3) and atomic volumes. All these quantities are very characteristic as expressing fundamental properties of elements.

Comparing the curves for densities, atomic volumes and magnetic properties of lanthanoids and actinoids, we find the division of elements into  $l_{\lambda}$  - multiplets to be really significant. This division corresponds, in particular, to that proposed by Hayssinski [7], whose separation of actinoids in two families is roughly the same as ours.

Thus, our classification is corroborated in considerable detail by experimental data shown on figures 1-7. Joining of elements into  $(\lambda, l_{\lambda})$  - multiplets enables us to single out of Mendeleevian periods families of elements with properties regularly changing (and for  $\lambda \geq 2$

altogether similar). Proximity of neighbouring elements within periods, noticed long ago, appears thus as a regularity inherent to the periodic system, like the analogy of elements constituting groups.

We see our division of elements into small multiplets to be in good agreement with the experiment.

The part played by big multiplets (i.e. by the quantum number  $\nu$ ) may be shown, for instance, as follows. Let us apply to an atom with the address  $(\nu, \lambda, L_\lambda, \partial e)$  the horizontal operator  $\Gamma$ . Then, for fixed  $\lambda, L_\lambda, \partial e$  we get atoms with other values of  $\nu$  and come to a dependence

$$Q^{(1)}(\nu) = Q(\nu, \lambda_1, L_{\lambda_1}, \partial e_1).$$

Taking another line of the table (i.e. other values of  $\lambda, L_\lambda, \partial e$ ) we must have a different regularity:

$$Q^{(2)}(\nu) = Q(\nu, \lambda_2, L_{\lambda_2}, \partial e_2).$$

The regularities appearing when  $\nu$  is changing are well known: each of the functions  $Q^{(1)}(\nu), Q^{(2)}(\nu) \dots$  describes a Mendeleevian series of homologues. Such a series takes up a line in the table II. It is clear that changing the parameters  $\lambda, L_\lambda, \partial e$  we must get another kind of regularity, the analogy being thus broken. The fact that just elements with the nearest properties are sent one into another by the "horizontal" operator described above, is by no means accidental. Here, apparently, a general principle is evidenced guiding the search of nearest analogues

in the group classification of particles (cf. [5], p.326).

We see that every big multiplet contains exactly one representative of each series of Mendeleevian analogues (if only  $\nu$  is sufficiently great to ensure that this big multiplet intersects the corresponding line of the table).

This means that, with the mentioned limitation as to the lengths of big multiplets, each of them consists of "specimens" taken one by one from every of Mendeleevian series. This is exactly the meaning of periodicity, from the point of the present theory.

One of the merits of the classification given by table II is that it points out possible analogies between elements where there is no grounds to expect them proceeding from the conventional tables.

Note, for example, the well-known duality of properties in the series H, He, Be, Al, Th, U, Pu a.s.o., which makes their arrangement in a conventional table rather ambiguous. Thus, Th, Pa and U, being analogues of Ce, Pr and Nd, are also analogues of Hf, Ta and W, which are elements of the IVb and VIb subgroups (cf. fig. 1). This duality is reflected by our classification as degeneracy in  $\lambda$  for greater  $\nu$ 's, as noted above. From this point of view, actinoids are not to be considered as homologues of lanthanoids only. The rapprochement of properties between neighbouring multiplets for greater  $\nu$  and  $\lambda$ , which was described above, supports the assumption that actinoids must have properties similar to those of lanthanoids and, besides that, of transition elements making the groups with  $\nu = 6$  and  $\lambda = 2$ . This circumstance represents the classical forms of the table as somewhat restricted.

The existing correlations are, especially for elements

with greater  $Z$ , too complicated and varied to be described by any of the conventional tables. It seems therefore probable that research of heavy elements necessitates a table of elements based on new principles.

