Table 1 Saturated aliphatic (alkane/alkyl) group frequencies

Group frequency (cm^{-1})	Functional group/assignment
	Methyl ($-CH_3$)
2970–2950/2880–2860	Methyl C–H asym./sym. stretch
1470–1430/1380–1370	Methyl C–H asym./sym. bend
1385–1380/1370–1365	*gem*-Dimethyl or "iso"- (doublet)
1395–1385/1365	Trimethyl or "*tert*-butyl" (multiplet)
	Methylene ($>CH_2$)
2935–2915/2865–2845	Methylene C–H asym./sym. stretch
1485–1445	Methylene C–H bend
750–720	Methylene $-(CH_2)_n-$ rocking ($n \geq 3$)
1055–1000/1005–925	Cyclohexane ring vibrations
	Methyne ($>CH-$)
2900–2880	Methyne C–H stretch
1350–1330	Methyne C–H bend
1300–700	Skeletal C–C vibrations
	Special methyl ($-CH_3$) frequencies
2850–2815	Methoxy, methyl ether O–CH_3, C–H stretch
2820–2780	Methylamino, N–CH_3, C–H stretch

Table 2 Olefinic (alkene) group frequencies

Origin	Group frequency, wavenumber (cm^{-1})	Assignment
C=C	1680–1620	Alkenyl C=C stretch
	1625	Aryl-substituted C=C
	1600	Conjugated C=C
C–H	3095–3075 +3040–3010	Terminal (vinyl) C–H stretch
	3095–3075	Pendant (vinylidene) C–H stretch
	3040–3010	Medial, *cis*- or *trans*-C–H stretch
C–H	1420–1410	Vinyl C–H in-plane bend
	1310–1290	Vinylidene C–H in-plane bend
C–H	995–985 + 915–890	Vinyl C–H out-of-plane bend
	895–885	Vinylidene C–H out-of-plane bend
C–H	970–960	*trans*-C–H out-of-plane bend
	700 (broad)	*cis*-C–H out-of-plane bend

Table 4 Acetylenic (alkyne) group frequencies

Origin	Group frequency, wavenumber (cm^{-1})	Assignment
C≡C	2140–2100	Terminal alkyne (monosubstituted)
C≡C	2260–2190	Medial alkyne (disubstituted)
C–H	3320–3310	Alkyne C–H stretch
C–H	680–610	Alkyne C–H bend
C–H	630 (typical)	Alkyne C–H bend

C–C stretch: ~1350–1000 cm^{-1}
C=C stretch: 1680–1620 cm^{-1}
C≡C stretch: 2260–2100 cm^{-1}

Table 3 Aromatic ring (aryl) group frequencies

Origin	Group frequency, wavenumber (cm^{-1})	Assignment
C=C–C[a]	1615–1580	Aromatic ring stretch
C=C–C[a]	1510–1450	Aromatic ring stretch
C–H	3130–3070	Aromatic C–H stretch
C–H	1225–950 (several)	Aromatic C–H in-plane bend
C–H	900–670 (several)	Aromatic C–H out-of-plane bend
	770–730 + 710–690	Monosubstitution (phenyl)
	770–735	1,2-Disubstitution (ortho)
	810–750 + 900–860	1,3-Disubstitution (meta)
	860–800	1,4-Disubstitution (para)
"Combi"[b]	2000–1660 (several)	Aromatic combination bands

[a] C=C–C used as an approximation of the unique aromatic ring bonding.
[b] "Combi" denotes assignment to combination bands.

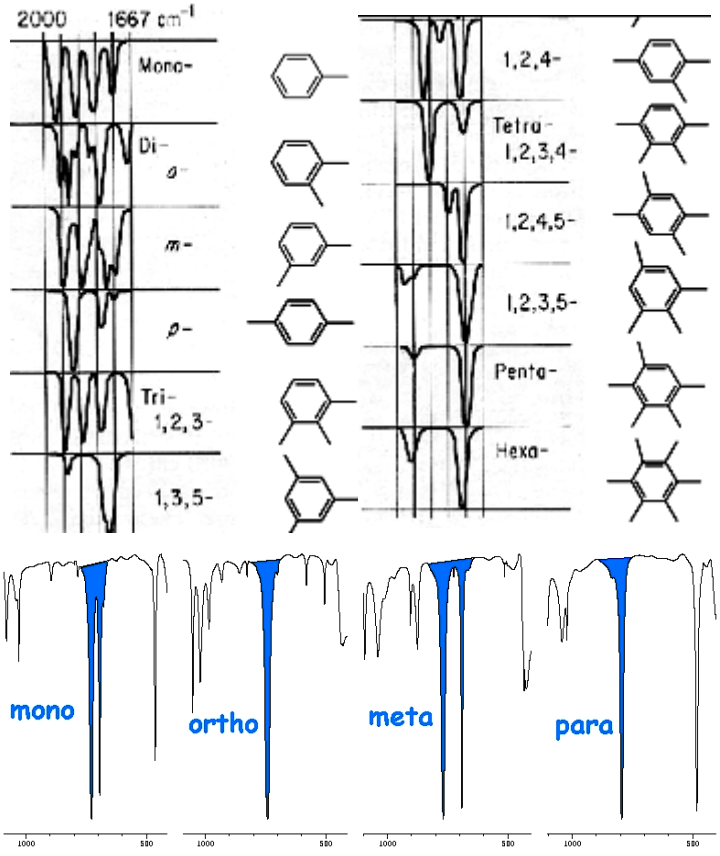


Table 5 Aliphatic organohalogen compound group frequencies

Origin	Group frequency, wavenumber (cm^{-1})[a]	Assignment
C–F	1150–1000	Aliphatic fluoro compounds, C–F stretch
C–Cl	800–700	Aliphatic chloro compounds, C–Cl stretch
C–Br	700–600	Aliphatic bromo compounds, C–Br stretch
C–I	600–500	Aliphatic iodo compounds, C–I stretch

[a] Note that the ranges quoted serve as a guide only; the actual ranges are influenced by carbon chain length, the actual number of halogen substituents, and the molecular conformations present.

Table 6 Alcohol and hydroxy compound group frequencies

Origin	Group frequency, wavenumber (cm^{-1})	Assignment
O–H	3570–3200 (broad)	Hydroxy group, H-bonded OH stretch
	3400–3200	Normal "polymeric" OH stretch
	3550–3450	Dimeric OH stretch
	3570–3540	Internally bonded OH stretch
O–H	3645–3600 (narrow)	Nonbonded hydroxy group, OH stretch
	3645–3630	Primary alcohol, OH stretch
	3635–3620	Secondary alcohol, OH stretch
	3620–3540	Tertiary alcohol, OH stretch
	3640–3530[a]	Phenols, OH stretch
O–H	1350–1260	Primary or secondary, OH in-plane bend
	1410–1310	Phenol or tertiary alcohol, OH bend
	720–590	Alcohol, OH out-of-plane bend
C–O	~1050[b]	Primary alcohol, C–O stretch
	~1100[b]	Secondary alcohol, C–O stretch
	~1150[b]	Tertiary alcohol, C–O stretch
	~1200[b]	Phenol, C–O stretch

[a] Frequency influenced by nature and position of other ring substituents.
[b] Approximate center of range for the group frequency.

Table 7 Ether and oxy compound group frequencies

Origin	Group frequency, wavenumber (cm^{-1})	Assignment
C–H	2820–2810	Methoxy, C–H stretch (CH_3–O–)
C–O–C	1150–1050	Alkyl-substituted ether, C–O stretch
C–O–C	1140–1070	Cyclic ethers, large rings, C–O stretch
ϕ–O–H	1270–1230	Aromatic ethers, aryl–O stretch
C–O–	~1250 + 890–800[a]	Epoxy and oxirane rings
C–O–O–C	890–820[a]	Peroxides, C–O–O– stretch

[a] Typically very weak, and not very characteristic in the infrared. Tend to be more characteristic in the Raman spectrum.

Table 8 Amine and amino compound group frequencies

Origin	Group frequency, wavenumber (cm^{-1})	Assignment
		Primary amino
N–H	3400–3380 +3345–3325	Aliphatic primary amine, NH stretch
N–H	3510–3460 +3415–3380	Aromatic primary amine, NH stretch
N–H	1650–1590	Primary amine, NH bend
C–N	1090–1020	Primary amine, CN stretch
		Secondary amino
>N–H	3360–3310	Aliphatic secondary amine, NH stretch
>N–H	~3450	Aromatic secondary amine, NH stretch
>N–H	3490–3430	Heterocyclic amine, NH stretch
=N–H	3350–3320	Imino compounds, NH stretch
>N–H	1650–1550	Secondary amine, NH bend
C–N	1190–1130	Secondary amine, CN stretch
		Tertiary amino
C–N	1210–1150	Tertiary amine, CN stretch
		Aromatic amino
C–N	1340–1250	Aromatic primary amine, CN stretch
C–N	1350–1280	Aromatic secondary amine, CN stretch
C–N	1360–1310	Aromatic tertiary amine, CN stretch

Table 9 Example carbonyl compound group frequencies

Group frequency (cm^{-1})	Functional group
1610–1550/1420–1300	Carboxylate (carboxylic acid salt)
1680–1630	Amide
1690–1675/(1650–1600)[a]	Quinone or conjugated ketone
1725–1700	Carboxylic acid
1725–1705	Ketone
1740–1725/(2800–2700)[b]	Aldehyde
1750–1725	Ester
1735	Six-membered ring lactone
1760–1740	Alkyl carbonate
1815–1770	Acid (acyl) halide
1820–1775	Aryl carbonate
1850–1800/1790–1740	Open-chain acid anhydride
1870–1820/1800–1775	Five-membered ring anhydride
2100–1800	Transition metal carbonyls

[a] Lower frequency band is from the conjugated double bond.
[b] Higher frequency band characteristic of aldehydes, associated with the terminal aldehydic C–H stretch.

Table 10 Examples of nitrogen multiple and cumulated double bond compound group frequencies

Group frequency (cm^{-1})	Functional group/assignment
2280–2240	Aliphatic cyanide/nitrile
2240–2220	Aromatic cyanide/nitrile
2260–2240/1190–1080	Cyanate (–OCN and C–OCN stretch)
2276–2240	Isocyanate (–N=C=O asym. stretch)
2175–2140	Thiocyanate (–SCN)
2150–1990	Isothiocyanate (–NCS)
1690–1590	Open-chain imino (–C=N–)
1630–1575	Open-chain azo (–N=N–)

Table 11 Example group frequencies for simple hetero-oxy compounds

Group frequency (cm^{-1})	Functional group/assignment
	Nitrogen-oxy compounds
1560–1540/1380–1350[a]	Aliphatic nitro compounds
1555–1485/1355–1320[a]	Aromatic nitro compounds
1640–1620/1285–1270[a]	Organic nitrates
	Phosphorus-oxy compounds
1350–1250	Organic phosphates (P=O stretch)
1050–990	Aliphatic phosphates (P–O–C stretch)
1240–1190/995–850	Aromatic phosphates (P–O–C stretch)
	Sulfur-oxy compounds
1335–1300/1170–1135[a]	Dialkyl/aryl sulfones
1420–1370/1200–1180[a]	Organic sulfates
1365–1340/1200–1100[a]	Sulfonates
	Silicon-oxy compounds
1095–1075/1055–1020	Organic siloxane or silicone (Si–O–Si)
1110–1080	Organic siloxane or silicone (Si–O–C)

[a] Asymmetric/symmetric XO_2 stretch (NO_2 and SO_2).

Table 12 Common group frequencies for thiols and thio-substituted compounds

Group frequency (cm^{-1})	Functional group/assignment
2600–2550	Thiols (S–H stretch)
710–685	Thiol or thioether, CH_2–S– (C–S stretch)
660–630	Thioethers, CH_3–S– (C–S stretch)
715–670	Aryl thioethers, ϕ–S (C–S stretch)
705–570	Disulfides (C–S stretch)
620–600	Disulfides (S–S stretch)
500–430	Aryl disulfides (S–S stretch)
500–470	Polysulfides (S–S stretch)

Table 13 Example group frequencies for common inorganic ions

Group frequency (cm^{-1})	Functional group/assignment
1490–1410/880–860[a]	Carbonate ion
1130–1080/680–610[a]	Sulfate ion
1380–1350/840–815[a]	Nitrate ion
1100–1000	Phosphate ion
1100–900	Silicate ion
3300–3030/1430–1390[a]	Ammonium ion
2200–2000	Cyanide ion, thiocyanate ion, and related ions

[a] Typically, the first absorption is intense and broad, and the second has weak to medium intensity and is narrow. Both often exist as multiple band structures, and this may be used to characterize individual compounds.

