

Completing the Shell Model of the Atom

The table below gives ionization energies for the elements Na through Ar.

Element	Ionization Energies in MJ/mol				
	1s	2s	2p	3s	3p
Na	104	6.84	3.67	0.50	
Mg	126	9.07	5.31	0.74	
Al	151	12.1	7.79	1.09	0.58
Si	178	15.1	10.3	1.46	0.79
P	208	18.7	13.5	1.95	1.01
S	239	22.7	16.5	2.05	1.00
Cl	273	26.8	20.2	2.44	1.25
Ar	309	31.5	24.1	2.82	1.52

Shown here is equivalent information for the PES spectrum of potassium, K.

	1s	2s	2p	3s	3p	???
Ionization Energy (MJ/mol)	347	37.1	29.1	3.93	2.38	0.42
Relative Abundance	2	2	6	2	6	1

Questions to Consider

- Using Coulomb's law, explain the trend in the ionization energies for Na as you move from a 1s electron to a 3s electron.

There are two effects here. First, a 1s electron is closer to the nucleus than a 3s electron, which makes V smaller and makes V , and, thus, the ionization energy larger. Second, the effective nuclear charge for a 1s electron in Na is greater than for a 3s electron, which makes q_+ larger and makes V , and, thus, the ionization energy larger.

- Explain the trend in the ionization energies for a 1s electron as you move from Na to Ar.

There are two effects here. First, the effective nuclear charge for a 1s electron in Ar is greater than for a 1s electron in Na, which makes q_+ larger and makes V , and, thus, the ionization energy larger. Second, the greater the effective nuclear charge, the more closely the nucleus pulls the electron toward it, decreasing the distance, d , and increasing V , and, therefore, the ionization energy.

- The first five peaks in potassium's PES spectrum are identified as 1s, 2s, 2p, 3s, and 3p. Are their ionization energies consistent with those for the elements Na \rightarrow Ar? Briefly explain.

Yes. Each ionization energy is slightly larger than the corresponding value for Ar, consistent with the greater charge for potassium's nucleus.

- The shell/subshell for the sixth peak in potassium's PES spectrum is not identified. Is this electron in a new subshell of the $n = 3$ shell (the 3d subshell) or is it in the first subshell of the $n = 4$ shell (a 4s subshell)? Look for patterns as you move between subshells of a given shell (e.g. 2s \rightarrow 2p or 3s \rightarrow 3p) and as you move between shells (e.g. 1s \rightarrow 2s or 2s \rightarrow 3s). Although you may know the answer from an earlier chemistry course, justify your answer here using an argument based on ionization energies. Write the electron configuration for K.

The trends in IEs suggest that electrons in the same shell have similar IEs and that each new shell produces a significant change in IE. For example, the 2s and 2p electrons in K have IEs of 37.1 and 29.1,

but the IEs for the 2s and 3s electrons are 37.1 and 3.93, respectively. An IE of 0.42 is inconsistent with a 3s or 3p electron and must come from a new shell; thus, we predict that it is a 4s electron, not a 3d electron. The electron configuration for potassium is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$.

5. The PES spectrum for scandium, Sc, has seven peaks with the following energies and relative abundances of electrons.

	1s	2s	2p	3s	3p	???	4s
Ionization Energy (MJ/mol)	433	48.5	39.2	5.44	3.24	0.77	0.63
Relative Abundance	2	2	6	2	6	1	2

The second-to-last peak in the PES spectrum for Sc is either a 3d or a 4p subshell. Which is it? Although you may know the answer from an earlier chemistry course, justify your answer using an argument based on ionization energies. Write the electron configuration for Sc.

This is a bit trickier because the IE is closer in magnitude to a 4s electron than it is to a 3s or 3p electron; however, we expect the IE for a 4s electron to be less than that for a 4p electron given the trend we see for other shells. The peak, therefore, must be for a 3d electron. It seems the presence of the two 4s electrons decreases the ionization energy for the 3d subshell, an observation to which we will soon return. The electron configuration for Sc is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$.

6. Many transition metals form a stable +2 cation. For example, in the first row of the transition metals we find Ti^{2+} , V^{2+} , Cr^{2+} , Mn^{2+} , Fe^{2+} , Co^{2+} , Ni^{2+} , Cu^{2+} , and Zn^{2+} . Explain why so many of these transition metals easily form a +2 cation.

The fact that a 3d electron has a greater ionization energy than a 4s electron when both are present means the most easily removed electrons for these transition metals are the two 4s electrons. It isn't surprising, therefore, that transition metals easily form a +2 ion as these two electrons have the smallest ionization energy.