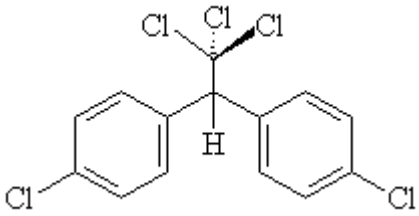
WUCT: Chemistry of Farming Sample Question

1. DDT, or dichlorodiphenyltrichloroethane, is an organochlorine which was developed as an insecticide. It has become infamous in history for its detrimental environmental impacts. Although DDT contains several components, the major component (77%) is the *p,p'* isomer, which is shown below.



   a. DDT is highly hydrophobic and insoluble in water, despite the existence of several chlorine atoms. Using the structure above, explain this phenomena.

Even though the chlorine atoms are electronegative and add polarity to the compound, the benzenes themselves are highly hydrophobic and nonpolar. The electronegativity difference between C and H is very small and the difference between C and C is zero. In addition, the molecule above is symmetrical, which may contribute to the fact that there is no dipole moment horizontally, only upward toward the chlorine atoms.

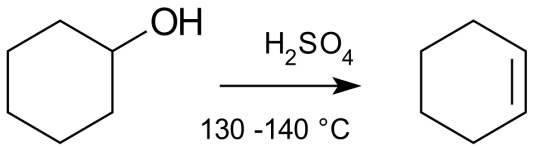
   b. On the structure above, label every carbon atom with its hybridization and geometry.

Two carbon atoms in the center - sp^3, tetrahedral
Carbon atoms in the benzene ring - sp^2, trigonal planar

   c. Write the molecular formula for the DDT structure shown above.

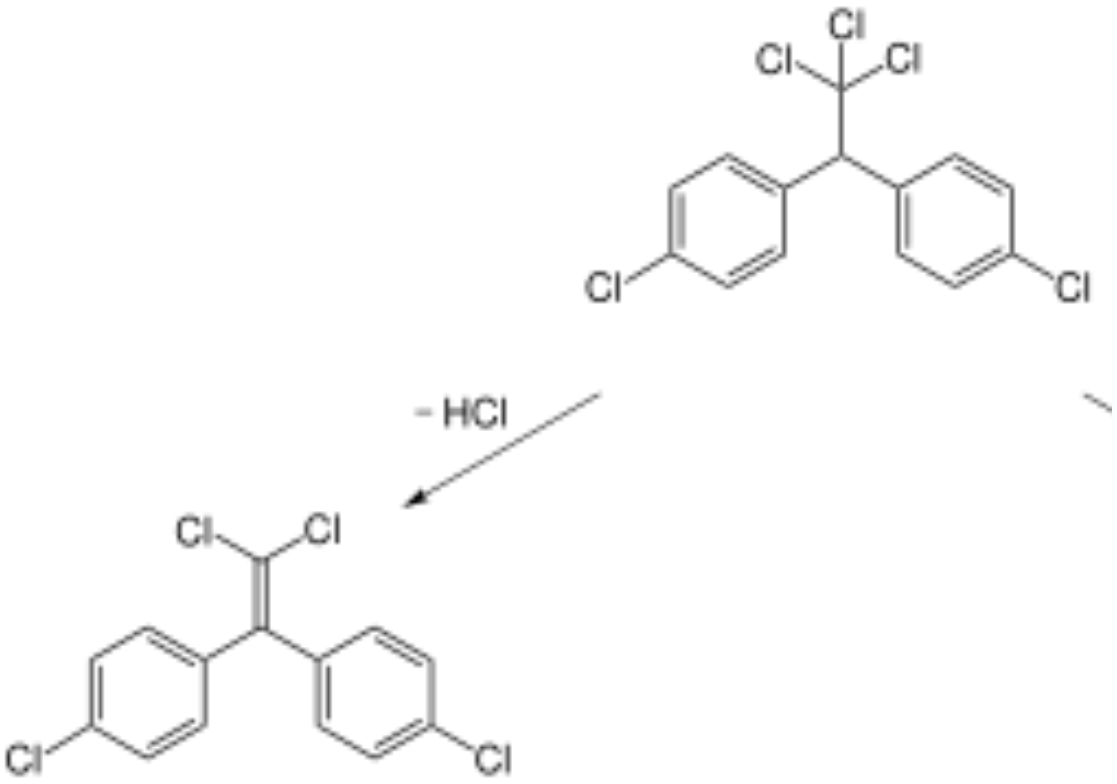
$C_{14}H_9Cl_5$

d. An elimination reaction is an organic reaction in which two substituents are removed from a molecule and a double bond is formed between the two. An example of an elimination reaction is shown below, where the two substituents are hydroxide and hydrogen groups.