Step 1: Overall Spectrum Appearance

Diagnostic Step 2: Testing for Organics and Hydrocarbons – Absorptions in the Region 3200–2700 cm^{-1}

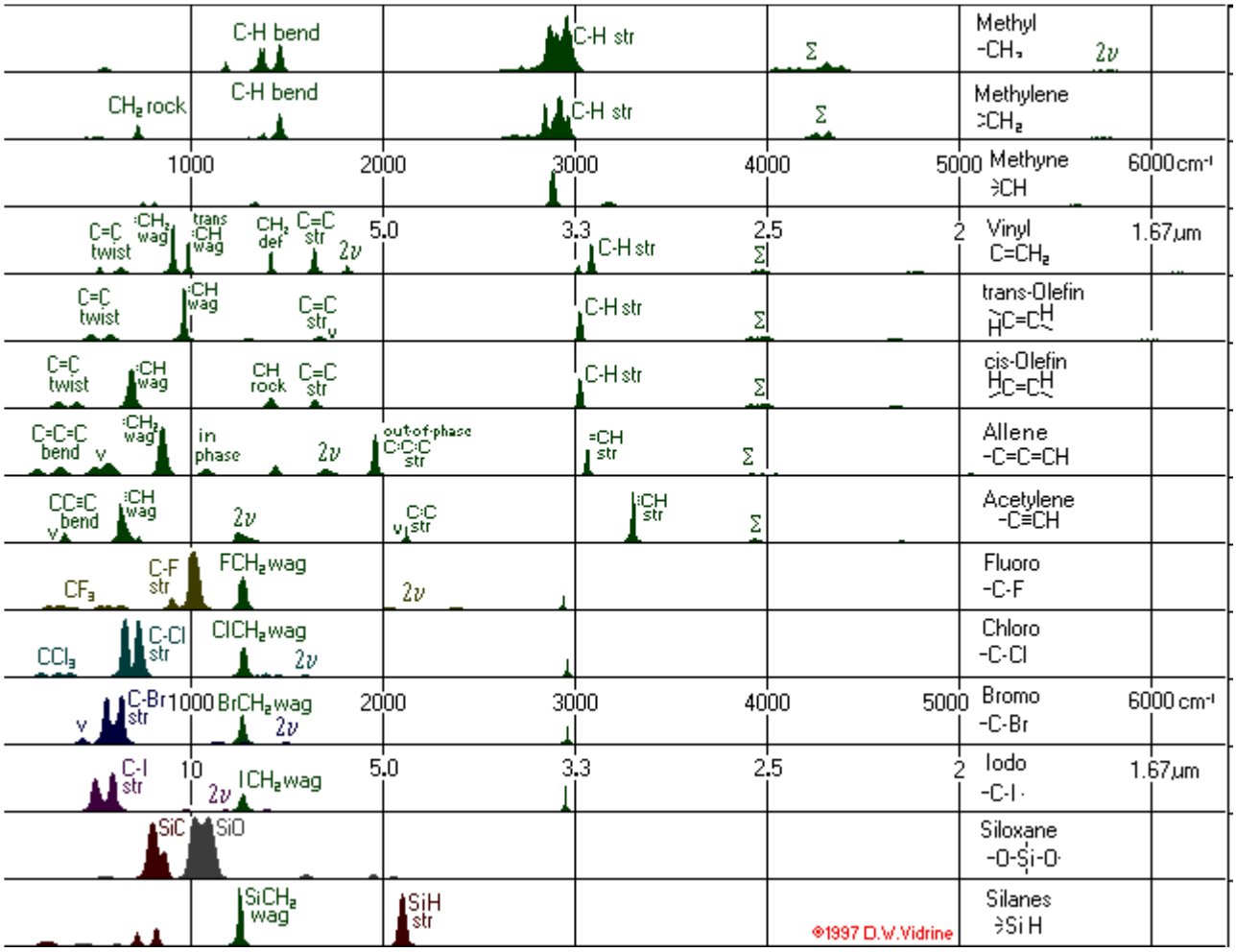
Diagnostic Step 3: Testing for Hydroxy or Amino Groups – Absorptions in the Region 3650–3250 cm^{-1}

Diagnostic Step 4: Testing for Carbonyl Compounds – Absorptions in the Region 1850–1650 cm^{-1}

Diagnostic Step 5: Testing for Unsaturation – Weak to Moderate Absorption in the Region 1670–1620 cm^{-1}

Diagnostic Step 6: Testing for Aromatics – Well-defined Absorptions in the Region 1615–1495 cm^{-1}

Diagnostic Step 7: Testing for Multiple Bonding (Often with a Bond Order of 2 or Higher) – Absorption in the Region 2300–1990 cm^{-1}


C-H bend
C-H str
Σ
Methyl
-CH₃
2ν
CH₂ rock
C-H bend
C-H str
Σ
Methylene
>CH₂
1000
2000
3000
4000
5000
Methyne
≡CH
6000 cm⁻¹
C=C twist
=CH₂ wag
trans =CH wag
CH₂ def
C=C str
2ν
5.0
3.3
2.5
2
C-H str
Σ
Vinyl
C=CH₂
1.67 μm
C=C twist
=CH wag
C=C str
C-H str
Σ
trans-Olefin
C=C str
C-H str
Σ
cis-Olefin
C=C=C bend
ν
=CH₂ wag
in phase
2ν
out-of-phase C=C=C str
=CH str
Σ
Allene
-C=C=CH
CC≡C bend
ν
≡CH wag
2ν
C≡C ν str
≡CH str
Σ
Acetylene
-C≡CH
CF₃
C-F str
FCH₂ wag
2ν
Fluoro
-C-F
CCl₃
C-Cl str
ClCH₂ wag
2ν
Chloro
-C-Cl
ν
C-Br str
BrCH₂ wag
2ν
Bromo
-C-Br
C-I str
ICH₂ wag
2ν
Iodo
-C-I
SiC
SiO
Siloxane
-O-Si-O-
SiCH₂ wag
SiH str
Silanes
≡Si H
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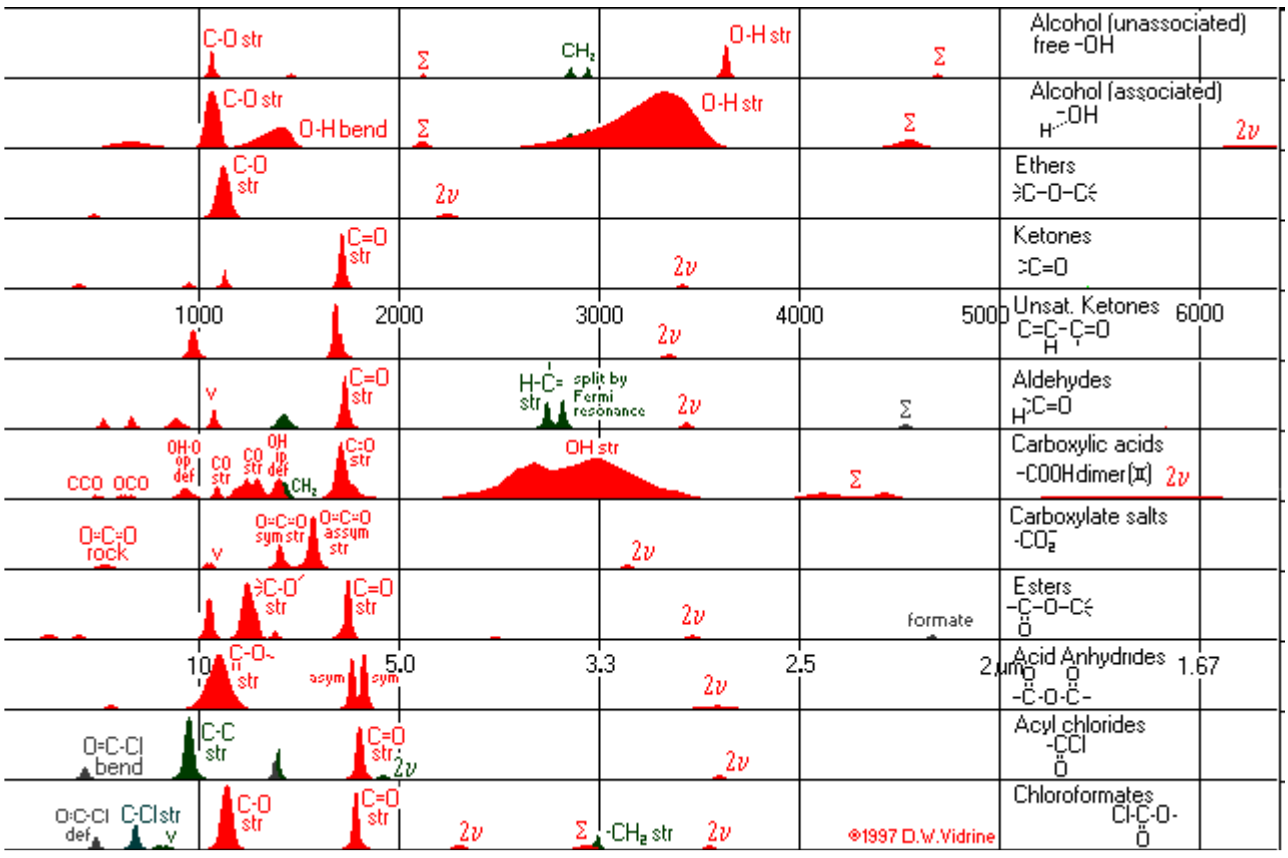
C-O str
Σ
CH₂
O-H str
Σ
Alcohol (unassociated)
free -OH
C-O str
O-H bend
Σ
O-H str
Σ
Alcohol (associated)
2ν
C-O str
2ν
Ethers
>C-O-C<
C=O str
2ν
Ketones
>C=O
1000
2000
3000
4000
5000
6000
2ν
Unsat. Ketones
C=C-C=O
ν
C=O str
H-C= str
split by Fermi resonance
2ν
Σ
Aldehydes
H-C=O
OH-O op def
CO str
C-O str
OH ip def
CH₂
C=O str
OH str
Σ
Carboxylic acids
-COOH dimer (x) 2ν
CCO OCO
O=C=O rock
ν
O=C=O sym str
O=C=O assym str
2ν
Carboxylate salts
-CO₂⁻
>C-O str
C=O str
2ν
formate
Esters
10
C-O-C str
asym
sym
5.0
3.3
2.5
2 μm
2ν
Acid Anhydrides
1.67
O=C-Cl bend
C-C str
C=O str
2ν
2ν
Acyl chlorides
-COCl
O=C-Cl def
C-Cl str
ν
C-O str
C=O str
2ν
Σ
-CH₂ str
2ν
Chloroformates
Cl-C-O-
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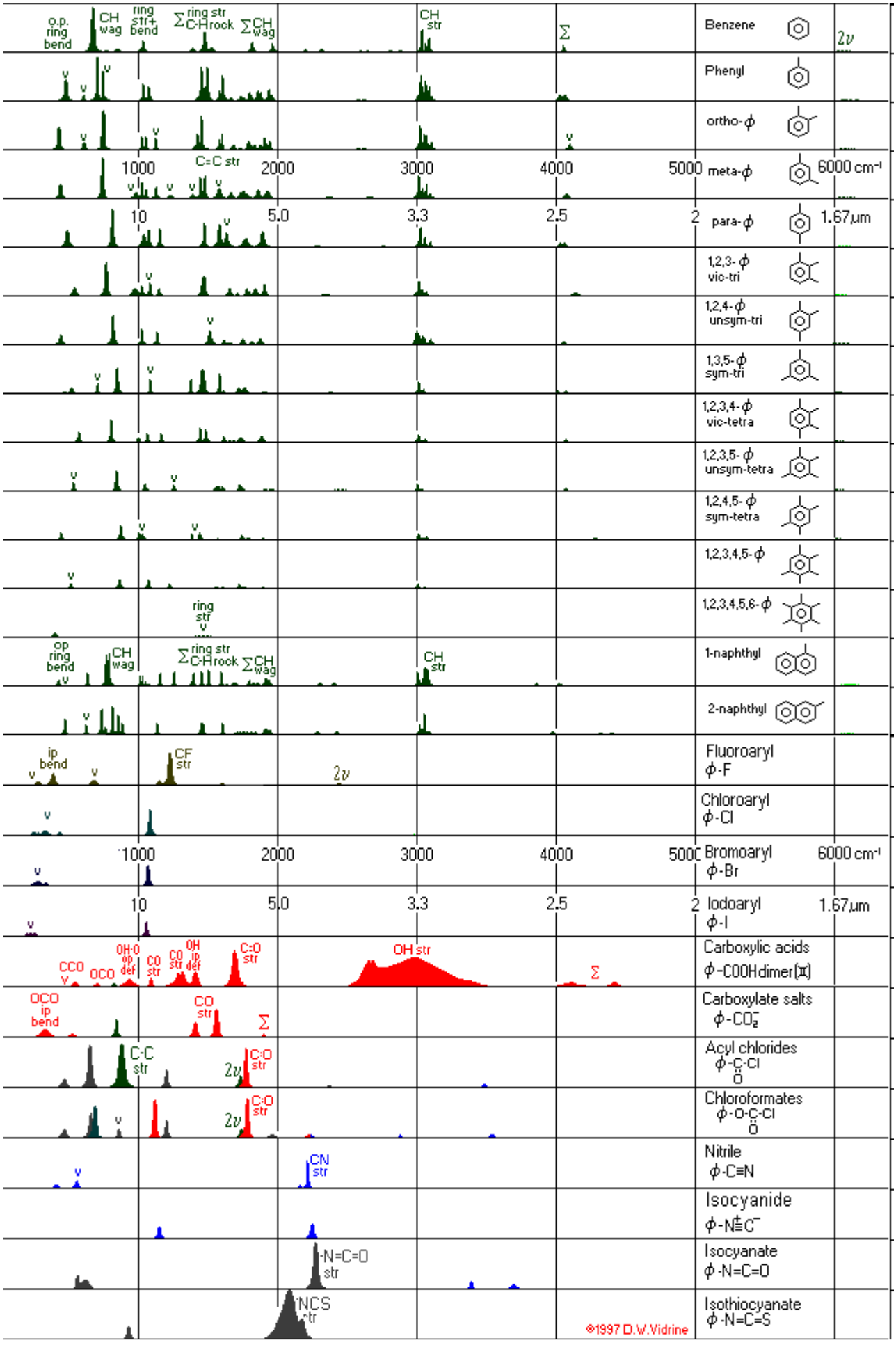
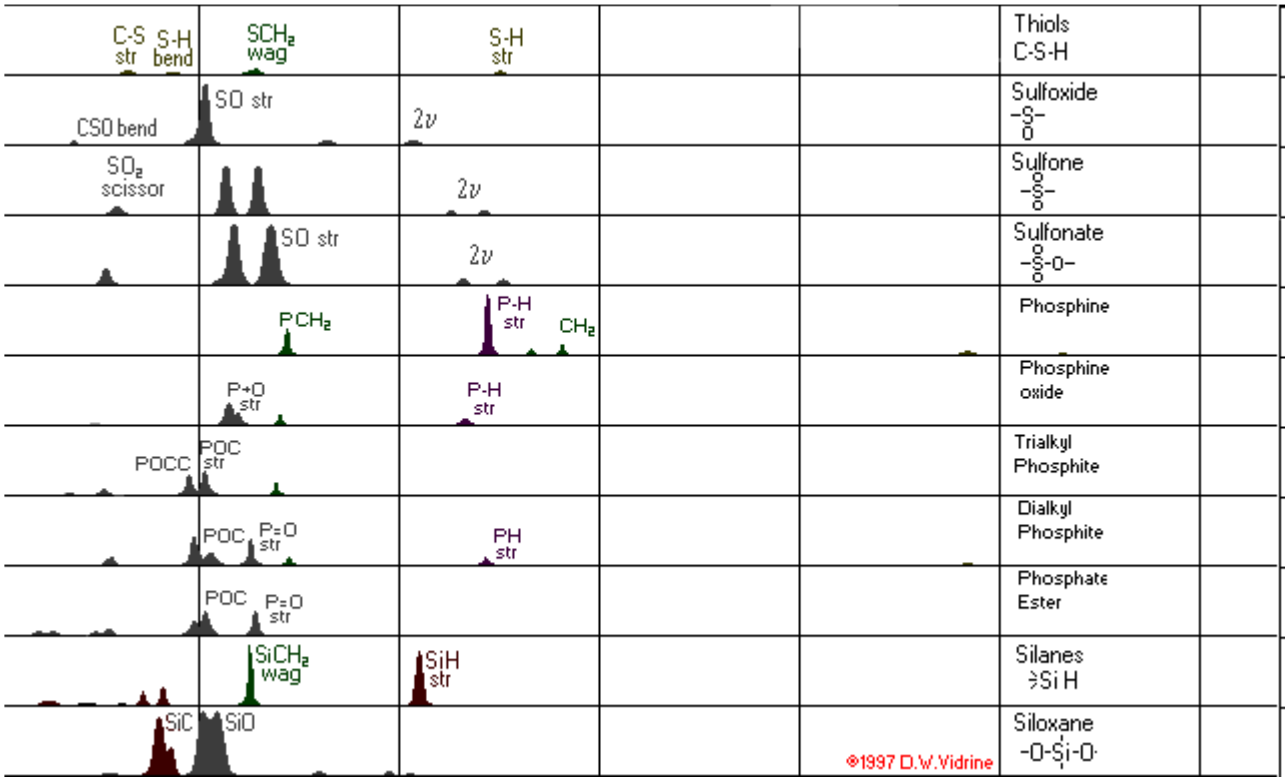

