CHEMISTRY 253
Spring, 2015 - Dixon
Last Group Assignment - Key

1. Ethanol (C_2H_5OH) has some advantages and disadvantages as a fuel. It is relatively easy to produce from sugars and starch. One way to overcome some disadvantages of ethanol as a fuel is to convert some ethanol to acetic acid (CH_3COOH) and to combine acetic acid with ethanol to form ethyl acetate ($C_2H_5O_2CCH_3$). 8 pts

compound	melting point	boiling point	octanol water partition coefficient
ethanol	-114°C	78.4°C	0.50
ethyl acetate	-119°C	77°C	4.6

a) By looking at the stoichiometry of the reaction of ethyl acetate with oxygen (vs. ethanol), which appears to be a more energy dense fuel? (you can also compare the reactions with coal – C or methane if that helps).
Reaction stoichiometry:
ethyl acetate: $C_2H_5O_2CCH_3 + 5O_2 \rightarrow 4CO_2 + 4H_2O$ so 5 mol O_2 per 4 mol CO_2 - which is the same as for carbon
ethanol: $C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O$ so 3 mol O_2 per 2 mol CO_2 – which is a higher ratio ***indicating greater energy density in ethanol****.*

b) Give one property of ethyl acetate is likely to overcome a disadvantage of using ethanol.
While the melting and boiling points are very similar, ethyl acetate is much less polar (higher K_{ow}). This will decrease problems of corrosion and retention of water that occurs with ethanol. A secondary advantage would be that the vapor pressure of ethyl acetate is not much reduced in gasoline vs. as a pure compound, while ethanol is more volatile in gasoline, requiring greater reformulation of gasoline.

2. Many insecticides have low oral LD_{50} values but high dermal LD_{50} values for humans. (12 pts)
a) Does this make the dermal route or the oral route more dangerous for humans?
A low LD_{50} value is more toxic (lower concentration needed to kill someone) so the oral route is more dangerous.
b) Insect's "skin" is much more porous than that of humans. How will that affect the toxicity of methyl parathion in insects.
The dermal (or equivalent) route for insects will be easier, making methyl parathion more toxic in insects.

c) Methyl parathion, which has an oral LD_{50} of 14 mg/kg, accidently contaminated wheat flour so that 0.08% by mass of the wheat flour was methyl parathion. How many grams of contaminated wheat would be needed to be consumed to cause a lethal dose in a "typical" 38 kg boy.
mass of wheat = (14 mg/kg)(38 kg)/(0.08/100) = ***665 g. of wheat.***