Engel 9.16

**Background.** Engel provides a formula in problem 9.15 that gives the energy of a one-electron atom as a function of the principal quantum number, \( n \), and the atomic number, \( Z \). The ionization potential (IP) of the atom is the negative of this energy.

**Problem.** The first IP of Li, a three-electron atom, is 5.39 eV. Use this value and the energy formula described above to calculate \( Z_{\text{eff}} \). This "effective" nuclear charge (really an "effective" atomic number because it must be multiplied by \(-q_e\) to obtain the nuclear charge) can be viewed as the nuclear charge that binds the 2s electron to the atom.

**Answer.** Because we are interested in the 2s electron, \( n = 2 \). Defining needed constants ...

\[
\begin{align*}
\text{In}[51]:= & \quad \text{Clear}[\text{Zeff}, \text{IP}, \text{qe}, \epsilon_0, a_0, n] \\
\text{IP} &= 5.39 \\
\text{qe} &= -1.6022 \times 10^{-19} \\
\epsilon_0 &= 8.8542 \times 10^{-12} \\
a_0 &= 5.2918 \times 10^{-11} \\
n &= 2
\end{align*}
\]

\[
\text{Out}[52]= 5.39 \\
\text{Out}[53]= -1.6022 \times 10^{-19} \\
\text{Out}[54]= 8.8542 \times 10^{-12} \\
\text{Out}[55]= 5.2918 \times 10^{-11} \\
\text{Out}[56]= 2
\]

Convert IP from eV to J by multiplying by \(1.6022 \times 10^{-19}\) (note that this conversion factor is just \(-q_e\)).

\[
\text{In}[57]:= \quad \text{IP} = \text{IP} \times (-\text{qe})
\]

\[
\text{Out}[57]= 8.63586 \times 10^{-19}
\]

Rearranging Engel's energy formula from problem 9.15 and solving for \( Z \) we obtain

\[
\text{In}[58]:= \quad Z = \sqrt{\frac{\text{IP} \pi \epsilon_0 a_0 n^2}{\text{qe}^2}}
\]

\[
\text{Out}[58]= 1.25882
\]

Li's atomic number is 3. The atomic number experienced by the 2s electron is much smaller, 1.26. From this result, it appears that the 2s electron experiences Coulombic effects from the entire atomic core, where the core's charge is roughly equivalent to the sum of the charges of its constituent particles: nucleus (+3), 1s core electron #1 (-1), and 1s core electron #2 (-1).