Slater's Rules for Effective Nuclear Charge

Skills to Develop

- Describe how to calculate the shielding constant using Slater's rules
- Identify a periodic trend for effective nuclear charge
- Calculate effective nuclear charge

Effective nuclear charge is really important, because it determines the size and energy of orbitals, which determine most properties of atoms. So it's useful to be able to predict effective nuclear charge! Slater's rules give a simple approximation of effective nuclear charge that works pretty well.

Based on the last section, we can expect that effective nuclear charge will depend on the number of electrons that might get between, so it depends on the electron we are looking at. For any electron, to find the effective nuclear charge it feels, we need to know how many other electrons might get in the way, and how much time it spends near the nucleus. Based on these, we will calculate a **shielding constant**, S. Then,

$$Z_{eff} = Z - S \tag{1}$$

where Z is the actual nuclear charge (which is the same as the atomic number) and Z_{eff} is the effective nuclear charge.

To calculate S, we will write out all the electrons in atom until we get to the group of the electron we want, like this:

(1s)(2s,2p)(3s,3p)(3d)(4s,4p)(4d)(4f)(5s,5p) etc.

1. Each other electron (not counting the one we have picked) in the same group () as the chosen electron, contributes 0.35 to S. (This means electrons in the same group shield each other 35%.
2. If the chosen electron is d or f, every electron in groups to the left contributes 1.00 to S. (This means that d and f electrons are shielded 100% by electrons with lower n or same n and lower ℓ.)
3. If the chosen electron is s or p, all the electrons in the next lower shell (n - 1) contribute 0.85 to S. (This means that s and p electrons are shielded 85% by the electrons one shell lower.) And all the electrons in even lower shells contribute 1.00 to S. (All electrons in shells n - 2 or lower shield 100%.)

The outcome of this is that Z_{eff} changes suddenly when going from one period to another. As you go from Li to Be, Z_{eff} (for the new electron) increases, because you add one proton (Z + 1) and it is only shielded 35% (S + 0.35). When you get to B, you added one proton, and it still shields 35%. So Z_{eff} increases until you go from Ne to Na. Now, suddenly, the (1s) electrons shield 100% instead of 85%, and the (2s,2p) shield 85% instead of 35%! So Z_{eff} goes down suddenly. From Na to Ar, Z_{eff} increases slowly again. From Ar to K, it drops again.

For an example, let's calculate Z_{eff} for a d electron in Zn, atomic number 30. Notice that although 4s is filled, we don't include it because it comes to the right of the d electrons we are looking at.

(1s)(2s,2p)(3s,3p)(3d)

$$S = 18(1) + 9(0.35) = 21.15 \tag{2}$$

$$Z_{eff} = 31 - 26 = 5 \tag{3}$$

You can see that just like changing periods (going to a new shell), going from the d-block to the p-block also gives a drop in Z_{eff} (partly because you actually are going to a new shell, as well as subshell).

Contributors and Attributions

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