Our classification procedure results in an unambiguous arrangement of elements, known or yet undiscovered, into a table displaying their affinities, known of possible. This may facilitate identification of synthesized elements. It is of interest to compare the arrangement of elements thus obtained, for  $104 \leq Z \leq 170$ , with the forecasts of Seaborg [ 8 ], based on quantum mechanical calculations of electronic shells. For  $104 \leq Z \leq 120$  our arrangement coincides with that proposed by Seaborg. But, contrary to his predictions, it is apparent from the table II that elements with  $121 \leq Z \leq 138$  form a new family, having no homologues between known elements. Very likely, this family is divided in two multiplets, strongly degenerate in their properties, with  $l_1 = 9/2$  and  $l_2 = 7/2$ . As to the family of superactinoids predicted by Seaborg, elements of which are to resemble, to a certain extent, actinoids, it contains in accordance with table II not elements with  $122 \leq Z \leq 153$ , but only those with  $139 \leq Z \leq 152$ . The subsequent elements, for  $153 \leq Z \leq 170$ , are to be homologues of elements with  $104 \leq Z \leq 120$ .

Note, that differences in properties of elements with atomic numbers from 113 to 118 are expected to be considerably larger than those for  $103 \leq Z \leq 112$ . As to elements with  $121 \leq Z \leq 138$ , these are probably extremely similar.

It should be noted that the element 164 corresponds to strong stability of the nucleus. It is remarkable that cen-

ters of nuclear stability, both known or predicted, such as silicon ( $Z = 14$ ), tin ( $Z = 50$ ), lead ( $Z = 82$ ), the 114-th and 164-th elements, are members of ( $\lambda = 1$ ) multiplets with  $l_\lambda = 1/2$ ,  $s_e = -1/2$ . Only helium ( $Z = 2$ ), oxygen ( $Z = 8$ ) and calcium ( $Z = 20$ ) belong to the same family, with  $\lambda = 0$ . This correspondence would be incomprehensible, if the group symmetry description presented above should be interpreted as symmetry of electronic shells. It is not surprising, however, if we keep to the conception expressed in [3], which considers group symmetry proposed therein to describe atoms as a whole.



	$\nu=1$	$\nu=2$	$\nu=3$	$\nu=4$	$\nu=5$	$\nu=6$	$\nu=7$
$\lambda=0$	H He	Li Be	Na Mg	K Ca	Rb Sr	Cs Ba	Fr Ra
		B C	Al Si	Ga Ge	In Sn	Tl Pb	$\chi=-1/2$ $\chi=1/2$
$\lambda=1$		N O F Ne	P S Cl Ar	As Se Br Kr	Sb Te I Xe	Bi Po At Rn	$\chi=-3/2$ $\chi=-1/2$ $\chi=1/2$ $\chi=3/2$
			Sc Ti V Cr	Y Zr Nb Mo	Lu Hf Ta W	Lw Ku	
$\lambda=2$			Mn Fe Co Ni Cu Zn	Tc Ru Rh Pd Ag Cd	Re Os Ir Pt Au Hg		
				La Ce Pr Nd Pm Sm	Ac Th Pa U Np Pu		
$\lambda=3$				Eu Gd Tb Dy Ho Er Tm Yb	Am Cm Bk Cf Es Fm Md No		

