ON REACTIVITY OF CHEMICAL ELEMENTS

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Abstract

In this paper, data on the electron configuration of atoms was used to predict the reactivity of chemical elements belonging to different blocks, S, P, D, F and DF. The study of elements of S-block and some elements of P- and D-blocks showed that the total amount (TA) of outer electrons usually correspond to maximum number of reactive valent electrons. Exceptions to this rule are described. The phenomenon of passivity of paired s-electrons for higher p- and d-elements was discussed. The relationship between total amount of outer electrons and average number of reactive electrons for the elements of D8–D12 groups was calculated. In addition, the specific electron structure was studied to predict the reactivity of lanthanides and actinides belonging to F-and DF-blocks.

Keywords: Chemical elements, Electron configuration, Total amount of outer electrons, Reactive electrons, Chemical properties, Reactivity, Discussion

INTRODUCTION

As is known, the chemical properties of an element are depended on electron structure of last energy level or outer electron shell of atom [1]. During chemical reactions, the nuclei of atoms remain unchanged, and only the structure of the electron shells changes due to the redistribution of electrons between the atoms. The ability of atoms to donate or attach electrons determines its chemical properties. The electron has a dual wave-particle nature. Due to the wave properties, electrons in an atom can have well-defined energy values, which depend on the distance to the nucleus.

The state of each electron in an atom is usually described with the help of four quantum numbers [2]: principal (n), orbital (l), magnetic (m) and spin (s). The first three characterize the movement of an electron in space, and the fourth around its own axis. The principal quantum number (n) determines the energy level of electrons, as well as the distance from the nucleus and size of the electron cloud. It takes integer values (n = 1, 2, 3, etc.) and corresponds to the period number in table of elements.

Electrons with similar energy values form an energy level corresponding to principal quantum number, **n** (1, 2 , 3, etc.). Each **n**-level contains a strictly defined number of electrons (N), maximum of $N=2n^2$. Besides, energy levels are subdivided into s-, p-, d- and f- sublevels (electron orbitals); where, number of these orbitals on the **n**-level is equal to principal quantum number, **n**.

The orbital quantum number (l) characterizes the geometric shape of the orbitals. It accepts integers from 0 to (n - 1). Each value of the orbital quantum number corresponds to a special form orbital. A set of orbitals with the same **n**-value is called the energy level, with can have a different l-sublevels. At the first energy level (n = 1), the orbital quantum number takes a single value, l = 0. Thus, on the first energy level, is only one sublevel, 1s, having orbital of spherical form. On the second energy level (n = 2), the orbital quantum number can take on two values: l = 0, 2s-orbital, a sphere larger than 1s-orbital; and l = 1, 2p-orbital of dumbbell form. On the third energy level (n = 3), the orbital quantum number takes three values: l = 0, 3s-spherical orbital; l = 1, 3p-orbital -

a dumbbell of a larger size than 2p-orbital; and l = 2, 3d, is a complex orbital. On the fourth energy level (n = 4), four orbitals may be present, 4s, 4p, 4d and 4f.

The magnetic quantum number (m) characterizes the position of the electronic orbital in space and takes integer values from -l to + l, including 0. This means that for each form of orbitals there are m = (2l + 1) energetically equivalent orientations in space. For the s-orbital, l = 0 that corresponds to m = 0; this position is one (sphere) because the sphere cannot have different orientations in space. For the p-orbitals (l = 1), three equivalent orientations in the space exist (m= 3) -1, 0 and +1. For d-orbitals (l = 2), five equivalent orientations in space exist (m = 5) -2, -1, 0, +1 and +2, whole for f=orbital (l=3), seven equivalent orientations in space exist. Thus, the s-sublevel can have one s-orbital, while the p-sublevel can have three p-orbitals, the d-sublevel – five d-orbitals and the f-sublevel - 7 f-orbitals. Since each orbital can contain a maximum of two electrons, the maximum number of electrons on single s-orbital is 2, on three p-orbitals is 6, of five d-orbitals is 10, and on seven f-orbitals is 14.

The spin quantum number characterizes the magnetic moment arising when the electron rotates around its axis. Accepts only two values +1/2 and –1/2 corresponding to opposite directions of rotation.

