In this section of Resonance, we invite readers to pose questions likely to be raised in a classroom situation. We may suggest strategies for dealing with them, or invite responses, or both. “Classroom” is equally a forum for raising broader issues and sharing personal experiences and viewpoints on matters related to teaching and learning science.

Young-tableaux: A Tetris-Brick Game for Getting Atomic Term Symbols*

Getting all the possible term symbols for a given electronic configuration by listing all the microstates is a very tiring and at times, boring job. In the present article, group theory has been used to construct the atomic term symbols under the $LS$ coupling scheme. It is shown that with the use of Young-tableau, getting term symbols become a Tetris brick game, where one needs to add boxes of right shapes to get term-symbols.

Introduction

In most of the standard physical chemistry textbooks, atomic term symbols are deduced by tabulating the microstates associated with the corresponding electronic configuration (Box 1). This enumeration is a straightforward but mostly a tedious job, especially as the angular momentum and the number of unpaired electrons of the electronic configuration increase.

A different and quick approach to get all possible term-symbols is by using group theory. Besides being more elegant than enumer-

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Box 1. Counting the Microstates

Given $N$ degenerate atomic orbitals (for $d$, it is 5; for $p$, it is 3, etc.) and $k$ electrons, there are $2^NC_k$ ways electrons can be filled in $N$ orbitals without violating Pauli principle. Each unique electronic configuration among $2^NC_k$ configurations is known as a microstate.

Unfortunately, permutation as well as continuous group, both are not a part of even specialized group theory courses in chemistry. If a student understands the importance of the symmetry in defining atomic state, they can easily generalize it to other cases, where symmetry is the only way to define the spectroscopic state. One problem in introducing the group theoretical technique for getting atomic term symbol in chemistry class is, it requires a good knowledge of permutation as well as continuous groups. Unfortunately, both are not a part of even specialized group theory courses in chemistry. Consequently, this method is usually not discussed in chemistry classes even at the Master’s level. Therefore, it is highly desirable to deduce term symbols using group theory in such a way that students understand the importance of symmetry in defining the electronic state without being lost in the technicality of group theory. Author’s personal experience in class as an instructor is that it can be done using the Young-tableau (Box 2) representation of permutation groups.

Box 2. Young tableaux

A Young diagram is a finite collection of boxes arranged in left-justified rows, with the row sizes not increasing. It is closely related to the partition of numbers. If one partition number $n$ in terms of integers say $\lambda_1, \lambda_2, \lambda_3 \cdots \lambda_n$ such that $\lambda_1 \geq \lambda_2 \geq \lambda_3 \cdots \geq \lambda_n$ and they satisfy $\lambda_1 + \lambda_2 + \cdots = n$, then Young diagram associated to the partition $n$ will have $\lambda_1$ boxes in the first row, $\lambda_2$ boxes in the second row and so on. A Young-tableau is obtained by filling the boxes of a Young diagram with numbers. In the present article, a notation $[\lambda_1, \lambda_2, \lambda_3, \cdots]$ means $\lambda_1$ boxes in first row, $\lambda_2$ in second row, etc. Therefore, the horizontal bars means only single non-zero entry in notation i.e. [30], [40], [20], etc. A vertical bar means that all the entries in the notation is one i.e. [11], [111], [11111], etc.
We will show in the present article that if one uses Young-tableau representation of permutation groups, students just require a few geometrical rules to construct boxes and deduce atomic term-symbols.

For the illustration, we choose equivalent electrons in Russel–Saunders coupling scheme (Box 3).

**Box 3. Russel–Saunders Coupling**

In many-electron atoms, there are different ways to combine the angular momenta associated with the orbital and spin motions. In the Russel–Saunders scheme, one assumed that spin-spin and orbital-orbital interactions are much stronger than spin-orbit interactions. Therefore, first the spin and orbital parts were combined separately and then the resultant total spin and orbital angular momentum were combined. This is found to give a good approximation for first row transition series where, the spin-orbit coupling can generally be ignored.

Let us start with $p^2$ electronic configuration. A simple quantum mechanical addition rule for angular momentum (Box 4) will predict the possible orbital angular momentum to be 0, 1 and 2, which are usually represented by $S$, $P$ and $D$ symbols respectively.

