Teacher Guide: The Drug Lab Evidence

Time: 4–5 days
Grades: 11 and 12 (2nd-year Chemistry)

Objectives

1. Students will solve a forensics case using their knowledge of chemistry (for Chapter 7 performance assessment, this includes naming compounds, organic functional group naming and identification, infrared spectroscopy, and thin layer chromatography).
2. Students will assemble their evidence and present their case at the end of the year.
3. Students will answer four questions:

Part I

1. Can any of the compounds be matched with unknowns from previous evidence?

Part II

2. How much total caffeine could be extracted from the coffee found in the basement?

Part III

3. Which substances were found in the unknown drug?

Part IV

4. Which suspect pen(s) match the ink on file from the drug logbook?

Preparation

Part I

You will need to make an evidence folder for each student group with the three unlabeled IR spectra. Students will create a data table to show which peaks from the IR spectra match which frequencies based on their knowledge of the organic compound and its various functional groups. You will also need to provide students with a chart of typical IR spectra absorption frequencies. The IR Spectra and frequency charts are provided at the end of this teacher guide.

Part II

Dissolve 50 g of instant caffeinated coffee in 1000ml of distilled water. You may have to heat the water to get all of the coffee to dissolve. Each group will use 100ml of this coffee solution for the lab.

Part III

For this activity, the unknown solution will contain caffeine and aspirin. One possible explanation for this combination would be a migraine medicine.

Part IV

You must use THREE different pens of the same color to produce three different TLC chromatographs *(i.e.* felt tip, marker, and ballpoint pen). Put each pen in a labeled baggie with a Forensics Tag detailing where each pen was found and from which suspect it came. You will also need to make evidence samples to which students can match their TLC samples in order to determine which suspect pens match the ink found in the drug log. Since students rotate from station to station for this lab assessment, you will only need one evidence folder with the evidence ink samples in it.

Question Guidelines

For calculations, formulas, and work, see the student example at the end of the chapter.

Part I

1. The Unknown #2 on Larry J. from *Performance Assessment #2: The Chemical Evidence* can be identified as caffeine.

Part II

1. Yes, they should be able to extract caffeine crystals.
2. Depends on the amount the students are able to extract from the coffee solution
3. Discolored if not properly decanted.

Part III

1. Caffeine and aspirin were present in the unknown drug.

Part IV

1. The pens of Larry and Gladys match the ink samples from the logbook.

Materials

In addition to the materials listed within the student assessment handout, the following materials will also be needed:

- Suspect File E
- Student Assessment Handout
- IR Spectra of caffeine, aspirin, and acetaminophen (included at the end of the teacher guide)
- TLC materials (Flinn Scientific, Inc. FB1648: Identification of Unknown Substances II)

- Ink evidence folder from the drug logbook (2)
- Suspect pens (3)

Teacher Hints

Part III

- While you may want to include some evidence of a suspect and/or victim having migraines, this may not be the only drug that Gerald was making in the drug lab, so we wanted to keep it general for the students to be able to create their final scenarios.

Possible Scenario

Gladys and her son were using the basement of the lake house to synthesize their own drugs. Her son, Gerald, would make the drugs, and then Gladys would sell them to her customers on the side. When Gladys rented the lake house to the victim, she did not inform her son. The victim walked into the lake house, only to find a surprised Gerald working away in the basement. After she discovered what he was doing, she threatened to inform the police. Gerald killed the victim. Afraid of going to jail, he called his mom. Gladys helped her son dispose of the body and much of the evidence; however, they couldn't get rid of everything. Larry J., while snooping around the lake house trying to find any clues as to his wife's death, came across the drug lab in the lake house basement. He was then killed (could also be a drug deal gone bad since Larry's name was found in the book). The police were then called to the scene where they found the final pieces of evidence.

