Key for Practice Problem for Slater's Rules

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

element	Z_{eff} (theory)	electron configuration	Z_{eff} (calc)	Δ
Li	1.28	$1s^2 2s^1$	1.30	0.02
Be	1.91	$1s^2 2s^2$	1.95	0.04
B	2.42	$1s^2 2s^2 2p^1$	2.60	0.18
C	3.14	$1s^2 2s^2 2p^2$	3.25	0.11
N	3.83	$1s^2 2s^2 2p^3$	3.90	0.07
O	4.45	$1s^2 2s^2 2p^4$	4.55	0.10
F	5.10	$1s^2 2s^2 2p^5$	5.20	0.10

Values for Z_{eff} are calculated for a $2s$ or a $2p$ electron using the following formula

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

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.