More thoughts on Ionic bonding

We have seen that the potential energy as a function of distance for our ionic bonding model has three parts.

$\Delta E_{\infty} = IE + EA$ the energy difference between the ions and the neutral atoms at infinite separation. This is equal to the IE for the cation (positive) + the EA for the anion (negative)

$\Delta E_{Coulomb}(R) = \dfrac{q_1 q_2}{4\pi\varepsilon_0 R}$ the Coulomb potential term that is distance dependant (and will be negative since the two charges will have opposite sign)

$\Delta E_{\mathrm{Repulsion}}(R) = Ae^{-\alpha R}$ Where A is a constant that deals with the magnitude of the repulsion and alpha is a constant the determines the distance dependence.

It can be a challenge to see if this model is working quantitatively as we need to get some data to try it out.

Let's examine the following data for NaCl.

The equilibrium bond distance is 2.365 Å.

The bond dissociation energy is 4.27 eV
The ionization energy of Na is 5.14 eV
The electron affinity of Cl is 3.62 eV

1 eV = 1.602×10^{-19} J

What is ΔE_{∞}?

What is $\Delta E_{Coulomb}(R_e)$ at the equilibrium bond length?

If you assume the difference between these two and the dissociation energy is the result of the repulsion term, how large is this term?

The challenge with our interpreting the repulsion term is that is has two unknown constants.

Use the fact that the potential is a minimum at 2.365Å and the value of $\Delta E_{\text{Repulsion}}(R_e)$ at the equilibrium distance to determine both A and alpha. (note: this will require some calculus).