Key for A Deeper Look at Shell Model Worksheet

The table below gives the ionization energies for elements in the third row of the periodic table (all values in MJ/mol; 1 MJ = 10^6 J).

element	Z	$1s$	$2s$	$2p$	$3s$	$3p$
Na	11	104	6.84	3.67	**0.50**	
Mg	12	126	9.07	5.32	**0.74**	
Al	13	151	12.1	7.79	1.09	**0.58**
Si	14	178	15.1	10.3	1.46	**0.79**
P	15	208	18.7	13.5	1.95	**1.01**
S	16	239	22.7	16.5	2.05	**1.00**
Cl	17	273	26.8	20.2	2.44	**1.25**
Ar	18	309	31.5	24.1	2.82	**1.52**

What is the electron configuration for aluminum? Which of these electrons are core? Which are valence?

- The electron configuration is $1s^2 2s^2 2p^6 3s^2 3p^1$. The valence electrons are $3s$ and $3p$ as these have the largest value for n; all other electrons are core.

For a valence electron in an $n = 3$ shell there are eight core electrons in shells closer to the nucleus. As a result, an $n = 3$ valence electron will not experience the full charge of the nucleus; instead it "sees" an effective nuclear charge, Z_{eff}, where

$$Z_{eff} = Z - \text{number of core electrons}$$

What is Z_{eff} for a valence electron in Al?

- For aluminum, we have $Z_{eff} = Z - \text{number of core electrons} = 13 - 10 = 3$.

Using Coulomb's law, explain the trend in the ionization energies for Na as you move from a $1s$ electron to a $2s$ electron to a $3s$ electron.

- An $n = 1$ electron is closer to the nucleus than an $n = 2$ electron, which, in turn, is closer to the nucleus than an $n = 3$ electron; thus, the binding energy of a $1s$ electron is greater than that for a $2s$ electron, which, in turn is greater than that for a $3s$ electron. In addition, Z_{eff} for an $n = 1$ electron is 11, for an $n = 2$ electron it is $11 - 2 = 9$, and for an $n = 3$ electron it is $11 - 10 = 1$.

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

- As we move from left-to-right in a row, the charge on the nucleus increases from 11 for Na to 18 for Ar (and the effective nuclear charge increases from $11 - 10$ for Na to $18 - 10 = 8$ for Ar. From Coulomb's law, the greater the charge on the nucleus, the larger the energy, E, and the greater the binding energy.

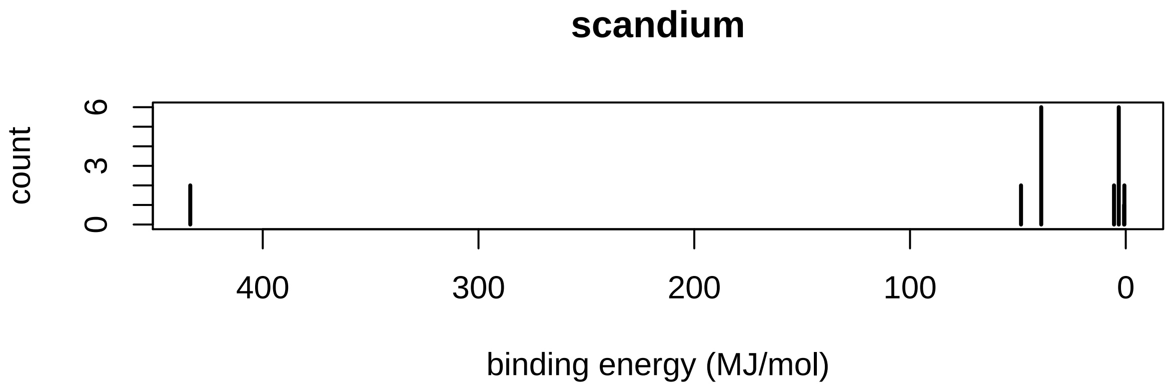
Identify each element's first ionization energy and, using Coulomb's law, explain the trend in their values.

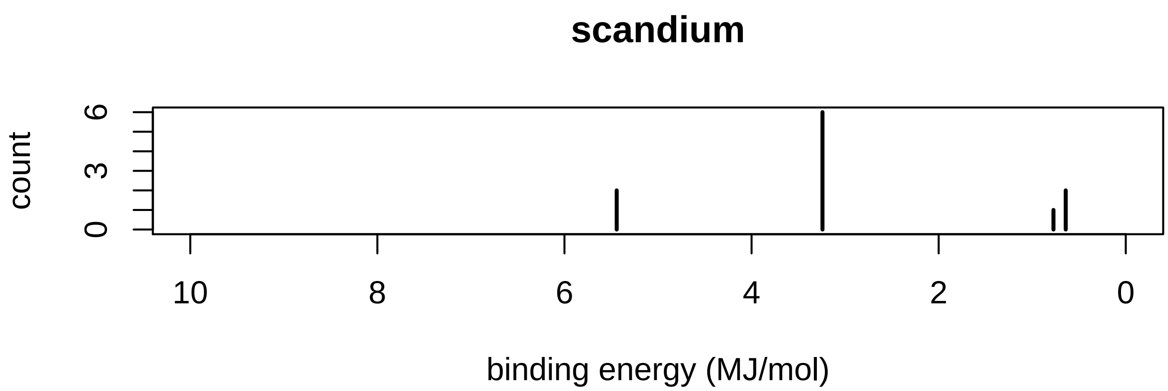
- The first ionization, IE_1, for each element is for the electron that is easiest to remove; this is the right-most ionization energy for each element, which is shown in **bold** above. In general, we see that IE_1 increases from Na $\longrightarrow$ Ar, as we expect given the increase in the charge on the nucleus. There are "glitches" in this trend that we need to explain as we move from Mg $\longrightarrow$ Al and as we move from P $\longrightarrow$ S; in both cases, the ionization energy becomes smaller rather than larger. We don't yet have a way to explain this, but it not unreasonable to assume it is related in some way to Z_{eff}.

The ionization energies for argon's $3s$ and $3p$ electrons are not the same. Given that the average distance of each electron from the nucleus is essentially the same, what problem does this present for our current model of the atom?

- This presents us with the following problem: if the distance is the same, then Coulomb's law requires that a $3p$ electron sense a smaller Z_{eff} than does a $3s$ electron; however, our current model that defined Z_{eff} as $Z -$ number of core electrons suggest that the $3s$ and $3p$ electrons have identical values for Z_{eff}.

The photoelectron spectrum for scandium, Sc, is shown below. The full spectrum is shown on the top and, although difficult to see, it has seven peaks. The spectrum on the bottom provides a close-up view of the four lowest-energy peaks.





The two lowest energy peaks in the spectrum have ionization energies of 0.77 and 0.63 MJ/mol, respectively, and counts of 1 and 2 electrons, respectively. One of these peaks is a $4s$ shell/subshell and the other is a $3d$ shell/subshell. Which is which? What leads you to this conclusion? What problem does this present for our current model of the atom?

- Based on our data for the elements H $\longrightarrow$ Ar we can reasonably expect that ionization energies decrease as we go from $n = 3$ to $n = 4$; thus, it is reasonable to identify the peak at 0.63 MJ/mol as a $4s$ electron. This does create an interesting problem for us as this is the first time we see a new shell accepting an electron before the earlier shells are full.