o.p. ring bend
CH wag
ring str+ bend
Σ ring str C-H rock
Σ CH wag
CH str
Σ
2ν
Benzene
Phenyl
ortho-ϕ
meta-ϕ
para-ϕ
1,2,3-ϕ vic-tri
1,2,4-ϕ unsym-tri
1,3,5-ϕ sym-tri
1,2,3,4-ϕ vic-tetra
1,2,3,5-ϕ unsym-tetra
1,2,4,5-ϕ sym-tetra
1,2,3,4,5-ϕ
1,2,3,4,5,6-ϕ
ring str
C=C str
1000
2000
3000
4000
5000
6000 cm⁻¹
10
5.0
3.3
2.5
2
1.67μm
op ring bend
1-naphthyl
2-naphthyl
ip bend
CF str
Fluoroaryl ϕ-F
Chloroaryl ϕ-Cl
Bromoaryl ϕ-Br
Iodoaryl ϕ-I
OH·O op def
CCO
OCO
CO str
OH ip def
C=O str
OH str
Carboxylic acids ϕ-COOH dimer(¤)
OCO ip bend
Carboxylate salts ϕ-CO2−
C-C str
Acyl chlorides ϕ-C(=O)-Cl
Chloroformates ϕ-O-C(=O)-Cl
CN str
Nitrile ϕ-C≡N
Isocyanide ϕ-N≡C
-N=C=O str
Isocyanate ϕ-N=C=O
NCS str
Isothiocyanate ϕ-N=C=S
©1997 D.W.Vidrine


C-S str
S-H bend
SCH2 wag
S-H str
Thiols
C-S-H
CSO bend
SO str
2ν
Sulfoxide
SO2 scissor
2ν
Sulfone
SO str
2ν
Sulfonate
PCH2
P-H str
CH2
Phosphine
P→O str
P-H str
Phosphine oxide
POCC
POC str
Trialkyl Phosphite
POC
P=O str
PH str
Dialkyl Phosphite
POC
P=O str
Phosphate Ester
SiCH2 wag
SiH str
Silanes
SiC
SiO
Siloxane
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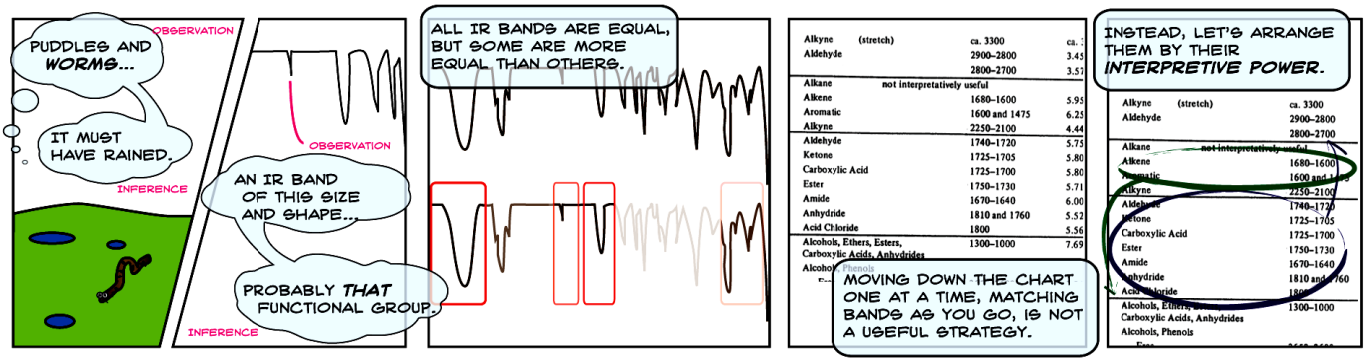
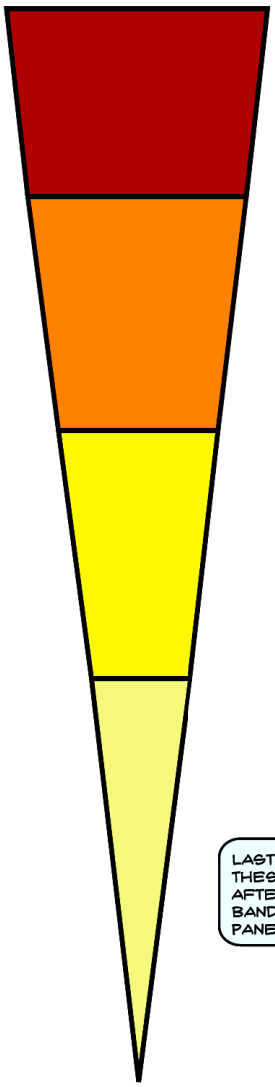
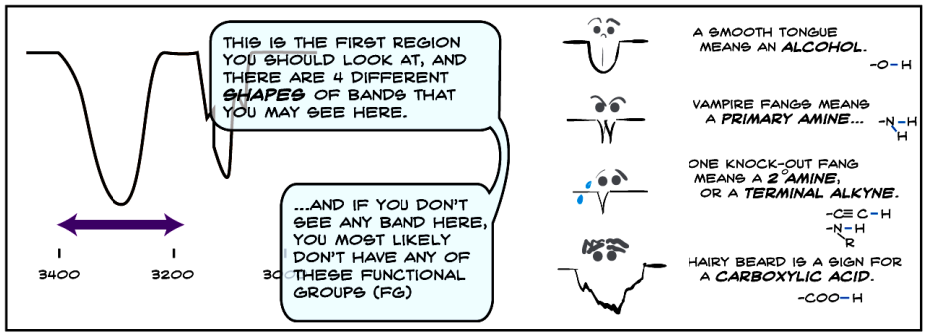
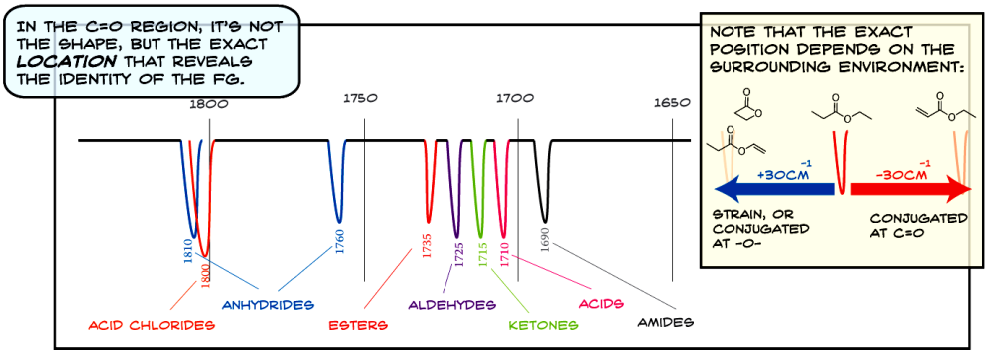