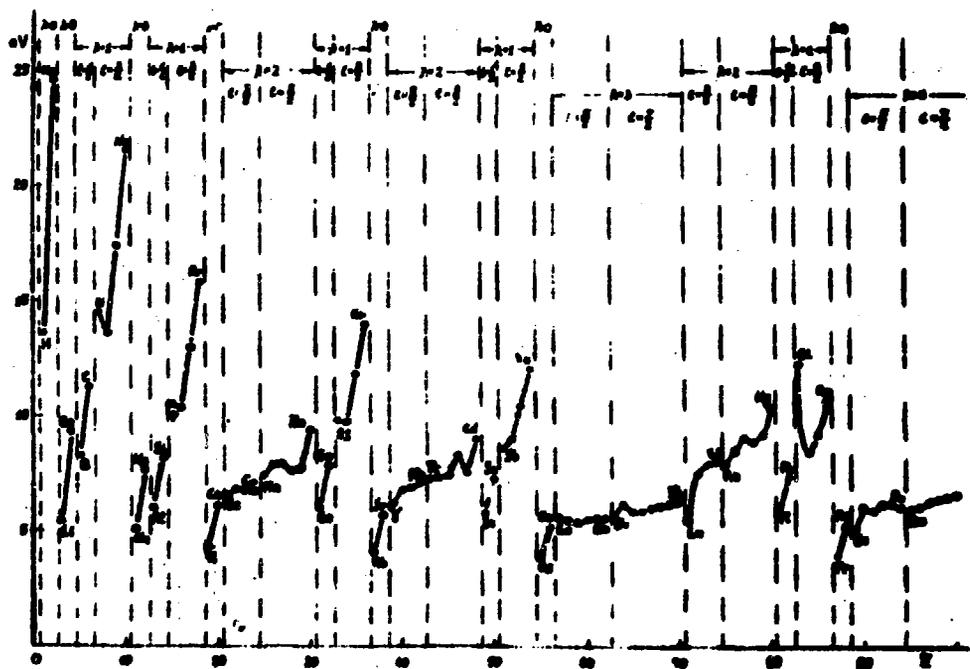


Fig.1. First ionization potentials of elements. Character of alteration of the ionisation potential is similar in identically labelled ( , )-multiplets. Extremal values correspond, as a rule, to the bounds of the multiplets. Local extrema are distinctly seen on passage from  $l = 1/2$  to  $l = 3/2$ . Approximation of properties for increasing  $l$  is manifest, differences between ionisation potentials being 5-10 eV for elements with  $l = 1$ , 2-3 eV for elements with  $l = 2$  and appr. 1 eV for elements with  $l = 3$ . "Degeneracy" for increasing  $l$  is also apparent.