The filling of orbitals with electrons obeys the following principles [3]:

1. When filling the electron orbitals, the Pauli principle is fulfilled, the consequence of which is that the energy level **n** can contain no more than $2n^2$ electrons located on the sublevels (orbitals).
2. Filling occurs starting with the minimum principal quantum number **n**=1
3. Inside the level having the principal quantum number n, the s-orbital is filled first, then the other orbitals
4. Within the one sublevel (orbital), electrons are arranged in such a way that their total spin is maximum, i.e. the orbital should contain the largest number of unpaired electrons (the Hund rule).
5. According to Madelung –Janet- Klechkowski rule, the filling of orbitals occurs so that (n + l) would be minimal. For a given value (n + l), the orbital with a smaller n has the lowest energy.

As a result, the filling order of orbitals will be the following:

1s; 2s, 2p; 3s, 3p; 4s, 3d, 4p; 5s, 4d, 5p; 6s, 4f, 5d, 6p; 7s, 5f, 6d, 7p; etc.

However, the further research revealed some additional rules that need to be considered in the case of transition metals. For example, if an element has a configuration of outer shell $(n-1)d^c$, ns^2 ($c<10$), then one electron can jump from s to d orbital. Similar additional rule apples also in the case of some lanthanides and actinides, when one electron jumps from $(n-2)f^k$ to $(n-1)d^c$ orbital.

The main purpose of this paper was to use the electron configuration of elements to predict their reactivity.

ELECTRON CONFIGURATION AND REACTIVITY

The data on electron configuration and filling order of orbitals [3, 4], along with block classification [5, 6], make it possible to subdivide all chemical elements into S-, P-, D, F- and DF-blocks, depending on the presence of the last filled orbital, s, p, d, f or df (Table 1).

Table1. Electron configuration (EC) of outer shell, last filled orbital (LFO) and total amount of outer electrons (TA) for elements belonging to different blocks

Block	EC	LFO	TA
S & s	ns^a	s	a
P	ns^a .. np^b	p	a + b
D	ns^a $(n-1)d^c$	d	a + c
F	ns^a $(n-2)f^k$	f	a + k
DF	ns^a $(n-2)f^k$ $(n-1)d^c$	d-f	a + c + k

Some lanthanides and actinides were allocated to a special DF-block for the following reason. Although the filling shells with electrons ends by d-orbital, unlike the d-elements, the df-elements have an incompletely filled (n-2)f-orbital. This leads to significant differences in the properties of df- elements from both d- and f-elements.

Using the block classification of chemical elements, the updated version of periodic table has been proposed (Figure 1). This table have the following specific features:

- The first period contains two elements, H and He, belonging to groups s1 and s2; moreover, the amount of s-electrons of these elements corresponds to TA numbering of the groups, 1 and 2, respectively.
- In the left side of the table there are groups of elements of S-block, and in the right side groups of elements of P-block; the elements of D-block are located in the middle, whereas the elements belonging to F- and DF-blocks at the bottom of the table.
- The TA-numbering (1 to 8) of such groups of elements as s1, s2, S1, S2 and P3 to P8 indicates the total amount of outer s- and p-electrons of these elements (see Table 1). Since s1- and S1-groups contain one outer s-electron, and other S- and P-groups contain two outer s-electrons, the difference between TA and amount of outer s-electrons (SA) gives the amount of outer p-electrons.
- The TA-numbering of groups of elements belonging to D-, F- and DF-blocks indicates the total amount of outer electrons of these elements (see Table 1). As is known, Pd has zero amount of outer s-electrons, i.e. SA=0, whereas Nb, Cr, Mo, Ru, Rh, Pt and all elements of D11-group have SA=1. Other elements of D-, F- and DF-groups have SA=2. Considering this fact, one can calculate the amount of outer d- or f-, or the sum of d and f-electrons, as the difference between TA and SA.
- DF-block includes some actinides and lanthanides having both d-and f- electrons on the outer shells.
- Some researchers consider that elements of the D12 group do not refer to transition metals, since they have a completely filled 10-electron d-orbital. However, although elements of the D11-group also have 10 electrons on the d-orbital, they are attributed to transition metals. Regardless of whether the elements of 12 column are transition, post-transition metals or main elements, they can be uniquely attributed to D-block, since these elements has d-orbital, though filled.
- Each group comprises elements with similar chemical properties.
- The number of periods (from 1 to 7) corresponds to the principal quantum number (n). Each period of this table begins with hydrogen (first period) or with alkali metal having one outer s-electron, and ends with noble gas having a completely filled outer electron shell. Thus, after the transition from one period to another is a cyclic or periodic variation of the properties of elements.

