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A magic trick for determination of ground state term of s , p & d -orbital electrons

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ABSTRACT

The term symbol is a shortened depiction of the total angular momentum quantum numbers in a multi-electron atom in quantum mechanics. Besides, a term symbol can also describe even a single electron. Both the electronic configuration and term symbol of an atom illustrate each energy level of an atom because the energy level also alters with the change in the total angular momentum and spin. L-S coupling (also well-known as Russell-Saunders coupling) is understood by the traditional atomic term symbols. Among many term symbols, the most stable i.e. ground state symbol is predicted with the help of Hund's rule. The present paper describes an interesting activity and deals with the new and easy trick to be used for writing a ground state term symbol of an electron present in any one of the s , p & d -orbital electrons. Besides, this trick also facilitates active learning in classrooms. Moreover, it is also very useful for the fast calculation of spin multiplicity and the total angular momentum of f -orbital electrons. Besides, it may also be useful in the future for the fast calculation of spin multiplicity and the total angular momentum of g -orbital electrons.

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Capsule Summary: A magic trick for determination of ground state term of s , p & d -orbital electrons was used to calculate spin multiplicity and the total angular momentum of f -orbital electrons. Besides, it may also be useful for the fast calculation of spin multiplicity and the total angular momentum of g -orbital electrons.

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INTRODUCTION

There are many term symbols for an electronic configuration because of many microstates. The main thing to be kept in mind is that only one term symbol is written for the ground state of the given element. This term symbol is called the ground state term (GST) symbol. The compound systems such as atomic nuclei, or mesons or molecules are described by term symbol. For molecules, the component of orbital angular momenta is designated by Greek letters to designate. Every energy level is determined by a definite term. This determination is totally based on an

empirical observation also known as Rydberg-Ritz combination principle. According to this principle, the wavenumbers of lines obtained in the spectrum can be stated as the distinction of 2 terms (Atkins et al., 2006). After that, the Bohr model summarized it again by multiplying hc , with both the spectral wavenumbers and quantized energy levels.

It should be noted that the same term symbol (for each column in the s -block and p -block elements) is acquired by neutral atoms of the chemical elements. On the other hand, d -block and f -block elements do not do so, and the term symbol differs with the change in ground state

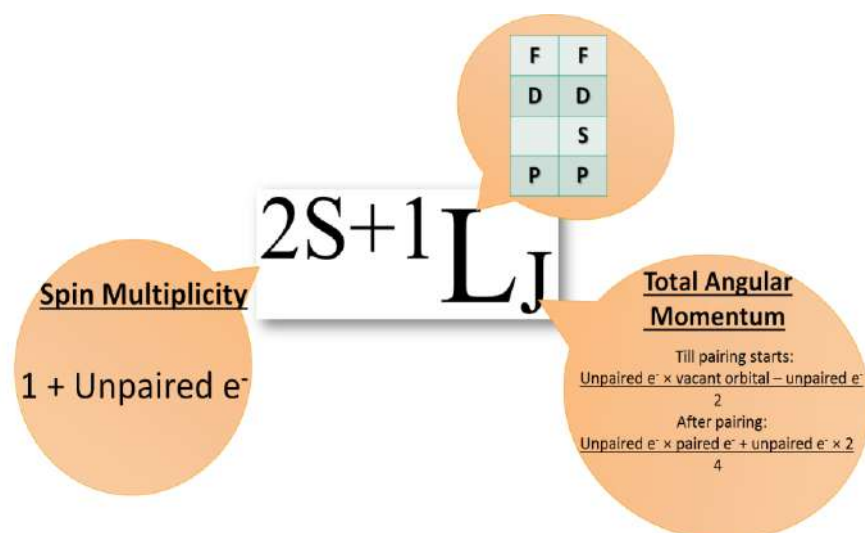


Fig. 1: Trick for getting ground state term.

electronic configuration. The GST symbol is written with the help of $2S+1L_J$ which involves following terms.