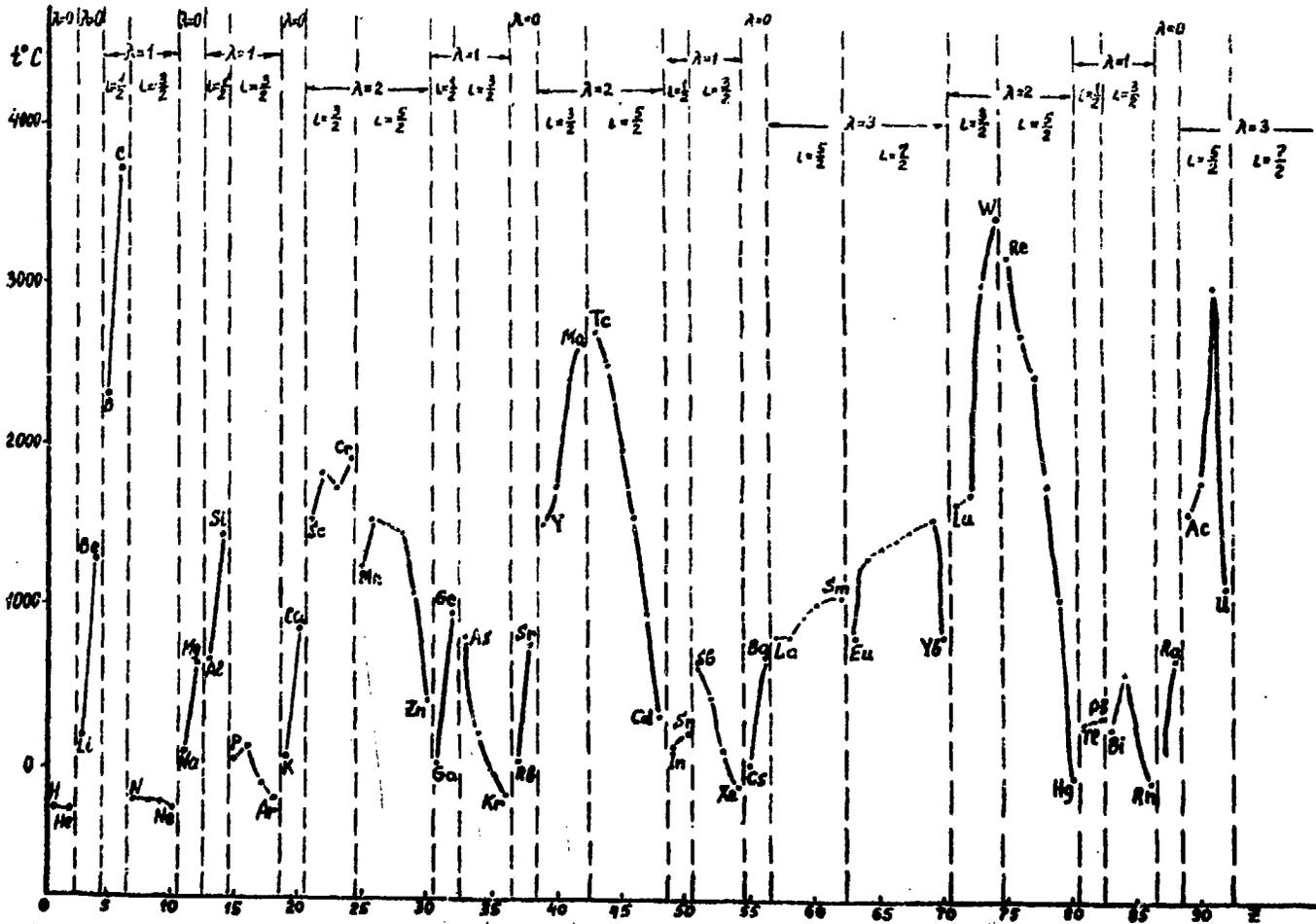


FIG. 2. Melting heats of elements.



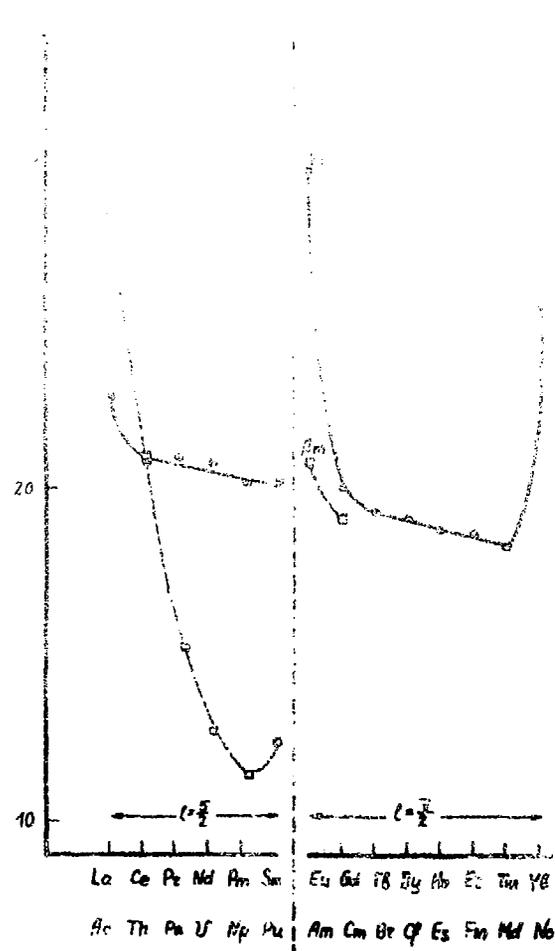
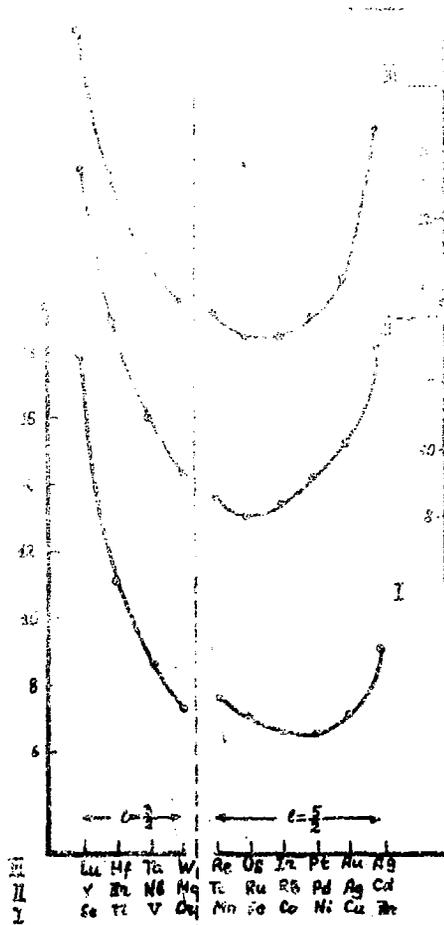


