Experiment 6:
Infrared Spectroscopy Tutorial

Preparation

There are no prelab questions and the instructor led tutorial during the in-person lab is optional.

Review Sections 12.5-12.8 on interpreting infrared spectra in the course textbook.

The tutorial can be found as an online resource.

Objectives

The purpose of this experiment is to improve your skill in

1. identifying the functional group or groups present in a compound, given a list of the most prominent absorptions in the infrared spectrum and a table of characteristic absorption frequencies.

2. identifying the broad regions of the infrared spectrum to determine the presence of functional groups, such as alcohols, amines, and carbonyl groups, in an unknown compound.

Interpretation of Infrared Spectra

The laboratory instructors will provide a brief infrared tutorial and workshop within the lab class. However, much of this experiment is not wet benchtop chemistry and can be done at home.

1. Review the Theory on Infrared Spectroscopy
2. Review the Listing of Organic Functional Groups and their corresponding Infrared Spectra.
3. Perform the Sample Infrared Spectrum Problems.
4. Answer four (4) of the 'Exp. 6 Infrared Unknown Downloads.'
   The Unknown Spectra can be at:

Introduction to Infrared Spectroscopy- Theory and Practice

Electromagnetic Radiation

As you read this page, uncountable numbers of photons or 'light particles' are reflecting off its surface and are being absorbed by pigments (i.e. complex organic molecules) in the rod and cone cells in the retina of your eye. Where the ink (i.e. complex organic dye) has absorbed the photons, you perceive a dark area (i.e. letters) due to the lack of photons from that point on the paper.

On a deeper level, photons (and electrons) are actually wave/particle dualities as described by quantum physics. Photons carry only a discrete amount of energy, called quanta, but the amount of energy of a quanta is defined by the equation, $e = h \upsilon = h c/l$
where:

- e = the energy of 1 photon (quanta)
- h = Planck's constant (6.62×10^{-27} erg sec)
- υ = Frequency in hertz (cycles or l per sec)
- c = Speed of light (3×10^{10} cm per sec)
- l = Wavelength in cm

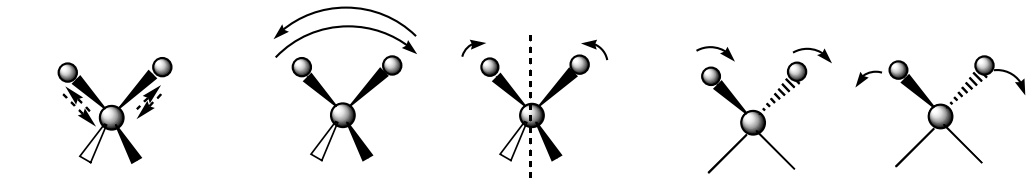
Thus, the amount of energy carried by a photon varies directly with its frequency, and because of the relationship between frequency and wavelength, varies inversely with its wavelength. Photons also behave like waves of electromagnetic energy traveling at the speed of light.

Practically speaking however, you need only understand that photons are the messengers that carry the electromagnetic force between electrons and other elementary particles. Electrons, whether free or bound in a covalent bond, are capable of absorbing (or emitting) photons and changing their energy state. This leads to different types of excitation (nuclear transformations, electronic, rotational, nuclear spin changes, bond deformation) depending on the amount of energy carried by the photon. High-energy photons (x-ray, gamma ray, and cosmic ray) can cause ionization of the molecule, while UV photons are involved in electronic interactions. Remember it is the interaction of electrons (via photons) in the outer cloud surrounding atoms that forms the foundation of all chemical reactions.

Infrared Radiation

Infrared radiation is composed of photons with a specific range of wavelengths (7.8×10^{-5} cm to 10^{-2} cm) and frequencies (~10^{14} to 10^{12} Hz). This range includes the near infrared, the infrared and far-infrared regions. The actual wavelengths of interest to most organic chemists are 1.667×10^{-3} cm to 2.5×10^{-4} cm (the 'infrared' region). These wavelengths (λ) are most often expressed as there corresponding wave number (n) where $n = 1/\lambda$, with n measured in cm^{-1}. (e.g. l2.5 to 16.6 μm = 4000 to 600 cm^{-1}).

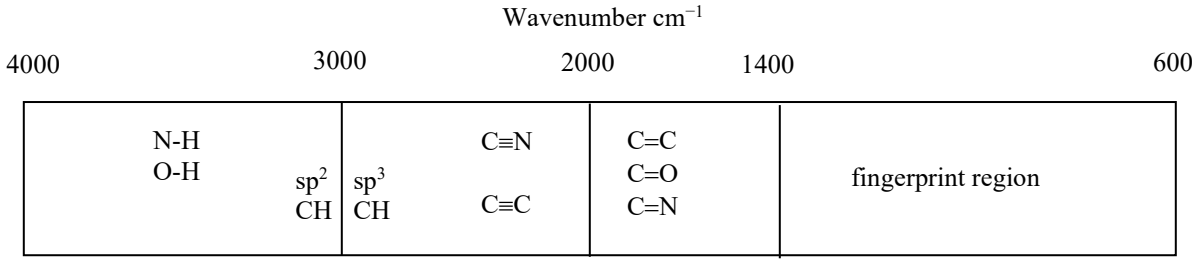
Infrared carries relatively low levels of energy (e.g. ~1 to 10 kcal/mol) which, when absorbed, result in only bond vibrations like stretching and bending, e.g., rocking, scissoring, wagging, and twisting (i.e., bond deformations).



SomeTypes of Bending Vibrations

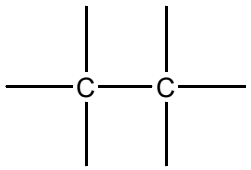
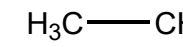
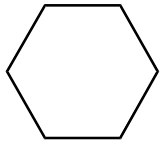
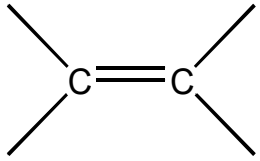
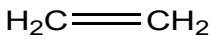
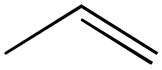
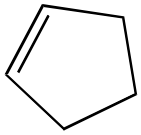
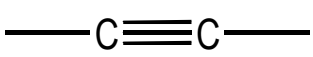
Every molecule, depending on its make-up, is capable of absorbing infrared photons and increasing the intensity of its molecular motions. Different functional groups within the molecule will absorb photons at different infrared wavelengths. Thus, when a spectroscopic wavelength scan is performed on an organic molecule, certain □ will be absorbed while other □ will pass through. Once we have the infrared spectrum of a compound, the spectrum can be analyzed and compared with known infrared absorptions for particular functional groups (see Table 6.1).

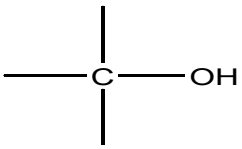
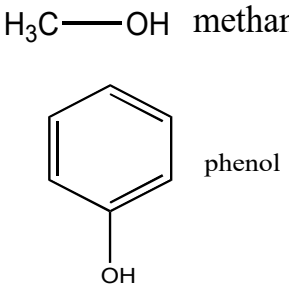
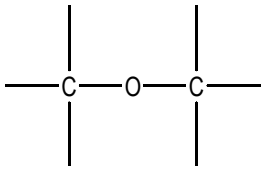
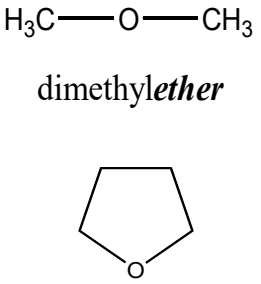
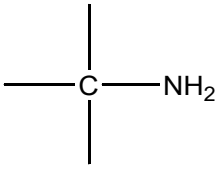
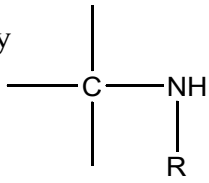
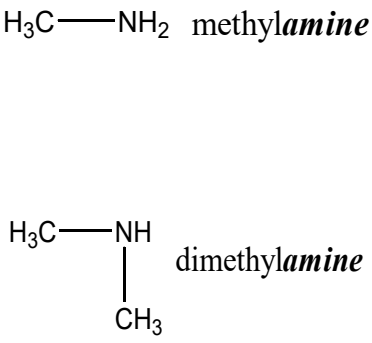
The infrared spectrum for a particular molecule can be very complex, consisting of many absorption bands because of the many possible motions each atom can undergo (a non-linear molecule has 3N-6 normal modes of vibration where N = the number of atoms in the molecule). When analyzing a spectrum, it is important to look at four different regions of the spectrum for the presence or absence of specific absorption peaks. **Note:** you are not required to analyze the fingerprint region.



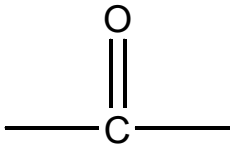
The following pages contain information to help you understand and interpret infrared spectra.

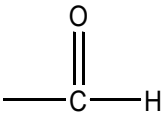
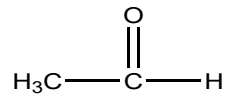
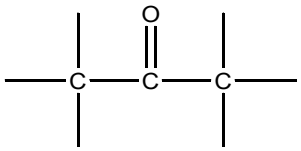
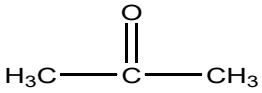
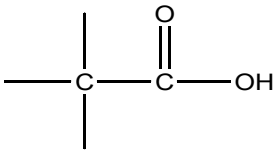
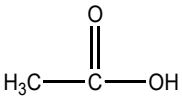
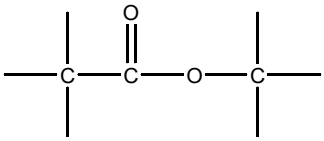
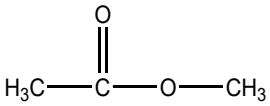
1. a chart showing the structures of various functional groups, which you need to know.
2. the wavenumbers of the functional groups, to help you locate pertinent absorption bands on an infrared spectrum.
3. Diagrams of the shapes and intensities of various infrared absorption bands, which will help in your interpretation of infrared spectra.
4. Finally, your instructor will lead you through the interpretation of sample infrared spectra representative of various functional groups. Unknown spectra are included to allow you to practice on your own. There is a great deal of information to learn, but the more you practice, the easier it becomes to interpret infrared spectra

