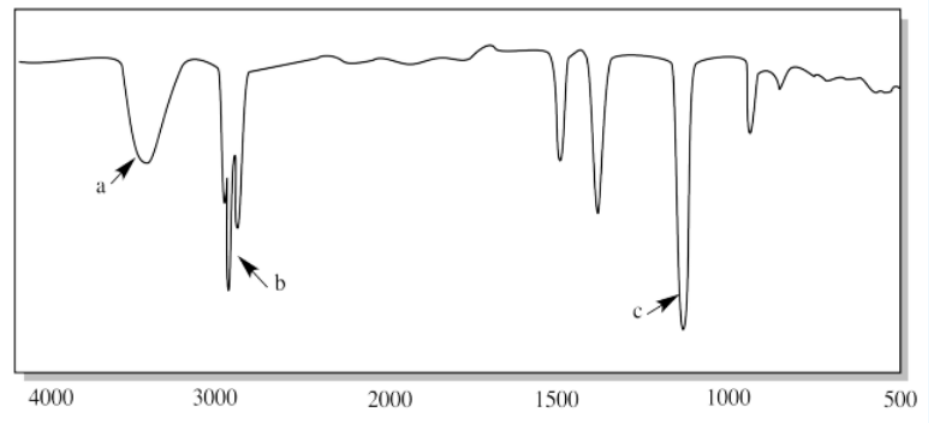
3.10: Additional Problems

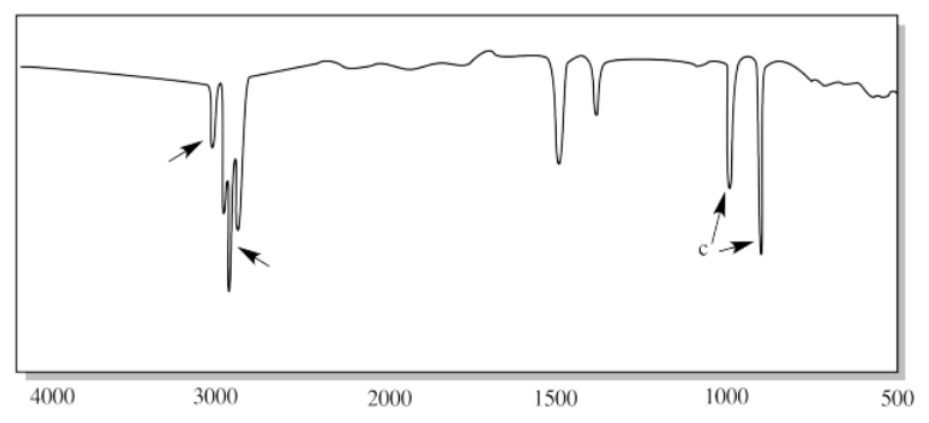
Exercise 3.10.1

For each of the following hand-drawn cartoons of IR spectra, identify the bond(s) that correspond to the indicated peaks.

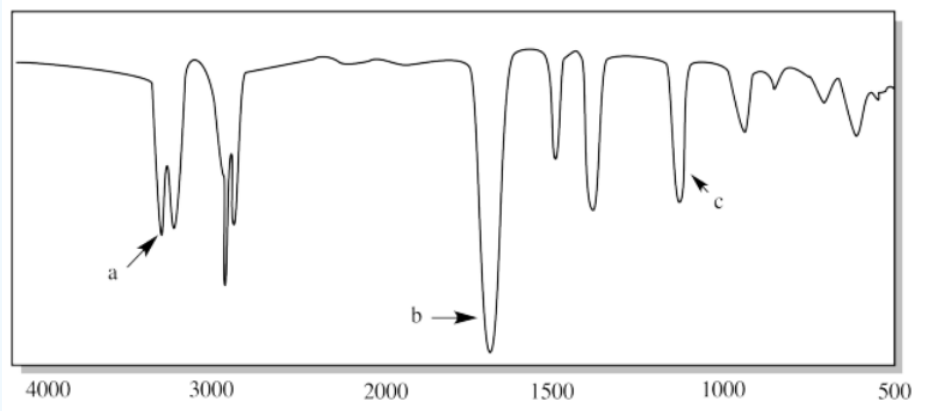
i.



