Engel 9.15

Problem. Engel provides a formula for the energy of a one-electron atom as a function of the principal quantum number, *n*, and the atomic number, *Z*. The problem is to calculate ionization energies (IE) or ionization potentials (IP) for several one-electron atoms in their *ground states*: H, He^+, Li^{2+} and Be^{3+}. I added a second challenge to this: to compare your IP to experimental values.

Answer. The ionization potential (IP) of a one-electron atom equals the negative of the total energy. Therefore the energy formula provided by Engel is an IP formula once one reverses its sign. The *ground states* correspond to *n* = 1.

```
In[40]:= Clear[Z, qe, ϵ0, a0 ]
         Z = {1, 2, 3, 4}
         qe = -1.6022 × 10^-19
         ϵ0 = 8.8542 × 10^-12
         a0 = 5.2918 × 10^-11

Out[41]= {1, 2, 3, 4}

Out[42]= -1.6022×10^-19

Out[43]= 8.8542×10^-12

Out[44]= 5.2918×10^-11
```

Engel's energy formula (with the sign reversed and assuming *n* = 1 for the ground state atom)

```
In[45]:= Clear[IP]
```

$$IP = \frac{Z^2\, qe^2}{8\,\pi\,\epsilon0\, a0}$$

```
Out[46]= {2.17992×10^-18, 8.71969×10^-18, 1.96193×10^-17, 3.48787×10^-17}
```

These energies obtained above are in Joules. The conversion factor to eV is 1.6022×10^{-19} (notice that this is also the charge on a proton!).

In[47]:=
$$IP = \frac{IP}{-qe}$$

```
Out[47]= {13.6058, 54.4232, 122.452, 217.693}
```

These are the calculated ionization potentials in eV. Experimental values can be obtained from many sources.

One nice collection of atomic or "elemental" data is located at WebElements (http://www.webelements.com/). Click on the atom of interest and then click on **Ionization energies** (located under **Electronic properties** in the sidebar on the left). I found these data (in kJ/mol)

H 1st 1312.0

He 2nd	5250.5
Li 3rd	11815.0
Be 4th	21006.6

These experimental values can be converted to eV by 1) dividing them by Avogadro's number (gives IP in kJ), 2) multiplying by 1000 (gives IP in J), and dividing by -qe (gives IP in eV)

In[48]:=
```
Clear[exptIP]
exptIP = {1312.0, 5250.5, 11815.0, 21006.6}
```
$$\text{exptIP} = \frac{\text{exptIP}}{6.0221\times 10^{23}}\,1000\left(\frac{1}{-\text{qe}}\right)$$

Out[49]= {1312., 5250.5, 11815., 21006.6}

Out[50]= {13.5978, 54.4172, 122.453, 217.716}

The experimental values agree well (<<1% rel. error) with the calculated values.