

The entire mass spectrometer is kept at high vacuum (10^{-6} torr) to ensure that the mean free path of the ions is large. The source ionizes the eluant stream of molecules from the gas chromatograph by electron bombardment. The ion beam is focused and accelerated into the mass analyzer by electrostatic lenses. The ion masses are sorted by a quadrupole mass analyzer. The sorted ions are detected by an ion multiplier. The distribution of mass fragments and the isotopic ratios between groups of related mass peaks allow the identification of compounds eluting from the GC.

Theory

Fragmentation Patterns

The ion source produces ions by electron bombardment. The most common source uses 70 eV electrons. The simplest ionizing event is



where the product ion gives rise to the parent peak in the mass spectrum. The parent peak, if it is present, automatically gives the molecular weight of the compound, since only a single electron has been removed during the ionizing collision. However, 70 eV is more than enough energy to rupture bonds, and commonly many fragment ions are produced in the source. The types of fragment ions can be predicted using familiar rules concerning carbonium ion stability studied in organic chemistry. The following are a few general rules concerning fragment ion formation.

1. Cleavage is favored at branched carbon atoms: tertiary, secondary, primary, with the positive charge staying with the branched carbon (the more stable carbonium ion).
2. Double bonds favor cleavage beta to the bond.
3. A substance having a strong parent peak often contains a ring, and the more stable the ring the larger the peak.
4. Ring compounds usually contain peaks at the mass number characteristic of the ring.
5. Saturated rings lose side chains at the alpha carbon. The peak corresponding to the loss of two ring atoms is much larger than for the loss of one ring atom.
6. In alkyl-substituted ring compounds, cleavage is most probable at the bond beta to the ring if the ring has a double bond next to the side chain.
7. A hetero-atom will induce cleavage at the bond beta to it.
8. Compounds containing a keto-group tend to break at this group, with the positive charge remaining with the carbonyl portion.
9. Loss of neutral species is common (H_2O from alcohols, HCN, CO)

For example, the spectrum of benzophenone, Figure 2, shows a strong parent peak, characteristic of conjugated ring systems ($m/z = 182$) as indicated by rule 3. The spectrum also shows a strong peak at $m/z = 77$ characteristic of aromatic compounds in general, as indicated by rule 4. The $m/z = 77$ phenyl ion is produced by the loss of a small neutral species, CO, as indicated by rule 9.