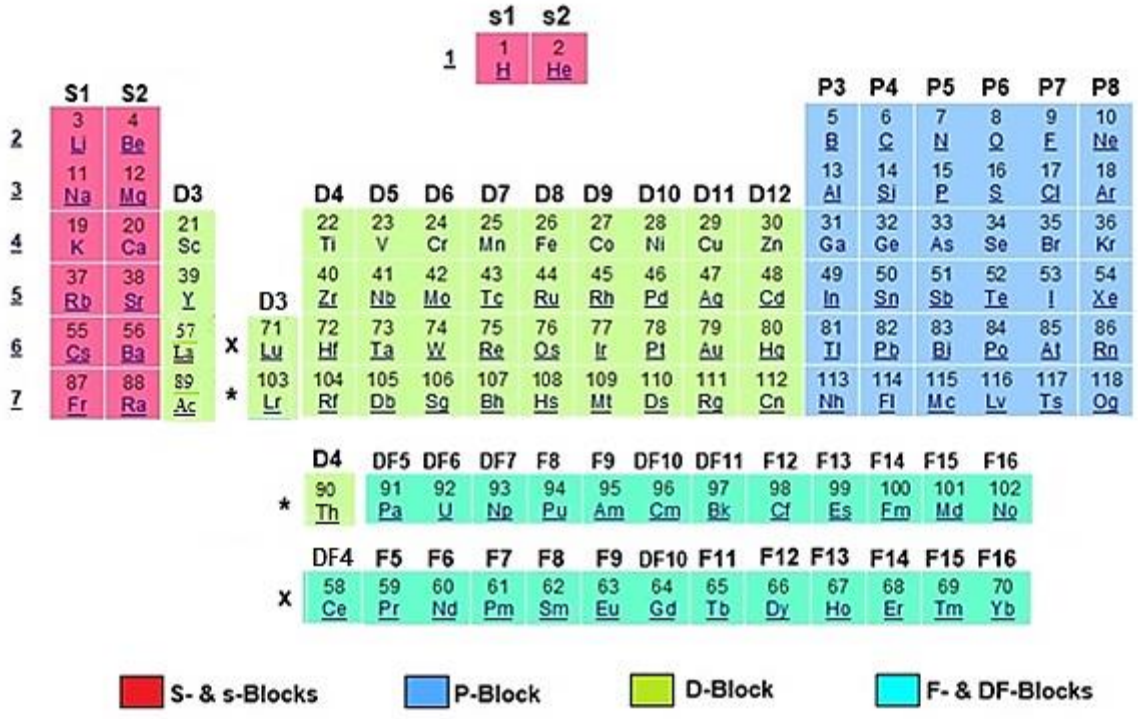

Figure 1. The updated version of periodic table with highlighted elements of different blocks

The advantage of such block table is that it allows to characterize the chemical properties of various elements. Firstly, it is clear that elements of s1, s2, S1 and S2 groups contain one or two of outermost s-electrons. It is also clear that elements of P_{TA} groups contain outer p- and s-electrons, the sum of which denote numbering of the group, TA. Moreover, except for some noble gases, the outer s- and/or p-electrons are valent electrons. Thus, hydrogen and elements of S1 and S2 groups can form mono- or bivalent compounds, respectively, e.g. HCl, LiCl, $CaCl_2$.

The elements of P3-P7 groups located in periods of 2 to 6 can donate the TA number (3 to 7) of p- and s-electrons, respectively, with the exception of fluorine and oxygen that do not possess electron donor properties. For example, the element of P5 group, phosphorus, containing two s- and three p- electrons on the outer shell can form pentavalent compounds, e.g. higher oxide, P_2O_5. On the other hand, if the p-element plays as electron acceptors, it can attach $N_a = (8\text{-TA})$ electrons, as for example, in the case of phosphine, PH_3.

Regarding the noble gases from the P8 group, it is known that they contain a stable completely filled outer shell built from two ns-electrons and six np-electrons, along with ten (n-1)d-electrons and fourteen (n-2)f-electrons for gases from periods 4 to 7. Despite such electron structure, there is evidence that some noble gases are not completely inert and can interact with strong oxidizing agents [7]. For example, xenon is oxidized by fluorine; and as a result, various fluorides, XeF_2, XeF_4 and XeF_6, were synthesized with the participation of outermost p-electrons of Xe. In addition, oxides of Xe were obtained, including the octavalent oxide, XeO_4, with the participation of all eight outer p-and s-electrons of Xe. Besides, diverse oxy-fluorides of Xe are known. Some other noble gases, such as krypton and radon, can also be oxidized by fluorine.

