Estimating Molecular Size and Bond Length

Introduction

Molecules are very small. Exactly how small was not definitively determined until early this century with the advent of X-ray diffraction, which probes molecules with photons that are similar in wavelength to the size of a molecule. There is a surprisingly simple way, however, to estimate the size of certain molecules, by taking advantage of their chemical properties and a little geometry. Some molecules form oils, which float on the surface of water. The fatty acid known as oleic acid ($C_{18}H_{34}O_2$), which is a major component of olive oil, is one such molecule. Oleic acid has a polar group on one end (such as O^-) that strongly attracts water, and the molecules align themselves so that they "stand on their heads." The small polar part of the molecule contacts the water while the remaining part of the molecule is hydrophobic and stays out of the water. Therefore, if a drop of this fatty acid is placed on the surface of the water, it spreads out in a monolayer, forming a cylinder whose height is equal to the length of the molecule. Recall that the volume (V) of a cylinder is $V = \pi r^2 h$, where r is the radius of the cylinder and h is its height. Therefore, as long as the volume of the drop is known and the diameter of the cylinder is measured, the height of the cylinder can be calculated.

Procedure

Show all calculations, diagrams, etc. in your notebook. You may not leave until all of the calculations have been completed.

<u>Volume of the Cylinder</u>: The volume of the cylinder is simply the volume of the oleic acid (and thus, the total number of oleic acid molecules) that will be added to the water. Later on, you will find the height of the cylinder formed by the oleic acid in one drop of solution, and so your first task is to find the volume of a single drop of oleic acid.

To do this, clean and dry a graduated cylinder. Count the number of drops it takes to fill the cylinder with exactly 2.0 mL of oleic acid solution. This solution is ~0.2% by volume dissolved in ethanol – be sure to obtain the exact percentage from the bottle! Remember that 1 mL = 1 cm^3. Repeat this process several times until you obtain a reproducible number of drops (±5 drops between trials) per 2.0 mL. Then, calculate the volume of a single drop of oleic acid solution.

The volume of the cylinder used in the next part is not the same as the volume calculated above, because the solution is part oleic acid and part ethanol. The ethanol will dissolve immediately in the water, leaving only the oleic acid on the surface. Thus, you should use the percentage of oleic acid to find the volume of oleic acid in one drop of solution.

<u>Diameter of the Cylinder:</u> Fill a pie pan with water. Sprinkle a light dusting of talc over the surface of the water so that you can better visualize your results. Then, add a drop of the oleic acid solution onto the surface water as close to the center of the pie pan as you can get. A circle should immediately form where the talc has been pushed out of the way. Carefully measure the diameter of the circle, which is the base of your cylinder. Repeat this procedure several times to get a good measurement of the diameter. Remember that the relevant formula calls for the radius, not the diameter.

<u>Height of the Cylinder:</u> Calculate the height of the cylinder from the volume equation given above. The height of the cylinder corresponds to the length of one oleic acid molecule. State whether or

not this length is reasonable. The structure of oleic acid is shown below. Assuming that the oleic acid has its -CO_2H end in the water, calculate the height of an oleic acid molecule.

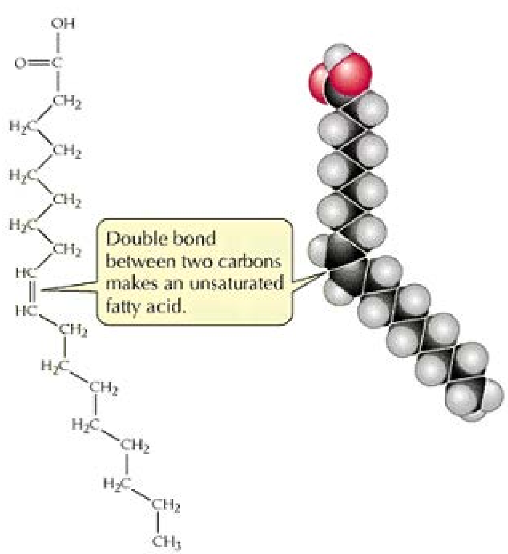
Estimating C-C bond length and C covalent radius in oleic acid: For all three of the following estimations, you will begin with the same assumption: namely, that the carbon at the polar end of the molecule is on the surface of the water, and the rest of the molecule sticks up in the air. From this point, there are three different ways of looking at the molecule, and you will explore them all:

1) First, estimate C-C bond length and covalent radius of C by assuming that the C-C-C bond angle in oleic acid is 180 degrees; that is, that the carbon atoms are simply stacked one upon the other. Use this picture to estimate the C-C bond length in oleic acid. Then, use your C-C bond length to estimate the covalent radius of a carbon atom. (How will this be related to the C-C bond length?) Assume that the carbon at the polar end is at the surface of the water.