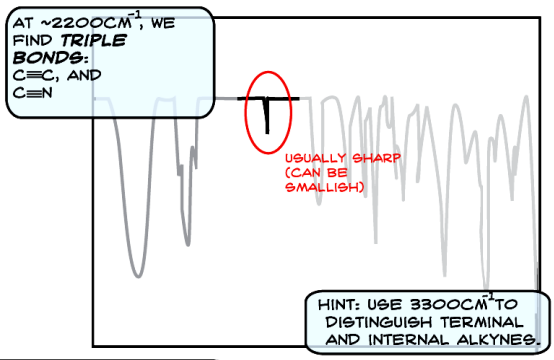
GREAT INTERPRETIVE POWER



WIMPY INTERPRETIVE POWER

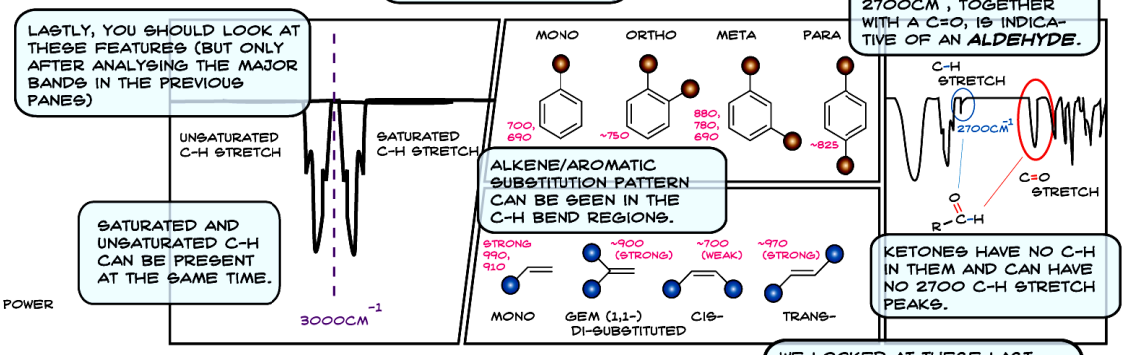






Interpreting IR spectra

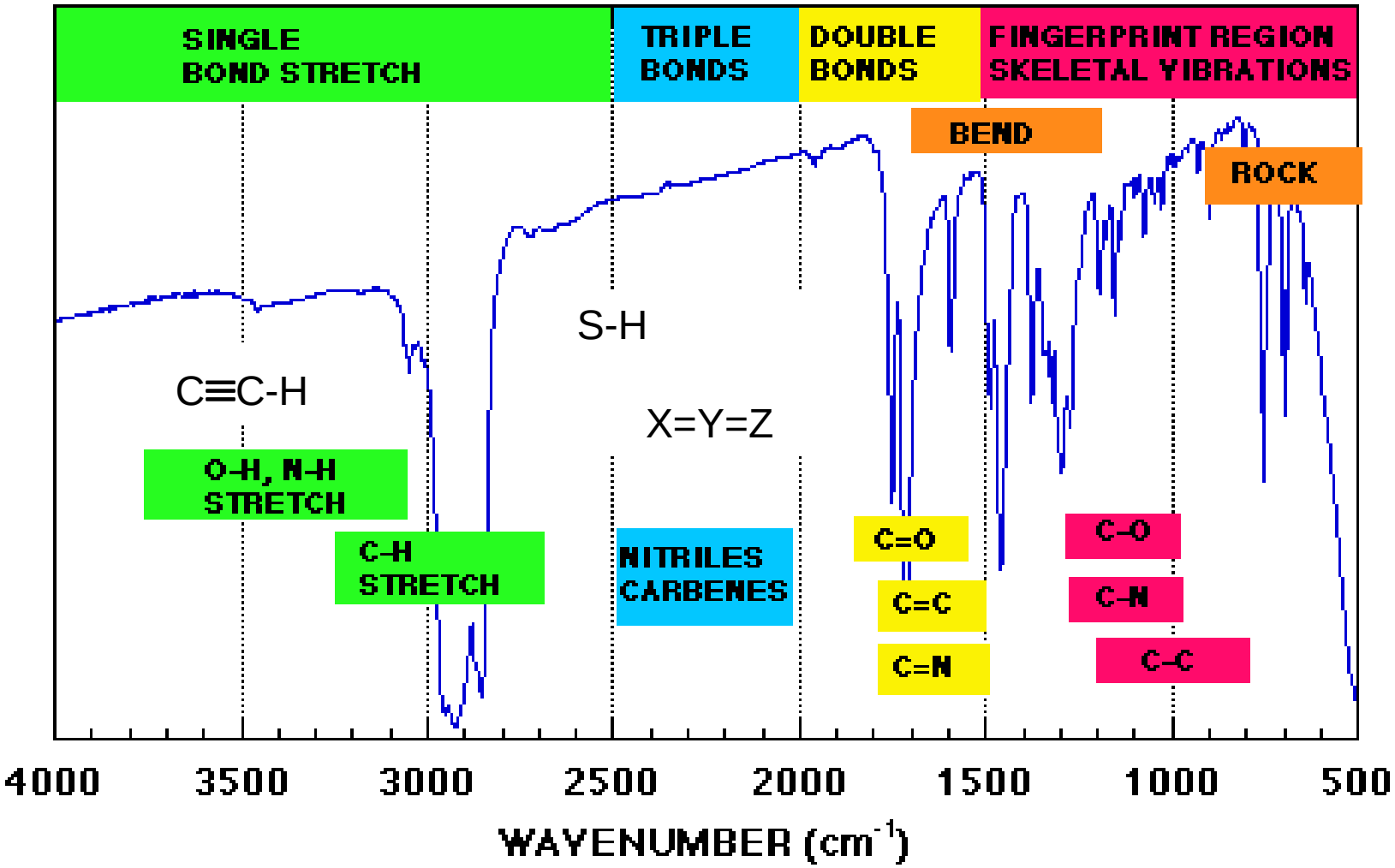
JON - JKWCHUI@UVIC.CA

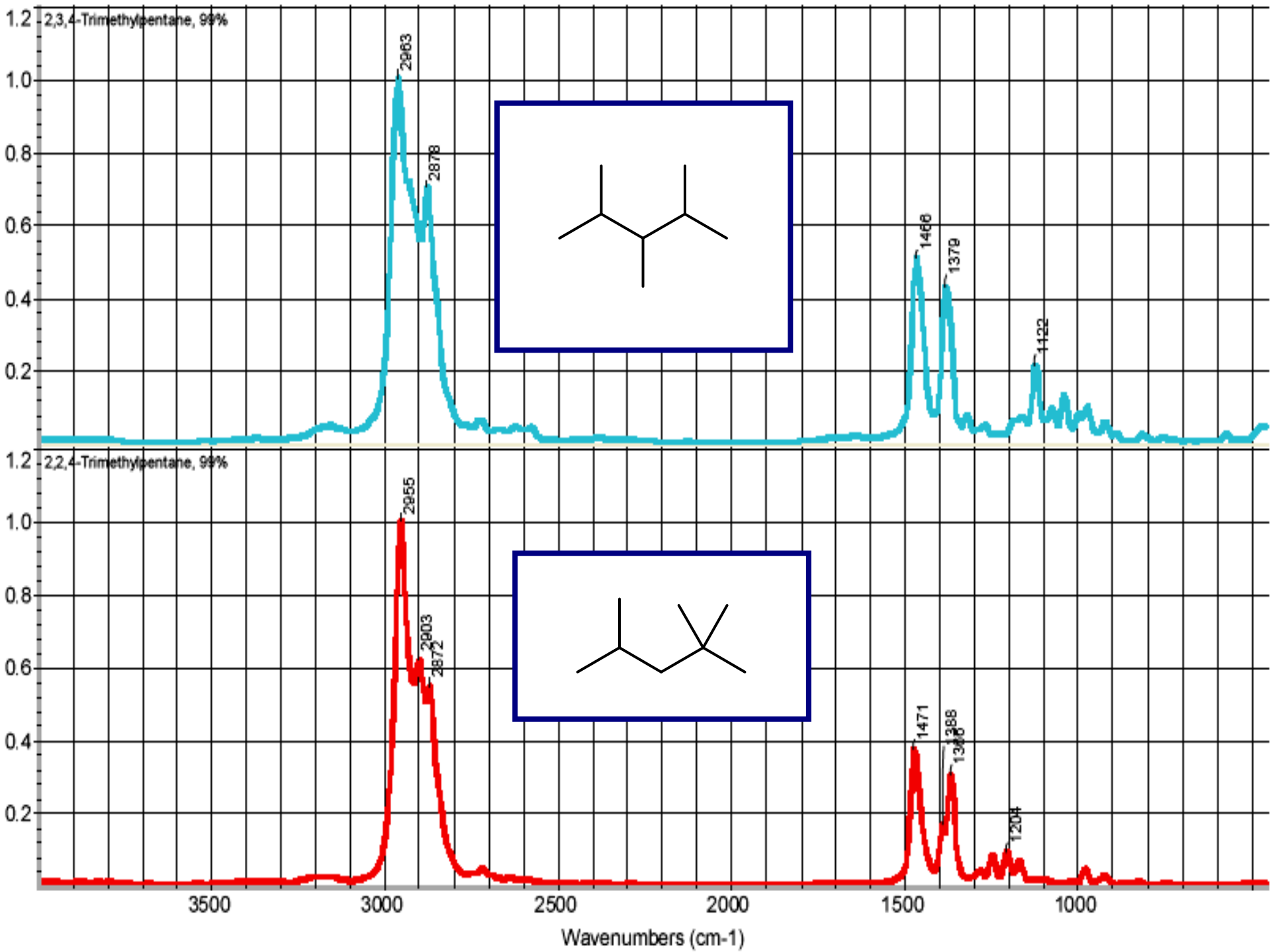


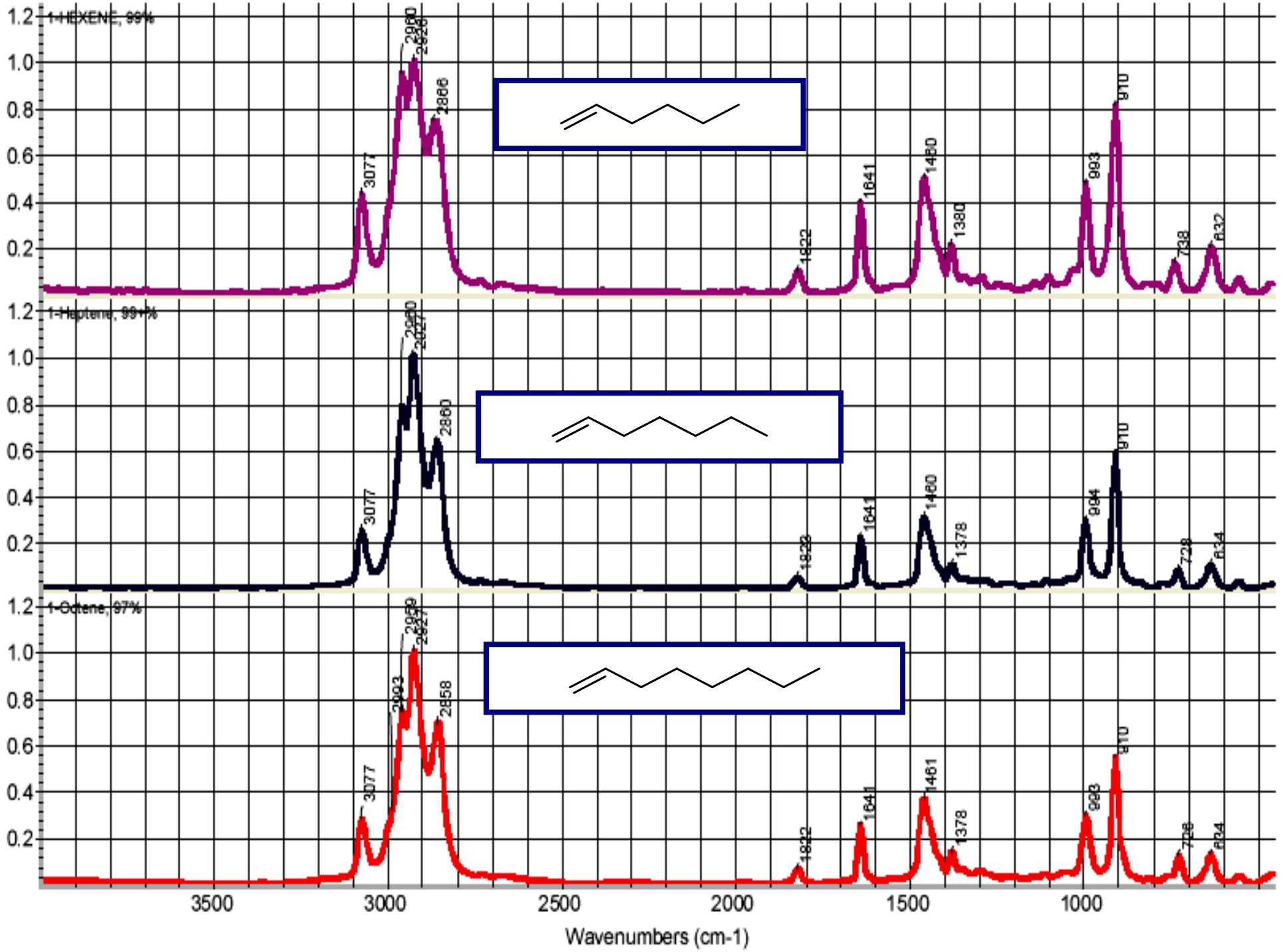
NOTES

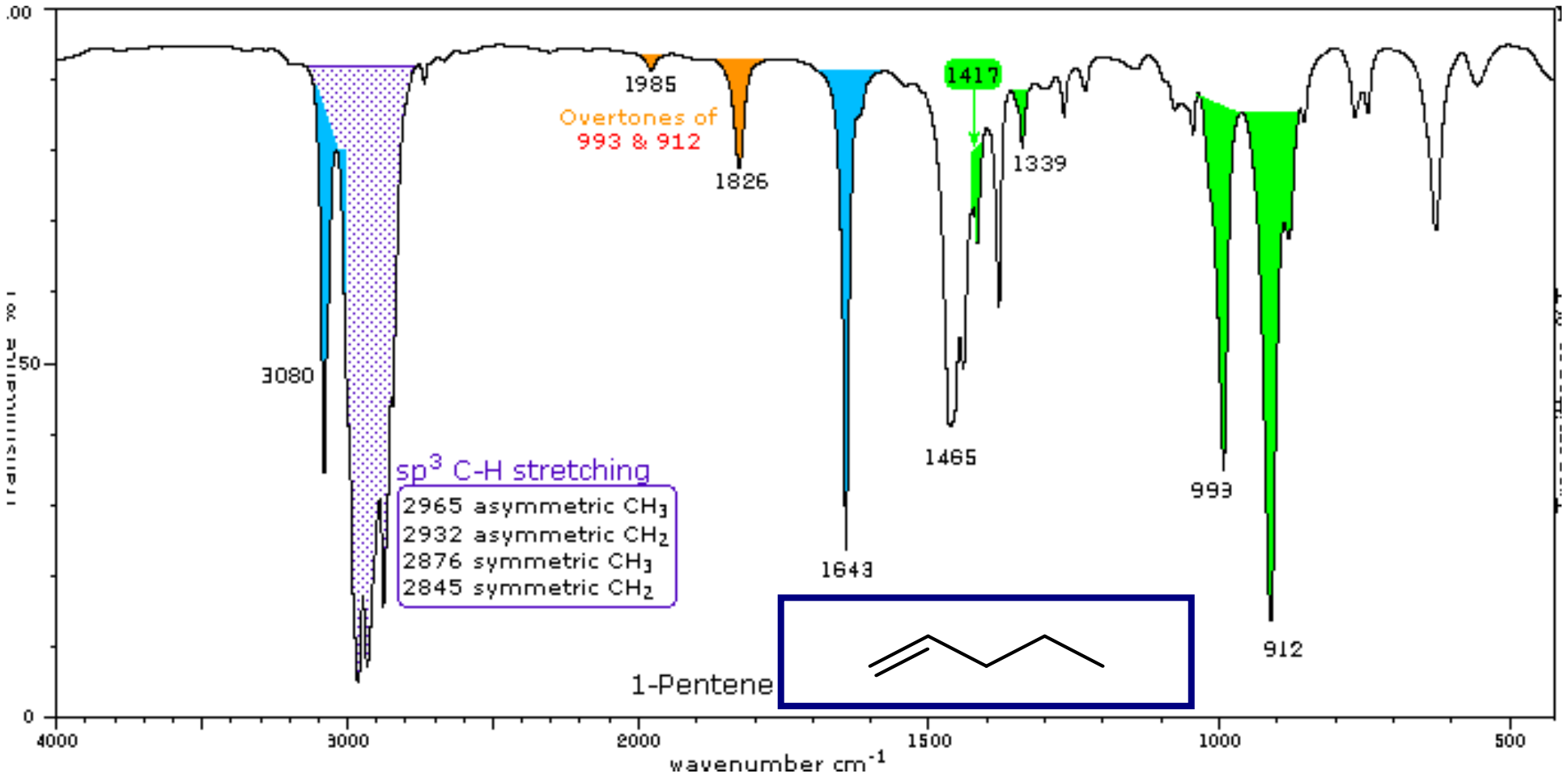
** IF YOU'RE NOT SURE WHAT THE DIFFERENCE BETWEEN AN ACID AND AN ALCOHOL IS, DO THE QUICK "FUNCTIONAL GROUP IDENTIFICATION" EXERCISE.

** ...IF YOU HAVE ONE FG. TWO 2°AMINE WOULD LOOK LIKE A 1 AMINE.


SINGLE BOND STRETCH
TRIPLE BONDS
DOUBLE BONDS
FINGERPRINT REGION SKELETAL VIBRATIONS
BEND
ROCK
S-H
C≡C-H
X=Y=Z
O-H, N-H STRETCH
C-H STRETCH
NITRILES CARBENES
C=O
C=C
C=N
C-O
C-N
C-C
4000
3500
3000
2500
2000
1500
1000
500
WAVENUMBER (cm-1)


2,3,4-Trimethylpentane, 99%
2963
2878
1466
1379
1122
2,2,4-Trimethylpentane, 99%
2955
2903
2872
1471
1388
1204
1.2
1.0
0.8
0.6
0.4
0.2
3500
3000
2500
2000
1500
1000
Wavenumbers (cm-1)


1-HEXENE, 99%
1-Heptene, 99+%
1-Octene, 97%
3077
2960
2928
2866
1822
1641
1460
1380
993
910
738
632
3077
2930
2860
1828
1641
1460
1378
994
910
728
634
3077
2959
2927
2858
1822
1641
1461
1378
993
910
728
634
1.2
1.0
0.8
0.6
0.4
0.2
3500
3000
2500
2000
1500
1000
Wavenumbers (cm-1)