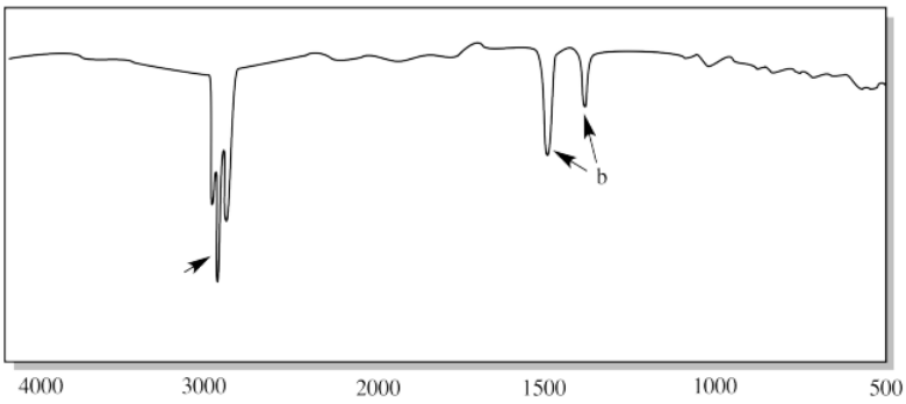
ii.



iii.



iv.


b
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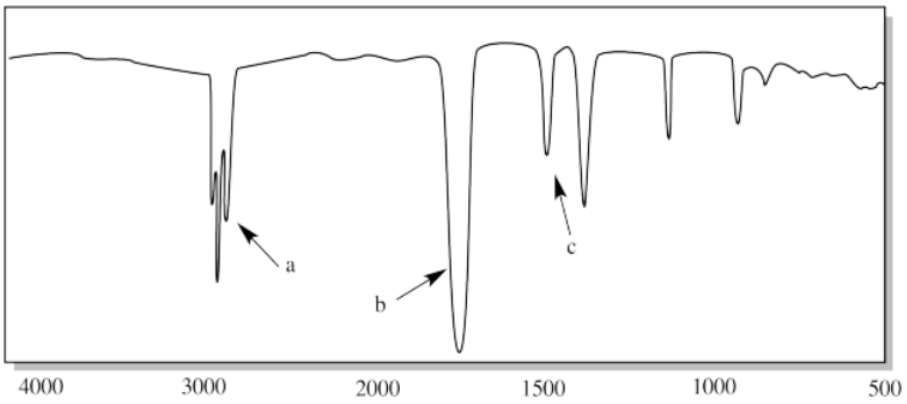
v.


a
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c
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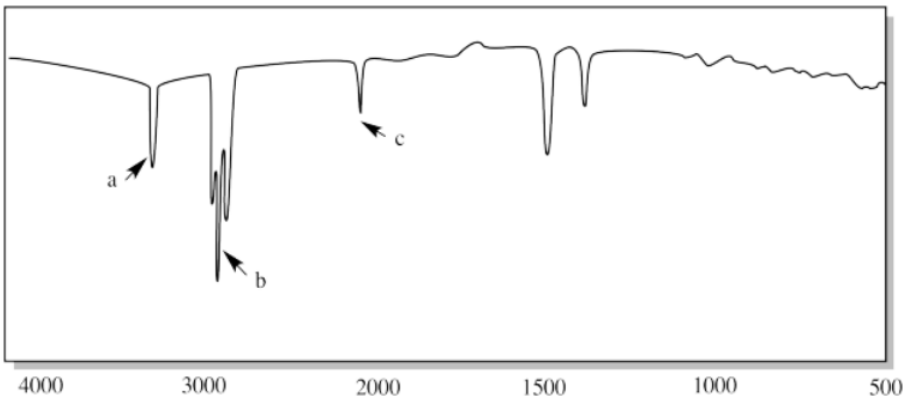
vi.