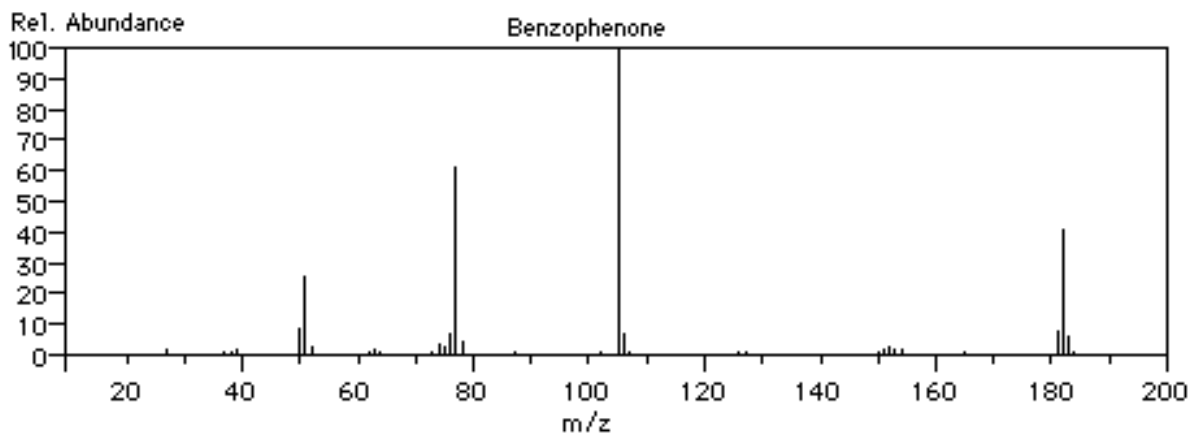
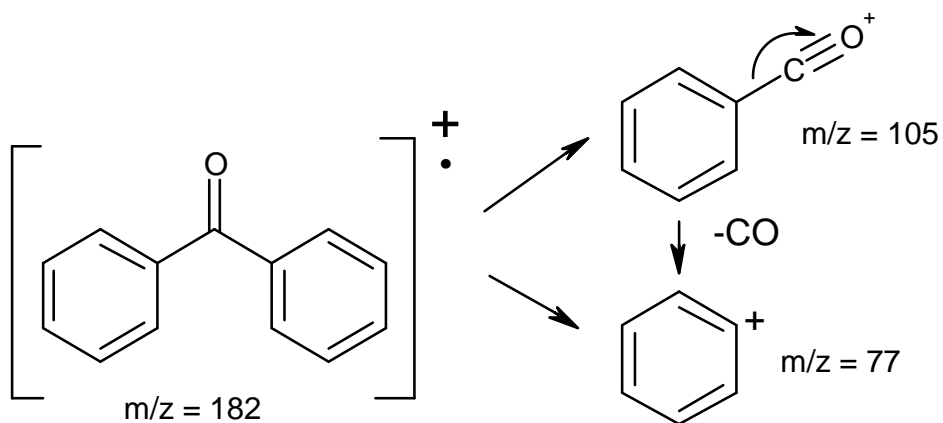
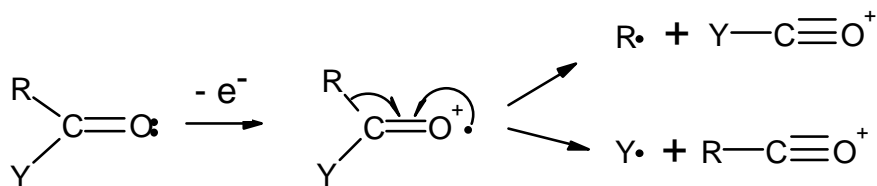


Figure 2.

The overall fragmentation process can be diagrammed as



For the present study rule 8 is the most important. That is, in ketones the fragmentation often proceeds in the following way.



In this case the acylium ion is formed, which is isoelectronic with $R-C\equiv N$, which is known to be very stable.

One complicating mechanism for ketones is the McLafferty rearrangement, which is an important mechanism in compounds that have hydrogen gamma to a carbonyl. The spectrum in Figure 3 of 4-methyl-2-pentanone is an example of this.

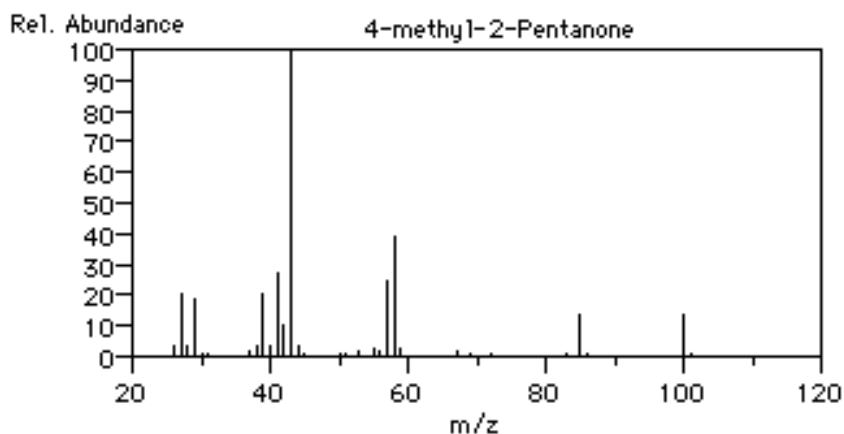
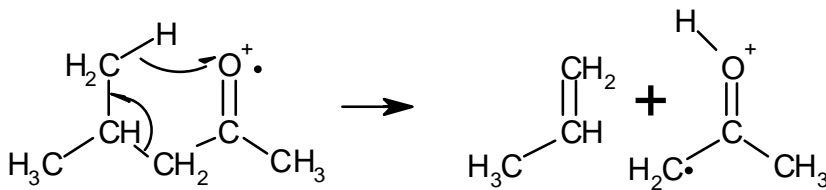


Figure 3.

