Take-Home Assignment 03

These two problems provide practice in using Slater's rules to estimate an element's effective nuclear charge and provide practice in interpreting the results of such calculations.

Problem 1. The table below reports theoretical values for the effective nuclear charge of the elements in the second row of the periodic table. Use Slater's rules to estimate Z_{eff} and report the difference between the estimated and the theoretical values: Δ = estimated Z_{eff} – theoretical Z_{eff}. Comment on your results.

			electrons				
element	Z	Z_{eff} (expt)	1*s*	2*s*	2*p*	Z_{eff} (Slater)	Δ
lithium (Li)	3	1.28	2	1	0	**1.30**	**0.02**
beryllium (Be)	4	1.91	2	2	0	**1.95**	**0.04**
boron (B)	5	2.42	2	2	1	**2.60**	**0.18**
carbon (C)	6	3.14	2	2	2	**3.25**	**0.11**
nitrogen (N)	7	3.83	2	2	3	**3.90**	**0.07**
oxygen (O)	8	4.45	2	2	4	**4.55**	**0.10**
fluorine (F)	9	5.10	2	2	5	**5.20**	**0.10**

Using Slater's rules, values for Z_{eff} are calculated for a 2*s* or 2*p* electron using the following formula

$$Z_{eff} = Z - (\text{number of } 2s \text{ and } 2p \text{ electrons} - 1)(0.35) - (2)(0.85)$$

Note that we subtract 1 from the total number of 2s and 2p electrons as the electron of interest cannot screen itself.

There are two things we see in these results. First, the estimated values for Z_{eff} are larger than the experimental (theoretical) values for Z_{eff}. Second, the smallest values for Δ are for the two elements that have *s* electrons only. Slater's rules assume that *s* and *p* electrons are equally effective at screening each other when *p* electrons are, in fact, less effective at screening; thus, Slater's rules tend to overestimate Z_{eff} when the valence shell includes *p* electrons. The effect is greatest with boron, which is the first element in this series to include a *p* electron.

Problem 2. Use Slater's rules to evaluate the following three possible electron configurations for scandium—[Ar]$4s^2 3d^1$, [Ar]$4s^1 3d^2$, and [Ar]$3d^3$—and comment on how your results support [Ar]$4s^2 3d^1$ as the expected electron configuration.

The values for Z_{eff} are shown here; note that you need to consider both the *s* and the *d* valence electrons.

[Ar]$4s^2 3d^1$, or in Slater's order $(1s^2)$ $(2s^2\ 2p^6)$ $(3s^2\ 3p^6)$ $(3d^1)$ $(4s^2)$

for a 4*s* electron $Z_{eff} = 21 - (1)(0.35) - (9)(0.85) - (10)(1.00) = 3.00$
for a 3*d* electron $Z_{eff} = 21 - (18)(1.00) = 3.00$

[Ar]$4s^1 3d^2$, or in Slater's order $(1s^2)$ $(2s^2\ 2p^6)$ $(3s^2\ 3p^6)$ $(3d^2)$ $(4s^1)$

for a $4s$ electron $Z_{eff} = 21 - (10)(0.85) - (10)(1.00) = 2.50$
for a $3d$ electron $Z_{eff} = 21 - (1)(0.35) - (18)(1.00) = 2.65$

[Ar]$3d^3$, or in Slater's order $(1s^2)$ $(2s^2\ 2p^6)$ $(3s^2\ 3p^6)$ $(3d^3)$

for a $3d$ electron $Z_{eff} = 21 - (2)(0.35) - (18)(1.00) = 2.30$

As greater values for Z_{eff} provide for a stronger attractive force for an electron (via Coulomb's law), the electron configuration with the greatest average Z_{eff} for its valence electrons will provide the most stable electron configuration. The average Z_{eff} for these three options, in order, are 3.00, 2.60, and 2.30; thus, [Ar]$4s^2 3d^1$ is the most stable electron configuration.