It is necessary to pay a special attention to p-elements with atomic numbers Z from 113 to 118, located in the 7th period. The peculiarity of their chemical properties is associated with the phenomenon of passivity of paired s-electrons [8]. The consequence of this phenomenon is that only the outer p-electrons of these elements are sufficient reactive to participate in chemical

reactions. Since the number of inactive s-electrons is 2, of the maximum number of reactive p-electrons can be found from the difference $N_r = (TA - 2)$.

When studying the chemical properties of metallic elements of D3-D7 groups, it can be concluded that TA numbering of the group corresponds to maximum number of all reactive d- and s-electrons or maximum valence of elements. For example, the element Sc from D3 group has three outer electrons, one d-electron and two s-electrons, and all these electrons are reactive. Consequently, Sc can form trivalent compounds, e.g. halides ScX_3. Another example is the element Re from D3 group, having seven outer electrons, which can form compounds with maximum valence of 7, e.g. higher oxide, Re_2O_7.

However, for groups D8 to D12, TA numbering, expressing the total amount of all external electrons, differs significantly from the maximum number of reactive electrons. Nevertheless, the relationship between total amount of outer electrons (TA) and average number of reactive electrons, N_r, for the elements of these groups can be calculated with deviation ±0.5 using the following correlation equation:

$N_r = 18.8 - 1.4TA.$

Although for elements belonging to D8, D9 and D10 groups the total number of outer electrons is 8 to 10, in fact only two elements, Ru and Os, really capable of forming stable octavalent compounds, such as MeO4. It has been also reported that iridium may have the highest oxidation state (+9) of all known elements [9]. However, this oxidation state was found for only one $[IrO_4]^+$ - cation under extreme conditions using supersonic laser evaporation of a metallic iridium target in a gas atmosphere of argon or helium containing a small amount of oxygen [10]. But, under normal conditions this cation does not exist, and therefore it cannot be isolated in the form of salt.

It should be noted that the completely filling of d-orbital does not guarantee its passivity. For example, the outer 10-eletron d-orbital, $(n-1)d^{10}$, of Pd and all elements of D11-group is a donor of d-electrons; as a result, these elements can form compounds (e.g. PdF_4, AuF, etc.) with the participation of d-electrons. As is known, the elements of D12-group also have the outer 10-eletron d-orbital, ns^2 $(n-1)d^{10}$; therefore, it is possible that the two reactive electrons of the elements of this group are d-electrons, and not s-electrons.

The F- and DF-groups comprising thirteen lanthanides can contain two 6s-electrons and 1 to 14 4f–electrons [11]. Besides the elements of DF-group contain additionally one 5d-electon. The data on the reactivity of lanthanides reveal that the maximum number of reactive electrons (N_r) varies from 3 and 4 independently on the total amount of outer electrons. For elements of F-groups, two 6s-electrons and one to two 4f-electrons participate in chemical reactions, while for elements of DF-groups (e.g. Ce), two 6s-electrons, one 4f-electron and one 5d-electron can be reactive. The remaining 4f-electrons of lanthanides are inactive.

A completely different result was obtained, when twelve actinides belonging to F- and DF-groups were studied [12]. As the total amount of outer electrons (TA) increases from 5 to 7, a proportional growth in number of reactive electrons (N_r) is observed at first, after which N_r drops to 3 (Figure 2). Thus, for actinides having TA from 5 to 7, all 7s- and 5f-electrons (along with one 6d-electron for df-elements) are reactive. Then, the number of reactive 5f-electrons decreases, and for actinides having TA from 10 to 16, only 1 to 3 5f-electrons are able to participate in chemical reactions. Actinide nobelium, for example, has 14 5f-electons, of which only one is reactive, while the remaining 13 5f-electrons are inactive.