The McLafferty rearrangement occurs through a 6-membered cyclic intermediate:



The ion produced has a mass of $m/z = 58$. This rearrangement is not seen in 3-pentanone, since there is no gamma hydrogen. The spectrum of 3-pentanone is shown in Figure 4. Notice that a strong peak occurs at $m/z = 57$ rather than 58.

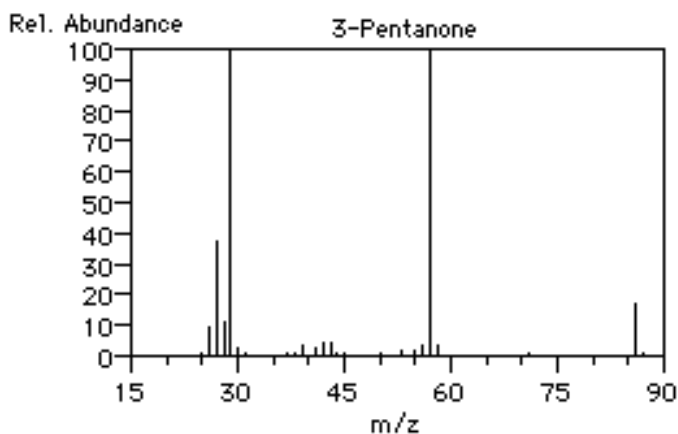


Figure 4.

Isotopic Peaks

Notice that in the preceding spectra, that the peaks occur in related groups rather than individually. This occurs because of the natural distribution of isotopes in the elements. The ratio of the heights of the isotope peaks are an excellent confirmation of the composition of fragment ions. In Table 1 is listed the natural isotopic abundance several elements. If we set the height of the ion peak containing the parent isotope to 100, then the height of the peak containing one atom of the more massive isotope will have a height:

$$\frac{\text{abundance of isotope}}{\text{abundance of parent isotope}} \times 100.$$

These numbers are listed in Table 1 as the $(M + 1)/M \times 100$ values, for isotopes with mass 1 greater than the parent, and as $(M + 2)/M \times 100$, for isotopes with mass 2 greater than the parent. For example, if we set the height of the $^{12}\text{CH}_4$ peak from methane to 100 then the contribution to the $M + 1$ peak from $^{13}\text{CH}_4$ will be 1.08%. Of course, the $M + 1$ peak will also have contributions from $^{12}\text{CH}_3\ ^2\text{H}$, which can occur in four different ways. The height of the $M + 1$ peak is then in total $1.08 + 4 \times 0.015 = 1.14\%$ of the parent peak.

Table 1. Isotopic Abundances.

	Isotopic abundance	Isotopic abundance	Isotopic abundance	$\frac{M + 1}{M} \times 100$	$\frac{M + 2}{M} \times 100$
^1H	99.985	^2H	0.015	0.015%	
^{12}C	98.892	^{13}C	1.068	1.08	
^{14}N	99.63	^{15}N	0.37	0.36	
^{16}O	99.76	^{17}O	0.037	0.04	0.20
		^{18}O	0.204		

An example of the usefulness of the isotopic peak ratio is as follows. There are 33 possible fragment ions that contain C, H, N and O with mass 168. Two of these are dinitrobenzene, $\text{C}_6\text{H}_4\text{N}_2\text{O}_4$, and $\text{C}_{12}\text{H}_{24}$. The height of the $M + 1$ peak for each of these ions will have the following contributions:

$\text{C}_6\text{H}_4\text{N}_2\text{O}_4$		$\text{C}_{12}\text{H}_{24}$	
^{13}C	: $6 \times 1.08 = 6.48$	^{13}C	: $12 \times 1.08 = 12.96$
^2H	: $4 \times 0.015 = 0.06$	^2H	: $24 \times 0.015 = 0.36$
^{15}N	: $2 \times 0.36 = 0.72$	total	$M+1/M$: 13.32%
^{17}O	: $4 \times 0.04 = 0.16$		
total	$M+1/M$: 7.42%		