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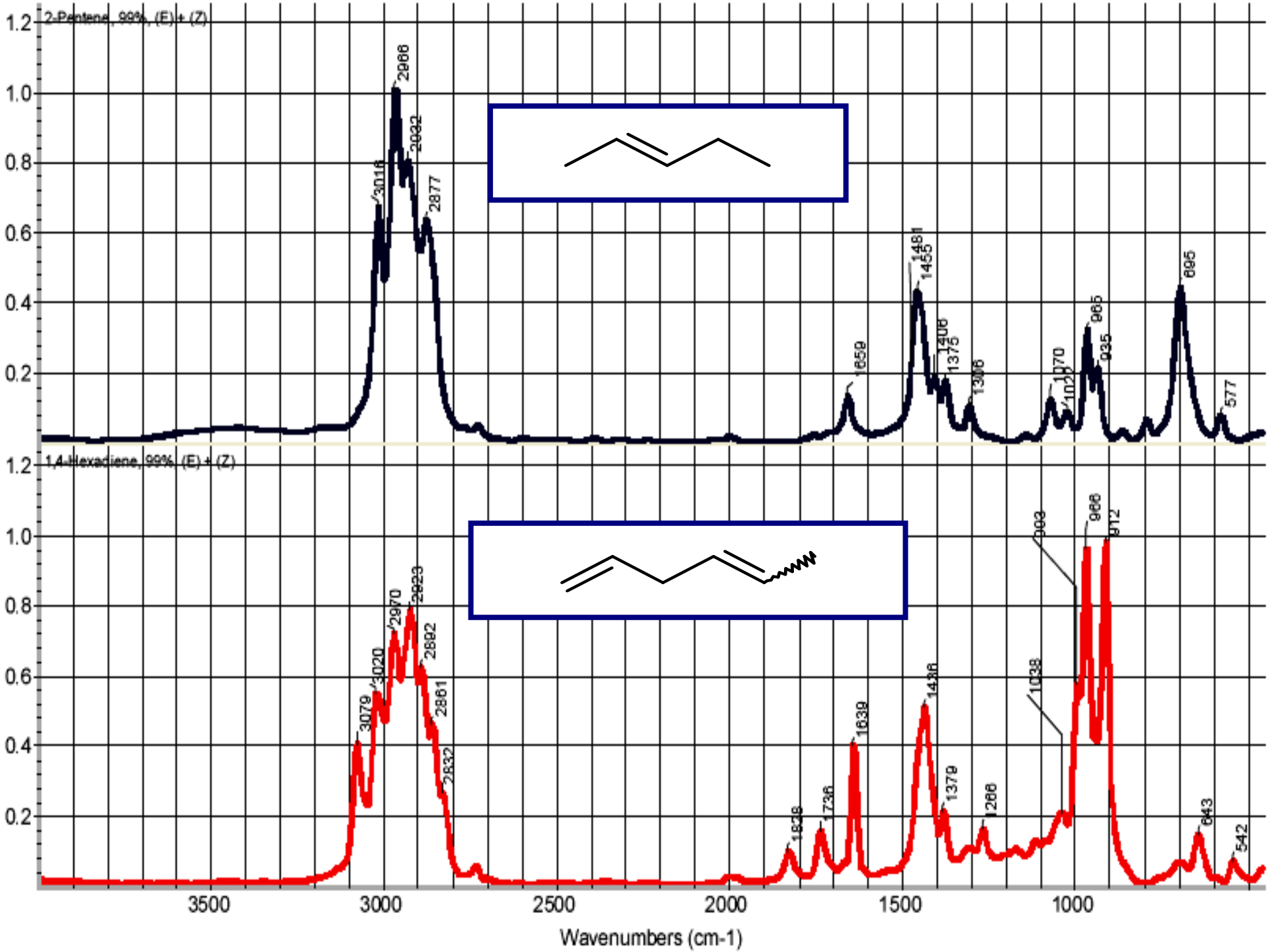
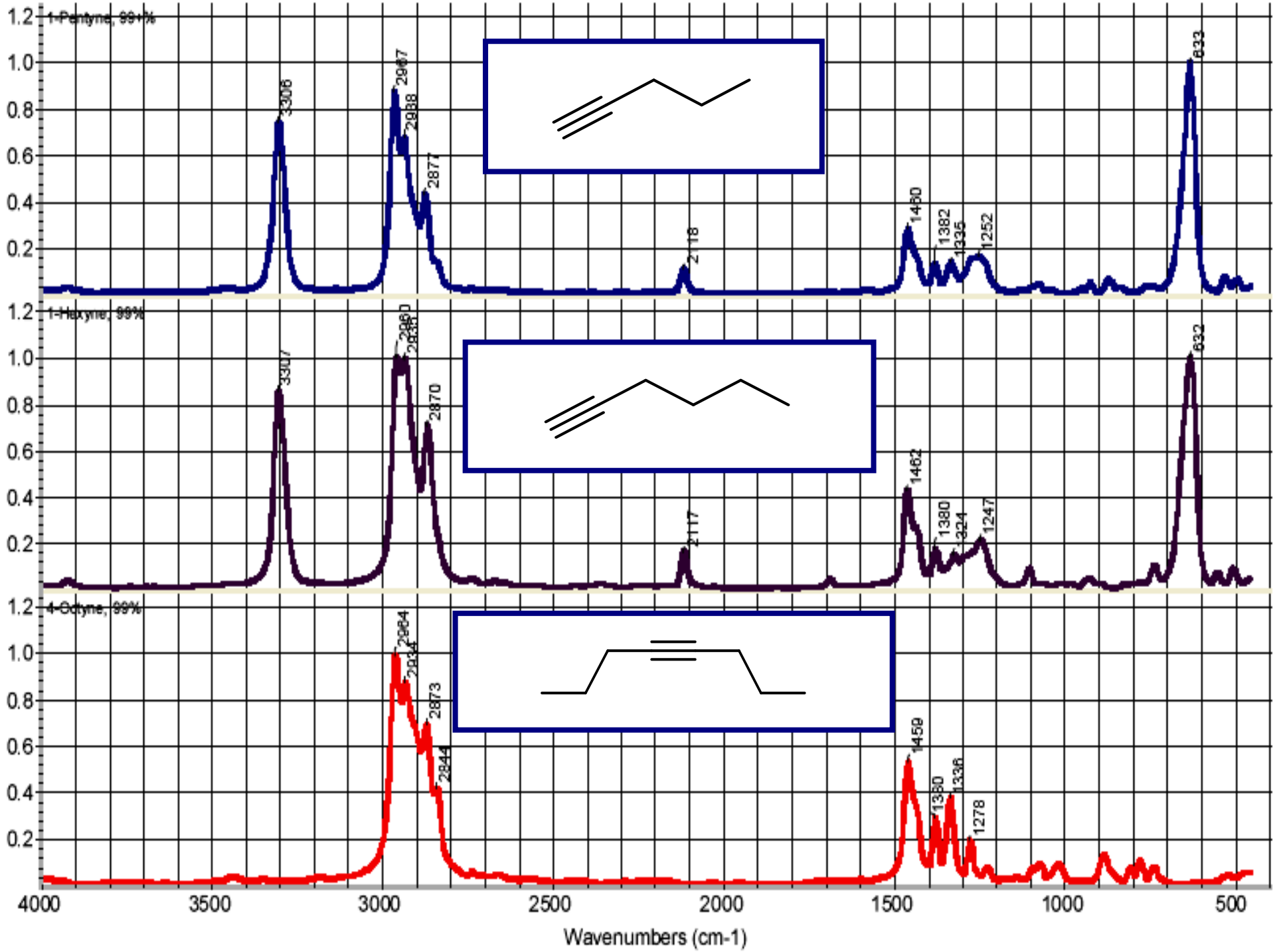
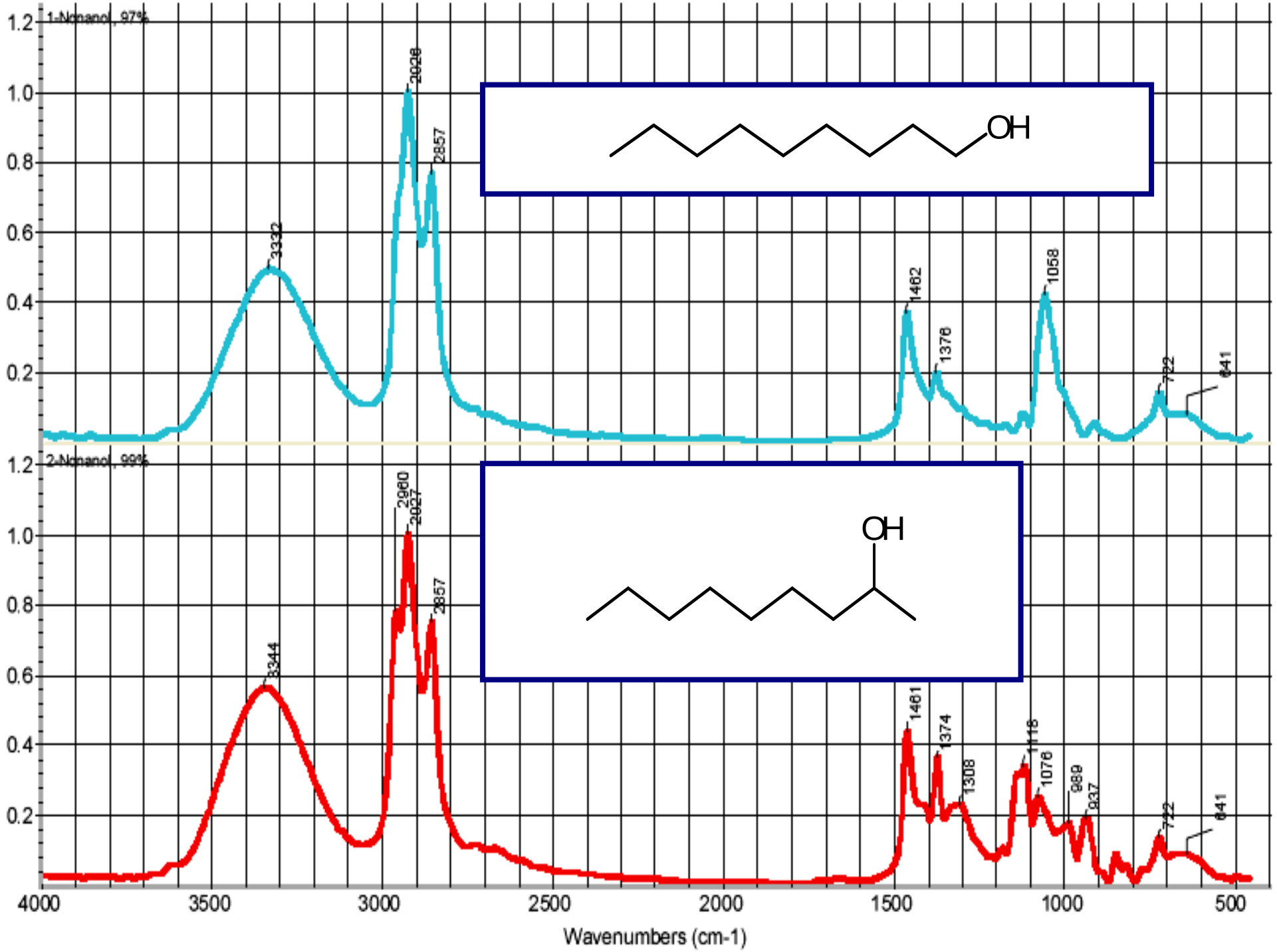
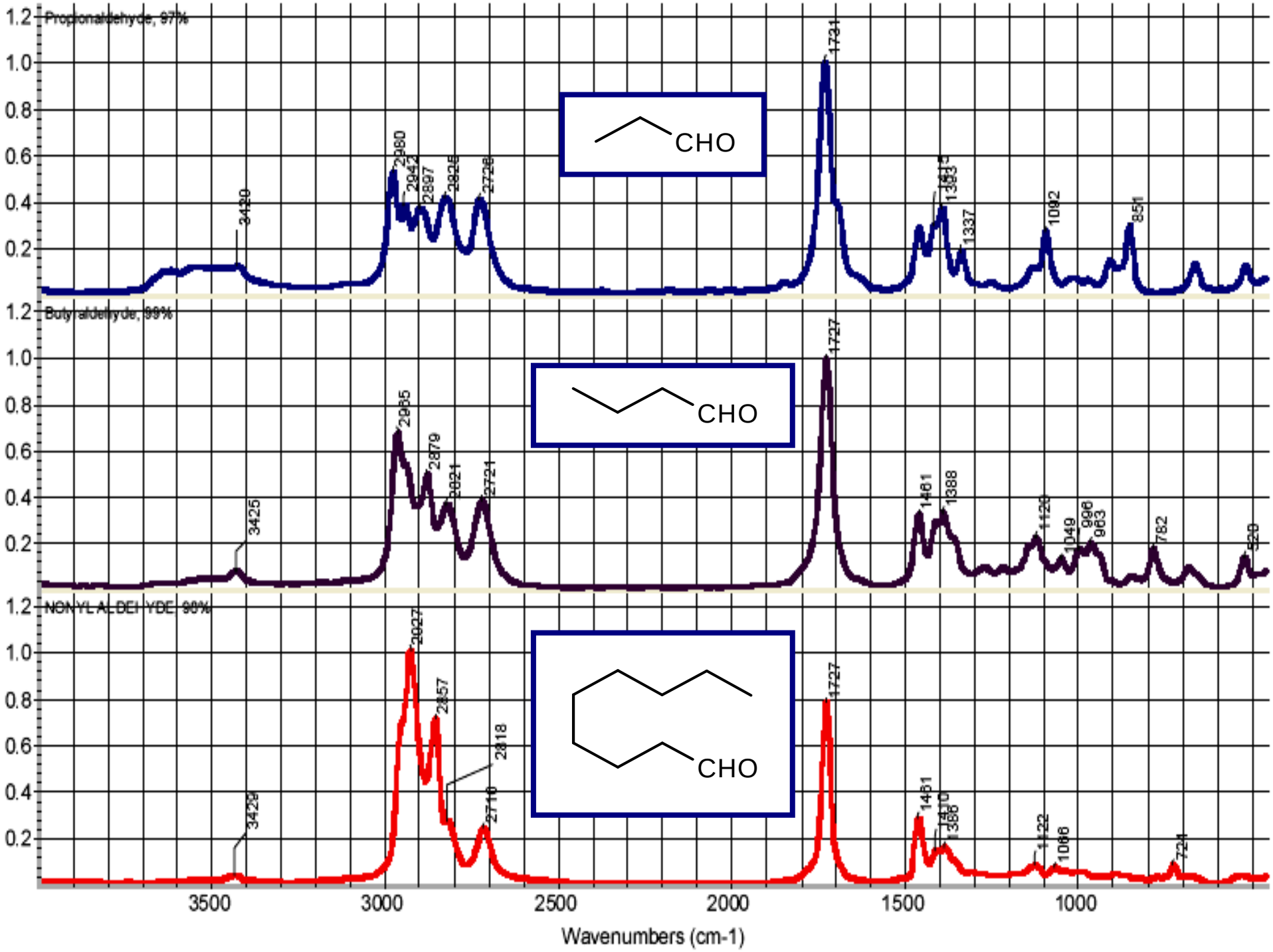
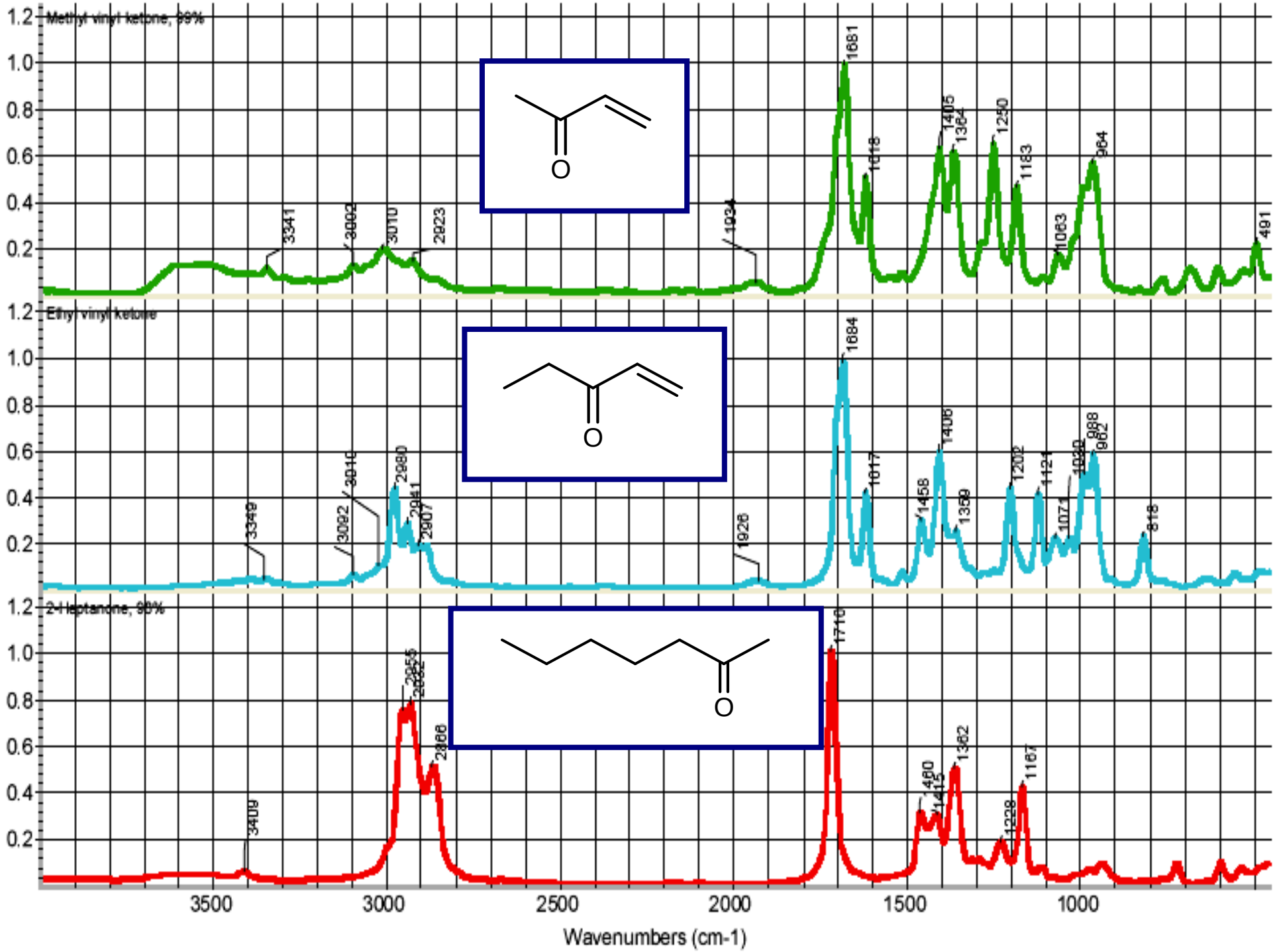
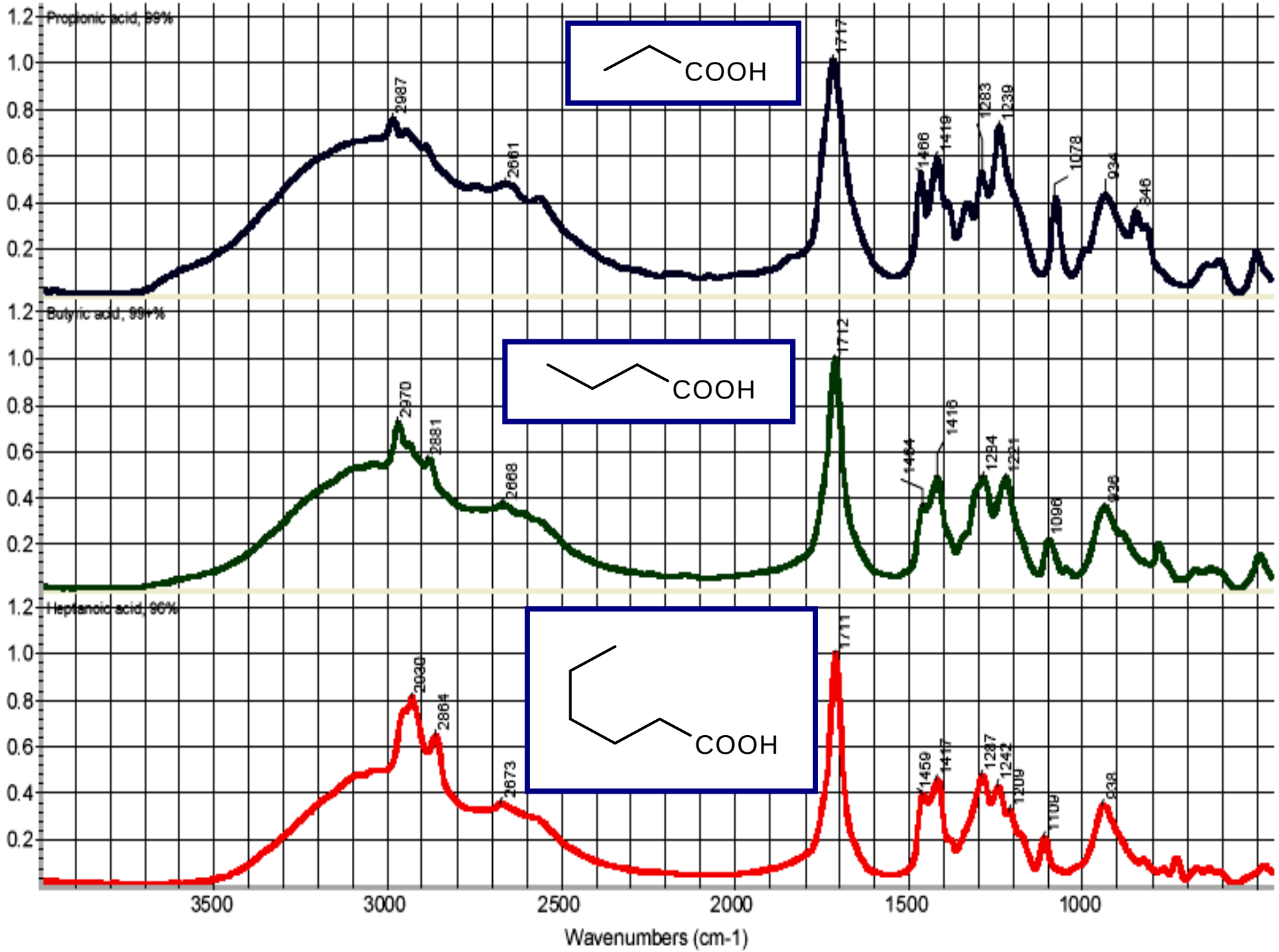

