1. (a) $C_3H_3Cl$; 3-chloropropyne

| | | |
|---|---|---|
| I.H.D.=2 | | 1 C≡C, or 2 C=C |
| ~2150 $cm^{-1}$ | moderate | C≡C |
| 3300 | strong | ≡C-H |
| 1270 | strong | -$CH_2$-Cl |
| 1375 & 1450 | MISSING | NO –$CH_3$ |
| 1600-1680 | MISSING | NO C=C |

1. (b) $C_{10}H_{14}$; *para*-isopropyltoluene ~or~ *p*-diethylbenzene ~or~ *p*-propyltoluene

| | | |
|---|---|---|
| I.H.D.=4 | | aromatic ring? |
| ~1375 & ~1450? | | C–H in –$CH_3$ |
| ~1465? | | C–H in –$CH_2$– |
| 1667-2000 | | *para*-substituted aromatic ring |
| 800-850 | | *para*-substituted aromatic ring |

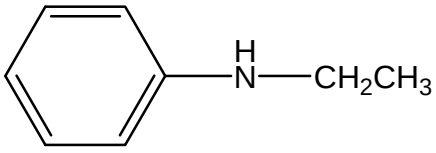
1. (c) $C_7H_9N$; *meta*-methylaniline

| | | |
|---|---|---|
| I.H.D.=4 | | aromatic ring? |
| 1667-2000 | | *meta*-substituted aromatic ring |
| 690 & 780 | | *meta*-substituted aromatic ring |
| 3300-3500 | 2 bands | primary amine |
| 1560-1640 | broad | primary amine |

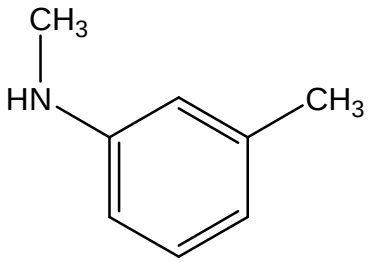
1. (d) $C_7H_8O$; *ortho*-methylphenol

| | | |
|---|---|---|
| I.H.D.=4 | | aromatic ring? |
| 1667-2000 | | *ortho*-substituted aromatic ring |
| 760 | | *ortho*-substituted aromatic ring |
| 3200-3600 | broad | alcohol or phenol |

1. (e) $C_8H_{11}N$; N-ethylaniline (phenylethylamine) (*or isomer shown on right*)




or

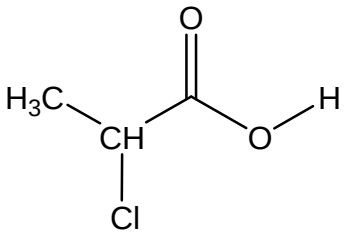



| | | |
|---|---|---|
| I.H.D.=4 | | aromatic ring? |
| 1667-2000 | | *mono*-substituted or *meta*- aromatic ring |
| 690 & 750 | | *mono*-substituted or *meta*- aromatic ring |
| 1500 | s | secondary amine |

1. (f) $C_7H_7Cl$; *ortho*-chlorotoluene

| | | |
|---|---|---|
| I.H.D.=4 | | aromatic ring? |
| 1667-2000 | | *ortho*-substituted aromatic ring |
| 750 | | *ortho*-substituted aromatic ring |

1. (g) $C_3H_5O_2Cl$; 2-chloropropanoic acid



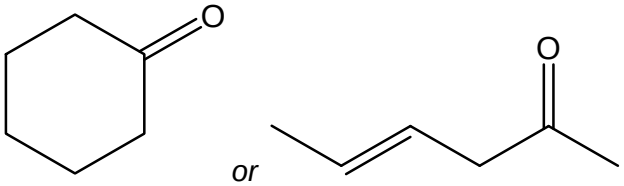
I.H.D.=1 ..... C=O?
1728 ..... s ..... carboxylic acid
2400-3600 ..... s, b ..... carboxylic acid
1775-1810 ..... MISSING ..... NO acid chloride
540-785 (strong) ..... MISSING ..... NO 1° or 3° C-Cl

1. (h) $C_5H_{12}O$; 1/2/3-methyl-1-butanol ~or~ 1,2-dimethyl-1-propanol

I.H.D.=0 ..... no double bonds; no rings
…-3600 ..... broad ..... alcohol or phenol
1060 ..... s ..... 1° alcohol
1465 ..... m/s ..... C–H in $CH_2$
1375 ..... m ..... C–H in $CH_3$
720 ..... MISSING ..... <4 $CH_2$ in 1 chain