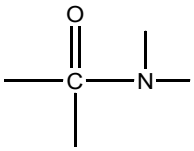
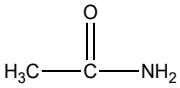
FAMILY NAME	FUNCTIONAL GROUP STRUCTURE	EXAMPLES AND NOMENCLATURE
Alkane	 sp^3 orbitals	 eth***ane***  pent***ane***  cyclohex***ane***
Alkene	 sp^2 orbitals	 eth***ene***  prop***ene***  cyclopent***ene***
Alkyne	 sp orbitals	 eth***yne*** (Acetylene)

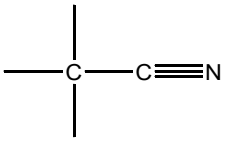
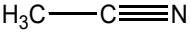
Alcohol		
Ether		
Amines	Primary  Secondary 	

Carbonyls:



Aldehyde		 ethan***al*** (Acetaldehyde)
Ketone		 propan***one*** (Acetone)
Carboxylic Acid		 ethan***oic acid*** (Acetic acid)
Ester		 methyl ethan***oate*** (Methyl acetate)

Amides		 ethan***amide*** (Acetamide)

Nitriles		 ethane***nitrile*** (Acetonitrile)

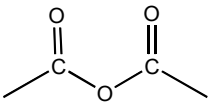
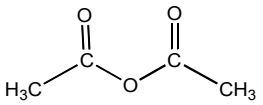
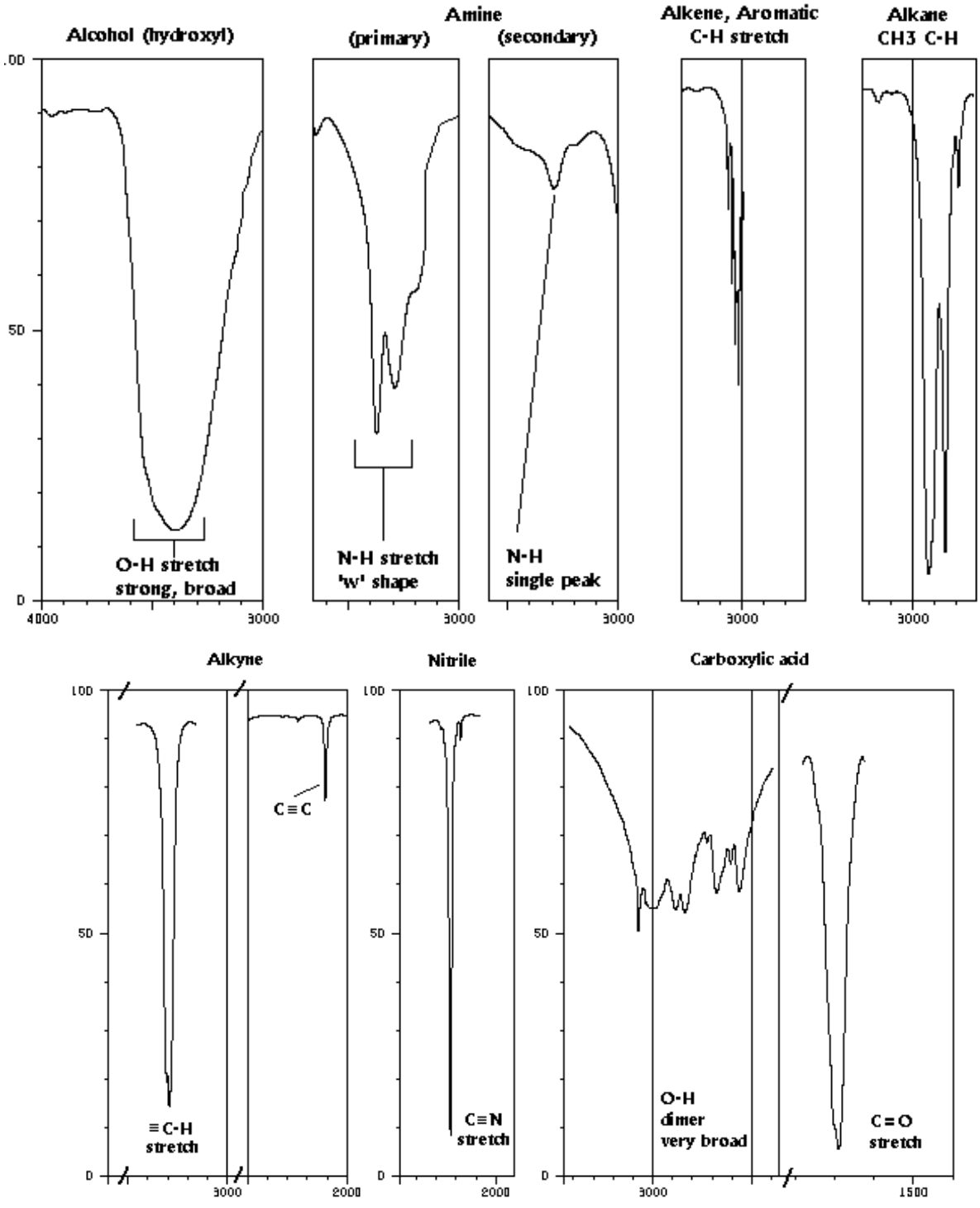
Anhydride		 acetic **anhydride**

Table 6.1 Correlation Table of Infrared Absorption and Functional Group.

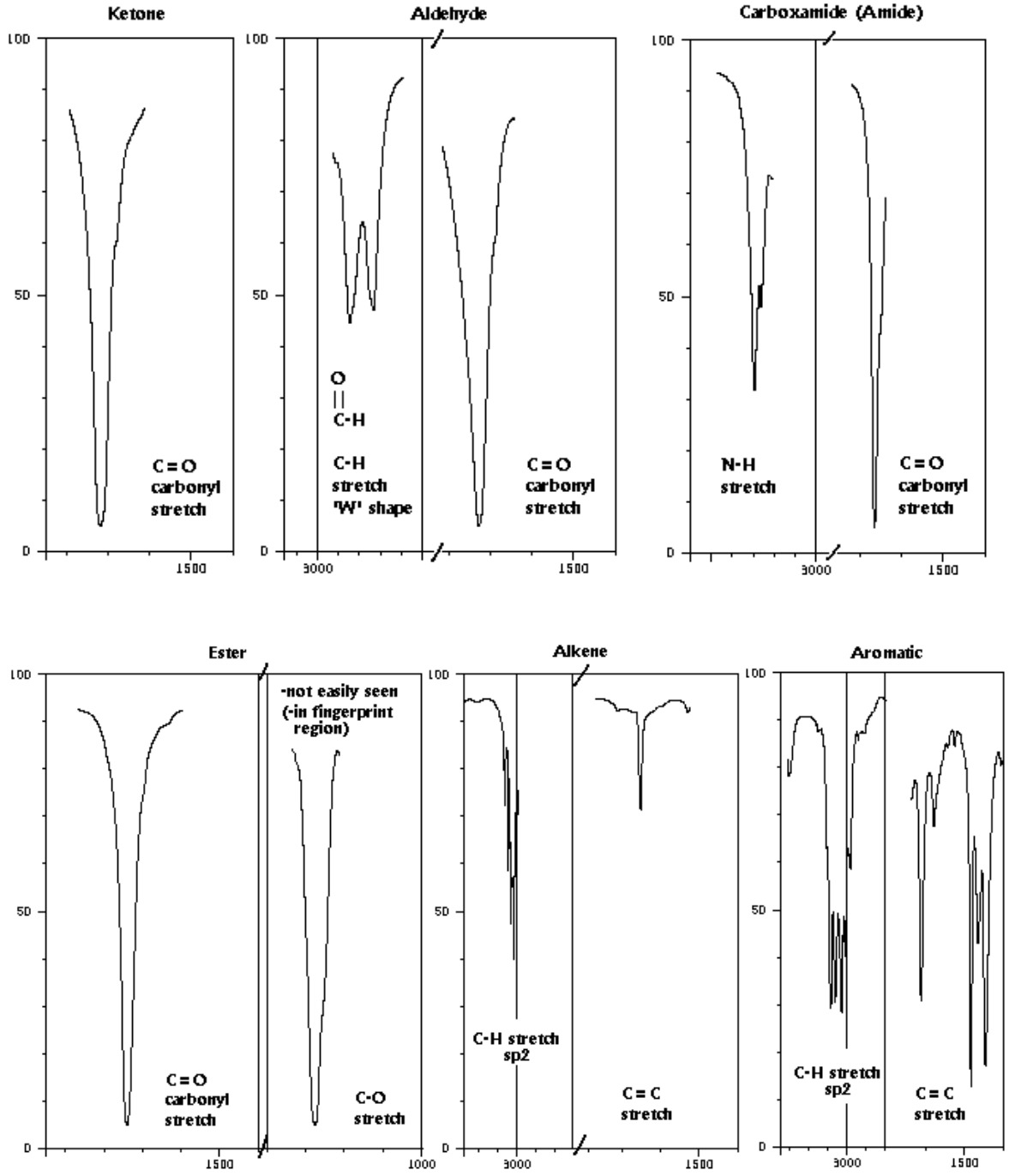
Type of Absorption	Wavenumber (cm^{-1})	Intensity of Absorption	Absorption of:
O-H stretch	3400-3640	strong, broad	alcohol
	2500-3300	strong, very broad	carboxylic acid
N-H stretch	3310-3350	medium ('W' shape)	amine (1^o)
C-H stretch	3300	strong	sp C-H of alkyne
	3030	medium	aromatic
	3020-3100	medium	sp^2 C-H of alkene
	2850-2960	medium to strong	sp^3 C-H of alkane
	2750 & 2850	weak-medium ('W' shape)	O=C-H of aldehyde
C≡N stretch	2210-2260	medium, sharp	nitrile
C≡C stretch	2100-2260	medium, sharp	alkyne
C=O stretch	1670-1780	strong, sharp	carbonyl
	1730-1750		ester
	1720-1740		aldehyde
	1705-1725		ketone
	1700-1725		carboxylic acid
	1640-1700		amide
	ca 1800 and 1760		anhydride
C=C stretch	1650-1670	weak-medium, sharp	alkene
	1600, 1500, 1450	strong sharp	aromatic
C=N stretch	1640-1670	medium, sharp	imine
N-H bend	1500-1650	medium to strong, sharp	amine and amide
N=O stretch	1500-1600 (1540) and 1320-1390	strong, sharp	nitro-compound
C-N stretch	1030, 1230	medium	amine
C-O stretch	1050-1150	strong	alcohol
	1250-1310	strong broad	ester-conjugated
	1240	strong, broad	ester-acetates
	1175	strong, broad	ester-unconjugated
C-Cl stretch (terminal)	600-800	strong	alkyl halide
Ar-Cl stretch	1000-1175	medium-strong	aryl halide
C-Br stretch (terminal)	500-760	strong	alkyl halide
C-I (terminal)	500	strong	alkyl halide

Note: when a C=C bond is in conjugation with a carbonyl, the observed carbonyl absorption frequency will be < ~ 30 cm^{-1}.