2-Pentene, 99%, (E) + (Z)
2966
3018
2932
2877
1659
1481
1455
1406
1375
1306
1070
1020
965
935
895
577
1,4-Hexadiene, 99%, (E) + (Z)
3079
3020
2970
2923
2882
2861
2832
1828
1736
1639
1436
1379
1266
1038
993
966
912
643
542
1.2
1.0
0.8
0.6
0.4
0.2
3500
3000
2500
2000
1500
1000
Wavenumbers (cm-1)

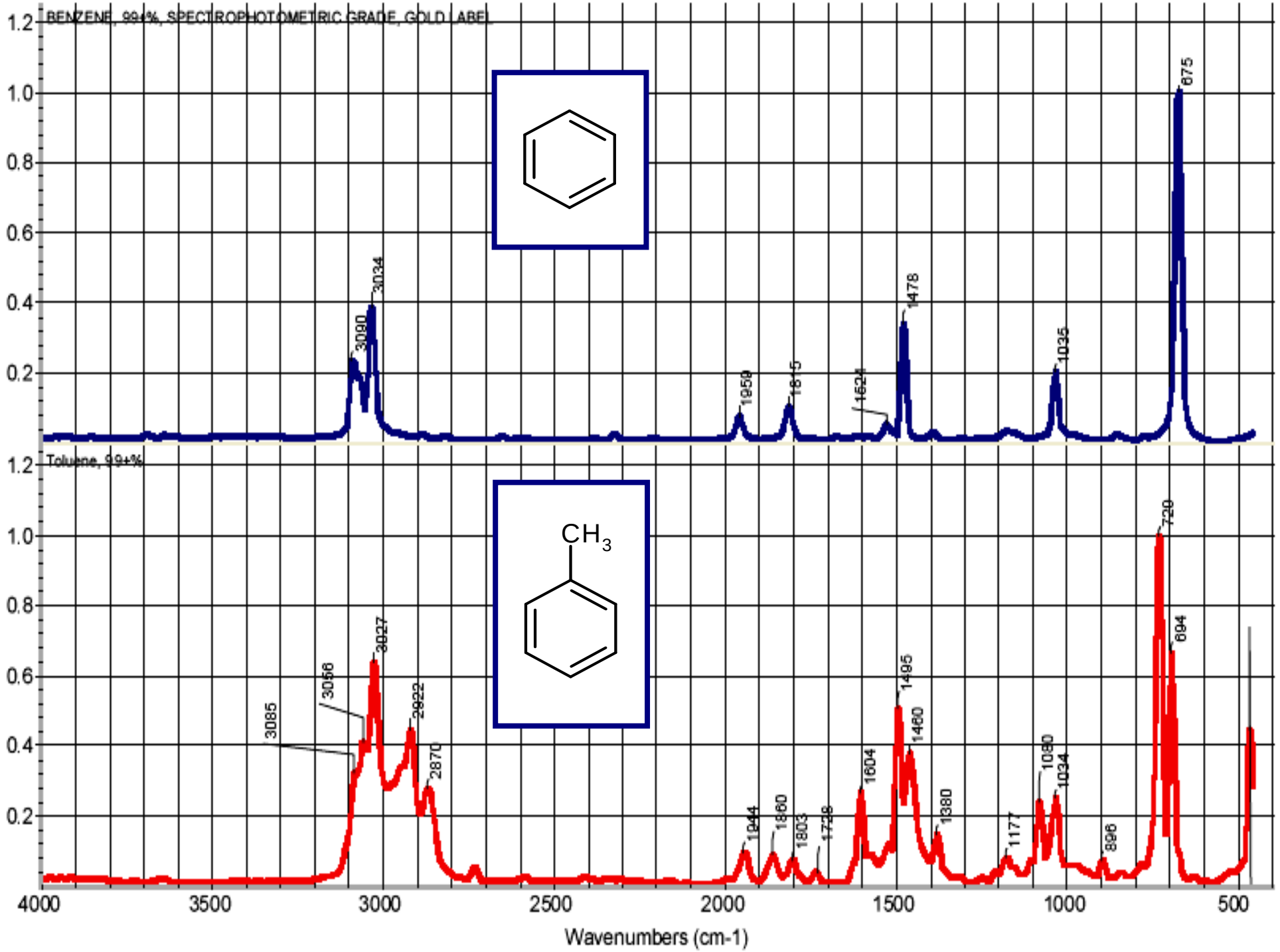

1-Pentyne, 99+%
3306
2967
2938
2877
2118
1458
1382
1335
1252
633
1-Hexyne, 99%
3307
2960
2870
2117
1462
1380
1324
1247
632
4-Octyne, 99%
2964
2873
2844
1459
1380
1336
1278
1.2
1.0
0.8
0.6
0.4
0.2
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

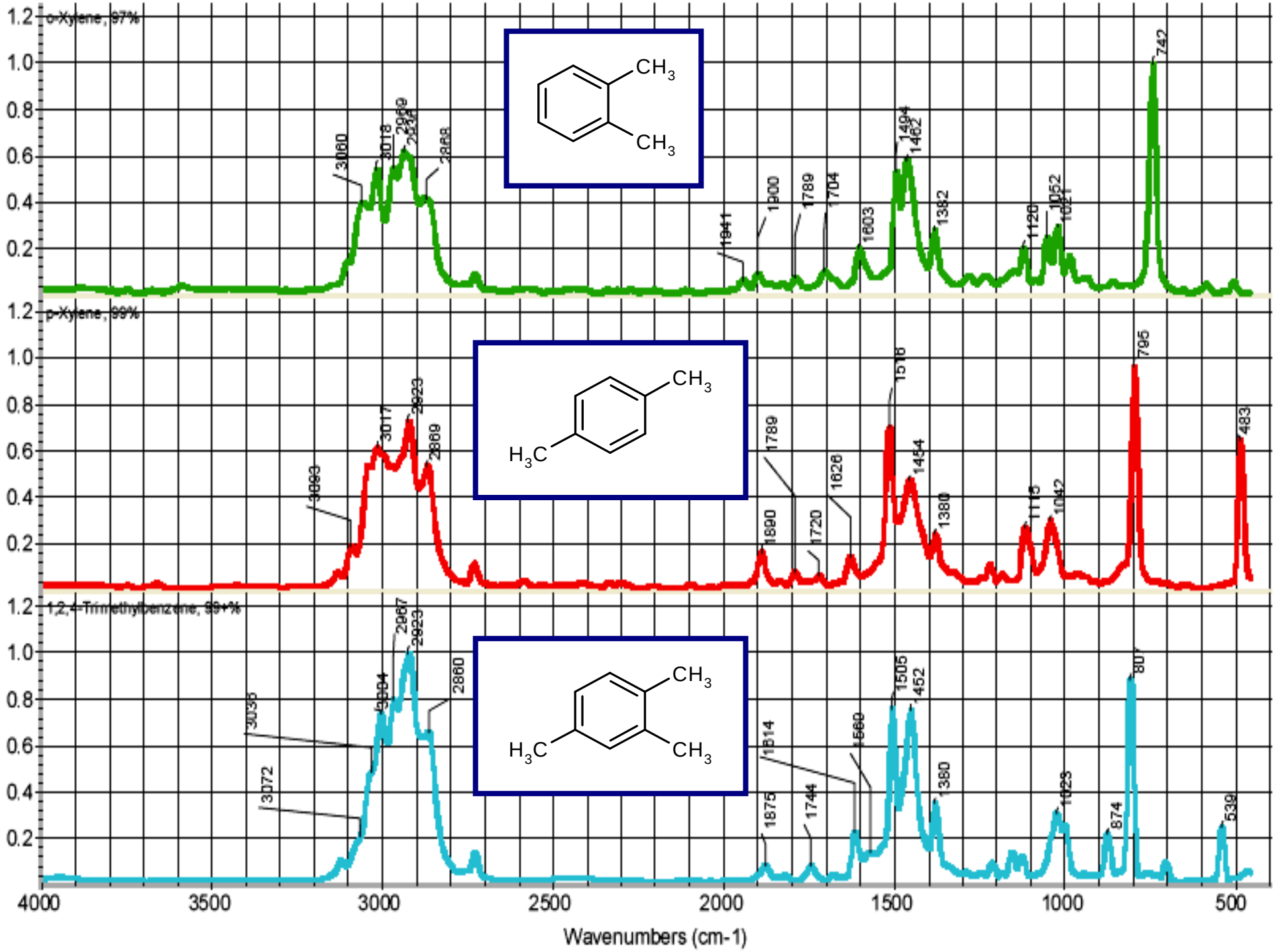

1-Nonanol, 97%
2928
2857
3332
1462
1376
1058
722
641
OH
2-Nonanol, 99%
2960
2927
2857
3344
1461
1374
1308
1116
1076
989
937
722
641
OH
1.2
1.0
0.8
0.6
0.4
0.2
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