The two fragment ions can be easily distinguished on the basis of the isotope ratios. Luckily, there are extensive tables of the possible formulas corresponding to different mass values, which include the $M + 1$ and $M + 2$ isotopic abundance ratios. An example is in Silverstein, Bassler and

Morrill's book, appendix a¹. The "Fragment Finder" application is also available on the CH341/342 Web page. The "Fragment Finder" gives the same information as Silverstein, Bassler and Morrill's appendix.

Procedure

Equipment

- 3 x screw cap bottles with aluminum foil septa
- 1 x 50-ul micropipet
- 1 x 100-ul micropipet

Instructions for using the Varian 3800/2000 gas chromatograph/mass spectrometer are included in the appendix.

GC/MS is exceedingly sensitive. To work within the range of the instrument, we will use the sampling technique called head space analysis. In head space analysis the vapor above a volatile sample is withdrawn by syringe and injected into the GC. In withdrawing samples, be very careful not to let the syringe needle touch the liquid or the walls of the sample bottle.

Using a clean pipet or syringe, pipet 20-50 ul of acetylacetone into one of the screw cap bottles and cap with an aluminum foil septum. This sample will be used to obtain the spectrum of pure acetylacetone. In the same way, prepare a sample of 2-pentanone

Pipet 20-50 ul of acetylacetone in the second screw cap bottle. Using a clean pipet or syringe, pipet 100 ul of D₂O into the sample bottle. Remember to immediately replace the cap on the bottle, to avoid hydrogen exchange with water vapor in the atmosphere. Cap the sample with an aluminum foil septum, and carefully mix the contents. Let this sample reach equilibrium for about 15-30 minutes before injection into the GC/MS. This volume ratio produces about a 10-fold excess of D₂O. The deuterium exchange will probably not appear to be as complete as this 10-fold excess might indicate. The deuterated acetylacetone can exchange with water vapor adsorbed on the surface of the syringe, the injector, in the column, and in the mass spectrometer.

While the D₂O/acetylacetone sample is equilibrating, obtain the spectrum of pure acetylacetone and 2-pentanone by head space sampling. Use an injection volume of 5-10 ul. Remember to use only a blunt tipped, conical needle syringe, to avoid destroying the Merlin valve GC inlet. Operate the injector with a 1/50 split ratio to avoid overloading the detector. That is, the injector should be set up to pass only about 1/50 of the injected sample into the column. The injector temperature should be 150°C and the oven temperature should be held constant at 50°C. Use a solvent delay of 2.0 min before the collection of mass spectra begins. Scan the spectrum from 40-300 m/z with a threshold of 1 and a sampling rate of 1 scan/sec. Print out several single spectra, with the peaks listed, to obtain estimates of the uncertainties in the isotope ratios. Also print out a 5 point averaged spectrum to see a spectrum with better signal to noise.

Obtain the spectrum of the deuterated acetylacetone.

Rinse the injection syringe 25 times with methanol. Using a cork borer, cut out new aluminum foil septa. Install the septa into the bottle caps, so that things are ready for the next group.

Report

For the neat, undeuterated samples: Assign all the prominent lines in the spectra. Make use of the isotope ratios and Silverstein, Bassler and Morrill: appendix a or the "Fragment Finder" Web

page to confirm your peak assignments. Estimate the uncertainty in the isotope ratios for acetylacetone from your replicate spectra.

Using the isotopic abundance (Table 1), calculate the $(M + 1)/M$ and $(M + 2)/M$ isotope ratios for the parent peak and the most intense peak in your spectrum of undeuterated acetylacetone. In effect, you are verifying the ratios in Silverstein, Bassler, and Morrill: appendix a or the on-line applet. Include your calculations in your report. Compare the calculated to the experimental $(M + 1)/M$ and $(M + 2)/M$ isotope ratios. Compare your calculated to the "Fragment Finder" $(M + 1)/M$ and $(M + 2)/M$ isotope ratios.