Fig.4. Atomic volumes of elements (quotients of atomic weights by densities) form a curve which is almost a mirror reflection of the density curve (see fig.5). For transition elements ( $\lambda = 2$ ) jumps between  $l, \lambda = 3/2$  and  $l, \lambda = 5/2$  are insignificant, but strongly pronounced for lanthanoids and actinoids ( $\lambda=3$ )

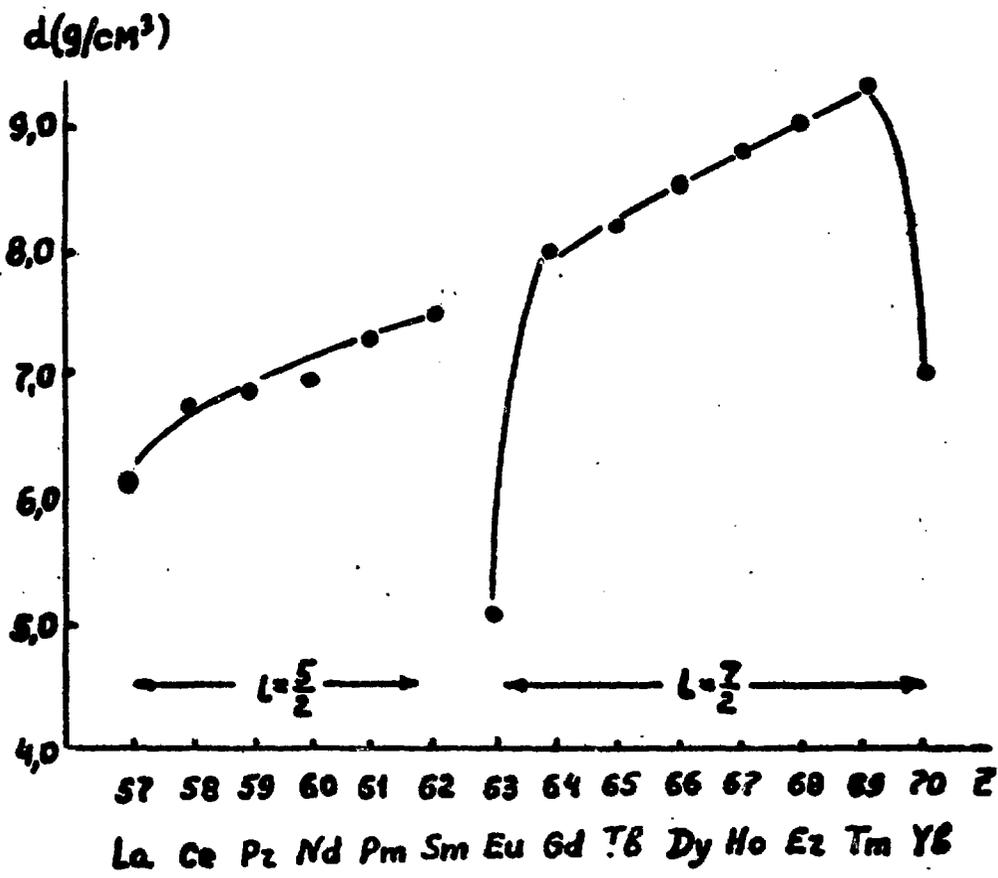


Fig. 5. Density of metallic lanthanoids.

Jump between  $L_2 = 5/2$  and  $L_2 = 7/2$  is very distinct.