a
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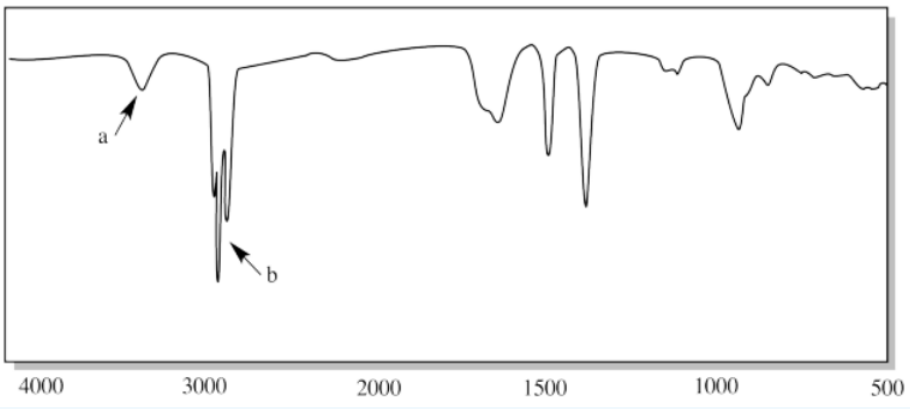
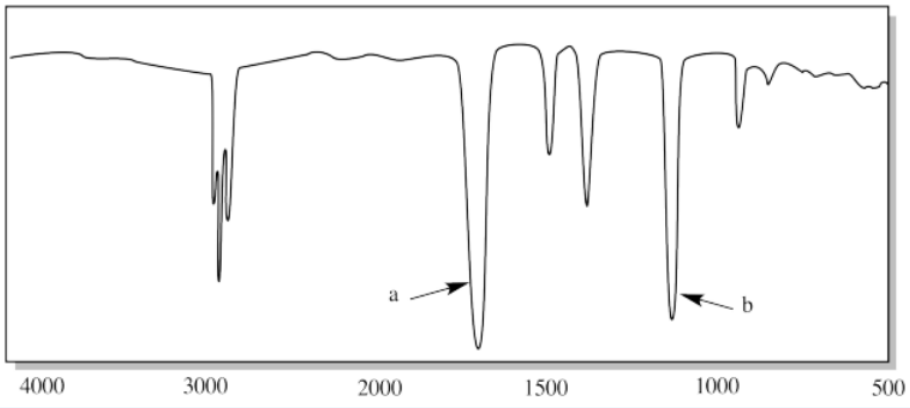
vii.


a
b
4000
3000
2000
1500
1000
500

viii.


a
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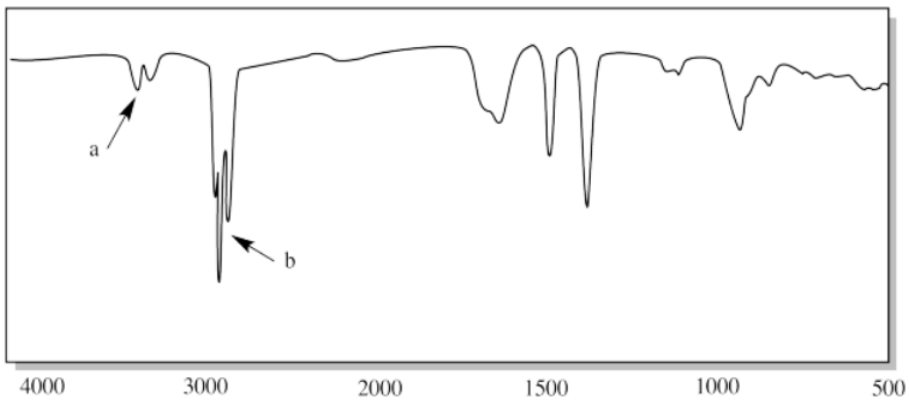
ix.


