

Term Symbols Example

C atom

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Carbon atom e^- config is $1s^2 2s^2 2p^2$

(1) Apply rule 1: $1s^2, 2s^2$ don't matter. We're left w/ $2p^2$.

(2) Consider what possible Slater determinants could be formed. For a p orbital, $l=1$, so $m_l = +1, 0, -1$.

<u>Det #</u>	<u>Det</u>	<u>M_L</u>	<u>M_S</u>
①	$2p \uparrow\uparrow \text{ --- } \text{ ---}$ $m_l = +1 \quad 0 \quad -1$	2	0
②	$\uparrow \uparrow \text{ ---}$	1	1
③	$\uparrow \uparrow\downarrow \text{ ---}$	1	0
④	$\uparrow \text{ --- } \uparrow$	0	1
⑤	$\uparrow \text{ --- } \uparrow\downarrow$	0	0
⑥	$\uparrow\downarrow \uparrow \text{ ---}$	1	0
⑦	$\uparrow\downarrow \text{ --- } \uparrow$	0	0
⑧	$\text{--- } \uparrow\uparrow \text{ ---}$	0	0
⋮	⋮		

there are more w/ $M_L, M_S < 0$... usually suffices to work w/ + ones, keep - in mind

(3) Use the Rules to Figure out which term symbols arise from this config.

Use corollary of Rule 3: The highest $M_L = 2$. \therefore Can't have $L > 2$. The highest $M_S = 1$. \therefore Can't have $S > 1$.

This gives us the following possible term symbols at this stage:

$$S = 0, 1 \quad (2S+1 = 1 \text{ or } 3)$$

$$L = 0, 1, 2$$

\Rightarrow $^1S, ^3S, ^1P, ^3P, ^1D, ^3D$.

But not all these are really possible. For example,

3D : Corollary says it must be possible to construct a Slater det. w/ $M_L = 2, M_S = 1$. But there's no such determinant! (would require 2 α spins in same orb). \therefore No 3D . Others still ok, for now...

Since we can make $\uparrow\uparrow$ ~~to~~ $M_L=2, M_S=0$,
 there must be an L-S eigenfunction w/ $L \geq 2, S \geq 0$.

But also we know $L < 3, S < 2$. The only
 term symbol in our list fitting this is 'D'.

\therefore This Slater det must belong to 'D'.

Now: other Slater det's also belong to this
 term symbol (because it's degenerate) —
 see Rule 2. We ~~do~~ need to figure out
 which ones & mark them out.

$$M_L = -L, -L+1, \dots, L-1, L \quad \text{or here } M_L = -2, -1, 0, 1, 2.$$

Likewise, $M_S = 0$. 'D' accts for the following

$$\text{determinants: } (M_L, M_S) = \underbrace{(2, 0), (1, 0), (0, 0), (-1, 0), (-2, 0)}$$

5 choices

$$5 = (2L+1)(2S+1)$$

\therefore Remove ①, ③, ⑤ (& the - ones not drawn
 in Slater det list).

Remaining det's:

		(M_L, M_S)
②	$\uparrow \uparrow -$	(1, 1)
④	$\uparrow - \uparrow$	(0, 1)
⑥	$\uparrow \uparrow -$	(1, 0)
⑦	$\uparrow - \uparrow$	(0, 0)
⑧	$- \uparrow -$	(0, 0)

Now go to the determinant w/ highest (M_L, M_S) left, which is ②, (1, 1). Apply Rule 3:

Must be an L-S state w/ $L \geq 1, S \geq 1$. out of our list of remaining term symbols,

($^1S, ^3S, ^1P, ^3P, \cancel{^1D} \rightarrow \text{did}$, $\cancel{^3D} \rightarrow \text{impossible}$),

we have to use only 3P for this ($L=1, S=1$).

For 3P , $M_L = -1, 0, 1$; $M_S = -1, 0, 1$. Therefore 3P accts for 9 Slater det's.

3P accts for Slater det's w/ $(M_L, M_S) =$
 $(1,1), (1,0), (1,-1), (0,1), (0,0), (0,-1), (-1,1), (-1,0),$
 $(-1,-1).$

Cross off ②, ④, ⑥, ⑦, (and the unwritten (-) ones). What Slater det's does this leave? Only $(0,0)$ ⑧ is left!

For remaining $(0,0)$ det ⑧, must have an $L-S$ state w/ $L=0, S=0$. What term symbols are left in our list?

$^1S, ^3S, ^1P$. It can't be 3S or 1P , because either of those take 3 det's, and we only have one left. \therefore It must be 1S ($L=0, S=0$).

Result: C atom $1s^2 2s^2 2p^2$ gives rise to term symbols $^1D, ^3P, ^1S$.