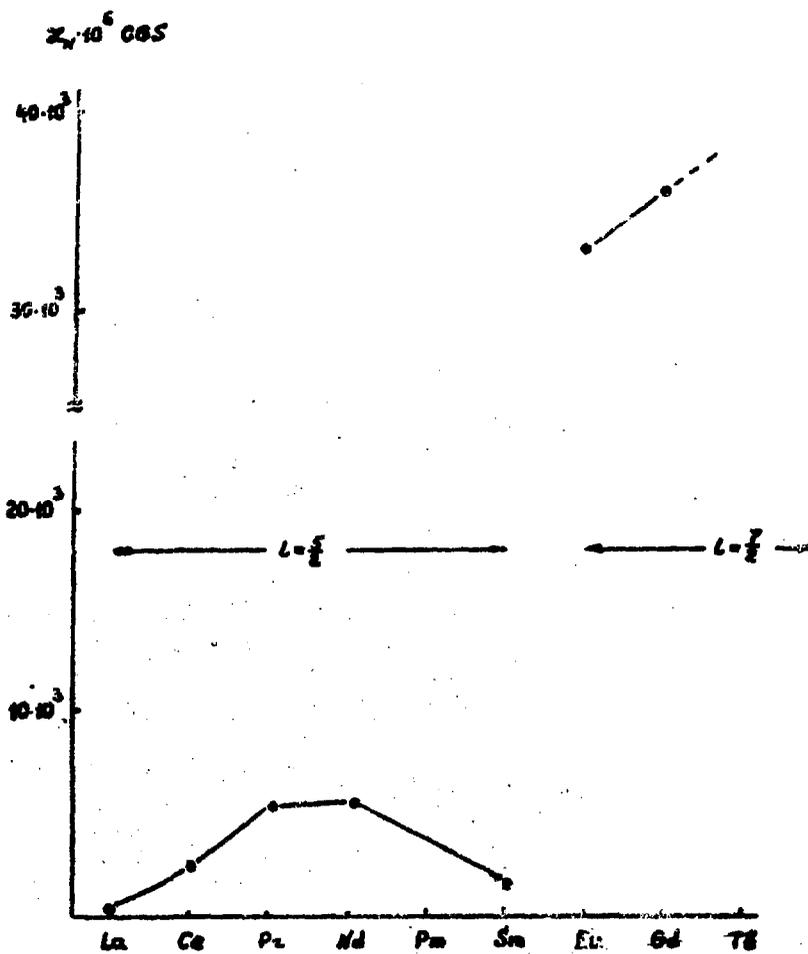


Fig. 6. Magnetic susceptibility of lanthanoids. The leapwise change of magnetic properties between  $L_{\lambda} = 5/2$  and  $L_{\lambda} = 7/2$  multiplets is evident.

