Homework 3: Problem 4.5

March 3, 2008

We're given the following data for polarizability:

Species	$\alpha 10^{25}$ cm^3
CH_4	26.0
C_2H_6	44.7
C_3H_8	62.9
CH_3Cl	45.6
CH_2Cl_2	64.8
$CHCl_3$	82.3
CCl_4	105.0

As suggested by the paragraph on page 174, assume that the polarizability is linearly proportional to the number of each atom type:

$$\alpha = \alpha_C n_C + \alpha_H n_H + \alpha_{Cl} n_{Cl} \text{ [+ 1 point]}$$

The easiest way to determine the unknown coefficients α_i is by minimizing the sum of squares in MATLAB. To do that, set up a matrix of number of atoms:

$$X = \begin{bmatrix} 1 & 4 & 0 \\ 2 & 6 & 0 \\ 3 & 8 & 0 \\ 1 & 3 & 1 \\ 1 & 2 & 2 \\ 1 & 1 & 3 \\ 1 & 0 & 4 \end{bmatrix}$$

Set up a similar column vector with the known polarizability. $X\backslash\alpha$ will give you the three coefficients:

$$\begin{aligned} n_C &= 11.275 \\ n_H &= 3.650 \\ n_{Cl} &= 23.095 \text{ [+ 3 points]} \end{aligned}$$

This result is consistent with the notion that larger atoms will be more polarizable. The result of this least sum of squares fit is:

Species	α	α_{fit}
CH_4	26.0	25.9
C_2H_6	44.7	44.5
C_3H_8	62.9	63.0
CH_3Cl	45.6	45.3
CH_2Cl_2	64.8	64.8
$CHCl_3$	82.3	84.2
CCl_4	105.0	103.4

Not a bad fit. Using these values, the predicted polarizabilities are:

$$\begin{aligned} C_4H_{10} &= 81.6E-25 \text{ [cm3] [+ 3 points]} \\ C_2H_5Cl &= 63.9E-25 \text{ [cm}^3\text{] [+ 3 points]} \end{aligned}$$

Make sure you include the $E-25$ to get full credit.