Comment on the importance of the McLafferty rearrangement in your peak assignments for acetylacetone and 2-pentanone. Why doesn't the McLafferty rearrangement occur in acetylacetone?

For the deuterated sample: Using your spectra decide if you can, indeed, determine which hydrogens readily exchange for deuterium.

Discuss the chemical significance of your results. For example, why is keto-enol tautomerization important? What kinds of compounds show keto-enol tautomerization? What other technique could you use to study keto-enol tautomerization?

Literature Cited

1. R. M. Silverstein, G. C. Bassler, T. C. Morrill, "Spectrometric Identification of Organic Compounds, 4th Ed.", Wiley, New York, NY, 1981. pp 46-89.

Appendix

Varian 3800/2000 GC/MS Operating Instructions

General Notes:

- * All mouse functions are accomplished with the left button unless specified.
- * The function of each icon can be listed by placing the cursor over the icon and waiting a second or two. The icon label will be listed on the screen.
- * Don't use the go-away box on the 3800.44 or 2000.40 control windows. Minimize them instead.
- * Do use the go-away box for the Review/Process Data- SatView window.

Procedure:

1. Check that the helium pressure gauge on the wall reads 40-80 psi.
3. On the computer, note the Varian Star Toolbar. This is a wide toolbar that runs down the left side of the screen. If the Varian Star toolbar runs across the bottom of the screen, click on the background of the toolbar and drag it to the left. Click on the System Control icon. This icon is at the top.
4. Pull down the Windows menu and select 3800.44 to display the GC control panel.
5. To select the desired method, click on the "Activate a Method" icon. This icon is an "open file folder" icon in the middle of the top icon bar, just to the right of the method pull down list. Find the CH341 folder; you may need to go up a level. In the CH341 folder, the method "acac.mth" has been specifically designed for the deuterium exchange lab. Click Open to continue. You should not need to change any settings.
6. Check the GC temperature zones, which are listed in the middle of the screen. The column oven should be 50°C, the front injector 150°C, and the middle injector 60°C. We will use the front injector for this lab. The oven temperature is set for 50°C. The total run time is 4.00 min. Check for the total run time, which is listed as the "End Time." Note the two status indicator lights: the Equilibrating/Ready light and the Fault/No Fault lights should both be green before beginning a run. These status indicators are in the upper left-hand block of the control window.
7. Minimize the 3800 control window.
8. Pull down the Windows menu and select 2000.40 to display the MS control panel.
9. Click on the Auto Tune button.
9. The tuning procedure calibrates the mass axis. Choose the "FC-43 mass calibration" tuning

mode in the pull-down list box in the middle of the window. Make sure the check box to the left of the pull-down list box is checked, and the other three check boxes are cleared. Click on Start Auto Tune. The system will open the calibration valve on the MS. This valve allows the vapor from a fluorinated organic liquid, FC-43, to enter the MS. The text box across the bottom the screen shows the progress of the Auto Tune procedure. After the procedure is complete, check to see that "Multipoint mass cal: completed" has been printed in the text box.

