Modern Physics Ch. 11: Problems 1,2,5

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1. Potassium Iodide a) This is just subtraction, following the description of ionic bond energies in the text. The ionization energy of K is $E_{iK} = 4.34$ eV and the electron affinity of I is $E_{aI} = 3.06$ eV and so the activation energy is

$$E_a = E_{iK} - E_{aI} = 1.28 \text{ eV}.$$

b) We need to solve

$$U(r) = 4\mathcal{E}\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + E_a$$

for the constants $\mathcal{E}, \sigma$ given at equilibrium $r_0 = 0.305$ nm and $U(r_0) = -3.37$ eV. We also know that $\frac{dU}{dr} = 0$ at $r = r_0$. So we take the derivative

$$\frac{dU}{dr} = \frac{d}{dr}\left(4\mathcal{E}(\sigma^{12}r^{-12} - \sigma^6 r^{-6}) + E_a\right)$$

after careful algebra:

$$= 24\mathcal{E}\sigma^6 r^{-7}(-2\sigma^6 r^{-6} + 1)$$

At $r = r_0$ this will be zero, so the quantity in parentheses must then be zero (everything else is nonzero constants).

$$1 - 2\sigma^6 r^{-6} = 0$$

and solving for σ:

$$\sigma = \left(\frac{1}{2}\right)^{1/6} r_0 = 0.272 \text{ nm}.$$

Then you plug into $U(r)$ all the known values at $r = r_0$ and solve for $\mathcal{E} = 4.65$ eV.

c) When I was preparing for class, I misread the problem. I thought it wanted the *energy* to disrupt the bond (that's easy, see p. 374). But we want the *force*.

This must be the maximum radial attractive force between the atoms. Recall that the force is the negative of the potential gradient:

$$F = -\frac{dU}{dr}.$$

We have this expression in part b) above (without the minus sign, which won't matter anyway, it only sets the direction). $-F = \frac{dU}{dr}$ So we have to take another derivative to find r_F, the point where the slope of the potential is greatest (outside r_0).

$$-\frac{dF}{dr} = 24\mathcal{E}\sigma^6 r^{-8}(-7 + 26\sigma^6 r^{-6})$$

at $r = r_F$ this will be zero, so this means again the part in parentheses is zero, so

$$r_F = (26\sigma^6/7)^{1/6} = 0.3385 \text{ nm}.$$

Then plug r_F into $-F = \frac{dU}{dr}$ and get the magnitude of $F = 6.57 \times 10^{-9}$ newtons. Whew! That was a job for Frink: I put in the values in eV and nm and got out an answer in N.

Here is a Frink transcript (`s` is σ, `E` is $\mathcal{E}$, `r` is r_F):

```
setPrecision[4]
r = ((26 * s^6)/7)^(1/6)
3.384864640124462e-10 m (length)

r -> "nm"
0.3385 nm

E = 4.65 eV
7.449e-19 m^2 s^-2 kg (energy)

F = 24*E*(s^6)*r^(-7)*( 1 - 2*s^6*r^(-6) )
6.570e-9 m s^-2 kg (force)

F -> "nN"
6.57 nN
```

2. NO reduced mass. We are told the frequency for the $\nu = 0$ to $\nu = 1$ transition is 5.63×10^{13} Hz. The effective spring constant is $K = 1530$ N/m from the table. Calculate the reduced mass μ using both the frequency and the reduced mass formula.

$$\mu = \frac{K}{\omega^2} = 1.223 \times 10^{-26} \text{ kg} = 7.363 \text{ amu}.$$

The reduced mass can also be gotten from the masses on the periodic table:

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = 7.468 \text{ amu},$$

just a few percent different.