

ENGR 240
Homework #2
Due: Wednesday, January 24, 2001

1. Two uncharged molecules exhibit van der Waals bonding between them, with attractive and repulsive energies (E_A and E_R) given by:

$$E_A = \frac{-8.4 \times 10^{-18} \text{ J} \cdot \text{\AA}^5}{r^5}$$

$$E_R = \frac{7.0 \times 10^{-14} \text{ J} \cdot \text{\AA}^{13}}{r^{13}}$$

where J is Joules, and

r is the interatomic separation distance in angstroms (\AA) [$1\text{\AA} = 10^{-10} \text{ m}$]

- a) Make a single computer generated plot (spreadsheet okay), that shows E_A , E_R , and E_N on the same set of axes, in the range $r = 3 \text{ \AA}$ to $r = 10 \text{ \AA}$. [If you are using a spreadsheet, to make it look smooth, start with a list of closely spaced r values (3.0, 3.1, 3.2.....10.0). Find out how to fill a list like this, you don't want to enter all these by hand!]
 - b) Calculate (mathematically find where the minimum is) the equilibrium interatomic spacing, r_0 , and locate this value on your plot.
 - c) Calculate the bond energy (E_0) in Joules.
 - d) What is the bond energy in kJ/mole (of bonds)?
2. State which is higher and briefly explain why:

Density of:

- a) phosphorous pentachloride (PCl_5)
- b) magnesium oxide (MgO)

3. State which is higher and briefly explain why:

Electrical conductivity of:

- a) calcium (Ca)
- b) calcium fluoride (CaF_2)