Table of Infrared Absorbances for Common Organic Functional Groups	
Functional Group	*Characteristic Absorption(s) in cm^{-1}*
Alkane C-H Stretch	2950-2850 (m or s)
Alkene C-H Stretch Alkene C=C Stretch	3100-3010 (m) 1680-1620 (v)
Alkyne C-H Stretch Alkyne C≡C Stretch	~3300 (s) 2260-2100 (v)
Aromatic C-H Stretch Aromatic C-H Bending Aromatic C=C Bending	~3030 (v) 860-680 (s) 1700-1500 (m)
Alcohol O-H Stretch	3550-3200 (broad, s)
Carboxylic Acid O-H Stretch Carboxylic Acid C=O Stretch	3000-2500 (broad, v) 1780-1710 (s)
Amine N-H Stretch	3500-3300 (m)
Aldehyde C=O Stretch	1740 –1690 (s)
Ketone C=O Stretch	1750-1735 (s)
Ester C=O Stretch	1750-1735 (s)
Amide C=O Stretch Amide N-H Stretch	1690-1630 (s) 3700-3500 (m)
Ether C-O Stretch	1200-1070

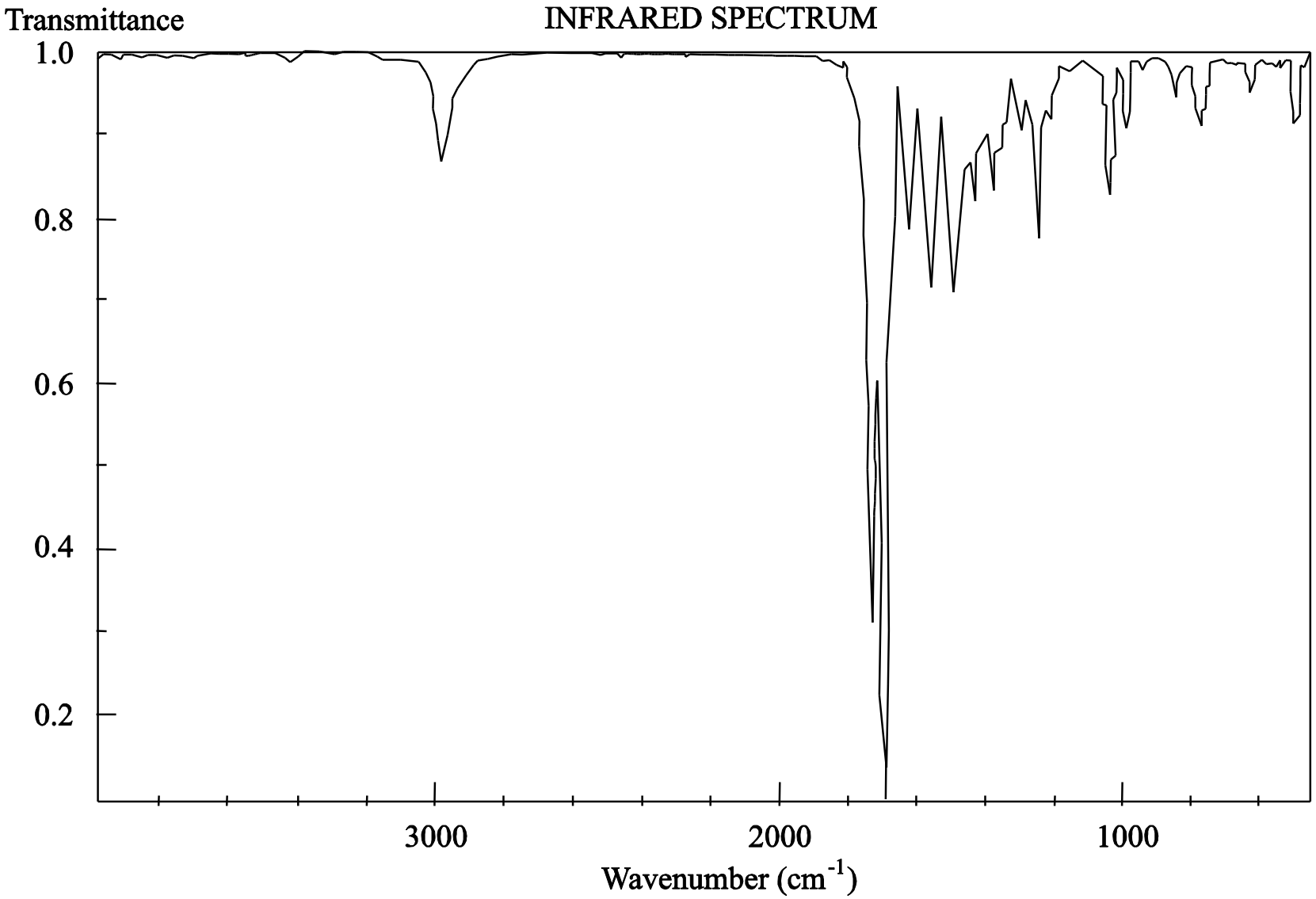
In the table above, signal intensity (peak height) is denoted by the following abbreviations:
w = weak, m = medium, s = strong, and v = variable.