DDT can undergo an elimination reaction, where the two substituents that are lost are hydrogen and chlorine. **Using structures, show the elimination reaction that DDT undergoes and the resultant molecule.**

Answer:



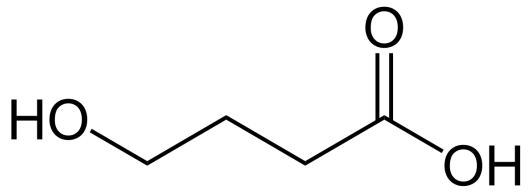
e. When DDT is synthesized, there are several impurities that must be removed before use. Agricultural chemists often use distillation to separate compounds. Explain the purpose of **vacuum distillation, boiling chips, and Bunsen burners** in distillation **respectively**.

Vacuum distillation is performed under reduced pressure to allow purification of compounds that may not be distilled at feasible pressures. Lowering the ambient pressure also lowers the boiling point, making it easier to distill compounds with high boiling points (typically above 150°C).

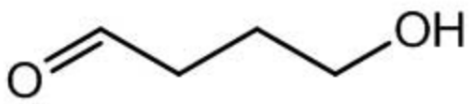
Boiling chips are tiny unevenly shaped pieces that make liquids boil more calmly. Also (not needed for credit) they provide nucleation sites to prevent superheating or bumping.

Bunsen burners are used to heat the solution to boiling temperatures.

f. Say that two compounds are involved in these agricultural separations are 4-hydroxybutanal and 4-hydroxybutanoic acid. The structures are shown below. Each is kept in a flask and distillation is performed to separate the two. Which compound will be remaining in the flask after the procedure is completed? Hint: think boiling points and polarity.



4-hydroxybutanal



4-hydroxybutanoic acid

Hydrogen bonding in the carboxylic acid group of the 4-hydroxybutanoic acid causes the molecule to have much more intramolecular bonding and thus have a higher boiling point. The carboxylic acid has more hydrogen bond donors and acceptors, another justification for why it will have a higher boiling point. Thus, 4-hydroxybutanoic acid will be remaining in the flask.

2. Determining favorabilities of different chemical reactions in agricultural chemistry is extremely important, whether this is in the form of Gibb's free energy, Ksp values, or entropy.

    a. Dissolving compounds is extremely important in agricultural chemistry. The molar solubilities and Ksp values for different compounds is important in understanding how much of a compound will dissolve in a solution.

    The Ksp value of PbI_2 in pure water at room temperature is 1.4×10^{-8}. An excess PbI_2 solution is added to two solutions.

    Solution 1 contains 50 mL of 0.10 M $Pb(NO_3)_2$ aqueous solution. Solution 2 contains 600 mL of 0.005 M KI aqueous solution.

    In which solution will more PbI_2 dissolve? Show all work.

Solution 1:

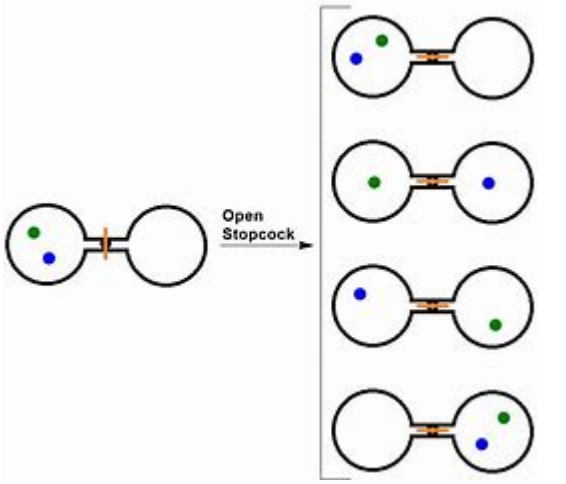
Initial	Change	End
50 mL 0.10 M Pb^{2+}	+x moles Pb^{2+} +2x moles I-	$1.4 \cdot 10^{-8} = [0.10\ M + x][2x]$

Solution 2:

Initial	Change	End
600 mL 0.005 M I^-	+x moles Pb^{2+} +2x moles I-	$1.4 \cdot 10^{-8} = [0.05\ M + 2x][x]$

[x] will be higher for solution 2, so PbI_2 will dissolve more in solution 2.
This can be understood intuitively, even though there is a greater volume of solution 2, the concentration is much lower so there will be more PbI_2 that can dissolve.

b. The following diagram shows the possible number of microstates for a two chamber container with two gas particles.



For two gas particles, there are four possible microstates. For a five atom system, how many possible microstates exist? Show all work

1 + 5 + 10 + 10 + 5 + 1 = 32

c. The efficiency of photosynthesis is a topic of great interest for agricultural chemists.

The reduction of each mole of CO_2 to hexose level requires 2 moles of NADPH. Forming 2 mol of NADPH needs 4 mol of electrons by photosystem I. Hence, eight photons total are needed to generate the required NADPH for reducing a single mole of CO_2 to the level of hexose.

The delta G^o for the reduction of CO_2 to the level of hexose is 477 kJ/mol. A mole of 660 nm photons has an energy content of 199 kJ

Determine the energy efficiency of photosynthesis under standard conditions.

8 mol of photons is equivalent to 1594 kJ (381 kcal) energy input. Thus, the overall efficiency of photosynthesis under standard conditions is at least 477/1594, or 30%.