Shapes of Infrared Absorption Bands Observed for Different Functional Groups



Typical Absorption Band Shapes (cont.)



How to Interpret an Infrared Spectrum

Step 1 Divide the infrared spectrum into four main areas (use pencil and ruler and take into account any off-shift in the spectrum's wavenumbers).

i) Above 3000 cm^{-1}
ii) Between 3000 and 2000 cm^{-1}
iii) Between 2000 and 1400 cm^{-1}
iv) Below 1400 cm^{-1} (fingerprint region)

Step 2 Starting at the left of the spectrum, examine the area **above 3000 cm^{-1}**, first looking in the region near 3300 cm^{-1} and record in tabular format the presence/absence of:

i) a broad, very strong absorption band of an **'O-H'**. If present, it means you know that your molecule is at least an **alcohol**.
ii) A broad, weak to medium strength, double or single absorption band of **'N-H'**. If present it means you have an **amine** (1° or 2°) or possibly an **amide**.
iii) A sharp, medium to strong, single absorption band of **'≡C-H'** of a **terminal alkyne**.
Note: If present, it means you should also see a 'C≡C' absorption near 2250 cm^{-1}.

After examining the region around 3300 cm^{-1}, look for any sharp, weak to medium absorption just above 3000 cm^{-1} (e.g., 3050 cm^{-1}) resulting from the 'C-H' stretch of a sp^2 hybridized carbon. If present, it means you have a **'C=C-H'** of an alkene or aromatic compound.

Step 3 Next examine the area between **3000 and 2000 cm^{-1}** and record the presence/absence of absorption bands or peaks.

i) First look just below 3000 cm^{-1} (e.g., 2850-2950 cm^{-1}) resulting from the 'C-H' stretch of a sp^3 hybridized carbon. If present, it means you are seeing the **'C-H'** stretch of an **$-CH_2$ or $-CH_3$** group. Note: This absorption is not very informative as most organic compounds have $-CH_2$ or $-CH_3$ groups.
ii) Then look for the extremely broad peak, actually starting at 3300 cm^{-1} and extending all the way to ~2500 cm^{-1}, caused by the **O-H dimer** between two **carboxylic acid** molecules (COOH). This absorption is probably the most difficult to see as other absorption peaks may be overlapping the broad peak.
iii) Finally look for a sharp, weak to medium peak caused by either **'C≡C'** or **'C≡N'**.
iv) If present, then the compound is an alkyne (might also have the 'C-H' of a terminal alkyne, see step 2 above) or a nitrile.

Step 4 Next examine the area between **2000 and 1400 cm^{-1}** and record the presence/absence of absorption bands or peaks.

i) First look near 1700 cm^{-1} (e.g. 1680-1750 cm^{-1}) for a sharp, strong peak resulting from the **'C=O'** stretch of a **carbonyl**. Note: This absorption is very informative and will be present if your compound is an aldehyde, ketone, ester, amide, or carboxylic acid.

ii) Next look near 1650 cm^{-1} (e.g. 1600-1670 cm^{-1}) for a sharp, weak peak resulting from the **'C=C'** stretch of an **alkene**.

iii) Finally look near 1600 cm^{-1} and 1500 cm^{-1} for a sharp, double peak resulting from the **'C=C'** stretch of an **aromatic ring**.

Step 5 If you dare, you may look in the **fingerprint region** (**area below 1400 cm^{-1}**) and record the presence of absorption bands or peaks.

i) First look near 1200 (1160-1310) cm^{-1} for a sharp, strong peak resulting from the **'C-O'** stretch of an **ester**.
Note: This absorption is very difficult to see and may or may not be present, i.e. conclusive if present, inconclusive if not present.

ii) If you suspect you have an aromatic ring (absorption bands at ~3030 and 1600 and 1500 cm^{-1} present), you may try to discern the substitution pattern of the benzene ring by looking at the strong absorption bands of the **ring 'C-H'** out-of-plane bending vibrations in the region 680-900 cm^{-1}.

Benzene Substitution Pattern	Ring 'C-H' Absorption Bands Present (cm^{-1})
monosubstituted	2 sharp peaks, 730-770, 690-710
ortho disubstituted	1 sharp peak, 735-770
meta disubstituted	3 sharp peaks, 860-900, 750-810, 680-725
para disubstituted	1 sharp peak, 800-860
1,2,3 trisubstituted	2 sharp peaks, 760-780, 705-745
1,3,5 trisubstituted	2 sharp peaks, 810-865, 675-730
1,2,4 trisubstituted	2 sharp peaks, 870-885, 805-825

Ref: McMurry, J., 1992. Organic Chemistry, 3rd ed, Brooks/Cole, p.549-550, (4th ed, p.559)
Nakanishi, K., 1964. Infrared Absorption Spectroscopy, Holden Day p.27.

iii) Again, if you have an aromatic, you may also try to discern the ring substitution pattern of the benzene ring by looking at the very weak overtone-combination absorption bands of the **ring 'C-H'** stretch vibrations in the region 1670-2000 cm^{-1}.

Benzene Substitution Pattern	Ring 'C-H' Overtone Bands Present (cm^{-1})
monosubstituted	4 weak equally spaced and shaped sharp peaks
ortho disubstituted	3 weak irregularly spaced/shaped sharp peaks
meta disubstituted	2 weak sharp peaks + one weak broad peak
para disubstituted	2 weak sharp peaks

iv) If you suspect you have a long straight chain (>4 C) alkane, (absorption bands at 2850-2950 cm^{-1} present but not much else), you may try to see the sharp, weak absorption due to the concerted rocking of >4 $-CH_2$ in a chain. It lies in the region 720 ± 10 cm^{-1}.

Step 6 Finally, you will summarize your results by making a statement about what functional groups you suspect to be present in the molecule or perhaps you will be asked to select from a list of suggested structures, which molecule most likely would generate the spectrum just analyzed.

Instructor Led Group Infrared Analysis Problems

Use the tables below to record your results of the 'Infrared Spectral Analyses' for the following compounds (infrared spectra appear on the following pages of this lab manual). Label the absorption bands.

Cyclohexanol	Absorption Band Code#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated
>3000 cm^{-1}	1	3331	broad	strong	O-H stretch alcohol
3000-2000 cm^{-1}	2	2932 & 2855	sharp	strong	C-H sp^3 stretch
2000-1500 cm^{-1}	none				
(Fingerprint)	*3*	*1068*	*sharp*	*strong*	C-O of alcohol

Functional Group absent: no ≡C-H, no N-H, no sp^2 H-C=, no C≡C, no C≡N, no C=O, no C=C alkene or aromatic

2-methyl-3-butyn-2-ol	Absorption Band Code#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated
>3000 cm^{-1}	1	~3380	broad	strong	O-H stretch alcohol
	2	3303	sharp	strong	
3000-2000 cm^{-1}	3	2876,2938,2987	sharp	med-str.	
	4	2120	sharp	weak	
2000-1500 cm^{-1}	none				

Functional Group absent: no N-H, no sp^2 H-C=, no C≡N, no C=O, no C=C alkene or aromatic

3-buten-2-ol	Absorption Band Code#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated
>3000 cm^{-1}	1	~3350	broad		
	2	3083 & 3012		strong	C-H _____stretch
3000-2000 cm^{-1}	3		sharp		C-H _____ stretch
2000-1500 cm^{-1}	4	1646			

Functional Group absent: no ≡C-H, no N-H, no C≡C, no C≡N, no C=O, no C=C aromatic

benzhydrol	Absorption Band Code#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated
>3000 cm^{-1}	1	3392-3359	broad		
	2	3049 & 3027	sharp		C-H _____stretch
3000-2000 cm^{-1}	3	2900	sharp		C-H _____stretch
2000-1500 cm^{-1}	4	1598,1495,1458	sharp		

Functional Group absent: no ≡C-H, no N-H, no C≡C, no C≡N, no C=O, no C=C alkene

Instructor Led Group Infrared Analysis Problems (cont.)

benzaldehyde	Absorption Band Code#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group absent: no O-H, no ≡C-H, no N-H, no sp^3 C-H, no C≡C, no C≡N, no C=C alkene

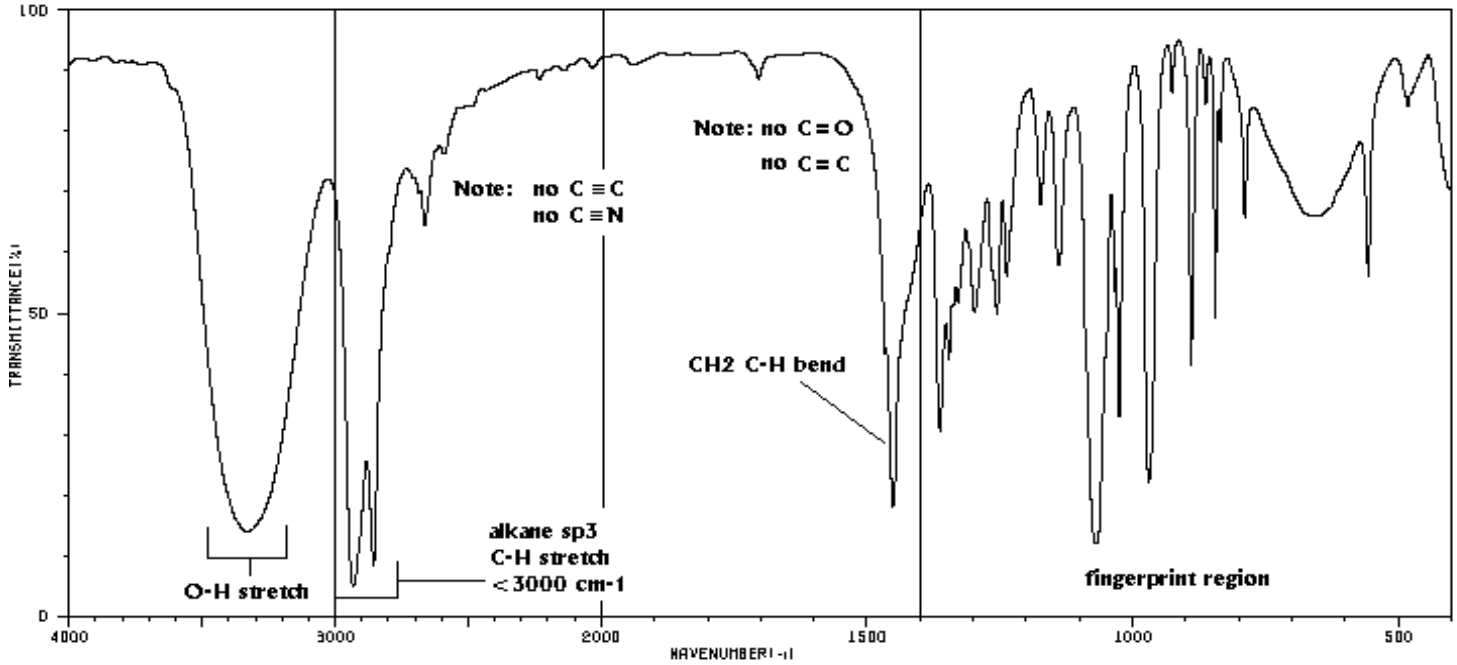
acetic acid	Absorption Band Code#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group absent:

