Determining the Carbon–Carbon Distance in an Organic Molecule with a Ruler

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This article describes how to estimate the carbon–carbon bond distance in the naphthalene molecule. The experimental results are good and the cost of the experiment is negligible. All the products and objects used can be obtained at home or purchased for little cost. The procedure is easily performed and can be done either at home or in the classroom, with the restriction that the mass of the naphthalene must be determined using an analytical or, at least, a precise balance. If there is not an appropriate balance, a neighborhood pharmacist could weigh the samples. Before performing the experiment, it is necessary for the students to be familiar with: the form and size of atoms and molecules; Avogadro's number; atomic and molecular masses; the chemical bond, with emphasis on the carbon–carbon bond; and liquid solutions and solution concentrations. It is also necessary for the students to know some trigonometry. This would be a good opportunity to interact with mathematics classes. The final result of this experiment, mainly considering the positive reaction of the students, is a real reward.

The fundamental idea of this procedure is based on the well-known experimental determination of Avogadro's number using an oil, such as oleic acid *(1)*. This experiment is based on Benjamim Franklin's famous experiment where a spoonful of olive oil was spread on the surface of Lake Clapham, near London. The oil spread out to an area of 100 m^2, forming a thin layer on the water surface. This idea was later used by Lord Rayleigh to determine the approximate size of a molecule. Assuming that the thin film formed on the water surface is monomolecular, by dividing the volume of the oil by the area of the film formed, the thickness of the film is obtained. This thickness is related to the size of the molecule.

There are many variations of this experiment in the literature. Some experiments are related to the determination of Avogadro's number *(1–5)* or to the determination of molecular shape or chain length *(6–9)* and one makes use of an analogy *(10)*. Nevertheless, all of the experiments that use chemicals *(1–9)* employ the whole surface, not considering the area occupied by solvent. Furthermore, none of the experiments are concerned with the bond length or use aromatic compounds as the solute; these are the principal differences between this article and the earlier articles.

In the experiment described here, the essential idea is that it is possible to spread the solvent and the solution on the water surface, since they have positive spreading coefficients *(11)* relating to water, forming a monolayer of planar molecules. By measuring the total surface occupied by these molecules, it is possible to determine the surface area of one molecule. Using this latter value, the bond distances can be calculated employing simple trigonometric relations.

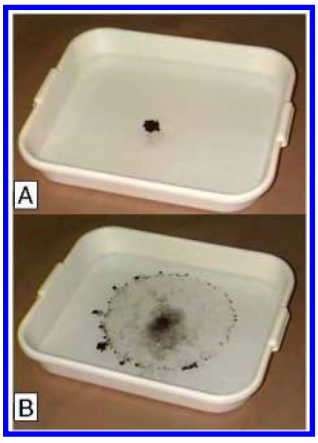

Figure 1. (A) The black spot formed by the carbon powder, placed onto the water at the center of the plastic tray. (B) The circle, delimited by the carbon powder, formed after the falling of one drop of liquid.

Materials

- Approximately 2 g of powdered carbon
- Baking tin or a plastic tray with the approximate dimensions of 65-cm long, 55-cm width, and 3-cm high
- Dropper that dispenses a drop volume between 0.015 and 0.025 mL
- 20 mL of ethyl alcohol (absolute ethyl alcohol is not necessary)
- 5- or 10-mL graduated cylinder
- One "ball" of naphthalene
- 40-cm plastic ruler

Procedure

A plastic tray is filled to a depth of 1 to 2 cm with water (tap water is adequate). A half teaspoon of carbon powder is carefully placed on the water surface at the center of the tray to form a black spot (Figure 1A). One drop of ethyl alcohol is dropped from the height of about 20 cm so that it falls in the middle of the black spot. Note that this height must be the same in every repetition. A circle immediately forms (Figure 1B). The diameter of the "maximum-size circle formed" is measured. The complete procedure is repeated at least five times, always using fresh water. If a plastic tray is used, it is not cleaned by rubbing with paper or other tissue as electrostatic charges can be formed that interfere with the size of the circle formed. The area of the circle is calculated, A_{eth}. In some cases the "circle" formed is not perfectly round. In such

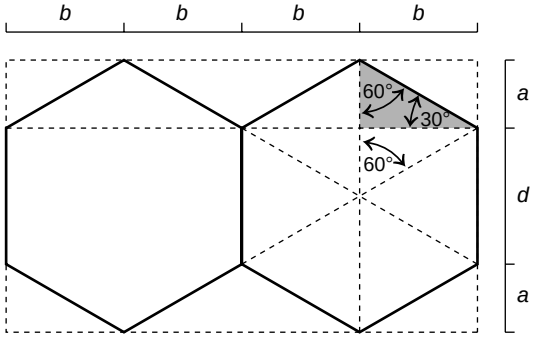

Figure 2. Simplified planar structure for the naphthalene molecule, as a rectangle, in order to calculate the carbon–carbon bond length.

Table 1. Diameters of the Circles Formed on the Surface of the Water

Trial	Diameter/cm	
	Ethyl Alcohol	Ethyl Alcohol and Naphthalene
1	30.0	35.0
2	31.0	35.6
3	31.0	35.6
4	30.0	35.0
5	29.0	34.6
6	31.0	35.0
Ave ± Mean Dev.	30.4 ± 0.4	35.0 ± 0.3

situations the diameter is measured in three or four different directions and the mean diameter is calculated.