10. Click on the Acquisition button, at the far right of the MS control window.

RUNNING A SAMPLE

1. The status indicators should both be green and be labeled Ready and No Faults.
2. The system is ready to begin. The start of data acquisition is signaled by the mechanical switch on the top of the injection port. When you press down on this switch with the syringe, data acquisition will begin.
3. Remember to use only a blunt tipped, conical needle syringe, to avoid destroying the Merlin GC inlet. Before the first use, flush out a gas tight syringe with methanol. Gas tight syringes have a Teflon tip on the end of the plunger. Be sure to eject the cleaning solvent into a waste container. Do not eject back into the source bottle as it will contaminate the entire bottle. Flush out the syringe at least 50 times with air to remove traces of solvent.
4. Flush out the syringe with your sample vapor at least three times.
5. Inject 5-10 uL of your sample by gently pushing the syringe needle into the injection port on the top of the GC. Be sure to push straight down and guide the needle in as it is very fragile and easily bent. Remove the syringe immediately after injection.
6. Note the data file name. This name will be listed in the upper-right corner of the acquisition dialog window. It will be in a form such as "2000.40012.SMS."
7. To view the data while it is being taken, click on the Hide Keypad button, which is on the left side in the middle of the control window. Pull down the adjacent list box and select Spectrum and Chromatogram. Both the yellow Spectrum and Chromatogram windows should be displayed. The relative heights of these windows can be adjusted by dragging the border between the two windows up and down. (Sometimes, this border is left too low so that only one window shows, even though you have chosen to display "Spectrum and Chromatogram." If this happens, move the mouse to the bottom of the yellow window until the cursor changes to "=". You can then drag the border up to reveal the second yellow window.)
8. After the solvent delay has passed, you will see the Total Ion Chromatogram accumulating on the screen. While it is running, you may adjust the graph parameters, including the vertical scaling using the slider at the far right of each yellow window. If you need to stop the run while it is in progress, click on the Show Keypad button, and then select Reset. To end early you will also

need to reset the GC. Pull down the Windows menu and choose 3800.40, and again click on Reset, and finally minimize the GC control window to return to MS data acquisition.

9. You can display information about the current MS scan by clicking the Scan Information icon. This icon looks like a small piece of white paper with tiny lettering. Clicking again hides this information box. You can display the current cursor m/z position and the corresponding data value by selecting the Cursor Display icon. This icon looks like a small mass spectrum with one red peak. Clicking again hides this information box.

Data Analysis

10. When the chromatographic peak returns to baseline or the run is completed, you can display the data in the Review/Process MS Data window. To open your data in the Review/Process MS window click on the small black icon that has a representation of the chromatogram in yellow and green. This small icon is in the middle of the screen above the yellow chromatogram window. (There are two other larger icons on the screen with the same symbol. These larger icons are used to enter the Review/Process MS Data application with a previously saved data file.)

11. In the SatView application window, pull down the Spectra menu and make sure that "Background Correct Spectra" is not checked. If it is checked selecting that entry will clear this mode.

12. Move the cursor over the chromatogram trace. Clicking the mouse will load the mass spectrum that was taken at that time into the window, on the left. Individual mass spectra or several consecutive spectra that have been averaged can be displayed. Pull down the Spectra menu, slide right on Spectrum Averaging and choose Single spectra. Click on the chromatogram trace to load single spectra for viewing. Now return to the Spectra menu, slide right on Spectrum Averaging and choose 5 point spectrum. Now clicking on the chromatogram trace will display the averaged result of 5 spectra centered on the time that you selected.

13. Areas of either the chromatogram or mass spectrum can be enlarged by highlighting a box around the area by holding the mouse button down and dragging around the area. Clicking the red A icon, above the spectrum window, will return to the full X and Y expansion.

14. To prepare for printing, press the right mouse button with the mouse in the mass spectrum window and slide right on Options. Make sure "print ions and intensities" is checked. This option produces a listing of the ion fragments and their abundances. You will need this tabulation to calculate M+1/M and M+2/M ratios. To print the mass spectrum, click right again and choose "Print Spectrum." In the print preview screen, click on the "print page" icon. This icon looks like a printer with a single sheet of paper. Click on the "Exit!" menu item to return to the data viewer.

15. When you are finished with data analysis, click the go-away box on the MultiChrom window and the SatView window.

16. You should now see the 2000.40 MS acquisition window. If necessary, click on the Show Keypad button to see the acquisition controls. Check the status indicators. If they are both green,

the system is ready for the next sample.

17. Rinse the injection syringe 25 times with methanol.

SHUT DOWN PROCEDURE

1. Minimize the 2000.44 acquisition control window.
2. Maximize the 3800.44 control window, or alternatively pull down the Windows menu and choose 3800.44.
3. If you are finished using the instrument for the day, click on the Activate a Method icon. (This icon is an “open file folder” icon in the middle of the top icon bar.) If you are in the CH341 folder; you will need to go up a level. Select the “standby” method. Click Open to continue. The standby method sets the oven at 50°C, the front injector at 200°C, and the middle injector to 50°C. The split vents are turned off to conserve on helium.