Table 7.2 "Infrared Absorption Frequencies Chart"

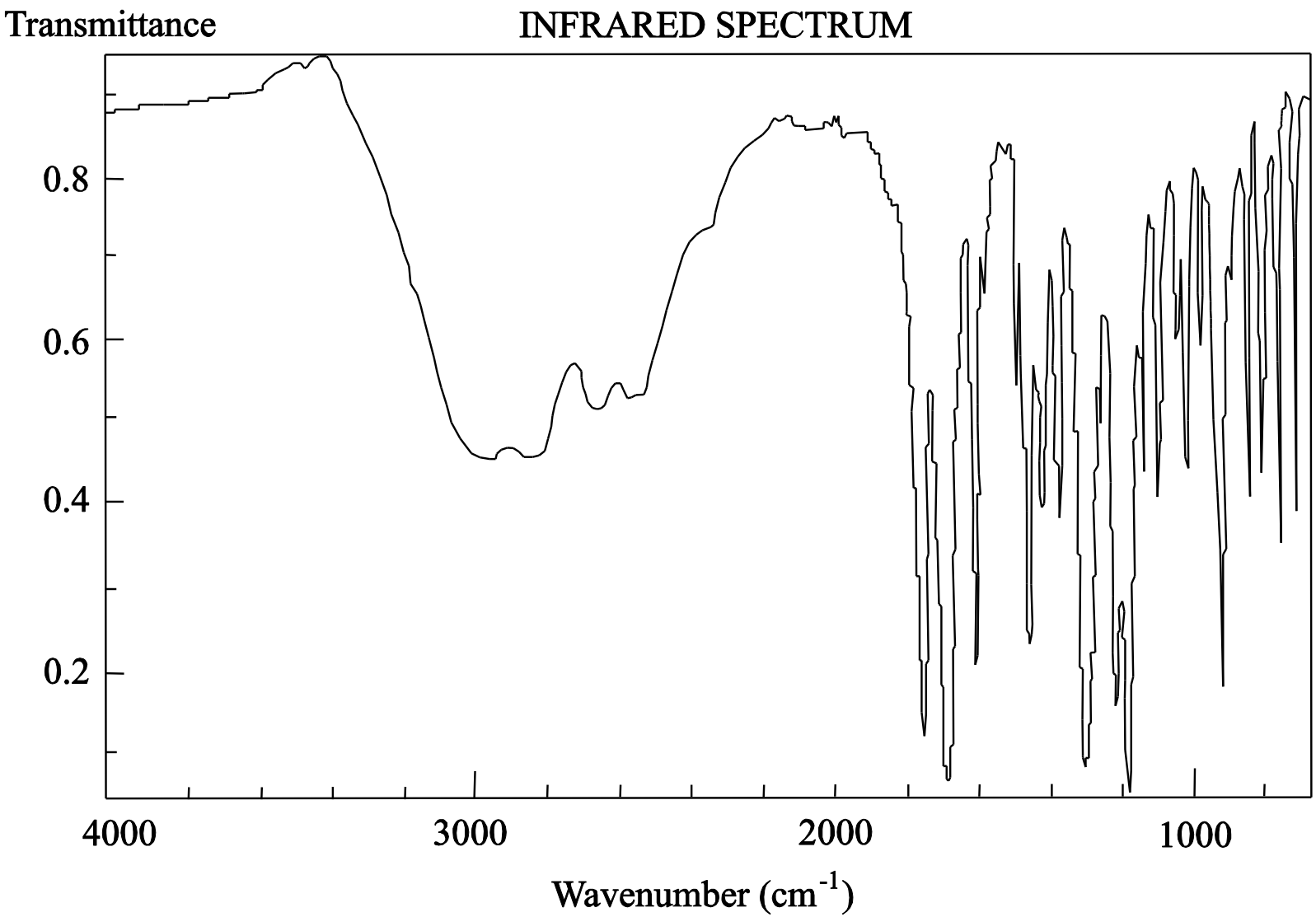
Functional Class	Characteristic Absorptions
Sulfur Functions	
S-H thiols	2550-2600 cm^{-1} (wk & shp)
S-OR esters	700-900 (str)
S-S disulfide	500-540 (wk)
C=S thiocarbonyl	1050-1200 (str)
S=O sulfoxide	1030-1060 (str)
sulfone	1325± 25 (as) & 1140± 20 (s) (both str)
sulfonic acid	1345 (str)
sulfonyl chloride	1365± 5 (as) & 1180± 10 (s) (both str)
sulfate	1350-1450 (str)
Phosphorous Functions	
P-H phosphine	2280-2440 cm^{-1} (med & shp) 950-1250 (wk) P-H bending
(O=)PO-H phosphonic acid	2550-2700 (med)
P-OR esters	900-1050 (str)
P=O phosphine oxide	1100-1200 (str)
phosphonate	1230-1260 (str)
phosphate	1100-1200 (str)
phosphoramide	1200-1275 (str)
Silicon Functions	
Si-H silane	2100-2360 cm^{-1} (str)
Si-OR	1000-11000 (str & brd)
Si-CH_3	1250± 10 (str & shp)
Oxidized Nitrogen Functions	
=NOH oxime	
O-H (stretch)	3550-3600 cm^{-1} (str)
C=N	1665± 15
N-O	945± 15
N-O amine oxide	
aliphatic	960± 20
aromatic	1250± 50
N=O nitroso	1550± 50 (str)
nitro	1530± 20 (as) & 1350± 30 (s)