a
b
4000
3000
2000
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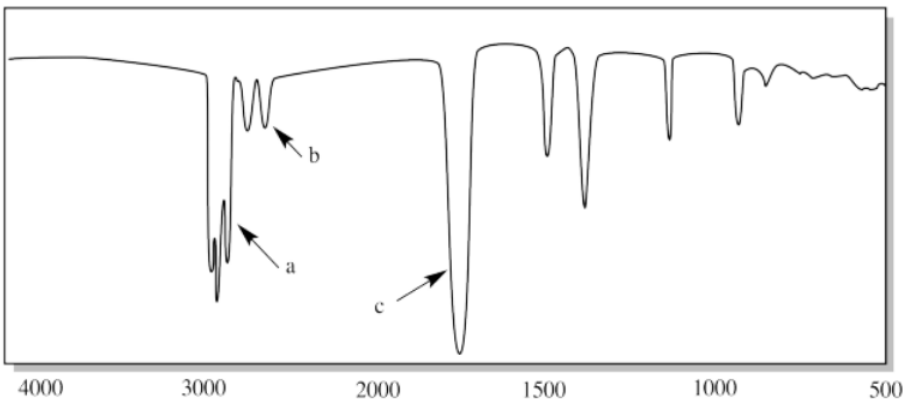
x.


b
a
c
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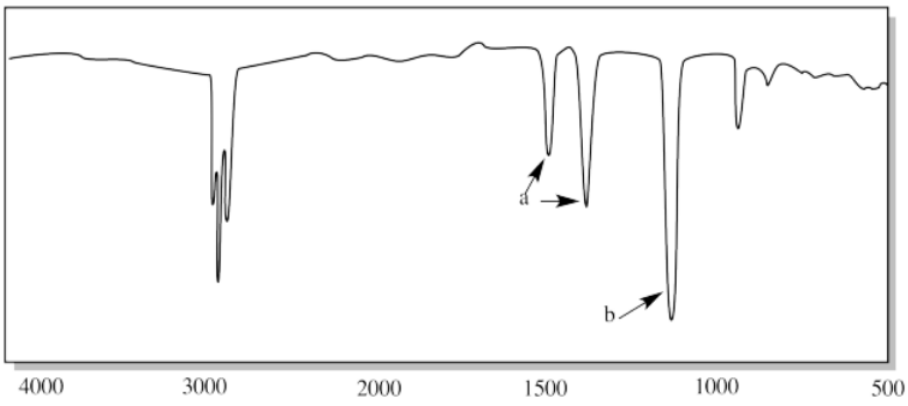
3000
2000
1500
1000
500

xi.


a
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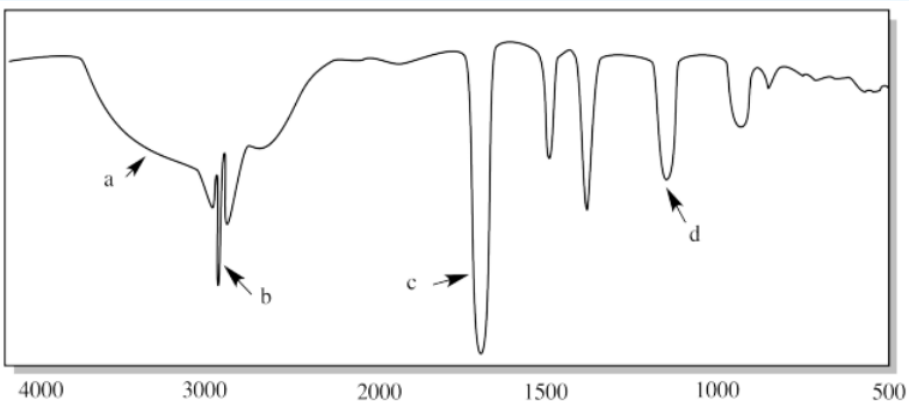
xii.