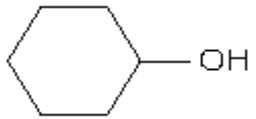
dibutylamine	Absorption Band Code#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group absent:

HIT-NO=1077	SCORE= ( )	SDBS-NO=581	IR-NIDA-09018 : LIQUID FILM
CYCLOHEXANOL			
$C_6H_{12}O$			



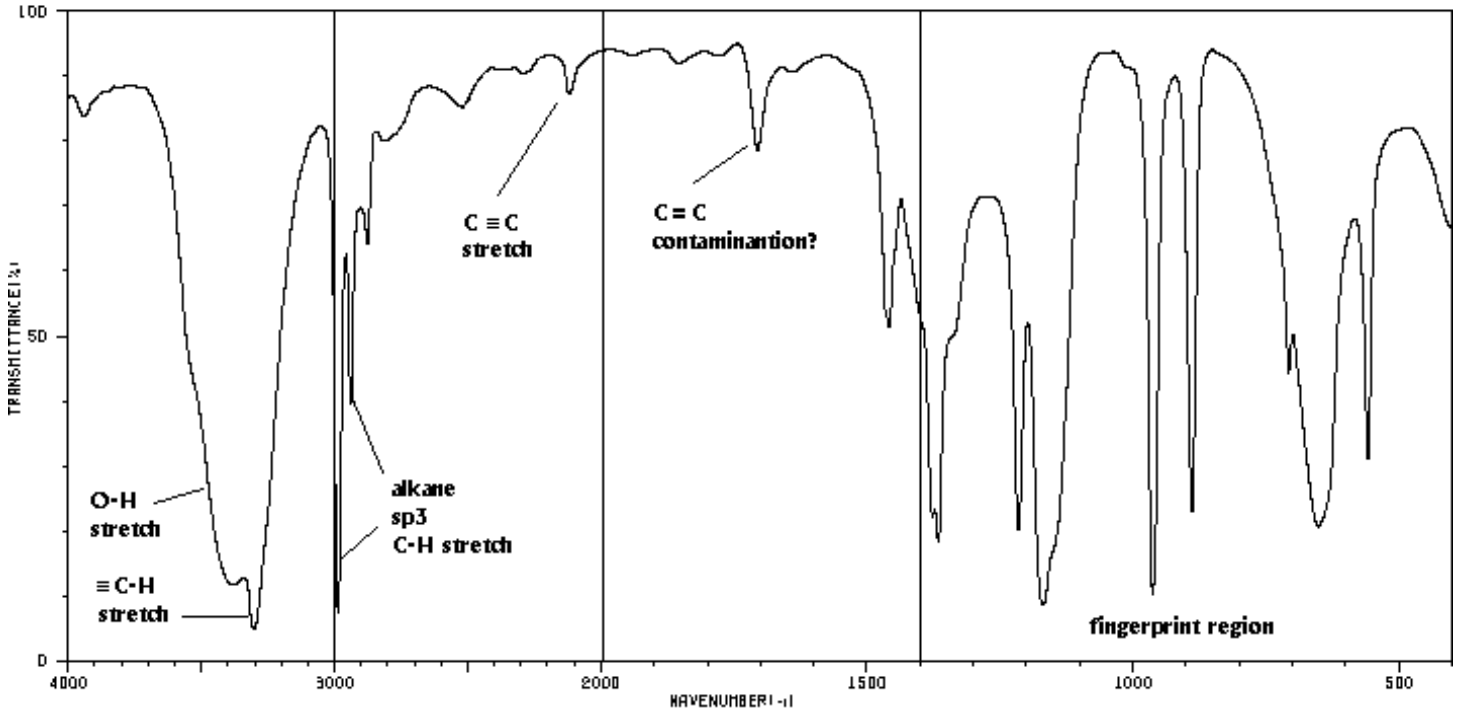
3331	13	1704	86	1266	47	970	21	667	64
2932	4	1467	42	1238	53	926	84	557	53
2855	6	1452	17	1174	86	890	39	462	61
2686	80	1363	29	1140	55	863	81		
2666	82	1346	41	1068	11	845	47		
2588	74	1329	50	1034	52	835	74		
2233	84	1298	49	1025	32	789	64		



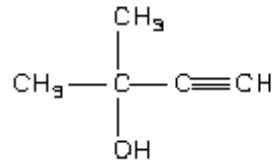
HIT-NO=2057	SCORE= ( )	SDBS-NO=2818	IR-NIDA-00603 : LIQUID FILM

2-METHYL-3-BUTYN-2-OL

C_5H_8O



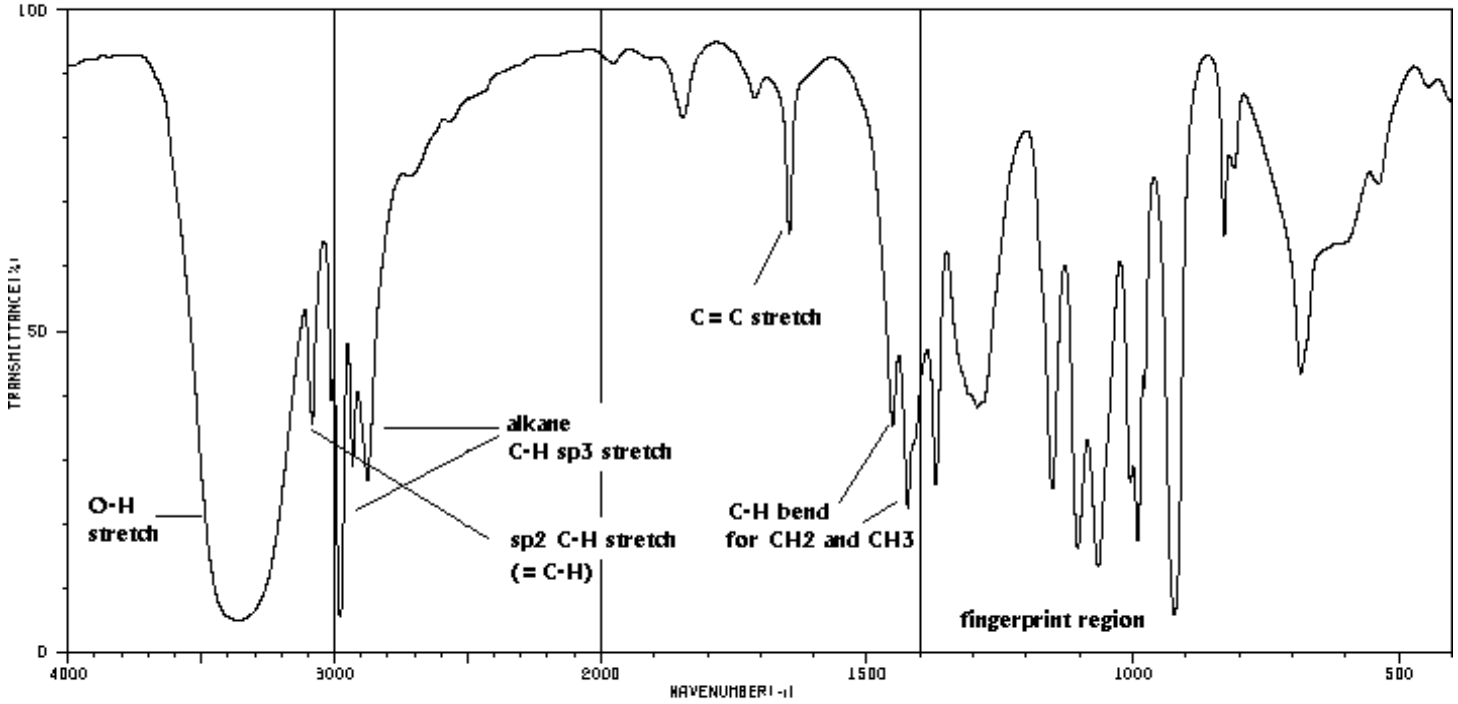
3939	81	2120	84	1170	8
3303	4	1706	74	963	10
2987	7	1465	52	889	22
2938	38	1459	49	708	42
2876	62	1378	21	652	20
2811	77	1368	17	556	30
2619	81	1216	19		



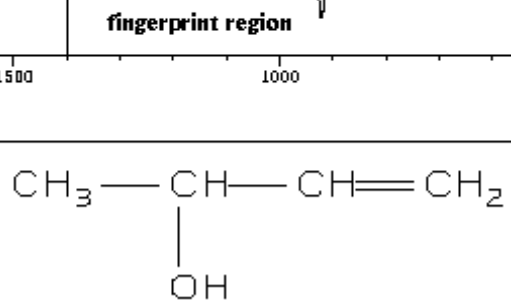
HIT-NO=1306	SCORE= ( )	SDBS-NO=1211	IR-NIDA-01713 : LIQUID FILM