Spin multiplicity ($2S+1$)

The spin multiplicity (calculated as ' $2S+1$ ') is written on the upper left side of the GST. The spin multiplicity is used to resolve of the number of probable angles of the spin angular momentum equivalent to a given total spin quantum number (S), for the identical spatial electronic wave-function. Singlet multiplicity is determined with $S=0$ and $2S+1 = 1$. On the other hand, doublet multiplicity is determined with $S=1/2$ and $2S+1 = 2$, etc (Verhoeven, 1996). For spin multiplicity calculation, there are some steps which are as follows:

- i. The spins of all electrons filled in orbitals are added.
- ii. After addition, obtained units are doubled.
- iii. In the last, 1 more digit is also added to the unit obtained in the second step to gain spin multiplicity.

Hence, the calculation for spin multiplicity is time-consuming in comparison to the trick given in the present paper.

Resultant orbital angular momentum (L)

The specific orbital angular momenta of electrons, ' l_i ', each of which may be 0, 1, 2, 3, 4in units of $h/2\pi$ for s, p, d, f, g.....orbitals individually, mix to give a resultant orbital angular momentum, L in units of $h/2\pi$. Like spin multiplicity calculation, orbital angular momentum calculation also involves the following steps:

- i. All the values of orbital angular momentum for each orbital filled with electrons are added.
- ii. After addition, the obtained unit determines the exact value of resultant orbital angular momentum as

we know that $L=0$ for S; $L=1$ for P; $L=2$ for D and so on.

Hence, the calculation for resultant orbital angular momentum is also time-consuming in comparison to the trick given in the present paper.

Total angular momentum (J)

The sum of the total spin angular momentum vector, S and the total orbital angular momentum vector, L determines the total angular momentum, ' J ' which is the best to be used to know where we are in the periodic table (Ali et al., 2017). The coupling of S and L is also known as Russell and Saunders coupling (Russell and Saunders, 1925). The consequence of these vector sums is listed in a code that is called a Russell-Saunders term symbol as shown in Eq. 1.

$$J = L + S, L + S - 1, L + S - 2, L + S - 3, \dots, |L - S| \quad (1)$$

The symbol $||$ indicates that the absolute value ($L - S$) is employed, i.e., no regard is paid to \pm sign. Thus, for $L = 2$ and $S = 1$, the possible J states are 3, 2 and 1 in units of $h/2\pi$.

Hence, for total angular momentum calculation, the following steps are involved which are as follows:

- i. Three steps for calculation of spin multiplicity as described above.
- ii. Two steps for calculation of orbital angular momentum as described above.
- iii. Coupling of spin angular momentum vector, S and the total orbital angular momentum vector, L .

Now, we can say that unlike spin multiplicity ($2S+1$) and resultant orbital angular momentum, L the calculation for total angular momentum is not as easy as it is thought. i.e. it is typical and takes more time as compared to the trick given in this paper.

F	F
D	D
	S
P	P

Fig. 2: Boxes with definite values to find resultant orbital angular momentum.