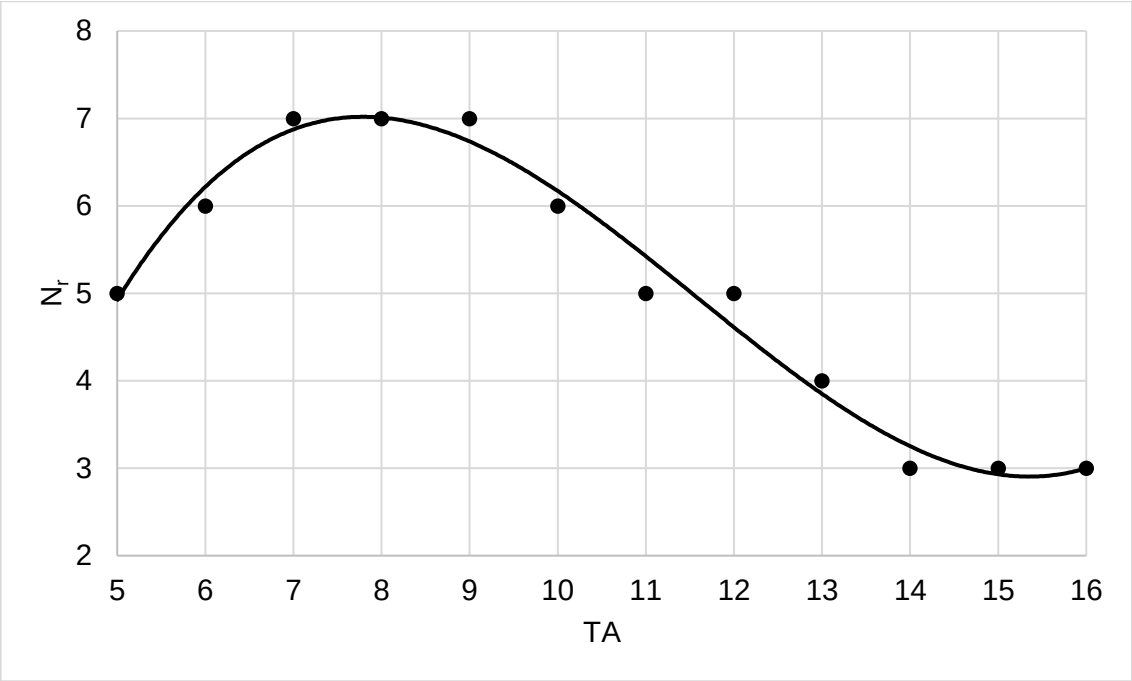

Figure 2. Dependence of number of reactive electrons on total amount of outer electrons of actinides

CONCLUSIONS

In this paper, data on the electron configuration of atoms was used to predict the reactivity of chemical elements belonging to different blocks, S, P, D, F and DF. The study of the number of reactive electrons that can participate in chemical reactions led to the following conclusions:

1). **Reactivity of s-electrons**

One $1s^1$ electron of hydrogen and all ns-electrons of elements belonging to groups S1, S2, D, F and DF, as well as ns-electrons of the most elements of P-groups, are reactive. In addition, the ns^2-electrons of Xe, and may be of Kr and Rn, also are reactive. The exception is inactive ns^2-electrons of such noble gases as He, Ne and Ar. Besides, the paired $7s^2$-electrons of P-elements with atomic numbers Z from 113 to 118 are inactive.

2). **Reactivity of p-electrons**

All p-electrons of elements belonging to P3-P7 groups are reactive. Besides, the p-electrons of Xe are reactive, while the p-electrons of Ne and Ar are inactive.

3). **Reactivity of d-electrons**

For elements belonging to D3-D7 groups, all d-electrons are reactive.

However, the elements belonging to D8-D11 groups show the following specific features. Increasing the total amount of all outer electrons (TA) or the average number of all d-electrons (DA) in the group reduces the average number of reactive d-electrons ($ND_{r,av}$) from 6 to 2. This behavior can be described by equations:

$ND_{r,av} = 14 - TA$ and $ND_{r,av} = 12 - DA$

4). **Reactivity of f-electrons of lanthanides**

Thirteen lanthanides can contain 1 to 14 4f–electrons. The data on the reactivity of lanthanides reveal that the number of 4f-reactive electrons (ND_r) can be from 2 to 1. Moreover, with an increase in the total amount of f-electrons (TF) of lanthanides, there is a tendency to decrease in the number of reactive f-electrons from 2 to 1 in accordance with the following equation:

$ND_r = 2.3 - 0.08TF.$

The remaining 4f-electrons of lanthanides are inactive.

5). **Reactivity of f-electrons of actinides**

Twelve actinides can contain 2 to 14 5f–electrons. In the series of first five actinides, the number of 5f-reactive electrons (ND_r) increases from 2 to 5. Then, when total amount of f-electrons exceeds six (TF > 6), the ND_r decreases from 5 to 1, according to equation:

$ND_r = 8 - 0.5\ TF.$

The remaining 5f-electrons of actinides are inactive.

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