3-BUTEN-2-OL

C_4H_8O



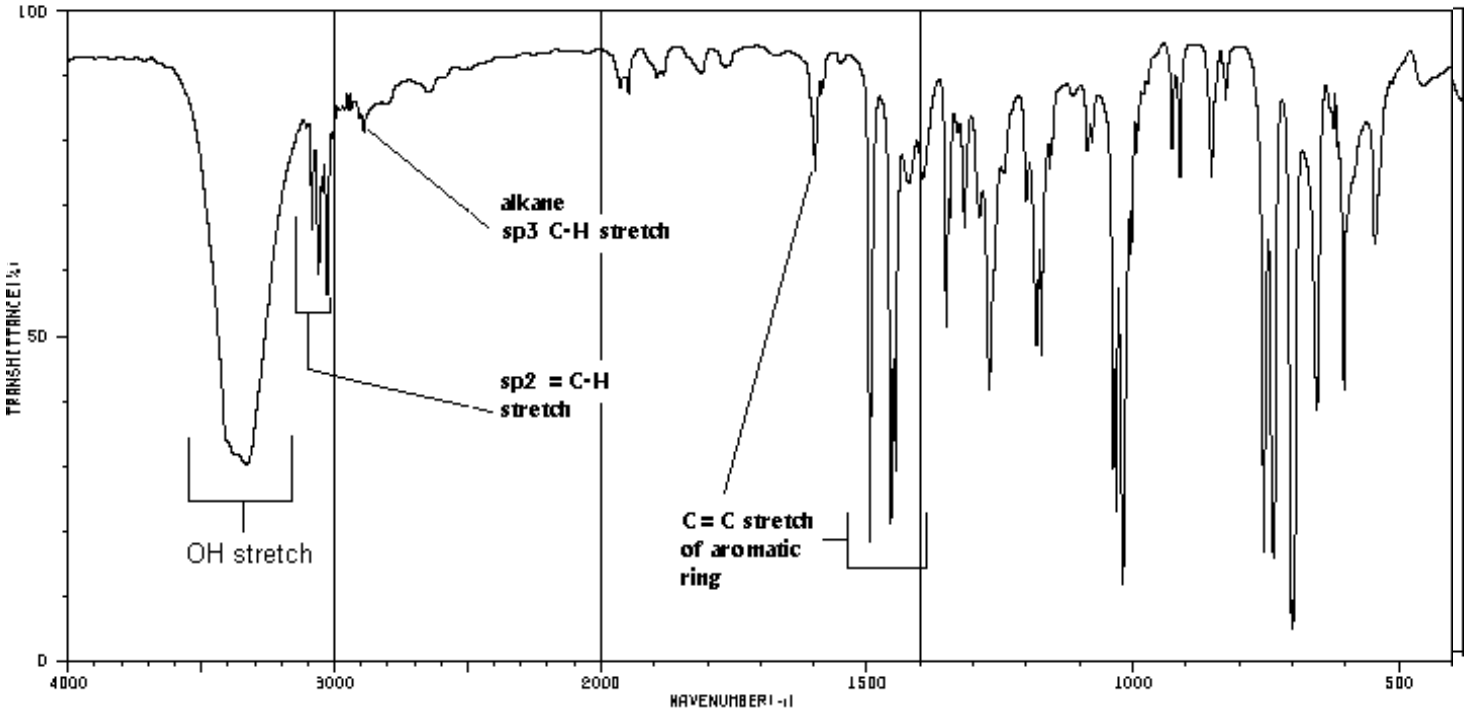
3083	33	1646	62	1066	12	686	41
3012	36	1452	33	1005	24	539	70
2979	4	1424	20	991	15	443	64
2932	26	1371	29	978	30		
2876	24	1292	35	922	5		
1646	79	1152	25	829	60		
1711	81	1103	14	810	72		



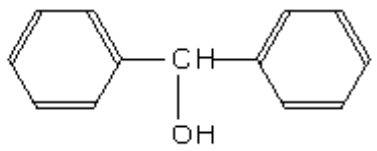
HIT-NO=1144	SCORE= ( )	SDBS-NO=869	IR-NIDA-47684 : KBR DISC

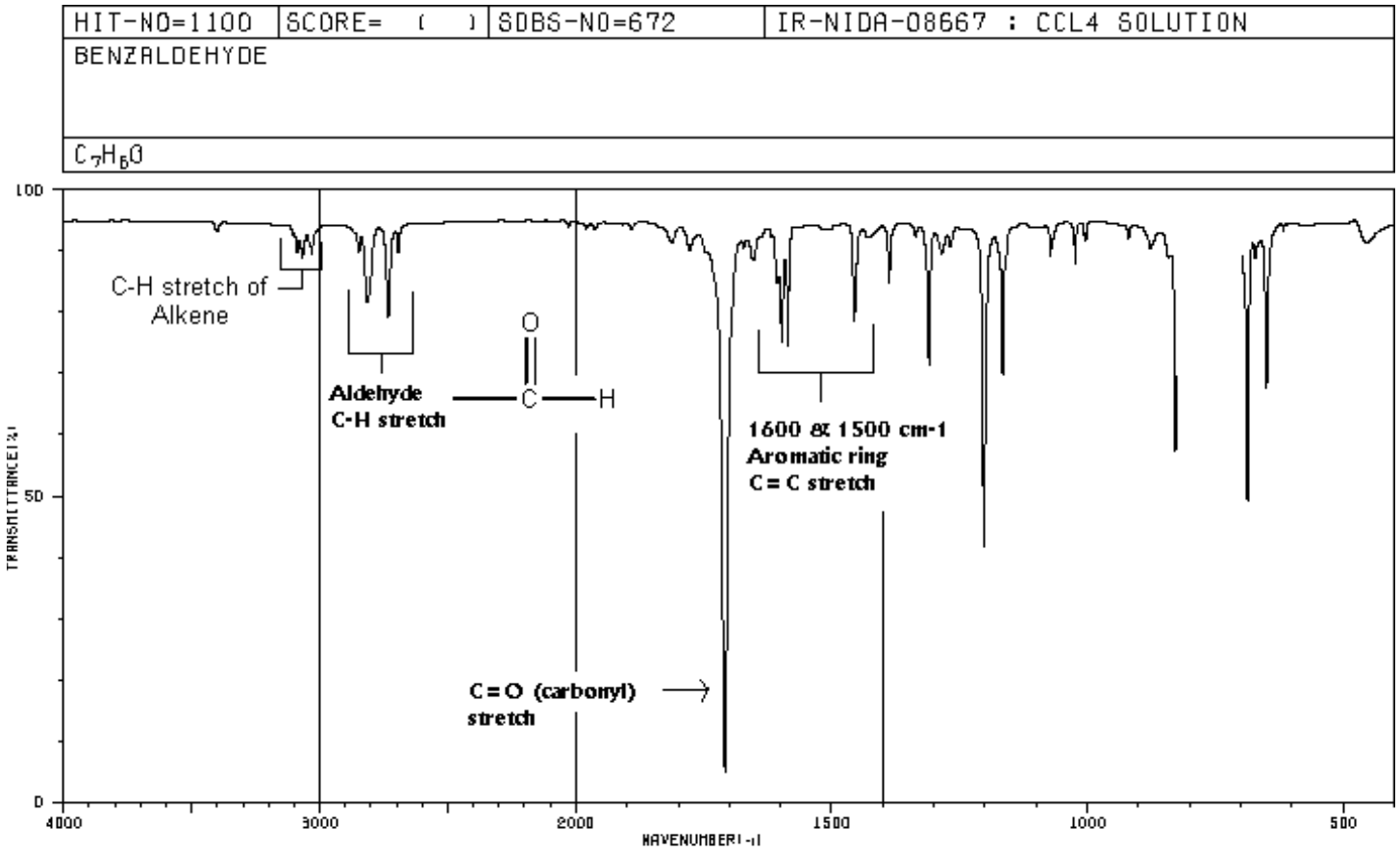
BENZHYDROL

$C_{13}H_{12}O$

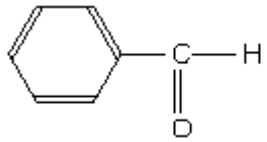


3392	26	1598	72	1345	66	1172	44	863	72
3359	30	1495	17	1317	64	1156	72	754	16
3331	29	1458	21	1289	86	1037	28	735	15
3086	64	1446	27	1271	39	1032	22	702	4
3059	57	1422	70	1244	72	1019	11	654	37
3049	70	1395	72	1201	88	1003	60	604	39
3027	63	1361	49	1182	46	912	72	645	62





