Spin-multiplicity value and its corresponding spin state was first discovered by Friedrich Hund in 1925. The formula which is generally used for the prediction of spin multiplicity value is \( \langle(2S+1)\rangle \), where

\[
\langle S \rangle = \langle \text{spin quantum #} \rangle \{ \sum m_s \} \label{eq1}
\]

is time consuming. To keep the matter in mind a simple innovative method\(^1,2,3\) has to be introduced for calculation of spin-multiplicity value and thus its corresponding spin state, shown in Table-1, in the easiest way by ignoring the calculation of total spin quantum number (Equation \ref{eq1}). First of all we should classify the species (atoms, molecules, ions or complexes) for which spin multiplicity value should be evaluated into three types based on the nature of alignment of unpaired electrons present in them.

### Species having unpaired electrons in upward alignment (\(\uparrow\))

In this case, spin multiplicity = (n+1); where n = number of unpaired electrons

- Spin multiplicity = (n + 1) = (1+1) = 2 (spin state = doublet); (2+1) = 3 (spin state = triplet) and (3 + 1) = 4 (spin state = quartet) respectively.
- Spin multiplicity = (n +1) = (2 + 1) = 3 (in this case ignore paired electrons) (spin state = triplet) and (1 + 1) = 2 (spin state = doublet)
- Spin multiplicity = (n +1) = (0 + 1) = 1 (spin state = singlet)
Species having unpaired electrons in downward alignment (↓)

In this case spin multiplicity = \((-n+1)\). Here (−ve) sign indicate downward arrow.

\[
\begin{array}{ccc}
\downarrow & \downarrow & \downarrow \\
\end{array}
\]

\[
\begin{array}{ccc}
\downarrow & \downarrow & \downarrow \\
\end{array}
\]

\[
\begin{array}{ccc}
\downarrow & \downarrow & \downarrow \\
\end{array}
\]

Spin multiplicity = \((-n + 1) = (-1 + 1) = 0; (-2 + 1) = -1\) and \((-3 + 1) = -2\) respectively.

\[
\begin{array}{ccc}
\uparrow\downarrow & \downarrow & \downarrow \\
\end{array}
\]

\[
\begin{array}{ccc}
\uparrow\downarrow & \uparrow\downarrow & \downarrow \\
\end{array}
\]

Spin multiplicity = \((-n + 1) = (-2 + 1) = -1\) (ignore paired electrons) and \((-1 + 1) = 0\) respectively.

Species having unpaired electrons in both mixed alignment (↑)(↓)

In this case spin multiplicity = \([(+n) + (-n) + 1]\), where, \(n\) = number of unpaired electrons in each alignment. Here, (+ve) sign and (−ve) sign indicate upward and downward alignment respectively.

\[
\begin{array}{ccc}
\uparrow & \downarrow & \\
\end{array}
\]

Here total no of unpaired electrons = 2 in which one having upward direction (+1) and other having downward mode (-1).

Hence Spin multiplicity = \([(+n) + (-n) + 1] = [(+1) + (-1) + 1] = 1\) (spin state = singlet)

\[
\begin{array}{ccc}
\uparrow & \uparrow & \downarrow \\
\end{array}
\]

Here the total no of unpaired electrons = 3 in which two unpaired electrons lie in upward (+2) and one unpaired electrons lie in downward (-1). Hence Spin multiplicity = \([(+n) + (-n) + 1] = [(+2) + (-1) + 1] = 2\) (spin state = doublet)

\[
\begin{array}{cccc}
\uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\
\end{array}
\]
Here the total no of unpaired electrons = 5 in which three unpaired electrons lie upward (+3) and two unpaired electrons lie downward (-2). Hence Spin multiplicity = [(+n) + (-n) + 1] = [(+3) + (-2) +1] = 2 (spin state = doublet)

Table 1: Spin multiplicity value and its corresponding spin state

<table>
<thead>
<tr>
<th>Spin multiplicity value</th>
<th>Spin state</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Singlet</td>
</tr>
<tr>
<td>2</td>
<td>Doublet</td>
</tr>
<tr>
<td>3</td>
<td>Triplet</td>
</tr>
<tr>
<td>4</td>
<td>Quartet</td>
</tr>
<tr>
<td>5</td>
<td>Quintet</td>
</tr>
</tbody>
</table>

References


External Links

- https://communities.acs.org/docs/DOC-46667
- https://communities.acs.org/docs/<wbr/>DOC-45853
- www.drarijitdaschem.in/Spin%2...13%20issue.pdf

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