	Stretching Vibrations			Bending Vibrations		
Functional Class	**Range (cm^{-1})**	**Intensity**	**Assignment**	**Range (cm^{-1})**	**Intensity**	**Assignment**
Alkanes	2850-3000	str	CH_3, CH_2 & CH 2 or 3 bands	1350-1470 1370-1390 720-725	med med wk	CH_2 & CH_3 deformation CH_3 deformation CH_2 rocking
Alkenes	3020-3100 1630-1680 1900-2000	med var str	=C-H & =CH_2 (usually sharp) C=C (symmetry reduces intensity) C=C asymmetric stretch	880-995 780-850 675-730	str med med	=C-H & =CH_2 (out-of-plane bending) cis-RCH=CHR
Alkynes	3300 2100-2250	str var	C-H (usually sharp) C≡C (symmetry reduces intensity)	600-700	str	C-H deformation
Arenes	3030 1600 & 1500	var med-wk	C-H (may be several bands) C=C (in ring) (2 bands) (3 if conjugated)	690-900	str-med	C-H bending & ring puckering
Alcohols & Phenols	3580-3650 3200-3550 970-1250	var str str	O-H (free), usually sharp O-H (H-bonded), usually broad C-O	1330-1430 650-770	med var-wk	O-H bending (in-plane) O-H bend (out-of-plane)
Amines	3400-3500 (dil. soln.) 3300-3400 (dil. soln.) 1000-1250	wk wk med	N-H (1°-amines), 2 bands N-H (2°-amines) C-N	1550-1650 660-900	med-str var	NH_2 scissoring (1°-amines) NH_2 & N-H wagging (shifts on H-bonding)
Aldehydes & Ketones	2690-2840(2 bands) 1720-1740 1710-1720 1690 1675 1745 1780	med str str str str str str	C-H (aldehyde C-H) C=O (saturated aldehyde) C=O (saturated ketone) aryl ketone α, β-unsaturation cyclopentanone cyclobutanone	1350-1360 1400-1450 1100	str str med	α-CH_3 bending α-CH_2 bending C-C-C bending
Carboxylic Acids & Derivatives	2500-3300 (acids) overlap C-H 1705-1720 (acids) 1210-1320 (acids) 1785-1815 (acyl halides) 1750 & 1820 (anhydrides) 1040-1100 1735-1750 (esters) 1000-1300 1630-1695(amides)	str str med-str str str str str str str	O-H (very broad) C=O (H-bonded) O-C (sometimes 2-peaks) C=O C=O (2-bands) O-C C=O O-C (2-bands) C=O (amide I band)	1395-1440 1590-1650 1500-1560	med med med	C-O-H bending N-H (1°-amide) II band N-H (2°-amide) II band
Nitriles	2240-2260	med	C≡N (sharp)			
Isocyanates, Isothiocyanates, Diimides, Azides, Ketenes	2100-2270	med	-N=C=O, -N=C=S -N=C=N-, -N_3, C=C=O			