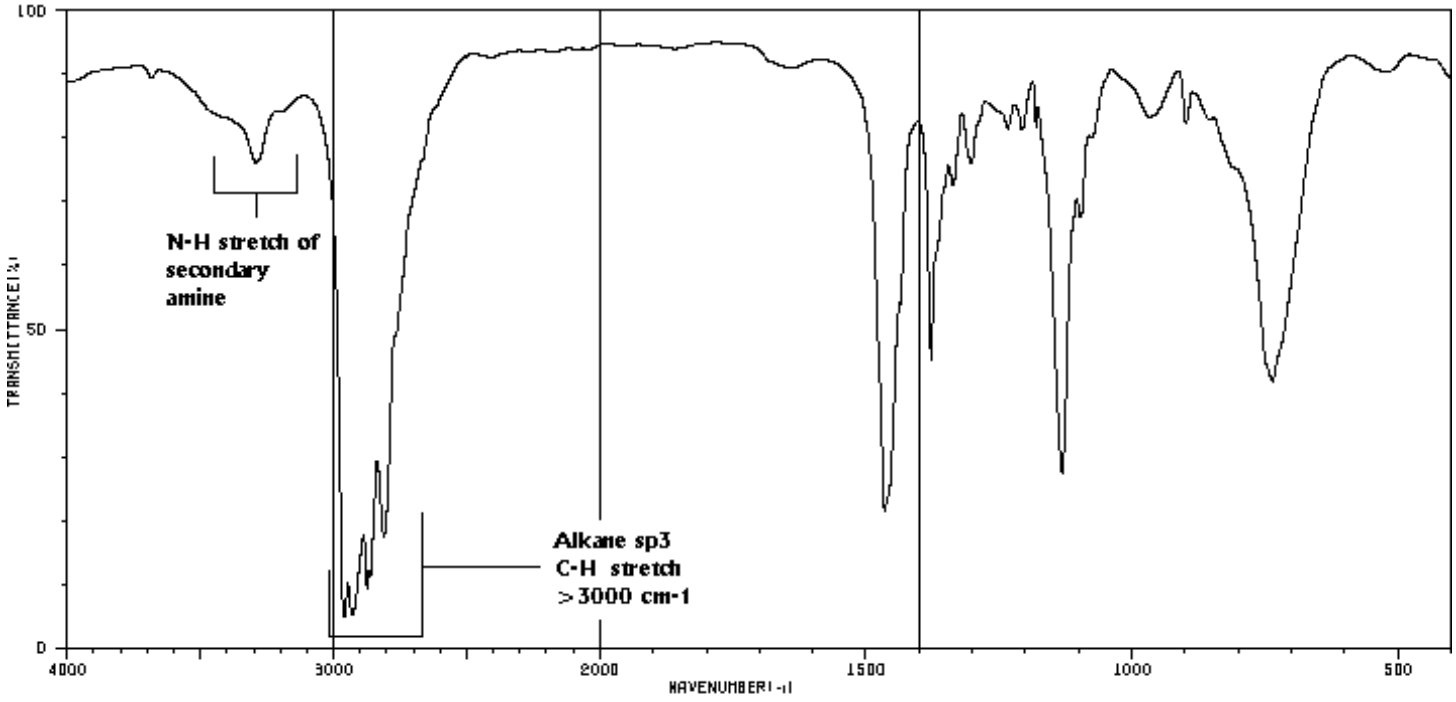
3088	86	1778	86	1388	81	1024	84
3068	86	1709	4	1310	68	828	55
3032	86	1653	84	1285	86	688	47
2847	86	1607	81	1203	39	673	86
2814	79	1598	72	1167	68	650	64
2732	77	1586	72	1160	84		
2693	86	1466	74	1072	86		



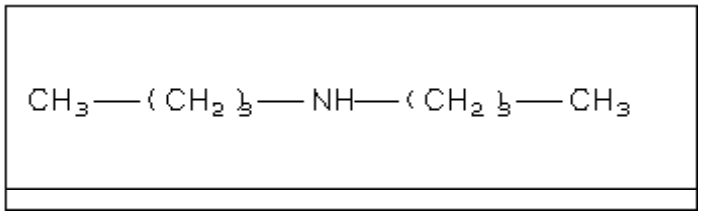
HIT-NO=1506	SCORE= ( )	SDBS-NO=1672	IR-NIDA-04481 : LIQUID FILM

DIBUTYLAMINE

$C_8H_{19}N$



3684	86	1466	20	1181	79
3290	72	1378	43	1131	26
2959	4	1338	70	1096	84
2929	6	1302	72	966	79
2874	9	1245	81	961	81
2862	10	1234	79	898	79
2810	16	1206	79	736	41
[illegible]	66	892	41		



Infrared Analysis Practice Problems

Use the tables below to record your results of the 'Infrared Spectral Analyses' of the provided known spectra in this lab manual.

benzaldehyde	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group(s) absent:

benzoic acid	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

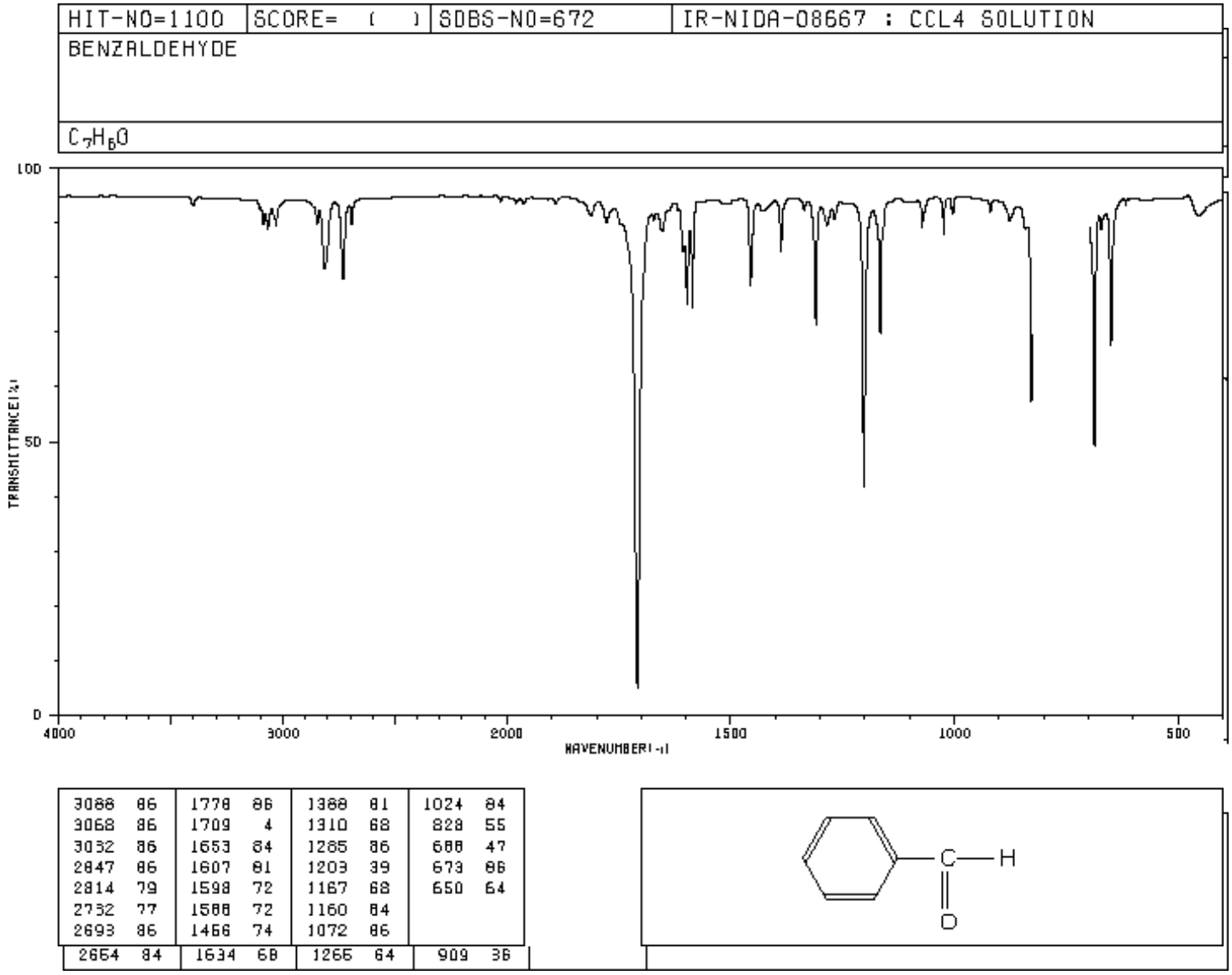
Functional Group(s) absent:

phenylacetylene	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group(s) absent:

styrene	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

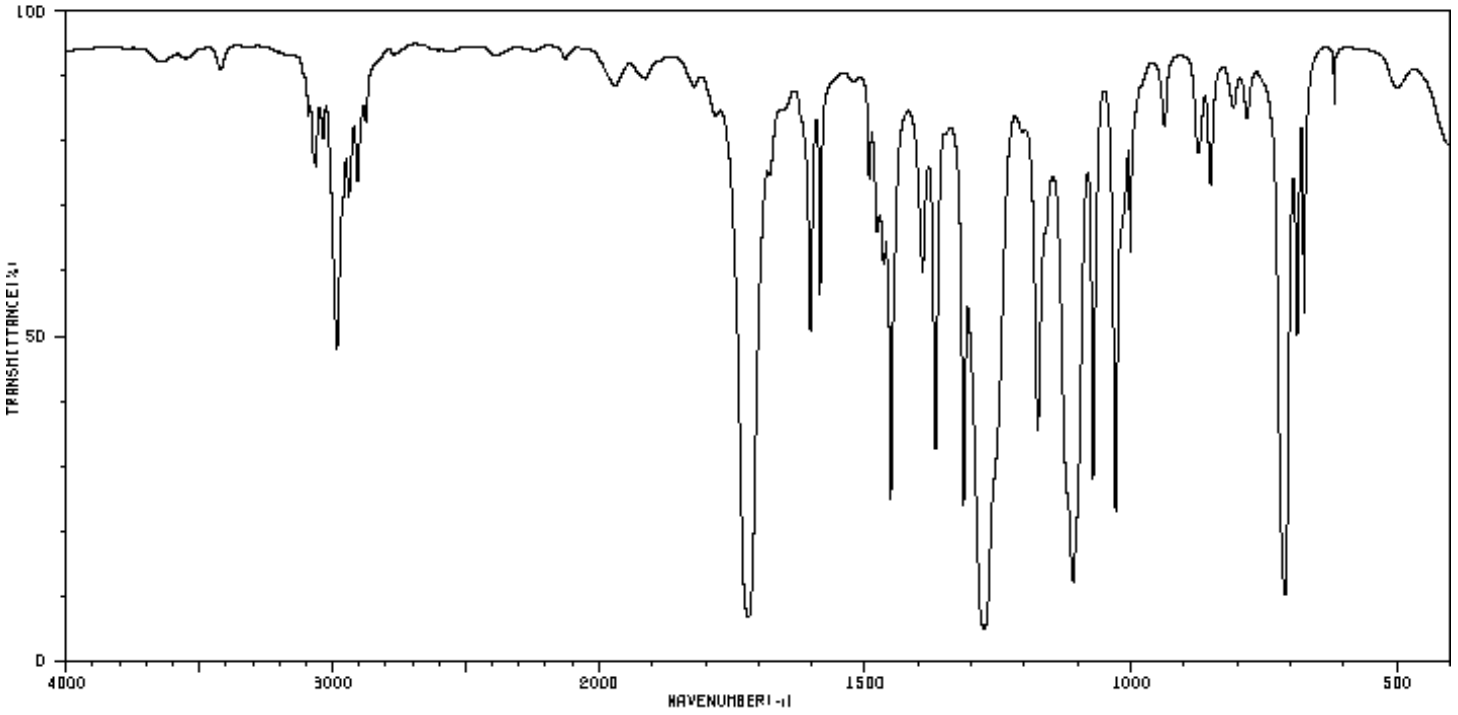
Functional Group(s) absen


HIT-NO=1100
SCORE= ( )
SDBS-NO=672
IR-NIDA-08667 : CCL4 SOLUTION
BENZALDEHYDE
C7H6O
100
50
0
TRANSMITTANCE[%]
4000
3000
2000
1500
1000
500
WAVENUMBER[cm-1]
3088 86
3068 86
3032 86
2847 86
2814 79
2732 77
2693 86
2664 84
1778 86
1709 4
1653 84
1607 81
1598 72
1586 72
1466 74
1634 68
1388 81
1310 68
1285 86
1203 39
1167 68
1160 84
1072 86
1265 64
1024 84
828 55
688 47
673 86
650 64
909 36
C
H
O