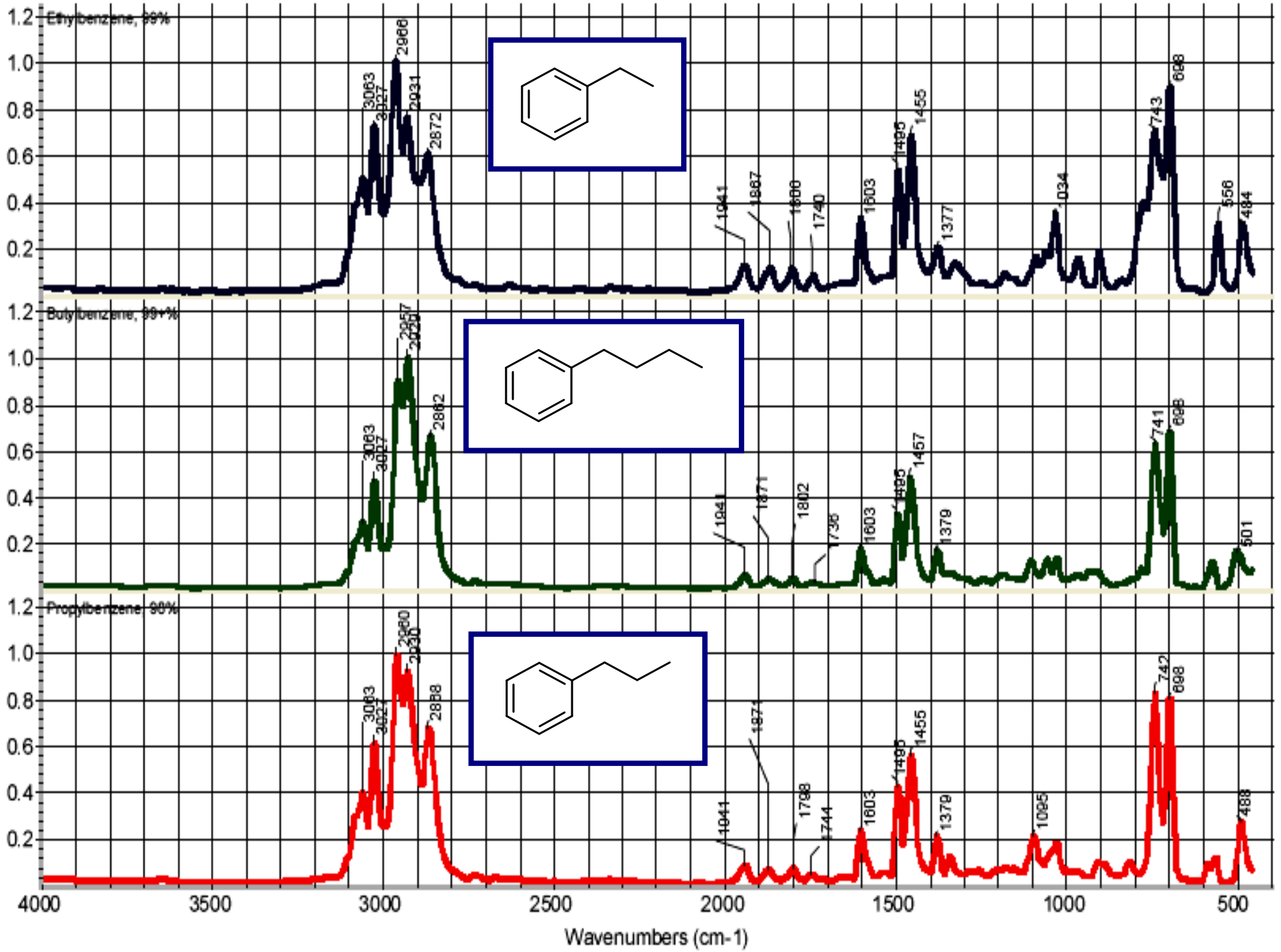

Propionaldehyde, 97%
CHO
3420
2980
2942
2897
2826
2726
1731
1463
1393
1337
1092
851
Butyraldehyde, 99%
CHO
3425
2965
2879
2821
2721
1727
1461
1388
1126
1049
996
963
762
539
NONYLALDEHYDE, 95%
CHO
3428
2927
2857
2818
2710
1727
1461
1410
1388
1122
1066
724
1.2
1.0
0.8
0.6
0.4
0.2
3500
3000
2500
2000
1500
1000
Wavenumbers (cm-1)

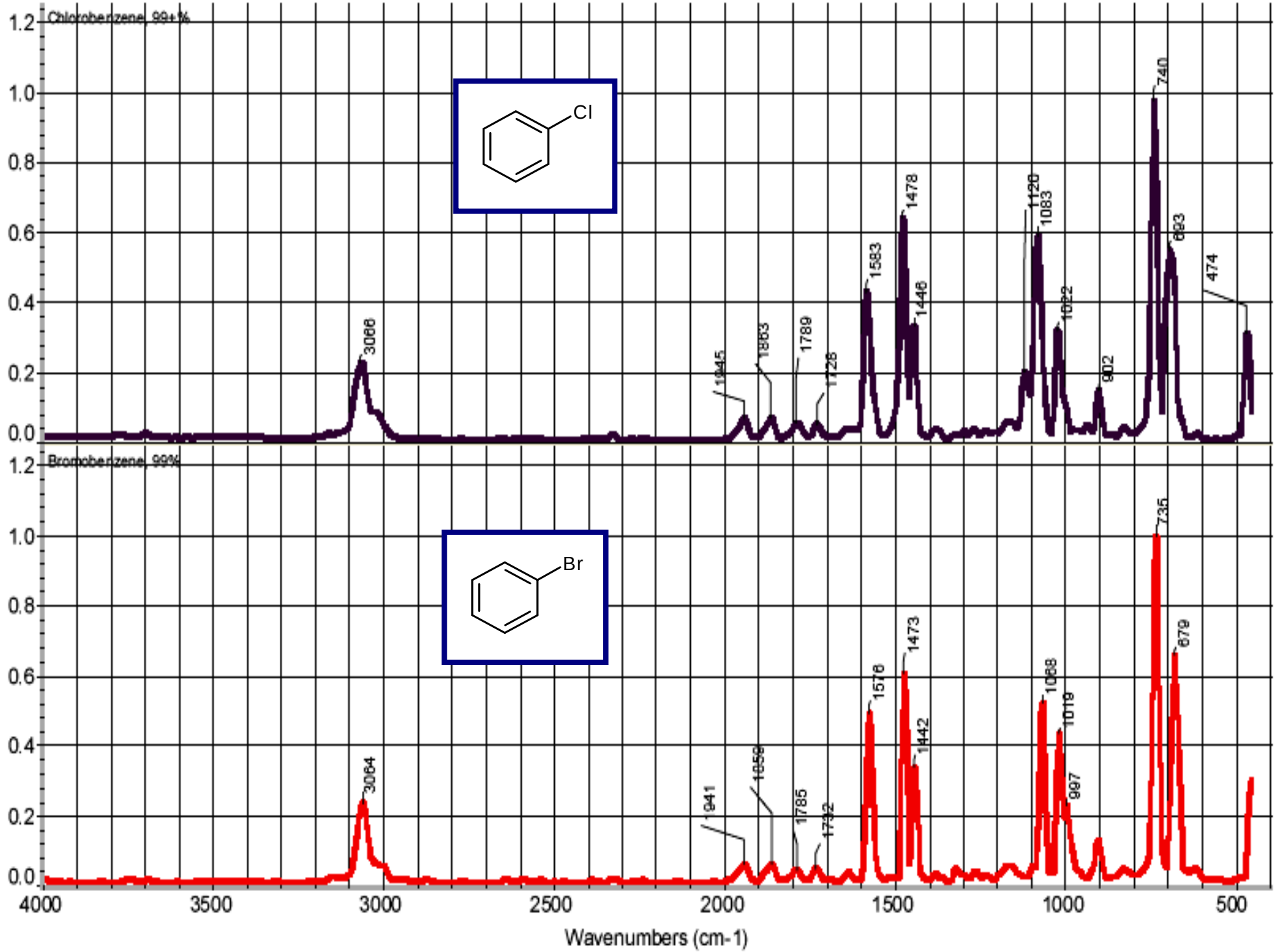

Methyl vinyl ketone, 99%
Ethyl vinyl ketone
2-Heptanone, 99%
1.2
1.0
0.8
0.6
0.4
0.2
3500
3000
2500
2000
1500
1000
Wavenumbers (cm-1)
O
O
O

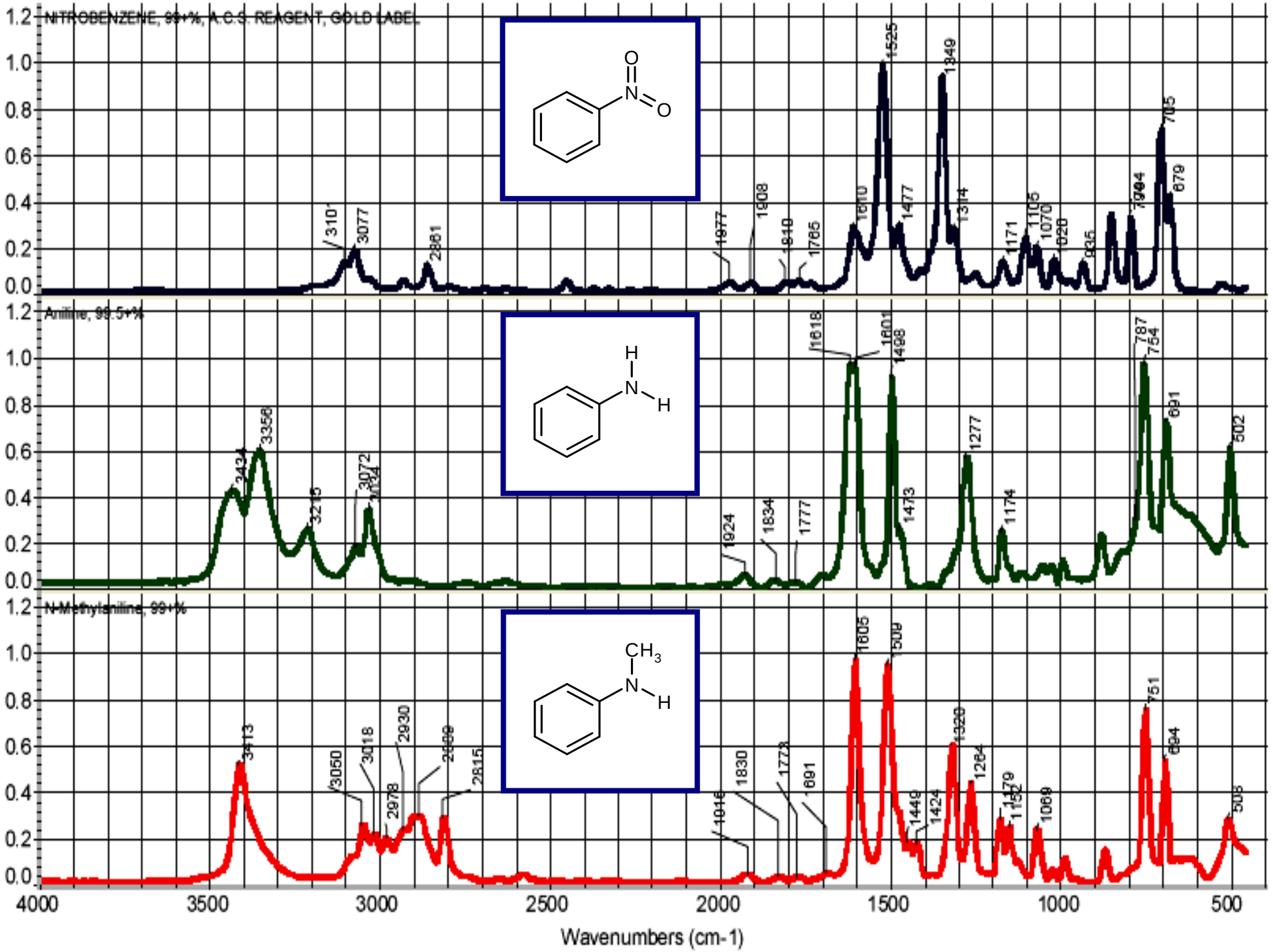

Propionic acid, 99%
COOH
2987
2661
1717
1466
1419
1283
1239
1078
934
846
Butyric acid, 99+%
COOH
2970
2881
2668
1712
1464
1418
1284
1221
1096
938
Heptanoic acid, 96%
COOH
2930
2864
2673
1711
1459
1417
1287
1242
1209
1108
938
1.2
1.0
0.8
0.6
0.4
0.2
3500
3000
2500
2000
1500
1000
Wavenumbers (cm-1)