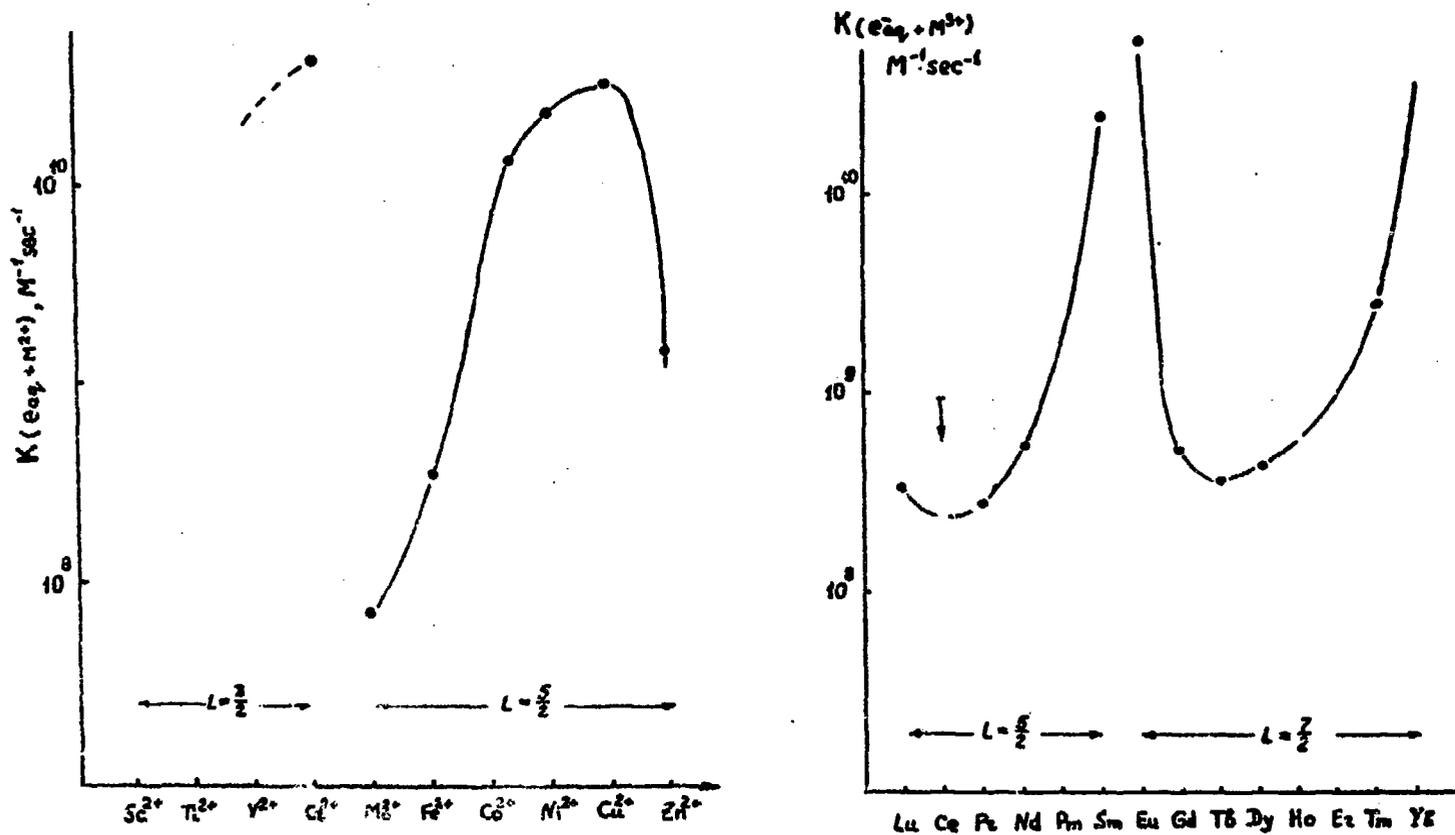


Fig.7. Rate constants of reactions of a hydrated electron with complex ions  $Me(H_2O)_6^{2+}$  of transition metals ( $\lambda = 2$ ) and lanthanoids ( $\lambda = 3, Me(H_2O)_9^{3+}$ ). Grouping of elements into  $(\lambda, l_\lambda)$ -multiplets is seen to be supported by chemical as well as physical properties of elements.

## References

1. Byakov V.M., Kulakov V.I., Rumer Y.B., Fet A.F. Group-theoretical Classification of Chemical Elements. I. Physical Foundations. M., Preprint ITEP, 1977, N 26.
2. Byakov V.M., Kulakov V.I., Rumer Y.B., Fet A.F. Group-theoretical Classification of Chemical Elements. II. Description of Applied Groups. M., Preprint ITEP, 1976, N 90.
3. Rumer V.B., Fet A.I. Teor. i Mat. Fiz., 1971, 9, p.203.
4. Fet A.I. Pisma v JETP . 1974, 20, p.24.
5. Fet A.I. Teor. i Mat. Fiz., 1975, 22, p.323.
6. Landau L.D., Lifshits E.M. Quantum Mechanics. M., "Nauka", 1974.
7. Haisinsky M. In "Centenary of Periodical Law of Chemical Elements". M., "Nauka", 1969, p.68.
8. Seaborg C. Ibid., p.21.
9. Energies of Chemical Bonds. Ionisation Potentials and Electron Affinity (V.N.Kondrajev, Ed.), M., "Nauka", 1974.
10. Physico-Chemical Properties of Elements (G.V.Samsonov, , Kiev, "Naukova Dumka", 1965.



**Индекс 3624**