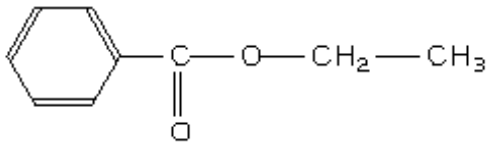
HIT-NO=1451	SCORE= ( )	SDBS-NO=1460	IR-NIDA-04316 : LIQUID FILM

ETHYL BENZOATE

$C_9H_{10}O_2$



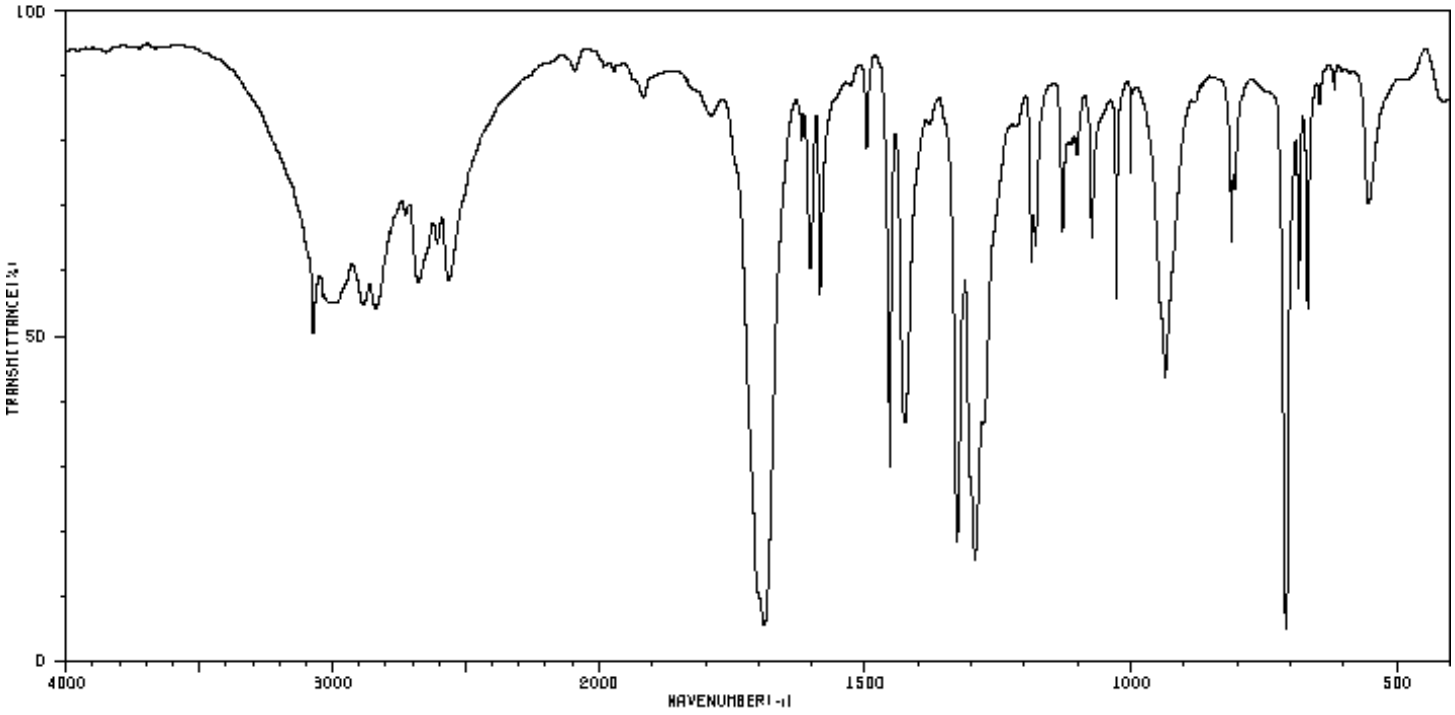
3091	81	1959	84	1466	68	1109	12	807	81
3064	72	1822	84	1452	23	1071	26	782	79
3035	77	1719	6	1392	57	1029	21	711	9
2983	46	1603	49	1368	31	1002	60	688	47
2939	68	1585	53	1315	23	937	79	675	52
2907	70	1492	72	1276	4	873	74	618	61
2874	79	1478	64	1176	34	861	70	506	84



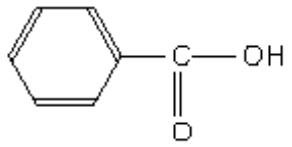
HIT-NO=1081	SCORE= ( )	SDBS-NO=673	IR-NIDA-63340 : KBR DISC

BENZOIC ACID

$C_7H_6O_2$



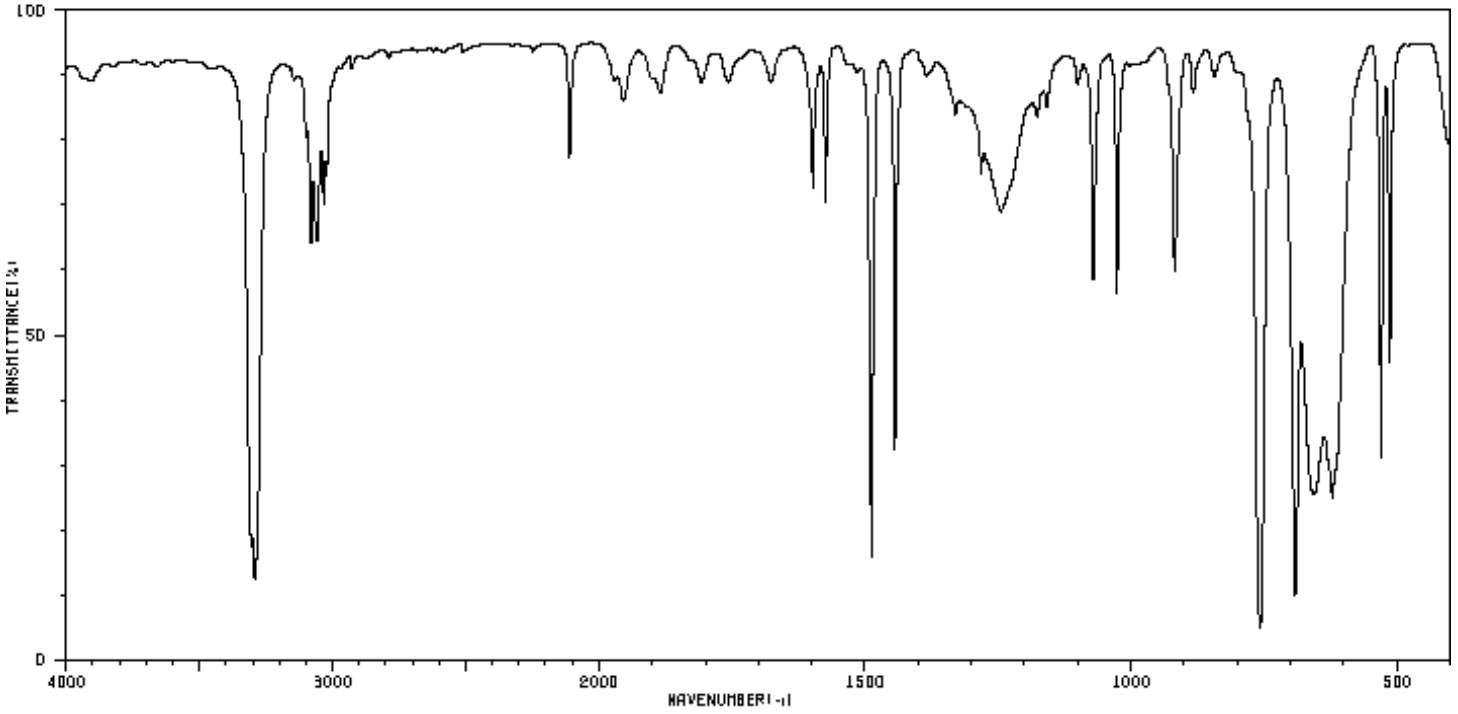
3073	49	2678	67	1426	36	1112	77	936	42
3012	53	2607	62	1327	17	1107	77	812	62
2998	53	2564	57	1294	14	1102	74	805	70
2985	53	1689	6	1187	58	1074	62	708	4
2886	52	1603	58	1180	60	1028	53	685	55
2838	52	1585	59	1129	64	1001	72	667	52
2726	66	1464	28	1118	77	943	60	664	68



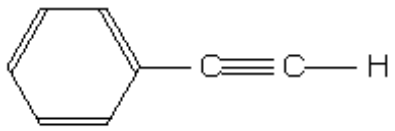
HIT-NO=1445	SCORE= ( )	SDBS-NO=1444	IR-NIDA-63379 : LIQUID FILM