**Box 4. Addition of Angular Momenta**

When two angular momenta $j_1$ and $j_2$ are added, the allowed values of $j$ corresponding to resultant angular quantum number is $j_1 + j_2$, $j_1 + j_2 - 1$, $j_1 + j_2 - 2$ ·······|$j_1 - j_2$|

Similarly, possible spin multiplicities will be 3 (triplet) and 1 (singlet). If one simply allows all the combinations of $\hat{S}$ and
\[ \hat{L}, \text{ the resulting terms will be } 1S, 3S, 1P, 3P, 1D \text{ and } 3D. \] A simple count of microstates can reveal the error in the method used. The total number of microstates from the above terms will be \[ 1 + 3 + 3 + 9 + 5 + 15 = 36, \] instead of 15 (according to \( 6C_2 \)). This error arises, as one cannot combine the spin and orbital angular momentum arbitrarily, one has to respect the Pauli exclusion principle. According to the exclusion principle, being fermions, the electronic states should be an antisymmetric wave-function (with the exchange of electrons, wavefunction changes its sign). The problem of getting the right term-symbol thus reduces to tagging different orbital and spin angular momentum wavefunctions with their symmetries and combining them in such a way that the resulting terms become consistent with the exclusion principle.

To illustrate the above point, let us reconsider the \( p^2 \) electronic configuration from the symmetry point of view. The resultant spin angular momentum for a two-electron system can be 0 (singlet) and 1 (triplet). It is known that in this case, odd (even) total spin angular momentum value corresponds to a symmetric (antisymmetric) wavefunction, whereas, for the orbital part, it is the opposite. Therefore, to make the whole wavefunction antisymmetric, the right combination will be \( 3P, 1S \) and \( 1D \). The case of two electrons is simple, since orbital as well as spin, both wavefunction are either totally symmetric or antisymmetric with respect to the permutation of electrons. This may not be the case for an electronic configuration consisting of more than two equivalent electrons. For example, for \( p^3 \) configuration, we can talk about symmetric or antisymmetric with respect to permutation of only, any two electrons among three. Consequently, we can expect three types of wavefunctions in this case; symmetric, antisymmetric and mixed-symmetric (Box 5). Symmetric means that wavefunction do not change sign for permutation of any two electrons among three, antisymmetric means that wavefunction always change sign no matter which two electrons you permute among three, and mixed-symmetry means that the wavefunction is symmetric for permutation of some two electrons among three and antisymmetric for some other two electrons among three.
Box 5. Pauli Exclusion Principle

Pauli exclusion principle demands that the overall wavefunction be antisymmetric with respect to the exchange of any two electrons. It does not mean that the components of wavefunction (here spin and orbit part) should also be antisymmetric. Therefore, spin and orbit part of wavefunction can be mixed-symmetric.

Now the question is, is there any easy way to know the symmetries of these wavefunctions and some rule to combine them in such a way that, the total wavefunction becomes antisymmetric? It is straightforward to combine totally symmetric and antisymmetric wavefunctions but combining mixed-symmetry wavefunctions require more work.

I hope the preceding para has convinced the readers that the problem of getting the right term symbol is closely linked to identifying the symmetries associated with the corresponding electronic configuration. It is known that all symmetry operations for a given symmetry of object, form a well-known mathematical structure known as ‘group’. Consequently, group theory is the mathematical language of symmetry. Therefore in science, whenever symmetry plays any role, group theory becomes helpful. (Reference [1] for a good introduction of group theory). Here also, group-theoretical tools become a natural choice to tag the spin as well as orbital wavefunction with right symmetry. Technically, one needs to use the permutation symmetry group for spin as well as orbital space function and then in this big permutation group search for those irreducible representations, which are antisymmetric. If we have to construct all the character tables explicitly, one cannot bypass the technicality of group-theory, but there is a way to do all this algebra using few rules to construct boxes.

This procedure has three steps:

1. Construct the Young diagram for spin-functions in such a way that we know the symmetries of different spin functions.
2. Identify the dual symmetry of the Young diagrams corresponding to the spin wavefunctions constructed in step one, so that combination of original and dual symmetry function can give desired antisymmetric wavefunction.

3. Identify those orbital-angular momentum wavefunctions, which are contained in this dual symmetry.

Let us do the first step for \( p^3 \) configuration. For three electrons, the Young diagram will consist of a total of three boxes. To construct them, the following rules will be used.

1. If the total number of boxes are \( n \) (which is here the total number of electrons), then possible Young diagrams will have, either \( n \) boxes in the first row; or \( n - 1 \) boxes in the first row and 1 box in the second row; \( \cdots \) so on till we get 1 column and \( n \) row.