Part 2: The Enthalpy of Sublimation of Camphor

Purpose: Determine the enthalpy of sublimation of camphor. Learn how to do solid sampling for mass spectrometry.

Introduction

Sublimation is the phase transition for the direct transfer of molecules from the solid to the vapor phase. Enthalpies of sublimation are a measure of the cohesive forces in the solid state. In molecular mechanics calculations of the enthalpy of formation, the result is for gas phase molecules. For many substances, the literature value for the enthalpy of formation is for the solid or liquid phase. To predict the enthalpy of formation of a liquid or a solid using a molecular mechanics calculation, the enthalpy of vaporization or sublimation must be subtracted from the gas phase enthalpy of formation. Camphor is a commonly used sample for At room temperature camphor is a solid, so the enthalpy of sublimation must be used when comparing to molecular mechanics calculations.

Theory

The relationship between vapor pressure and temperature is given by the Clausius-Clapeyron equation:

$$\ln \left(\frac{p_2}{p_1} \right) = \frac{-\Delta_{\text{sub}}H_m}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \quad (1)$$

The assumptions used in the derivation of Eq. 1 are that the vapor behaves as an ideal gas, the molar volume of the solid is much smaller than the vapor, and the enthalpy of vaporization is independent of temperature. Therefore, a plot of $\ln p$ versus $1/T$ will yield a straight line of slope $-\Delta_{\text{sub}}H_m/R$. Equation 1 is also used for vaporization of a liquid, where $\Delta_{\text{sub}}H_m$ is replaced by $\Delta_{\text{vap}}H_m$. Notice that Eq. 1 is independent of the units of the pressure. The pressure units cancel out. So any pressure units or any property proportional to pressure can be used, such as the total ion current from the mass spectrometer. The units of temperature are degrees K, since the units must cancel with R.

Equilibrium vapor pressure measurements for solids are very difficult, because the vapor pressure is so small. A mass spectrometer can be used to measure very small vapor pressures using a solids probe. One version of a solids probe is called a Chromatoprobe.

In the Chromatoprobe, the sample is held in a small tube that is placed in the injector of a gas chromatograph. As the injector is heated, solids sublime and are carried into a column. If a long column is used, mixtures can be separated as in normal GC/MS. The Chromatoprobe just substitutes for the normal injector. However, the Chromatoprobe can also be used to produce a constant stream of sample into the mass spectrometer. In this mode, a very short piece of fused silica tubing is used to connect the injector to the inlet of the mass spectrometer. No separation is achieved, however the sample is available for mass analysis for an extended time, instead of arriving at the mass spectrometer in one short peak.

The signal from the mass spectrometer using a Chromatoprobe will be proportional to the rate at which the sample sublimates. For this experiment, we need to measure the equilibrium vapor pressure and not the rate of vaporization. We can convert the rate measurement into an equilibrium measurement by using a clever trick, gaseous effusion.

*Effusion*¹

The mean speed of molecules in a gas is:

$$c = \left(\frac{8RT}{\pi M} \right)^{1/2} \quad (2)$$

where M is the molar mass. The rate at which molecules collide with the walls of the container is proportional to the velocity of the molecules towards the wall, the area of the wall, A , and the number of molecules per unit volume. The number of molecules per unit volume is the number density, d , which is determined by the pressure; $d = n N_A/V = p N_A/RT$. The collision frequency is then

$$f = \frac{1}{4} c d A = \frac{p N_A A}{(2\pi MRT)^{1/2}} \quad (3)$$

The $\frac{1}{4}$ adjusts the mean speed to the mean velocity towards the wall. When a gas is placed in a container with a small hole, molecules will leave the container at a slow rate that is given by the collision frequency with the cross sectional area of the hole. If the hole is much smaller than the sides of the container, this process is called effusion. The important result in Eq. 3 is that the effusion rate depends on the sample pressure. For a solid, this pressure is the sublimation pressure.