Unknown A is_____


INFRARED SPECTRUM
Transmittance
1.0
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)

Unknown B is_____


Transmittance
INFRARED SPECTRUM
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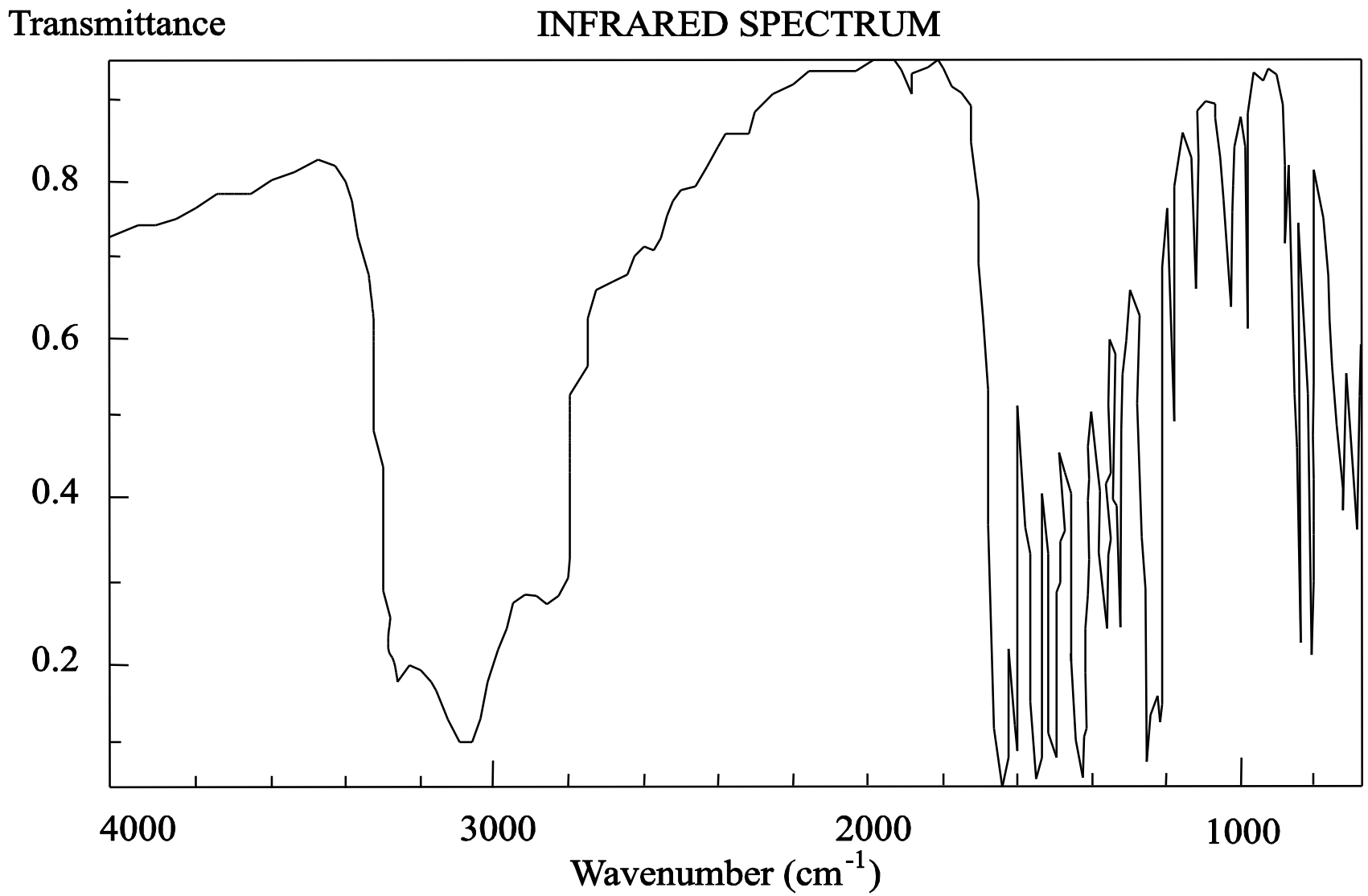
0.6
0.4
0.2
4000
3000
2000
1000
Wavenumber (cm-1)

Unknown C is_____


Transmittance
INFRARED SPECTRUM
0.8
0.6
0.4
0.2
4000
3000
2000
1000
Wavenumber (cm-1)