G. Term Symbol : Understanding spectroscopic Data

- A notation to label the energy levels of an atom

  generally, it is about the atom as a whole

- Notation provides information on

  (l, s, j) for H-atom

  (L, S, J) for atoms in general

Capital Letters are used for labelling atoms

L for quantum number of total orbital angular momentum

S for quantum number of total spin angular momentum

J for quantum number of $\vec{J} = \vec{L} + \vec{S}$

H-atom (simplest)

- One electron only (nothing to "total", e.g. electron's l is atom's L)

  $s = 1/2$ always, (total spin is single electron's spin) ($S = 1/2$ H-atom)

  $2s + 1 = 2$ (this will go into upper left-hand corner of term symbol)

  l (single electron's l is whole atom's L)

  $l = 0, 1, 2, 3, \ldots$

  Notation: s, p, d, f, ...

  } H-atom

- $\vec{J} = \vec{L} + \vec{S}$ ⇒ Quantum number j (multiple values) [with m_j's behind j]

  Atomic Term Symbol (H-atom)

$$\boxed{{}^{2s+1}l_j} \qquad \text{labels energy levels} \tag{28}$$

notation provides information on s, l, j

e.g. H-atom ground state → 1s ($n=1$, $\ell=0$)
→ $\ell=0 \Rightarrow$ "S" in the middle

one electron : $2s+1 = 2$ [go to upper left-hand corner]
(s ↑ spin ½)

$\ell=0$, $s=\frac{1}{2} \Rightarrow j=\frac{1}{2}$ only [go to lower right-hand corner]

G.S. of H-atom is described by electron configuration (1s)
and Term Symbol $^{2}S_{1/2}$ ($2 = 2\cdot\frac{1}{2}+1$; $S \leftarrow \ell=0$; $\frac{1}{2} \leftarrow j=\frac{1}{2}$) OR $1s\ ^{2}S_{1/2}$

An excited state : Crude description $2p \leftarrow \ell=1$ ("P" in the middle)
$j=\frac{3}{2}$, $j=\frac{1}{2}$ one-electron: $2\cdot\frac{1}{2}+1=2$ (upper LH corner)

Could be

$2p\ ^{2}P_{1/2}$ (2 states) OR $2p\ ^{2}P_{3/2}$ (4 states) ← Recall: fine structure [They have slightly different energies]

[Data Tables use these labels]

Making connections

This is the point of using (ℓ, m_ℓ, s, m_s) vs (ℓ, s, j, m_j)

- Since spin-orbit interaction is always there (except for atoms with total $\vec{S}=0$)

Using (ℓ, s, j, m_j) is a better choice

Term Symbol gives ℓ, s, j

[m_j comes in only when an external magnetic field is applied]

anomalous Zeeman effect

General Atoms

- $\vec{L} = \sum_{i} \vec{l}_i$ ← orbital AM of i^{th} electron; i ← all electrons
  ↖ then L^2 can take on $L(L+1)\hbar^2$

  ; $\vec{S} = \sum_{i} \vec{s}_i$ ← spin AM of i^{th} electron
  ↖ then S^2 can take on $S(S+1)\hbar^2$

[Values of L? By rule of adding AM's]

$L = 0, 1, 2, 3, \ldots$

Notation: S, P, D, F, ...

[Values of S? By adding AM's]

(2S+1) appears in upper LH corner

Term Symbol is $^{2S+1}L_J$ for all atoms

(29)

Sometimes, principle quantum number n is included as: $n\,^{2S+1}L_J$