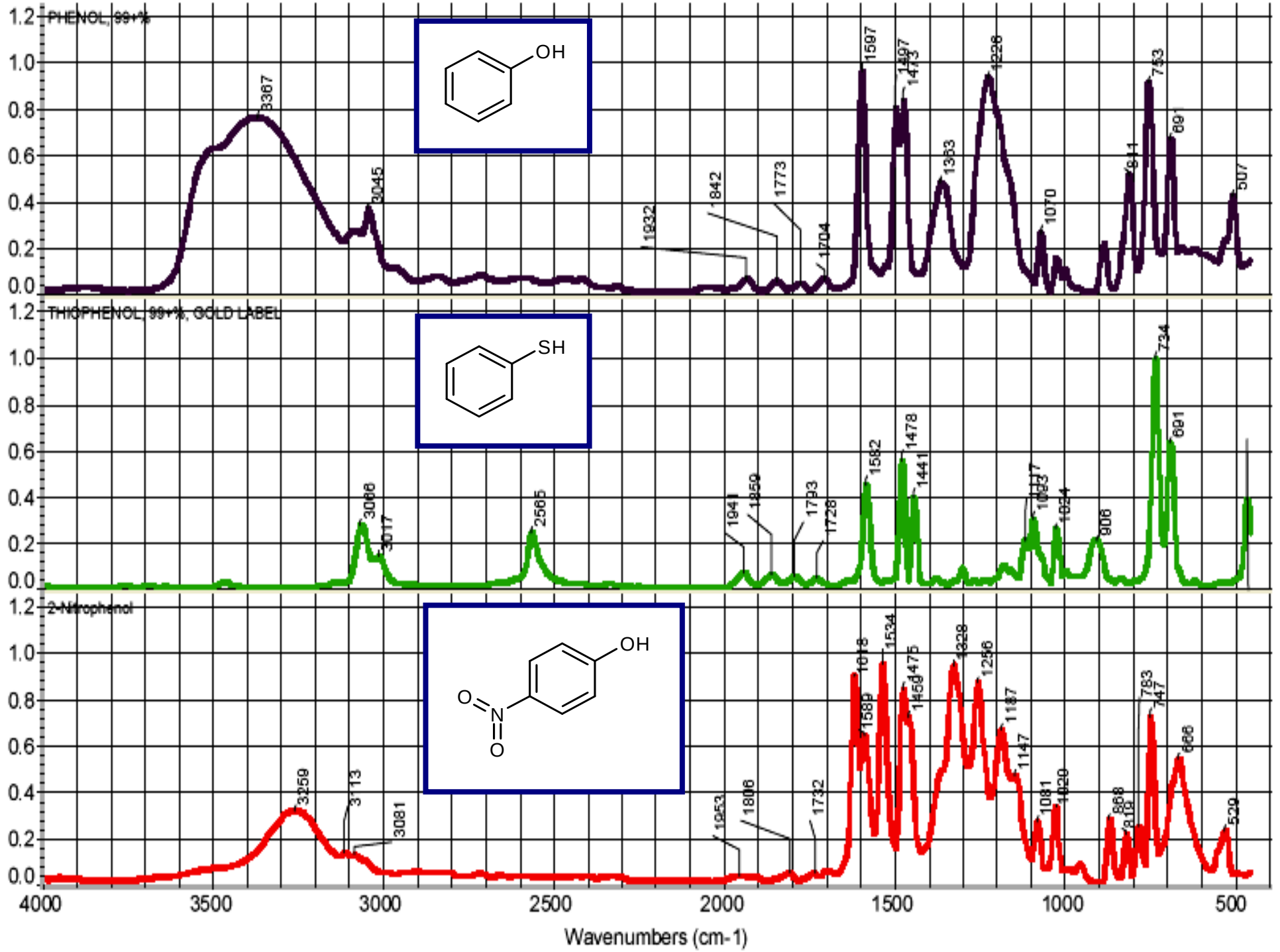

BENZENE, 99+%, SPECTROPHOTOMETRIC GRADE, GOLD LABEL
3090
3034
1959
1815
1624
1478
1035
675
Toluene, 99+%
CH3
3085
3056
3027
2922
2870
1944
1860
1803
1728
1604
1495
1460
1380
1177
1080
1034
896
720
694
1.2
1.0
0.8
0.6
0.4
0.2
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

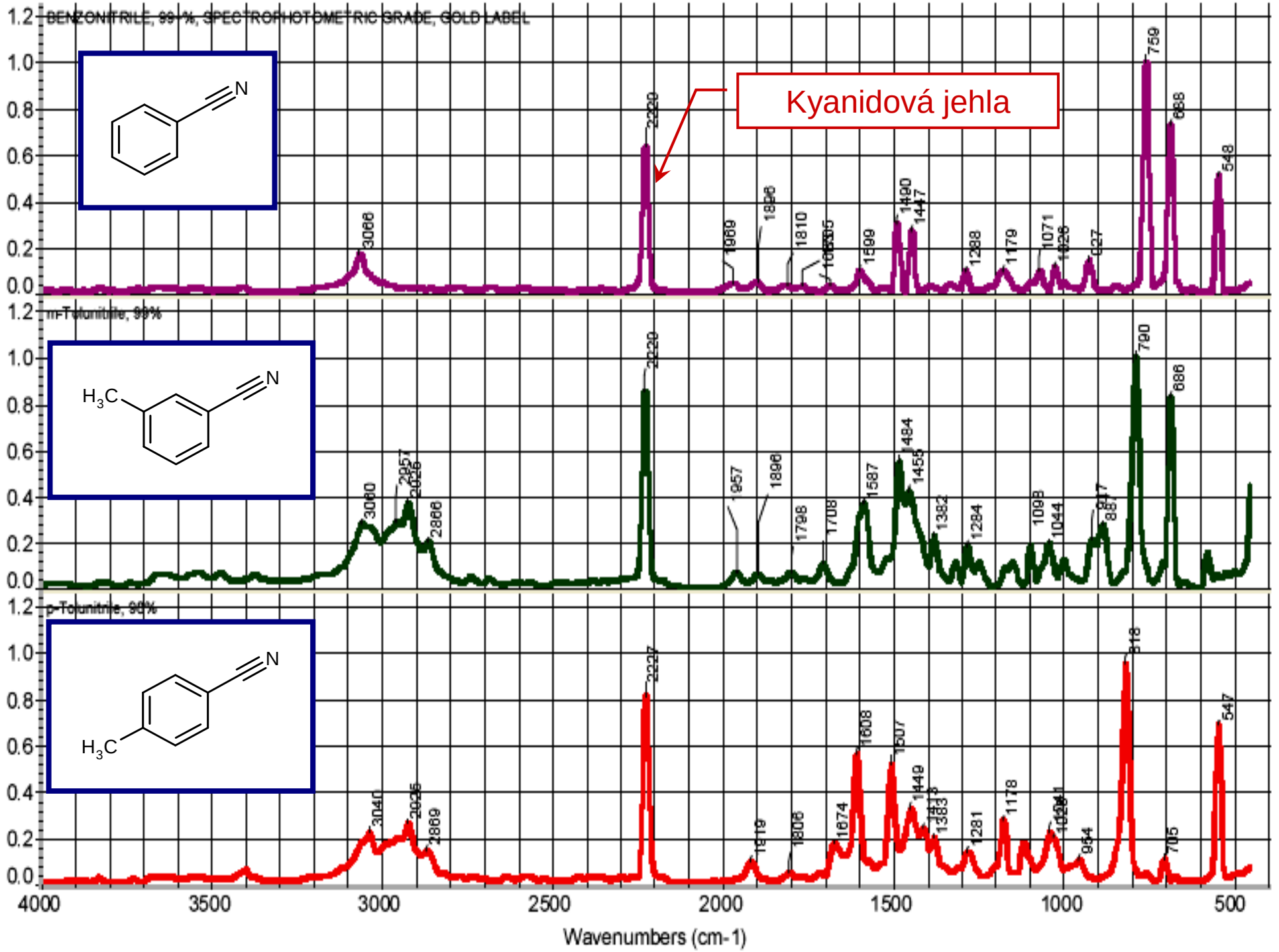

o-Xylene, 97%
p-Xylene, 99%
1,2,4-Trimethylbenzene, 99+%
CH3
CH3
H3C
CH3
H3C
CH3
3060
3018
2968
2924
2868
1941
1900
1789
1704
1603
1494
1462
1382
1126
1052
742
3093
3017
2923
2869
1890
1789
1720
1628
1516
1454
1380
1115
1042
795
483
3035
3072
2967
2923
2860
1875
1814
1744
1660
1505
1452
1380
1023
874
801
539
1.2
1.0
0.8
0.6
0.4
0.2
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

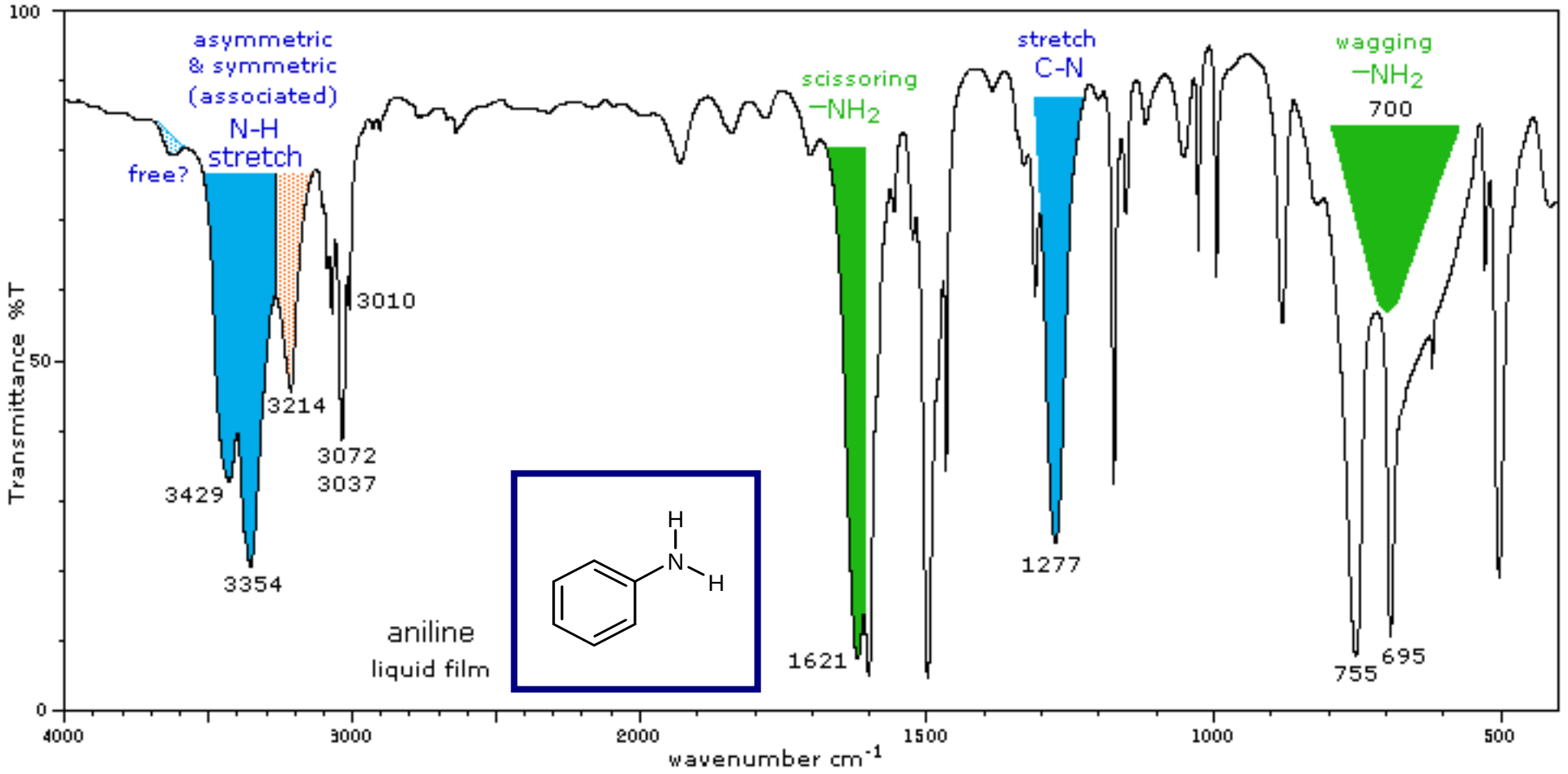

Ethylbenzene, 99%
Butylbenzene, 99+%
Propylbenzene, 98%
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500


Chlorobenzene, 99+%
Cl
3066
1945
1863
1789
1726
1583
1478
1446
1120
1083
1022
902
740
683
474
Bromobenzene, 99%
Br
3064
1941
1858
1785
1732
1576
1473
1442
1068
1019
997
735
679
1.2
1.0
0.8
0.6
0.4
0.2
0.0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)


NITROBENZENE, 99+%, A.C.S. REAGENT, GOLD LABEL
3101
3077
2861
1977
1908
1849
1765
1610
1525
1477
1349
1314
1171
1105
1070
1026
935
904
705
679
Aniline, 99.5+%
3424
3358
3215
3072
3054
1924
1834
1777
1618
1601
1498
1473
1277
1174
787
754
691
502
N-Methylaniline, 99+%
3413
3050
3018
2978
2930
2859
2815
1916
1830
1773
1691
1605
1509
1449
1424
1320
1264
1179
1152
1069
751
694
506
1.2
1.0
0.8
0.6
0.4
0.2
0.0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)


PHENOL, 99+%
OH
3367
3045
1932
1842
1773
1704
1597
1497
1443
1383
1226
1070
753
691
507
THIOPHENOL, 99+%, GOLD LABEL
SH
3066
3017
2565
1941
1859
1793
1728
1582
1478
1441
1117
1024
906
734
691
2-Nitrophenol
OH
O
N
O
3259
3113
3081
1953
1806
1732
1589
1534
1475
1450
1328
1296
1187
1147
1081
1020
868
819
783
747
666
529
1.2
1.0
0.8
0.6
0.4
0.2
0.0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)


BENZONITRILE, 99+%, SPECTROPHOTOMETRIC GRADE, GOLD LABEL
Kyanidová jehla
m-Tolunitrile, 99%
p-Tolunitrile, 99%
Wavenumbers (cm-1)



http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/InfraRed/infrared.htm