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3.1: SII ion

The electronic configuration is $1s^2 2s^2 2p^6 3s^2 3p^3$.

So we have three electrons in the shell, we have to guess how many configurations we could possibly rearrange them. We know that $m_\ell = -1, 0, 1$ and we know $m_s = -1/2, 1/2$. We have to distribute 3 electrons into 3×2 slots:

$$C^6_3 = \frac{6 \times 5 \times 4}{3!} = 20. \tag{1}$$

I crudely all the possibilities here, based on Pauli exclusion principle:

	A	B	C	D	E
1		ml		L	S
2	-1	0	1		
3	↑	↑	↑	0	1.5
4	↑	↓	↑	0	0.5
5	↑	↑	↓	0	0.5
6	↓	↑	↑	0	0.5
7	↑	↓	↓	0	-0.5
8	↓	↑	↓	0	-0.5
9	↓	↓	↑	0	-0.5
10	↓	↓	↓	0	-1.5
11	↑↓	↓		-2	-0.5
12	↑↓	↑		-2	0.5
13	↑	↑↓		-1	0.5
14	↓	↑↓		-1	-0.5
15		↓	↑↓	2	-0.5
16		↑	↑↓	2	0.5
17	↑↓		↓	-1	-0.5
18	↑↓		↑	-1	0.5
19		↑↓	↑	1	0.5
20		↑↓	↓	1	-0.5
21	↑		↑↓	1	0.5
22	↓		↑↓	1	-0.5

Figure 1: electron configuration

Of course we need to write into spectroscopic terms like:

$$^{2S+1}\mathcal{L}^p_{\mathcal{J}},$$

where $\mathcal{L} \in \{S, P, D, ...\}$ and $p \in \{\text{odd}, \text{blank}\}$, and $\mathcal{J} = S + L$.

Now we examine the total spin and total angular momentum in our list, and we get the last 2 columns in Fig 1.

We follow the procedure taught in the class, and write these possibilities into a cubic:

F	G	H	I	J
ml \ ms	-1.5	-0.5	0.5	1.5
-2		1	1	
-1		2	2	
0	1	3	3	1
1		2	2	
2		1	1	

After examining all possibilities with symmetric along m_ℓ and m_s, we can write down these three:

- The 5×2 matrix: $S = 1/2, L = 2, \mathcal{J} = 2 \pm 1/2$, thus ${}^2\mathrm{D}^{\mathrm{o}}_{3/2,5/2}$
- The 3×2 matrix: $S = 1/2, L = 1, \mathcal{J} = 1 \pm 1/2$, thus ${}^2\mathrm{P}^{\mathrm{o}}_{1/2,3/2}$
- The 1×4 matrix: $S = 3/2, L = 0, \mathcal{J} = 0 + 3/2$, thus ${}^4\mathrm{S}^{\mathrm{o}}_{3/2}$

Now we have to construct energy levels. Basically, there are 5 different level (including fine structure splitting) and any pair would be a valid transition. So, we would have $C^5_2 = 5!/3!/2! = 10$ transitions. The question is how we line up these states.

According Hund's rule, the term with maximum multiplicity ($2S+1$) has the lowest energy. So apparently we have ${}^4\mathrm{S}^{\mathrm{o}}_{3/2}$ to br the lowest. Also, the term with largest L has lowest energy. So we should line up the order as $P \to D \to S$. Third rule says the lowest $\mathcal{J}$ has the lowest energy. Thus, the order in our mind right now should look like:

$$ {}^2\mathrm{P}^{\mathrm{o}}_{3/2} \to {}^2\mathrm{P}^{\mathrm{o}}_{1/2} \Rightarrow {}^2\mathrm{D}^{\mathrm{o}}_{5/2} \to {}^2\mathrm{D}^{\mathrm{o}}_{3/2} \Rightarrow {}^4\mathrm{S}^{\mathrm{o}}_{3/2}, $$

where bigger arrows indicate larger energy gaps downwardly.

We should be able to draw these 10 transitions in our mind, but strictly speaking:

1. ${}^2\mathrm{P}^{\mathrm{o}}_{3/2} \to {}^2\mathrm{P}^{\mathrm{o}}_{1/2}$
2. ${}^2\mathrm{P}^{\mathrm{o}}_{3/2} \to {}^2\mathrm{D}^{\mathrm{o}}_{5/2}$
3. ${}^2\mathrm{P}^{\mathrm{o}}_{3/2} \to {}^2\mathrm{D}^{\mathrm{o}}_{3/2}$
4. ${}^2\mathrm{P}^{\mathrm{o}}_{3/2} \to {}^4\mathrm{S}^{\mathrm{o}}_{3/2}$

5. $^2\mathrm{P}^{\mathrm{o}}_{1/2} \to {}^2\mathrm{D}^{\mathrm{o}}_{5/2}$
6. $^2\mathrm{P}^{\mathrm{o}}_{1/2} \to {}^2\mathrm{D}^{\mathrm{o}}_{3/2}$
7. $^2\mathrm{P}^{\mathrm{o}}_{1/2} \to {}^4\mathrm{S}^{\mathrm{o}}_{3/2}$
8. $^2\mathrm{D}^{\mathrm{o}}_{5/2} \to {}^2\mathrm{D}^{\mathrm{o}}_{3/2}$
9. $^2\mathrm{D}^{\mathrm{o}}_{5/2} \to {}^4\mathrm{S}^{\mathrm{o}}_{3/2}$
10. $\mathrm{D}^{\mathrm{o}}_{3/2} \to {}^4\mathrm{S}^{\mathrm{o}}_{3/2}$.

3.2: Draine 4.1:

Those rules we should follow are listed in 6.7.1 in Draine. These are transitioning selection rules:

1. Parity must change.
2. $\Delta L = 0, \pm 1$
3. $\Delta J = 0, \pm 1$, but $J = 0 \to 0$ is forbidden.
4. Only one single-electron wave function $n\ell$ changes, with $\Delta \ell = \pm 1$.
5. $\Delta S = 0$: Spin does **not** change.

Notably, violating 5th rule is called semiforbidden or intercombination. And violating any of 1st to 4th rule says to be forbidden.

1. CIII: $^3\mathrm{P}^{\mathrm{o}}_1 \to {}^1\mathrm{S}_0$: it fulfills (1, 2, 3, 4) and violates 5, so semi-forbidden.
2. OIII: $^1\mathrm{D}_2 \to {}^3\mathrm{P}_2$: it violates 1, so forbidden.
3. OIII: $^1\mathrm{S}_0 \to {}^1\mathrm{D}_2$: it violates 1, so forbidden.
4. OIII: $^5\mathrm{S}^{\mathrm{o}}_2 \to {}^3\mathrm{P}_1$: it fulfills (1, 2, 3, 4) but violates 5, so semi-forbidden.
5. CIV: $^2\mathrm{P}^{\mathrm{o}}_{3/2} \to {}^2\mathrm{S}_{1/2}$: it fulfills (1, 2, 3, 4, 5), so allowed.
6. Ne II: $^2\mathrm{P}^{\mathrm{o}}_{1/2} \to {}^2\mathrm{P}^{\mathrm{o}}_{3/2}$: it violates 1, so forbidden.
7. O I: $^3\mathrm{S}^{\mathrm{o}}_1 \to {}^3\mathrm{P}_2$: it fulfills (1, 2, 3, 4, 5), so allowed.