2. If the number of objects to be filled in these boxes are \( m \) (in present case, these are two spins of an electron) then denote these \( m \) objects by number 1, 2, 3 \( \cdots \) \( m \) and fill these boxes in such a way that in row direction, number should not decrease (in row direction, next number should be greater than or equal to the preceding one), and in column direction, number should always increase.

Following above rules, total number of such possible boxes are shown in Figure 1.

**Figure 1.** Construction of Young-tableaux for spin with \( p^3 \) electronic configuration

\[
\begin{align*}
S &= \frac{3}{2} & S &= \frac{1}{2} \\
\frac{3}{2} &= 111 112 122 222 \\
\frac{1}{2} &= 11 12 22
\end{align*}
\]
In *Figure 1*, notation $[30]$ means 3 boxes in the first row and 0 in the second row. Similarly, $[21]$ means 2 boxes in the first row and 1 in the second row. One can see here, there is no vertical box, as it is impossible to fill a vertical box of three rows with number 1 and 2 in such a way that the number always increases. If we fill $[30]$ box with all the permutations of 1 and 2 in such way that number should not decrease, we will get 4 such boxes, similarly for $[21]$ box, one will get 2 such boxes. By correlating this number with spin multiplicities, one can see that $[30]$ represents the spin $\frac{3}{2}$ state, whereas $[21]$ represents the spin $\frac{1}{2}$ state. Here, we represented the spin wave-functions in terms of Young-tableaux.

The horizontal bar represents symmetric functions, while the vertical box represents antisymmetric functions. Therefore, $[30]$ is completely symmetric, whereas, $[21]$ is a mixed-symmetric function, and there is no antisymmetric function. The first step of the procedure is complete. The next task is to figure out the Young diagrams corresponding to the dual symmetries of spin functions.

It can be easily done by exchanging the rows with columns as shown in *Figure 2*. It is worth mentioning that in this transformation, the size of the row cannot increase, hence dual of $[21]$ remains $[21]$ rather becoming $[12]$.

Now, we are only left with the third step. We already know the required symmetry of space wavefunctions in the form of Young

![Young-tableaux](image)

The horizontal bar represents symmetric functions, while the vertical box represents antisymmetric functions.

*Figure 2.* Construction of dual Young-tableaux for spin with $p^3$ electronic configuration
diagrams. We need to convert it to \( S, P, D \cdots \) notations i.e. the irreducible representations (IR) of the rotation group. The basic connection is, single box of Young diagram correspond to corresponding rotational quantum number i.e. \( j \leftrightarrow [1] \). For \( p \) orbitals \( j = 1 \), therefore, \([1] \leftrightarrow P\) and our task is to figure out the rotational angular momentums IR contains in \([1^3]\) (it is a short notation for \([111]\)) and \([21]\):

\[
\begin{array}{c}
\begin{array}{c}
\text{?}
\end{array}
\end{array} =? \quad \begin{array}{c}
\begin{array}{c}
\text{?}
\end{array}
\end{array} =?.
\]

The main brick game starts now. As mentioned before, one need to construct \([1^3]\) and \([21]\) using our basic box \([1]\) and then we need to replace \([1]\) with \(P\). This has been done in Table 1.

**Table 1.** Construction of Young boxes for \( p^3 \) configuration.

The left hand side of Table 1 is obvious, as we are adding the boxes in such a manner that all the possible standard Young diagrams can be formed. In the right hand side, usual rule of adding angular momentum is employed. This recursive algebra can be made simple with two observations. First, in \([1] \otimes [1] = [20] \otimes [11]\) formation, \([20]\) is symmetric (horizontal box) and \([11]\) is anti-symmetric (vertical box), therefore \([20] = D \oplus S\) and \([11] = P\).

Another point that helps in simplifying this algebra is to notice the equivalence among different Young diagrams. Which means \([1^n] \equiv [1^{(2j+1)-n}]\) and \([1^{(2j+1)}] = [0] = S\). Therefore, in the case of \( p^3 \) where \( j = 1 \), \([1^3] = S\) and \([1^2] = [1] = P\). The term symbols for \( p^3 \) configuration is summarized in Table 2.

Now, let us try the \( d^3 \) configuration. The spin part will be all same
Table 2. Summary of term-symbol calculation for $p^3$ configuration.

<table>
<thead>
<tr>
<th>SPIN</th>
<th>SPACE</th>
<th>TERM-SYMBOL</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{3}{2}$</td>
<td>$S$</td>
<td>$^4S$</td>
</tr>
<tr>
<td>$\frac{1}{2}$</td>
<td>$P \oplus D$</td>
<td>$^2P, ^2D$</td>
</tr>
</tbody>
</table>

as $p^3$ case, only the last step will change (See Table 3).