2) It is known, though, that the C-C-C bond angle is not 180 degrees; instead, it is more like 109 degrees. Use this information to draw a stick model of the carbon atoms in oleic acid, beginning with the polar end of the molecule. How does this stick model relate to the height of the cylinder that you measured earlier? Now, use trigonometry on your diagram to estimate the C-C bond length and covalent radius of carbon. Did this method predict a longer, or a shorter, C-C bond length than the first method?

3) To further complicate matters, oleic acid has a *cis* double bond between carbon-9 and carbon-10 that puts a bend in the molecule, resulting in the picture shown below. Predict (do not calculate) whether this *cis* double bond would make your previous estimate of covalent bond length too small or too large.

(*b*) Oleic acid



Use the CRC handbook of Chemistry and Physics to look up the length of a C-C single bond (be sure to correctly cite your source in your lab report!). You are looking for a table called "Bond Lengths in

Crystalline Organic Compounds." Look for Csp^3-Csp^3, and then specifically C#-CH_2-CH_2-C#. This entry is closest to the C-C bonds in oleic acid. Report this value, then use this value to estimate the covalent radius of carbon (covalent radius = ½ C-C bond length). Note the units! Compare these numbers to your estimate of the C-C bond length and the covalent radius of a carbon atom according to your experiment. Which model did best? Which was not very good? Would you expect a calculation using the *cis* double bond to improve your best estimate, or to make it worse?

Scientific Communication: the Discussion Section

The purpose of the several-paragraph Discussion section is to interpret the meaning of your experimental results for the reader. Paragraphs in the Discussion section should be divided into **topics**, rather than **tasks**. A single paragraph over a specific topic identifies trends in your experimental data, explains the origin of those trends, and assesses the reliability of your results. You will repeat this process for each topic that you are asked to address. Each lab handout contains a number of additional questions to guide you through this process: please make sure that you use these resources!

A paragraph begins by identifying a trend in your data/observations as related to the requested topic. *(Example: "The pH of the acetic acid solution increased as sodium hydroxide was added to it.")* Next, explain the meaning and origin of that result or trend. *("A rise in pH indicates that a chemical reaction occurred between acetic acid and sodium hydroxide, removing acetic acid from the solution and so that the solution becomes more basic.")* After this, compare your results to any predictions you made based on hypotheses you had going into the experiment, and whether your results agree with these hypotheses. *("It is not surprising that a chemical reaction occurred between acetic acid and sodium hydroxide, because one is an acid and the other is a base. The acid (acetic acid) donates a proton to the base (sodium hydroxide), producing water, which has a neutral pH.)* **It is perfectly fine if you do NOT get the "expected" results; simply say so, and go on to write about whether it was your hypothesis that was problematic, or whether experimental problems kept you from getting good results.** Finally, end your paragraph with a reflection on the reliability of your assessment. Was the data precise (self-consistent) and accurate (consistent with others' measurements)? If so, state why you believe this is the case. If not, state **specific** experimental problems, known as "sources of error," that might cause you to question the reliability of your results. *(Example: "Although the pH was expected to increase due to the reaction between the H^+ of acetic acid and the OH^- of sodium hydroxide, the pH was not observed to increase when sodium hydroxide was added to acetic acid. However, the pH meter was observed to fluctuate wildly during the experimental trials, making it difficult to obtain a reliable reading. Furthermore, the pH readings between trials were not very consistent. These things may suggest that the pH meter was broken, and that the observations are unreliable.)*

Lastly, you may be asked to make predictions based on your data. You do not need to follow the preceding format when asked to make predictions. Simply state what you expect to happen. Then, use the rest of the paragraph to clearly explain why, on the basis of your experimental observations, you have made this prediction. Keep things clear and concise.

One final note regarding error: "human error," "measurement error" and "calculation error" are not acceptable sources of error. "Human error" is unacceptable because it is too vague. "Measurement error" and "calculation error" are not only too vague, but they are also unacceptable because they are factors you can control and fix. You should be able to make correct measurements in the laboratory, and you should have put in sufficient time and thought (and sought help where necessary) to ensure that you have performed calculations properly.

Discussion Points (up to 6)

- 6 – Overarching trend(s) in the data have been clearly identified; trends are interpreted as supporting or refuting a specific hypothesis; a satisfactory assessment of the reliability of results has been provided; specific sources of error in results have been identified.
- 5 – One of the level 6 items is unsatisfactory.
- 4 – Two of level 6 items are unsatisfactory.
- 3 – Three of the level 6 items are unsatisfactory.
- 2 – One of the level 6 items above is missing.
- 1 – Two of the above are missing.
- 0 – Discussion section is missing or lacking in substance.

Report 7 – Estimating Molecular Size and Bond Length (Formal Lab Report)

This is your first formal lab report. Section-specific instructions are found below. In addition, make sure that you consult the general directions for each section (found in a summary document on Angel) so that you are following the requested formatting and content guidelines.

The entire lab report should be double-spaced. Each section should be clearly delineated by a heading in bold-face or underlined type.

