

# 1 Morning class week 4 day 1: Effective nuclear charge

## 1. The second row elements Li, Be, B

- (a) In exactly the same way that last week we compared  $Z_{eff}$  for the Li and Be atoms, we can try to compare  $Z_{eff}$  for the Be and the B atoms. Unfortunately, to do so, we will have to make one additional (and fairly poor) approximation.

In the B atom, the outermost electrons are both  $2s$  and  $2p$  orbitals.  $2p$  orbitals are not spherical and hence do not follow Gauss's Law. In this problem set, we will be forced to make the simplifying, but not very satisfying, approximation that for shielding, we can think of electrons in  $p$  orbitals as if they had spherical charge distribution.

With that noted, we begin our analysis. In Figure 8-36, you can see that although the  $2s$  and  $2p$  orbitals have different energies, the difference in energy is not too big. Armed with this information and knowing the virial theorem, can we conclude the B  $2s$  and  $2p$  electrons have nearly the same electrostatic energies?

- (b) Using Coulomb's Law and your knowledge of the radial distribution functions can you conclude electrons in these orbitals spend a good portion of their time at roughly the same distance from the nucleus? Explain your reasoning.
- (c) What would be your guess as to the fraction of the time an electron in a B  $2s$  orbital is inside with respect to an electron in a B  $2p$  orbital and vice-a-versa?
- (d) Guess the effective nuclear charge of an electron in a B  $2s$  orbital.
- (e) Guess the effective nuclear charge for an electron in a B  $2p$  orbital.

2. **An initial estimate of second row element's effective charges** Using these same thoughts, estimate the effective nuclear charge for a  $2p$  electron for the six second row elements in the periodic table: B, C, N, O, F, and Ne. This group of six elements form the first complete row of the *main group* in the periodic table. Place your values in the table given below.

Element	Estimated Effective Charge	True Effective Charge
B		2.42
C		3.14
N		3.83
O		4.45
F		5.10
Ne		5.76

3. **An improved estimate of second row element's effective charges** An examination of this table shows the estimated effective charge is not very accurate when compared with the true effective charge. If instead of assuming that an outer shell  $2p$  electron shields another outer shell electron 50% of the time, we had chosen an alternate number, we might have obtained better numerical agreement. Calculate what the estimated effective charge would have been had we assumed that the highest energy  $2p$  electron spent one-third rather than

one-half of its time interior with respect to the other  $n = 2$  electrons. Place your new values in the table below.

Element	Revised Est. Effective Charge	True Effective Charge
B		2.42
C		3.14
N		3.83
O		4.45
F		5.10
Ne		5.76

4. **Effective charges for the alkali metals** It is approximately true that the  $1s$  orbital always lies closer than the  $2s$  orbital on this same atom, the  $2s$  orbital always lies closer than the  $3s$  orbital on this same atom, and so forth. Based on this assumption, please estimate the effective nuclear charge of electrons in the outermost shell for H, Li, Na, K, Rb, and Cs. Enter your estimates onto the table given below.

The graphs in Figure 8-35 show, however, that the electrons in an outer shell are not always on the exterior of earlier filled shells. A more accurate estimate is that the outermost  $s$  orbital is exterior to the interior orbitals only 85% of the time. Based on this revised estimate, please place revised values for the estimated effective nuclear charge in the table given below.

Element	Est. Effective Charge	Rev. Est. Effective Charge	True Effective Charge
H			1.00
Li			1.28
Na			2.51
K			3.50

5. **Effective charges for third main group elements** Now consider the third row of the main group series: Na, Mg, Al, Si, P, S, Cl, and Ar. In the table below, please use all the revisions applied in the last two problems in calculating the estimated effective nuclear charge for these elements.

Element	Rev. Est. Effective Charge	True Effective Charge
Na		2.51
Mg		3.31
Al		4.07
Si		4.29
P		4.89
S		5.48
Cl		6.12
Ar		6.76

6. Review what you have just learned.