Table 3. Construction of Young boxes for $d^3$ configuration.

Here, as $j = 2$, therefore, $1^3 \equiv 1^2 = P \oplus F$. So similar to the case of $p^3$ configuration, the term symbols for $d^3$ configuration will be as follows (Table 4).

Table 4. Summary of term-symbol calculation for $d^3$ configuration.

<table>
<thead>
<tr>
<th>SPIN</th>
<th>SPACE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{3}{2}$</td>
<td>$P \oplus F$</td>
</tr>
<tr>
<td>$\frac{1}{2}$</td>
<td>$P \oplus D \oplus D \oplus F \oplus G \oplus H$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TERM-SYMBOL</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^4P, ^4F$</td>
</tr>
<tr>
<td>$^2P, ^2D, ^2D, ^2F, ^2G, ^2H$</td>
</tr>
</tbody>
</table>

In $d^3$ configuration, $D^2$ term occurs twice. Therefore, one additional complication has been started; occurrence of some terms more than once. It usually makes this algebra more complicated for the higher terms. To illustrate it, let us take $d^5$ configuration. From the first and second steps, we will get the following boxes...
for spin functions.

\[
\begin{array}{ccc}
\text{Spin} & \text{box} & \text{dual box} \\
\hline
\frac{5}{2} & \begin{array}{c}
\square \\
\square \\
\square \\
\end{array} & \begin{array}{c}
\square \\
\square \\
\square \\
\end{array} \\
\frac{3}{2} & \begin{array}{c}
\square \\
\square \\
\end{array} & \begin{array}{c}
\square \\
\square \\
\end{array} \\
\frac{1}{2} & \begin{array}{c}
\square \\
\end{array} & \begin{array}{c}
\square \\
\end{array}
\end{array}
\]

The third step is summarized in the Table 5.

The last row of Table 5 requires little bit more attention. Before that we only needed to multiply one box to any regular Young-tableau, and the only thing we needed to care about was that the new shape should be a standard Young-tableau. The last step involved multiplication of two arbitrary Young-tableaux. Let us assume these two tableaux are \([\lambda_1, \lambda_2, \ldots, \lambda_n]\) and \([\mu_1, \mu_2, \ldots, \mu_n]\). The rules to combine them are as follows.

1. Label all \(\mu_1\) with the same symbol say \(\alpha\) and \(\mu_2\) with the same symbol say \(\beta\), etc. So each row in \(\mu\) boxes have the same symbol but symbols of one row is different from the other row, i.e.

\[
\begin{array}{ccc}
\alpha & \alpha & \alpha \\
\beta & \beta & \beta
\end{array}
\]

2. Now add it to \(\lambda\) in such a way that no two columns contain the same symbol.

3. If we read these symbols in final shape, right from each row, we should obtain a lattice permutation of \(\alpha^{\mu_1} \beta^{\mu_2} \cdots\).
Table 5. Summary of term-symbol calculation for $d^5$ configuration.
**Box 6. Lattice Permutation**

A lattice permutation is a string composed of positive integers, in which every prefix sub-string contains at least as many positive integers $i$ as integers $i + 1$. For example 2233232 is a lattice permutation, but 232322 is not a lattice permutation, since the sub-word 23233 contains more three's than two's.

To illustrate the above point, let us consider few examples below,

\[
\begin{array}{ccc}
1 & 2 & 2 \\
\alpha & \beta & \alpha \\
2 & 2 & 2 \\
\end{array} \otimes
\begin{array}{ccc}
1 & 1 & 1 \\
\alpha & \beta & \beta \\
2 & 2 & 2 \\
\end{array} =
\begin{array}{ccc}
1 & 2 & 1 \\
\alpha & \beta & \alpha \\
2 & 2 & 2 \\
\end{array} \oplus
\begin{array}{ccc}
1 & \alpha & 1 \\
\alpha & \beta & \beta \\
2 & 2 & 2 \\
\end{array}
\]

**Summary**

In the present article, group-theory has been used to construct atomic term symbols in $LS$ coupling scheme. It has been shown that due to Young-tableaux, it is possible to use group-theory without explicitly constructing the character table. I hope the present article will not only help student to write down quickly the term-symbols but also inspire them to learn group-theory to understand the present method explicitly.

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Suggested Reading