Make sure that your lab pages clearly describe your observations and laboratory procedure. This means that any information present in your report should also be present in your notebook. Failure to do this will keep you from earning full credit on your lab pages.

Introduction (3 pts): In two concise, well-written, narrative paragraphs, provide the following information:

- Background information: In one sentence, explain why oleic acid stands up on the surface of the water. Then, briefly describe the two ways that you modeled oleic acid. Include specific bond angles in your description.
- Summary of experiment and conclusions: Carefully and concisely (1-2 sentences) explain the goals of the experiment. End with a statement of the C-C bond length and covalent radius of carbon calculated using the 180 degree and 109 degree methods, and state which model produced a more accurate view of the molecule.

Experimental Procedure (3 pts): Attach a typed and double-spaced description of the experimental procedure, written in third person passive voice, giving specific details so that someone else could reproduce the experiments without knowing about the lab handout. This should take no more than ¾ of a page. You do not need to report any observations in this section; save the observations for the Results section.

Results (8 pts) Attach a typed, double-spaced Results section that includes the following information.

- A table of drops of oleic acid solution in 2.0 mL for each of your trials.
- Beneath the table, include a sample calculation for the volume of a single drop of solution (use the **average** number of drops from all trials) and the volume of oleic acid in one drop.
- A table containing columns for the diameter of the oleic acid cylinder measured in each trial and the average of all acceptable trials. Rows should be titled as follows:
- Below the table, show a calculation for the average cylinder volume. Use the average volume of one drop (mL), volume % of oleic acid solution, volume of oleic acid in 1 drop (cm^3)
- Then, show a calculation for the height of the cylinder using the average diameter of circle (cm), volume of cylinder (cm^3), and height of cylinder (cm and m). Report your answer in cm and in m.
- Draw a picture of oleic acid showing 180˚ bonding in the carbon atoms and a picture of oleic acid showing 109˚ bonding. Hand-drawn pictures are acceptable. On both pictures, clearly indicate the total height of the molecule (*h*) and the bond length between a pair of carbon atoms (*l*).
- A table reporting the C-C bond length and covalent radius of C as determined by the 180 degree and 109 degree pictures of bonding. Report these values in m, nm, pm, and angstroms (Å).
- Show a sample calculation of C-C bond length using the 180 degree bonding model.
- Show a sample calculation for your bond length assuming 109 degree bonding.

Discussion (6 pts) Address the following topics in your Discussion section in a way that satisfies the general requirements of a Discussion section (above, and in the summary document):

- (1 paragraph) State the trend observed in the C-C bond length as calculated using the 180˚ bonding model versus the 109˚. Compare both of these bond length values to that found earlier in the CRC Handbook. Which method produced a bond length closest to the experimentally-measured bond length (CRC)? Which method was better? Which method did you expect to be better, and why? End with an assessment of the reliability of your C-C bond lengths as based on the experimental measurement of the circle size. Do you, or do you not, expect your results to be reliable, and why?
- (1 paragraph) Make a prediction about the effect the *cis* double-bond geometry (picture shown in the Procedure section) in the oleic acid would have on your calculation of bond length. Explain your reasoning. Drawing another picture is highly recommended.
- (1 paragraph) Finally, make one more prediction about a different molecule. The structure of stearic acid is the same as that of oleic acid, except that it has a single bond in the middle instead of a double bond and is a straight molecule. Why do you think that stearic acid is a solid at room temperature and oleic acid, with its kink in the middle, is a liquid at room temperature? (Hint: which molecule can arrange itself better with respect to other molecules, and why?)

Conclusion (3 pts) End with restatement of the following information:

- The height of the molecule as calculated from your measurements.
- The C-C bond length as calculated by the 180 degree model and the 109 degree model.
- Which bonding model (180˚ or 109˚) produced the more accurate C-C bond length.

Chemistry 111L
Prelab Worksheet

Name ___________________________
Size of a Molecule

T8:00 T12:30 T6:30 W3:00 R8:00 R12:30 R6:30 circle your regular lab time

Davis Klein Osborne circle your **lecture** instructor

Keep an extra copy of this pre-lab assignment. You will need ALL of this information in the lab!

1. A drop of 0.20% oleic acid occupies a volume of 0.0375 mL. What is the volume (in cm^3 and in m^3) of pure oleic acid in the drop? Show all work. 1 mL = 1 cm^3. 100 cm^3 does NOT equal 1 m^3, so be careful!

2. Convert 5.0 nm into m, cm, nm Angstroms (Å), and pm.

3. Assume that you have an isosceles triangle, where angle CAB and angle ACB are the same. A drawing is shown below. Let the length AC equal 36 mm and the angle ABC equal 140°. What is the length of the line connecting A and B? All you need to do is some simple trigonometry. Begin by splitting the triangle into two right triangles with the line DB. You know the length of AD; you know the degrees of angle ABD. So use the formula opposite/hypotenuse = sin(angle) to calculate AB.