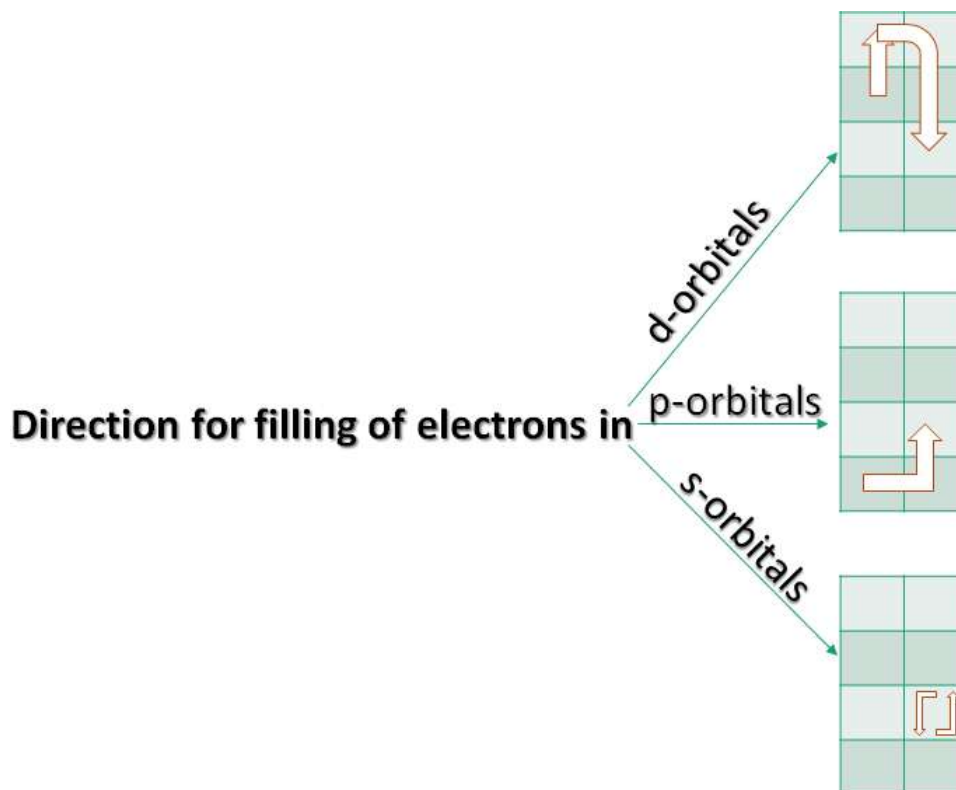


Fig. 3: Pattern of filling electrons in boxes.

Rules to find ground state term symbol

The term symbol for the ground state of an atom is calculated with the help of Hund's rules (Engel and Reid, 2006; Herzberg, 1944; Miessler and Tarr, 1999). The rules governing the term symbol for the ground state according to the L-S coupling scheme are given below:

- The spin multiplicity is maximized i.e., the electrons occupy degenerate orbitals to retain parallel spins as long as possible (Hund's rule).
- The orbital angular momentum is also maximized i.e., the orbitals are filled with the highest positive 'm' values first.

- If the sub-shell is less than half-filled, $J = L - S$ and if the sub-shell is more than half-filled, $J = L + S$.

An alternative method using group theory

Besides Hund's rule, another method utilized to find the GST was group theory (McDaniel, 1977). Having read this method, we observed that this method was too difficult to be understood. Besides, this method was also very time consuming especially for those whose background is not quantum chemistry.