1. (i) $C_6H_{10}O$; (multiple keto-alkene isomers possible, NOT conjugated; cyclohexanone is )

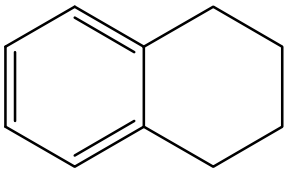
I.H.D.=2 ..... C=O + (ring ~or~ C=C)
1718 ..... s ..... ketone
*1715 ..... s ..... cyclohexanone (pretty close)*
reasonable deductions:



*or*

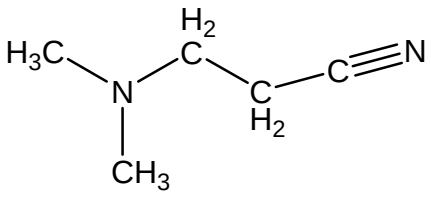
1650 ..... m ..... C=C ?
700 ..... MISSING ..... NOT *cis*-
990 ..... m/w ..... *trans*- ?
720 ..... MISSING ..... <4 $CH_2$ in 1 chain ?

1. (j) $C_{10}H_{12}$ (2 six-membered rings); 1,2,3,4-tetrahydronaphthalene



I.H.D.=5 ..... aromatic ring + ring?
1667-2000 ..... *ortho*-substituted aromatic ring
750 ..... *ortho*-substituted aromatic ring?

1. (k) $C_5H_{10}N_2$; 3-(dimethylamino)propanenitrile



I.H.D.=2 ..... 2 = bonds? 1 ≡ bond? 1 = + ring?
3300-3500 ..... MISSING ..... NO N-H
1560-1640 ..... MISSING ..... NOT 1° amine
1500 ..... MISSING ..... NOT 2° amine
1500 + 1560-1640 ..... MISSING ..... 3° amine
2250 ..... m ..... C≡N
1375 + 1450 ..... m ..... C–H in -$CH_3$
1465 ..... s ..... C–H in -$CH_2$-

2. citronellal
1720 ..... s ..... citronellal
1680-1700 ..... MISSING ..... NOT conjugated aldehyde
1725 ..... ..... aldehyde

3. $C_9H_8O$ (cinnamon oil); trans-3-phenyl-2-propenal
I.H.D.=6 ..... ..... aromatic ring + 2 double bonds?
3200-3600 ..... MISSING ..... NOT alcohol
1677 ..... s ..... conjugated C=O?
1620 ..... s ..... C=C
975 ..... m ..... *trans*-1,2-C=C
690 + 740 ..... m/s ..... monosubstituted aromatic ring

4. lower spectrum=*cis*- and upper spectrum = *trans*-3-hexene-1-ol
960 ..... s ..... *trans*-C=C
720 ..... m ..... *cis*-C=C

5. (a) B, ethyl cinnamate
1712 ..... s ..... conjugated C=O
1630 ..... s ..... C=C
(1735-1750 ..... ..... ester)

5. (b) C, cyclobutanone
1780 ..... s ..... ketone
1780 ..... s ..... cyclobutanone

5. (c) D, 2-ethylaniline
3380 + 3580 ..... m ..... 1° amine
750 ..... s ..... ortho-substituted aromatic ring

5. (d) A, propiophenone

| | | |
|---|---|---|
| 1688 | s | conjugated C=O |
| 1715 | MISSING | NOT unconjugated ketone |
| 1725 | MISSING | NOT unconjugated aldehyde |
| 2400-3600 | MISSSING | NOT carboxylic acid O-H |

5. (e) D, butanoic anhydride

| | | |
|---|---|---|
| 1750 + 1819 | s | acid anhydride |
| 550-730 | MISSING | NOT acid chloride |

REFERENCES:

1. *Introduction to Spectroscopy, 2nd edition*; Pavia, Lampman & Kriz; ch. 2

2. *Introduction to Organic Chemistry, 3rd Edition*; Brown & Poon; ch. 11

3. *The Organic Chem Lab Survival Manual, 7th Edition*; Zubrick; ch. 34

GRADING:

| QUESTION | POINTS EACH |
|---|---|
| 1(a) – 1(k) | 4 |
| 3 | 4 |
| 2 & 4 | 1 |
| 5(a) – 5(e) | 2 |

| QUESTION | TOTAL POINTS |
|---|---|
| 1(a) – 1(k) | (6 questions x 4 pts/each = ) 24 |
| 3 | (1 x 4 = ) 4 |
| 2 & 4 | (2 x 1 = ) 2 |
| 5(a) – 5(e) | (5 x 2 = ) 10 |
| **TOTAL** | **40** |