PHENYLACETYLENE

C_8H_6



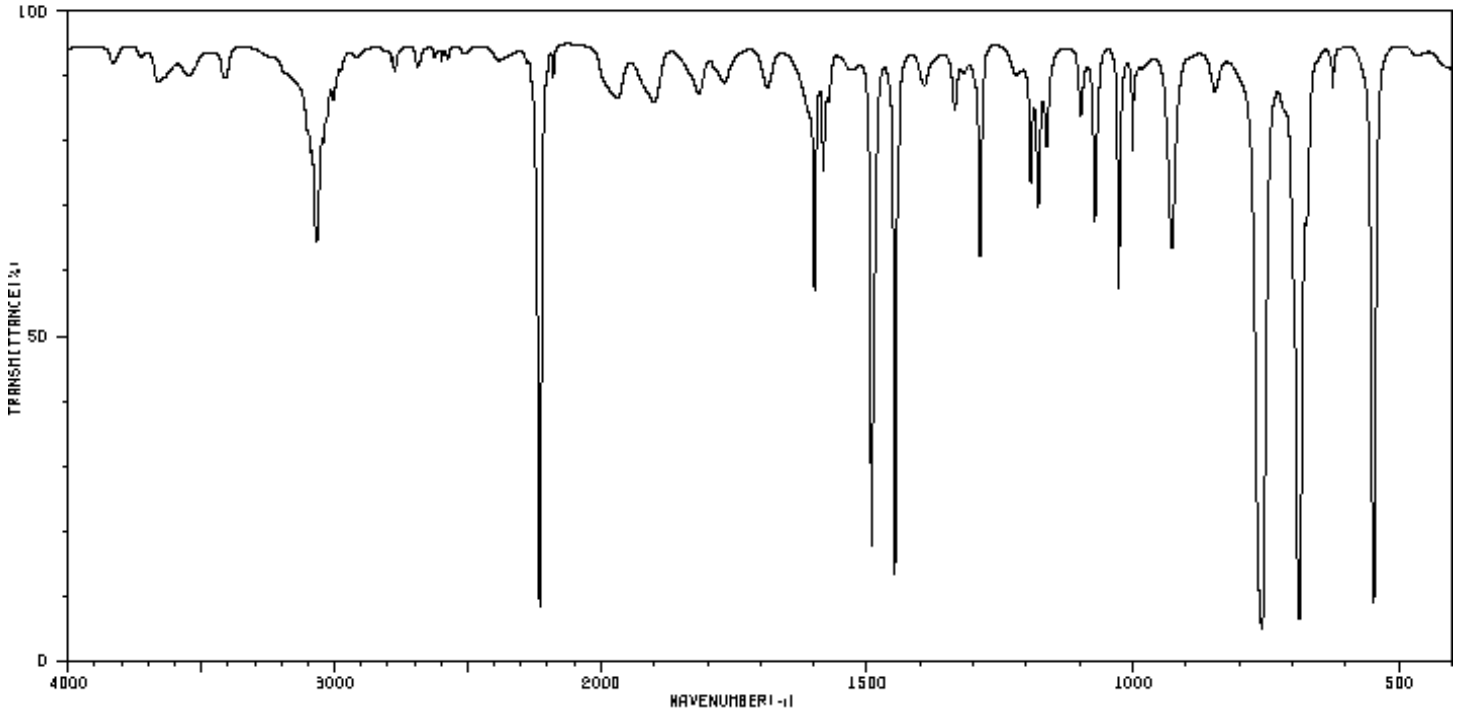
3906	86	2110	74	1674	68	1176	81	843	86
3306	16	1954	84	1488	15	1159	81	757	4
3291	12	1900	86	1444	31	1100	84	692	9
3081	62	1886	84	1386	86	1071	67	666	24
3058	62	1808	86	1331	81	1026	53	621	23
3034	68	1757	86	1282	72	918	57	530	30
3022	72	1698	70	1245	66	883	84	514	43



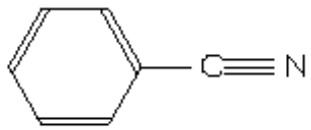
HIT-NO=1114	SCORE= ( )	SDBS-NO=669	IR-NIDA-05064 : LIQUID FILM

BENZONITRILE

C_7H_5N



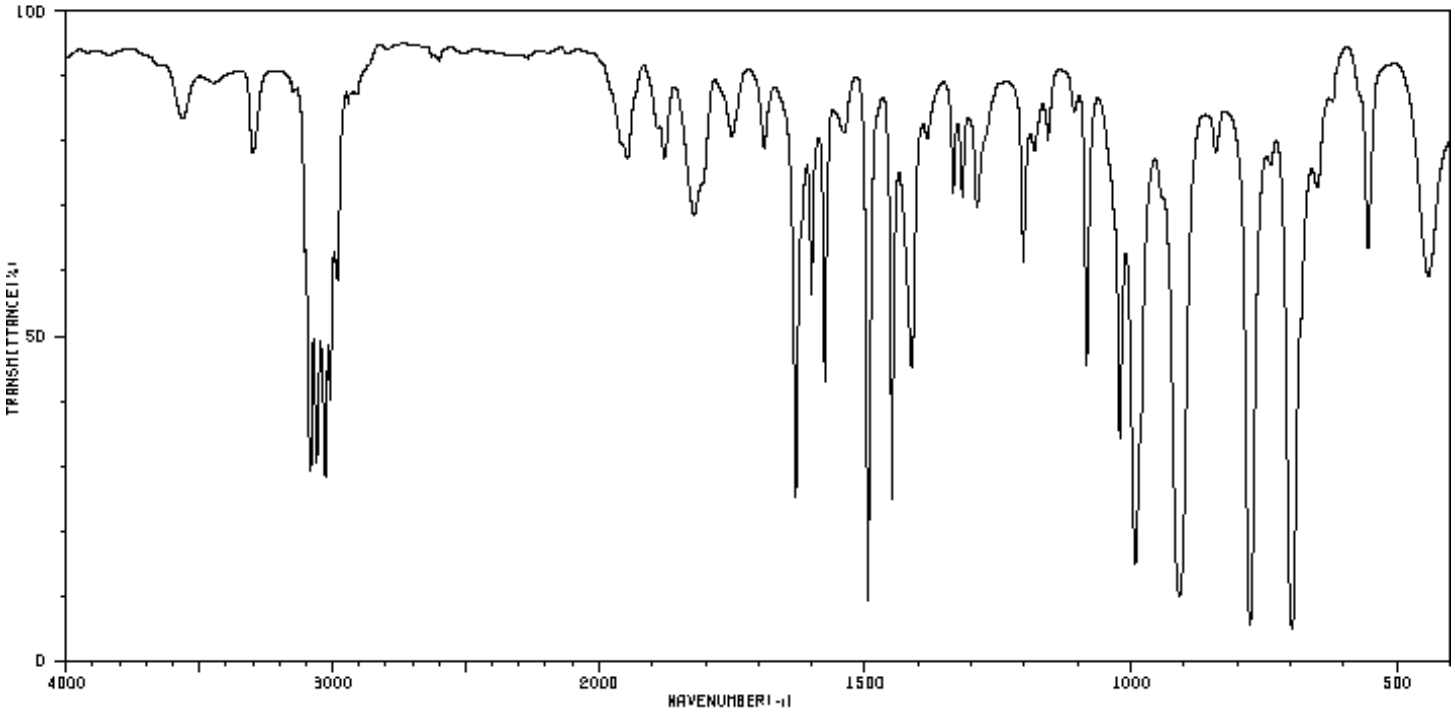
3646	86	2178	86	1582	72	1288	60	1001	74
3412	86	1969	84	1572	81	1193	70	927	60
3088	74	1899	81	1492	17	1178	66	846	64
3066	62	1816	84	1448	12	1163	77	758	4
3004	84	1768	86	1441	72	1098	81	688	6
2256	84	1688	84	1392	84	1072	64	625	64
2230	8	1599	66	1336	81	1027	66	548	8



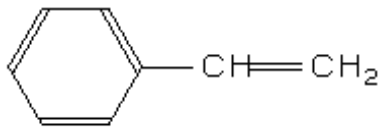
HIT-NO=2170	SCORE= ( )	SDBS-NO=3044	IR-NIDA-10290 : LIQUID FILM

STYRENE

C_8H_8



3299	74	1946	74	1495	9	1202	68	841	74
3082	28	1876	74	1449	23	1182	74	777	5
3060	29	1821	66	1412	43	1156	77	756	72
3027	27	1689	77	1383	77	1083	49	698	4
3009	38	1630	24	1334	70	1021	33	650	70
2980	57	1601	59	1317	66	992	14	555	60
1955	77	1575	41	1290	66	909	9	442	67



Write-up

Fill in the following form below and answer the post-lab questions. Use the Word version of the report form so you can add additional space for your answers. You will also need to download four (4) unknown spectra and include that in your report. When complete save as a PDF and email as an attachment to your Academic Expert for grading.

CHEM 350 Experiment 6 Report Form

Infrared Spectroscopy Tutorial

Date:_____

Student Name:_____ ID Number:_____

Infrared Knowns

Fill in the following three (3) analyses tables to reflect your characterization of the spectra provided (above).

cyclohexanone	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group(s) absent:

ethyl benzoate	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group(s) absent:

benzonitrile	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or ,weak)	Functional Group Indicated

Functional Group(s) absent:

Infrared Unknowns

Select four (4) unknowns from the ‘Exp. 6 Infrared Unknown Downloads’ list:

Download 4 of the possible 20 spectra (PDFs). Please neatly fill out the table on the unknown spectra and remember to fully label each of the absorption bands identified and identify the compound. If you find the tables on the PDFs too small use this Word template to give yourself more space to write/type.

Code: Name:	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group absent:

Code: Name:	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group absent:

Code: Name:	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

Functional Group absent:

Code: Name:	Absorption Band#	Wavenumber (cm^{-1})	Peak Shape (sharp, broad)	Peak Intensity (strong, medium or weak)	Functional Group Indicated

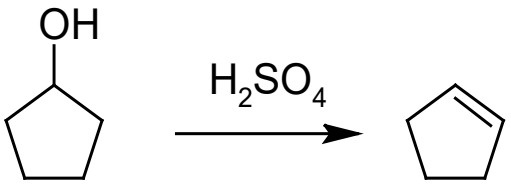
Functional Group absent:

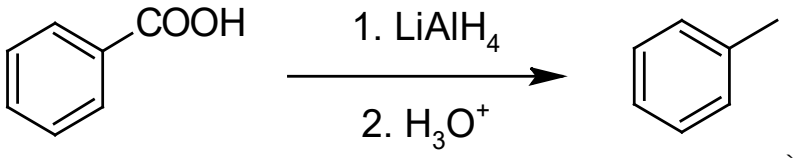
Questions

1. What are the major differences you would see in the infrared spectra of an alkane, alkene, and alkyne?

2. Consider the C=O absorption of three compounds: 2-butanone (1715 cm^{-1}), propanoyl chloride (1772 cm^{-1}), and propyl amide (1650 cm^{-1}). Explain the observed differences.

3. Describe how IR spectroscopy might be used to monitor the progress of each of the following reactions.





I certify that this submitted laboratory report represents entirely my own efforts. I have read and understand the Athabasca University policies regarding, and sanctions for, plagiarism.

Signature: _____ Date: _____