A simple trick for resolving of GST

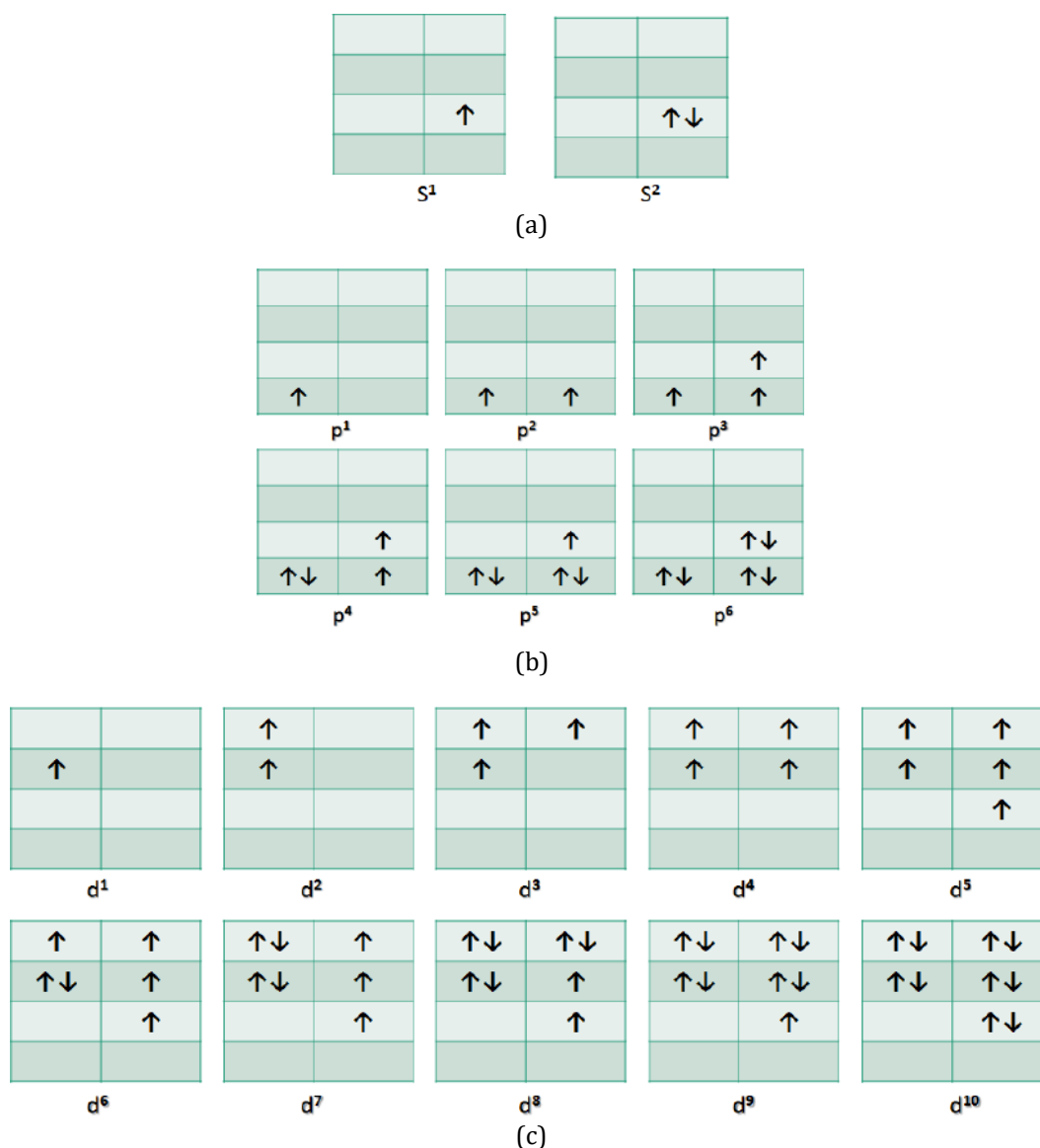


Fig. 4: Electrons filling pattern in boxes for (a) *s*-orbitals, (b) *p*-orbitals and (c) *d*-orbitals.

Having noticed the difficulties in the calculation, we gave an easy and simple trick (Fig. 1) to find the GST. This trick is based on time-consuming faults present in the methods described before. Besides, this trick may also be used to find spin multiplicity and total angular momentum of the electron present in 'g-orbitals' which are yet to be discovered. Hence, this is an easy, useful and acceptable modified short trick to find the GST easily. The salient features of this trick are as below:

Spin multiplicity ($2S+1$)

For spin multiplicity calculation, we had to follow all steps described above, but now no need to follow those steps if we are using the trick given in (Fig. 1). We have to count up

only the number of unpaired electrons to find spin multiplicity (Table 1).

Total angular momentum (*J*)

For total angular momentum, *J* of *s*, *p*, *d* and *f*-orbital electrons, we had to read and remember the whole section described above, but now no need to remember that section to find out total angular momentum. We have to remember only one trick presented in (Fig. 1). Besides, we must look at the number of paired electrons, unpaired electrons and vacant orbital for total angular momentum calculation. The most interesting point is that everybody knows how to fill electrons and how to count the paired and unpaired electrons, since the starting of chemistry basics.

