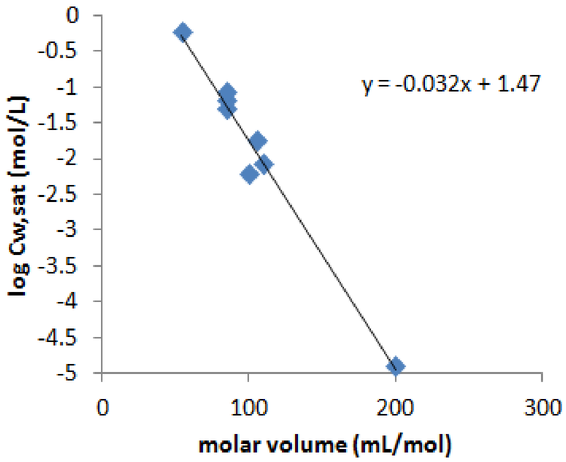
Environmental Chemistry, Homework set

Partitioning part 1 - Solutions

1. Aqueous solubility of chlorinated alkanes

Recall from the notes that within a class of compounds (here: chlorinated alkanes), there is a linear relationship between log C_w^{sat} and the molar volume. Plot the data from the table as follows:



We can thus establish the relationship: log C_w^{sat} = -0.032*(molar volume)+1.47

For dichloromethane we find: log C_w^{sat} = -0.594; C_w^{sat} = 0.25 mol/L.

Now we can determine the K_{ow} using the general relationship between K_{ow} and C_w^{sat}:

log $K_{i,ow}$=(-log $C_{i,w}{}^{sat}$+ 3.70+log MW_i)/1.08.

In this relationship, C_w^{sat} must be in units of ppm, whereby 1 ppm = 1 mg/L. So

C_w^{sat} =(0.25 mol/L)*(85 g/mol) = 21.25 g/L = 21250 ppm.

$K_{i,ow}$=(-log (21250)+ 3.70+log(85))/1.08 = 1.20; K_{ow} = 15.85

2. Benzene in groundwater

First calculate $K_{benzen,\ aw}$ at 5°C. This can be done using the relationship $\ln\frac{K_{12}(T_2)}{K_{12}(T_1)} = \frac{\Delta_{12}H}{R}\left(\frac{1}{T_1}-\frac{1}{T_2}\right)$

Or, more simply, from table 3.5 given in the notes, we know that – given a $\Delta_{12}H$ of 20 kJ/mol – K_{12} decreases by a factor of 1.33 for every 10°C decrease in temperature. So:

$K_{benzen,aw}$ (5°C)= $K_{benzen,aw}$ (25°C) /$(1.33)^2$=0.12 = $C_{benzen,\ air}$ / $C_{benzene,\ water}$

Since we know both $K_{benzene,\ aw}$ and $C_{benzene,\ water}$, we can calculate the concentration of benzene in air:

$C_{benzene,\ air}$ = $K_{benzene,\ aw}$ * 100 μg/L = 12 μg/L

We have 900 mL of air in the bottle, so the total mass of benzene in air is:

0.9 L * 12 μg/L = 10.8 μg

The mass of benzene in 100 mL water is:

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0.1 L * 100 μg/L = 10 μg

So total mass of benzene in the bottle is:

10.8 μg + 10 μg = 20.8 μg

Considering that all this benzene originally came from 100 mL of groundwater, the concentration of benzene in the original groundwater was 20.8 μg/ 100mL = 208 μg/L.

3. Disinfectant in air

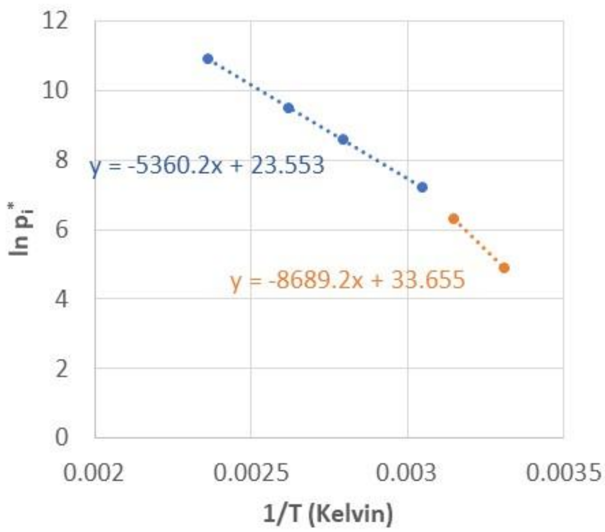
Recall the relationship between p_i^* and temperature:

$$\log p_i^* = -\frac{A}{2.303 * T} + B$$

Or on a natural log (ln) basis:

$$\ln p_i^* = -\frac{A}{T} + 2.303 * B$$

Plot ln p_i^* vs. 1/T (in Kelvin) to find p_i^* (separately for T > T_m, where 1,4-DCB is a liquid and T < T_m, where it is a solid). We find:



a) Inserting for T = 20 °C, we obtain: ln p_i^* = -8689.2*(1/293)+33.655 = 3.99; p_i^* = 54.5 Pa.

To calculate the concentration in air (in M), use the ideal gas law:

$$C_{i,a} = \frac{p_{i,a}}{RT}$$

Where R = 8314 M^{-1} Pa K^{-1} and T = 293 K. We find: $C_{i,a}$ = 22.4 μM

b) Inserting for T = 60 °C, we obtain: ln p_i^* = -5360.2*(1/333)+23.553 = 7.46; p_i^* = 1730.7 Pa

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Converting to concentration using T = 333 K we find $C_{i,a}$ = 625 μM