The procedure is repeated with a naphthalene solution (from 0.0120 to 0.0150 g of naphthalene in 10.0 mL of ethyl alcohol). The areas of the circles are calculated, $A_{\text{naph sol}}$.

The average area of the circle formed by ethyl alcohol is subtracted from the average area of the naphthalene solution circle, $A_{\text{naph sol}} - A_{\text{eth}}$. Supposing that the naphthalene forms a "monolayer", that is, all the naphthalene molecules are in direct contact with the water surface, this result gives the area occupied by a monolayer of naphthalene molecules on the water surface, A_{mono}. If this area is divided by the number of naphthalene molecules, the area of one molecule is obtained. Then, with simple trigonometrical relations, it is possible to calculate the carbon–carbon bond distance.

Hazards

Ethyl alcohol *(12a)* is a flammable solvent with high vapor pressure and a flash point at 13 °C. Avoid handling it close to a flame. There is no evidence for carcinogenicity from naphthalene *(12b)*. However, ingestion can cause headaches, nausea, vomiting, profuse perspiration, diarrhea, convulsions, and hematuria. Handle these chemicals in a well ventilated room and avoid contact with the skin.

Calculations

Area of a Single Naphthalene Molecule

The number of naphthalene molecules, n, that form the monolayer can be calculated by,

$$n = NVC$$

where N is Avogadro's number, V is the volume (in liter) of one drop of solution added, and C is the concentration (in mol per liter) of the naphthalene solution. The area of a single naphthalene molecule, *MA,* can be obtained by dividing the area of the naphthalene monolayer by the number of naphthalene molecules

$$A_{\text{mono}}/n = MA$$

If the value of *MA* is in units of cm^2, this value can be multiplied by 1×10^{16} to obtain the value of *MA* in angstroms per molecule.

Relationship between Area and C–C Bond

Consider that the naphthalene molecule is formed by two hexagonal rings (Figure 2) linked by one of their sides, all carbon–carbon bonds are bonds of the same length, and the molecule is planar and presumed, to an approximation, to be a rectangle (the area occupied by the hydrogen atoms is not considered). The molecular area, *MA,* can be calculated as,

$$MA = l \times m$$

where $l = 2a + d$ and $m = 4b$. From the shaded triangle in Figure 2,

$$a = d\sin(30) = 0.5d; \quad b = d\sin(60) = 0.866d$$

Therefore,

$$MA = (4 \times 0.866d)(2 \times 0.5d + d) = (3.46d)(2d) = 6.92d^2$$

Results

Using the experimental data summarized in Table 1, a carbon–carbon bond length of 1.67 Å (167 pm) is calculated. Considering the simplicity of the experiment and the approximations, the results are good; compare this value to the values for the length of the carbon–carbon aromatic bond in benzene, 1.397 Å (139.5 pm), and in toluene, 1.52 Å (152 pm) *(13)*.

The experiment was also performed with other aromatic compounds, such as phenanthrene (obtained length, 1.33 Å), anthracene (1.78 Å), benzene (1.47 Å), and toluene (1.57 Å). The carbon–carbon lengths in anthracene, phenanthrene, and naphthalene molecules were calculated using the semiempirical method PM3. The calculated values were 1.40 Å for all three cases.

Discussion

This experiment allows a wide discussion of chemical concepts. However, the discussion here will be limited to the essentials as most of the relevant information is easily found in chemistry textbooks. Ethyl alcohol is miscible with water as the result of hydrogen bonding. Its spreading coefficient is positive in liquid water, which means the spreading is accompanied by a decrease in free energy, that is, it is spontaneous *(11)*. For all solutes this coefficient is also positive.

Thus, when one drop of such a substance touches the water surface, the molecules rapidly interact with water molecules in the surface and also in the bulk. The effect on the surface is easily detected using a "marker" such as the carbon powder that is pushed by the spreading ethyl alcohol, forming a circle. Repeating the procedure in identical conditions, circles of the same size are expected.

If a very small quantity of another substance (naphthalene in this case) is dissolved in the ethyl alcohol, it can be assumed that the number of ethyl alcohol molecules in a drop vary so little that this change can be considered negligible in terms of the size of the circle formed by the ethyl alcohol "alone" on the water surface. However, if the added solute is insoluble in water, it will remain on the surface and will contribute to the size of the circle. In the present case as the naphthalene molecule is planar, it may be supposed that the molecules lie on the water surface according to the plane formed by the carbon atoms. Therefore, dividing this additional area by the number of solute molecules, the area of one molecule is obtained. Considering, as an approximation, that the naphthalene molecule is a rectangle, according to Figure 2, the calculations are simplified and the carbon–carbon bond distance can be obtained.

This approximation contains two principal errors. The first is the "extra" area included in the parallelogram that circumscribes the naphthalene molecule and the second is the hydrogen atoms that are not taken into consideration. In the final result, the proposed rectangle that passes through the external carbon atoms is actually bigger than the real one. This fact leads to a carbon–carbon distance a little higher than the actual value, as observed in our results.

[W]Supplemental Material

Instructions for the students are available in this issue of *JCE Online*.

Acknowledgments

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The structures of a number of the molecules discussed in this article are available in fully manipulable Chime format as *JCE* Featured Molecules in *JCE Online* (see page 912).