Table 1: Trick calculated spin multiplicity and total angular momentum

Orbitals	Electrons	Unpaired electrons	Paired electrons	Vacant orbitals	Trick calculated Value of $2S + 1$	Trick calculated Value* of J
s	s^1	1	0	0	2	1/2
	s^2	0	2	0	1	0
p	p^1	1	0	2	2	1/2
	p^2	2	0	1	3	0
	p^3	3	0	0	4	3/2
	p^4	2	2	0	3	2
	p^5	1	4	0	2	3/2
	p^6	0	6	0	1	0
d	d^1	1	0	4	2	3/2
	d^2	2	0	3	3	2
	d^3	3	0	2	4	3/2
	d^4	4	0	1	7	0
	d^5	5	0	0	6	5/2
	d^6	4	2	0	5	4
	d^7	3	4	0	4	9/2
	d^8	2	6	0	3	4
	d^9	1	8	0	2	5/2
	d^{10}	0	10	0	1	0
f	f^1	1	0	6	2	5/2
	f^2	2	0	5	3	4
	f^3	3	0	4	4	9/2
	f^4	4	0	3	5	4
	f^5	5	0	2	6	5/2
	f^6	6	0	1	7	0
	f^7	7	0	0	8	7/2
	f^8	6	2	0	7	6
	f^9	5	4	0	6	15/2
	f^{10}	4	6	0	5	8
	f^{11}	3	8	0	4	15/2
	f^{12}	2	10	0	3	6
	f^{13}	1	12	0	2	7/2
	f^{14}	0	14	0	1	0

*All the values of J will always be considered with positive sign even if they are negative.

Resultant orbital angular momentum (L)

For resultant orbital angular momentum of s , p & d -orbital electrons, we had to follow all steps described above, but now no need to follow those steps if we are using the trick given above to get resultant orbital angular momentum because two things which will give the exact value of resultant orbital angular momentum are (i) two columns of four boxes having a definite value each (Fig. 2) and (ii) pattern of filling of electrons in these boxes for given orbitals (Fig. 3 and 4). Hence, no need to remember orbital angular momentum values of s , p & d -orbitals. The most important, easy and interesting point is that you have to start electron filling from that box which has the same alphabet having similarity with the orbital name. For instance, suppose if we are given d -orbital electrons to find the value of resultant orbital angular momentum, then we

have to start electrons filling where 'D' is written first from; according to arrow notation given in (Fig. 3). In the same way, if we are given p -orbital electrons to find the value of resultant orbital angular momentum, then we have to start electrons filling where 'P' is written first from; according to arrow notation given in (Fig. 3), and so on.

Electrons filling pattern in the boxes

Electrons would be filled in given boxes for a given orbital according to the pattern shown in (Fig. 4).

Future perspective

Having read research papers regarding the ground state term symbols of f -orbitals, we observed that a trick for spin multiplicity and total angular momentum of f -orbital

electrons filled orbitals is easy to be given (Table 1), but the trick for resultant orbital angular momentum (L) for *f*-orbital electrons is too difficult to be given because many *f*-block elements show ambiguities in electronic configuration. Therefore, we gave this trick for the term symbol of electrons filled in orbital; not for the elements showing ambiguities in electronic configuration, because all calculations in this trick are based on the number of paired and unpaired electrons, not on the nature of elements. For instance, Chromium (${}_{24}\text{Cr}$) should have d^4 electronic configuration but it has d^5 electronic configuration, so this trick is applicable only for d^5 not for chromium (${}_{24}\text{Cr}$). Consequently, a trick-based calculation for the resultant orbital angular momentum (L) of *f*-orbitals electrons may also be given in the future as we did in the present paper.

CONCLUSIONS

The presented short trick has also established the correct values of the ground state term symbol for the electrons present in *s*, *p* & *d*-orbitals, spin multiplicity ($2S+1$) and total angular momentum (J) for *f*-orbital electrons. The presented trick for calculation of ground-state term symbol of the elements may also be applicable and useful to the scientific community whenever '*g*-block elements' would be discovered in the future. Moreover, this trick also saves time, and we may also calculate spin multiplicity and total angular momentum for '*g*-orbitals' in the future using this short trick. Additionally, it can also be used by the students working on quantum chemistry. Besides, the proposed trick will be useful in the learning process because it is very fast and time-saving.

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