a
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c
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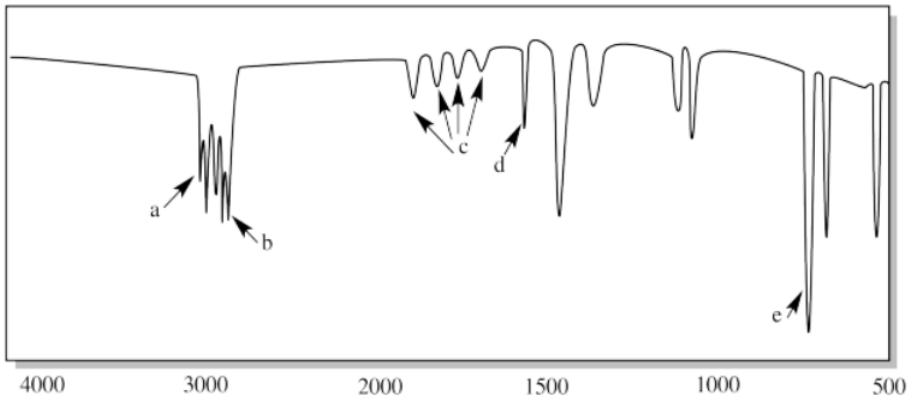
xiii.



Answer

i. a) O-H b) sp^3 C-H c) C-O

ii. a) sp^2 C-H b) sp^3 C-H c) C=C-H (oop bend)

iii. a) N-H (two of them) b) C=O c) C-N

iv. a) sp^3 C-H b) H-C-H (CH_2 bend)

v. a) sp^3 C-H b) C=O c) H-C-H (CH_2 bend)

vi. a) sp C-H b) sp^3 C-H c) C≡C

vii. a) N-H b) sp^3 C-H

viii. a) C=O b) C-O

ix. a) N-H (two of them) b) sp^3 C-H

x. a) sp^3 C-H b) aldehyde C-H c) C=O

xi. a) H-C-H (CH_2 bend) b) C-O

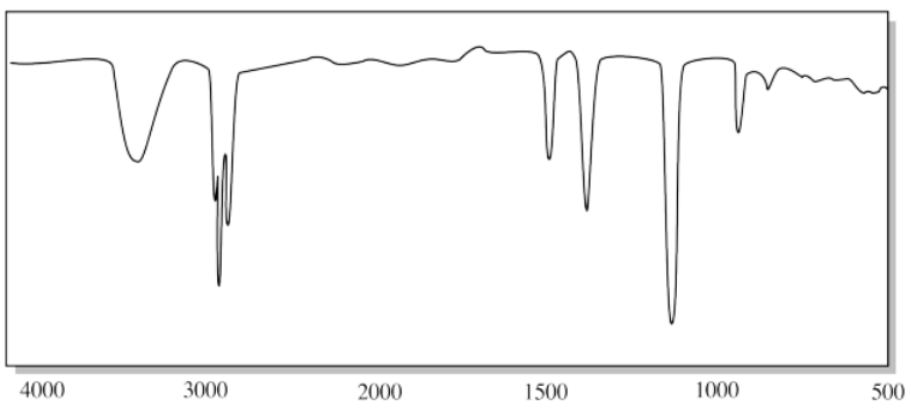
xii. a) O-H (very broad in CO_2H) b) sp^3 C-H c) C=O d) C-O

xiii. a) sp^2 C-H b) sp^3 C-H c) aromatic overtones d) C=C

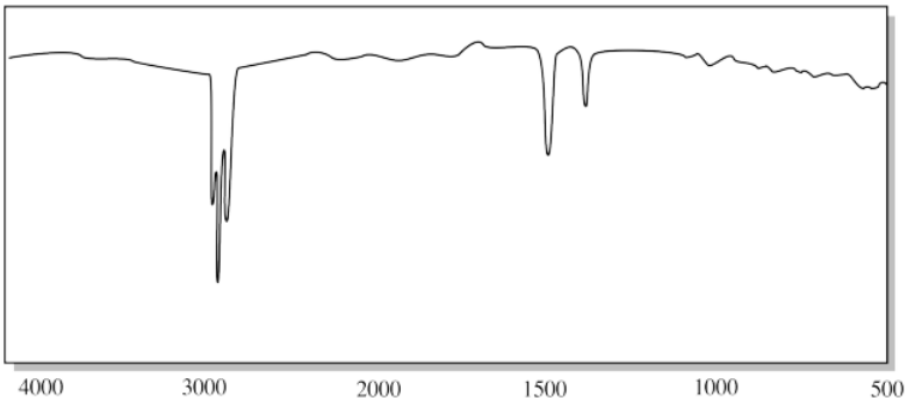
Exercise 3.10.2

For each of the following hand-drawn cartoons of IR spectra, identify the functional group suggested by the spectrum.