Put specifically into the terms of this experiment, placing a small hole in the container allows the solid to establish its equilibrium vapor pressure, while allowing a small amount of the gas to effuse out of the container to be analyzed by the mass spectrometer. This effusion trick works so long as the rate of sublimation is much greater than the rate of loss through the small hole.

The determination of $\Delta_{\text{sub}}H_m$ is then particularly simple. The sample is placed in the solid sampling probe of the mass spectrometer. A cap that has a very small hole is placed on the sample tube. The intensity of the mass spectral peaks are then monitored as a function of the temperature of the injector.

Procedure

Fingerprints contain oils that will contaminate the Chromatoprobe injector and produce a large background signal in your spectra. Handle the Chromatoprobe holder carefully to avoid touching the sample holder. Handle the sample tubes and cap with forceps.

1. Pull down the Windows menu and select 3800.44 to display the GC control panel.
5. To select the desired method, click on the “Activate a Method” icon. This icon is an “open file folder” icon in the middle of the top icon bar, just to the right of the method pull down list. Find the CH341 folder; you may need to go up a level. In the CH341 folder, the method “solid50splt50” is used for low temperature Chromatoprobe use. Click Open to continue.
6. Check the GC temperature zones, which are listed in the middle of the screen. The column oven should be 200°C, the front injector 200°C, and the middle injector 50°C. We will use the middle injector, which contains the Chromatoprobe, for this lab. The total run time is 10.0 min.

Check for the total run time, which is listed as the “End Time.” Note the two status indicator lights: the Equilibrating/Ready light and the Fault/No Fault lights should both be green before beginning a run. These status indicators are in the upper left-hand block of the control window.

7. Minimize the 3800 control window.

8. Pull down the Windows menu and select 2000.40 to display the MS control panel.

9. Click on the Acquisition button, at the far right of the MS control window, if the Acquisition window is not active.

10. Place a few small crystals of camphor in a Chromatoprobe sample tube. Place the aluminum cap onto the sample tube, and slip the sample tube into the Chromatoprobe holder.

11. Unscrew the cap from the Chromatoprobe injector, and carefully insert the holder into the injector. Tighten the holder. To see if the holder is tight enough, we need to check the inlet pressure for leaks. On the GC control panel, press the Flow/Pressure button. Use the “v” cursor button to select the middle (1079) injector. Press Enter. The status for the middle injector should now be shown. The injector pressure should be 35 psi and the Column flow should be 1.0 mL/min. If the pressure and flow are low, you need to tighten the Chromatoprobe holder.

12. Back on the data station, click on the Start Acquisition button. After a 1.5 min delay to allow air to flush from the system, spectra will be displayed.

13. Acquire spectra until the intensity is constant, then change the temperature. To change the injector temperature, on the GC press the Injector button. Use the “v” cursor button to select the middle (1079) injector. Press Enter. The current injector temperature will be highlighted. Type in a new value; 20°C higher. Press Enter. The intensity should increase and become constant. Repeat this step until you get near the melting point of camphor, 175°C.

If the intensity does not increase significantly, you have run out of sample. To change samples, on the data station, click on Reset before you loosen the Chromatoprobe holder, to avoid introducing air into the mass spectrometer.

14. Follow the data analysis instructions, above, to get the intensity of a given mass peak as a function of temperature.

Calculations

Plot the mass spectral intensity as discussed above. Determine the slope and intercept and their uncertainties using least squares curve fitting. Determine the enthalpy of sublimation from the slope and use propagation of errors to find the uncertainty in this result. This enthalpy is calculated for the average temperature of this experiment, roughly 110°C. We really need the enthalpy of sublimation at 298 K. Discuss how to convert your result to 298 K. Discuss the chemical significance of your result.

References

1. P. Atkins, "Physical Chemistry, 6th Ed." W. H. Freeman, New York, 1998, Chapt 24.1-2.