

Chemistry 3P51 – Fall 2013

Quantum Chemistry

Lecture No. 29

Nov 15th, 2013

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Objectives

- To remind the student the main ideas about term symbols
- To present Hund's to determine the most stable configuration

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Term symbols for atomic states

Because the orbital and spin angular momenta **L** and **S** interact, atomic states with different *L* and *S* have different energies. Atomic states that have the same electron configuration, same *L* value, same *S* value, and same energy constitute a **term**. Atomic terms are classified (and designated) according to *L* and *S*. The convention is to report the values of *L* and *S* for a given configuration as a **term symbol**

$$^{2S+1}L$$

in which the value of *L* is represented by a capital letter as follows:

<i>L</i> =	0	1	2	3	4	...
Symbol	S	P	D	F	G	...

The superscript $2S+1$ is the **spin multiplicity**:

$2S+1 =$	1	2	3	4	5	6
Name	singlet	doublet	triplet	quartet	quintet	sextet

Examples of terms: 2S , 3P , 1D .

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Table showing term symbols for some electron configurations

Terms for Equivalent Electrons	
Electron Configuration	Terms
$s^2; p^6; d^{10}; f^{14}$ (filled subshells)	1S
s^1	2S
$p^1; p^5$	2P
$p^2; p^4$	$^3P; ^1D; ^1S$
p^3	$^4S; ^2D; ^2P$
$d^1; d^9$	2D
$d^2; d^8$	$^3F; ^3P; ^1G; ^1D; ^1S$

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Hund's rules for the most stable states of a molecule

Given several term using the same orbitals, it is important to know their energies. This is determined using **Hund's rules**.

Hund's Rule No.1. The higher the multiplicity of a state, the lower its energy.

Hund's Rule No.2. Among states of equal multiplicity, the one with the highest value of L has the lowest energy.

Hund's Rule No.3. If spin-orbit effects are considered, then for given values of S and L , the state with the lowest value of J is the lowest energy state when the *unfilled* shell is less than half-filled. If the *subshell* is more than *half-filled*, the highest value of J is the lowest energy state.

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Summary

To summarize, given an electronic configuration:

1. We first determine all the term symbols.
2. The Hund's rules are applied in order to determine the symbol with the lowest energy.

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