a)



b)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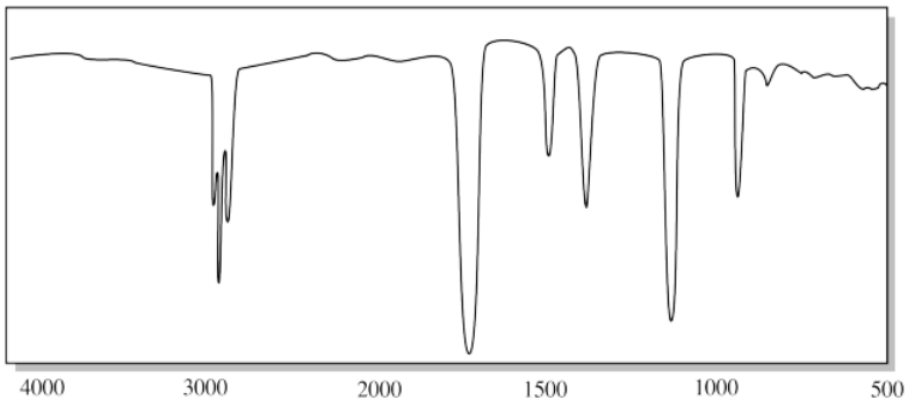
c)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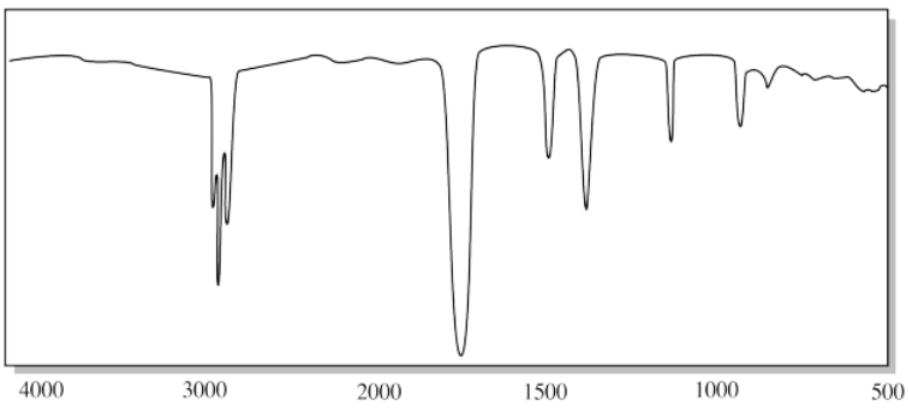
d)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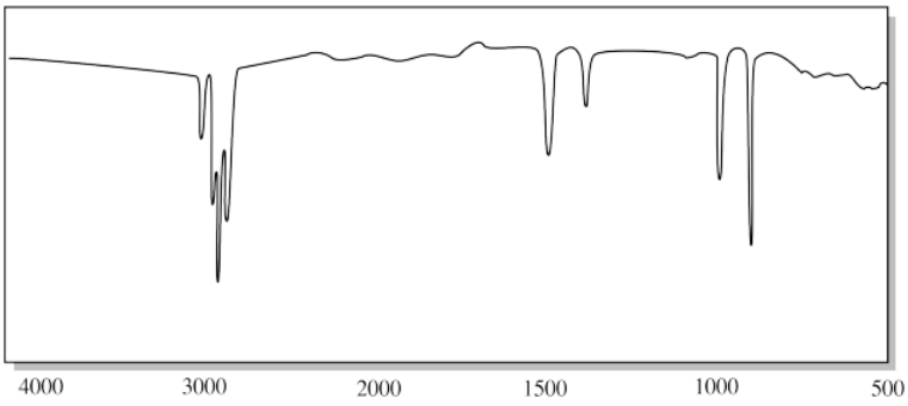
e)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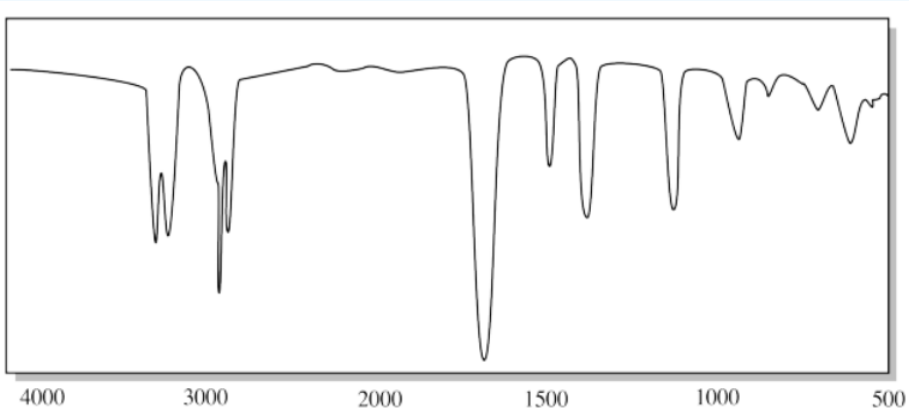
f)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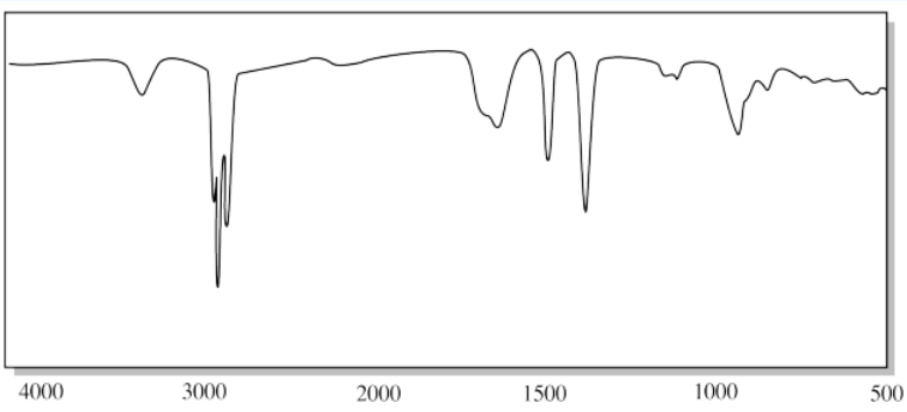
g)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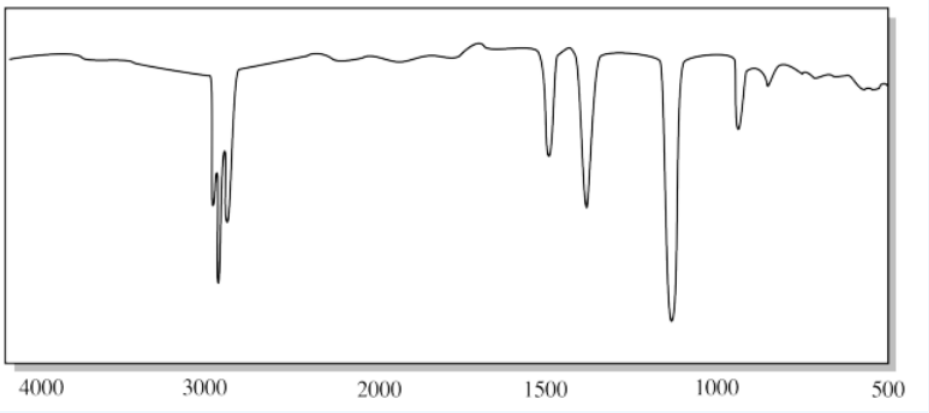
h)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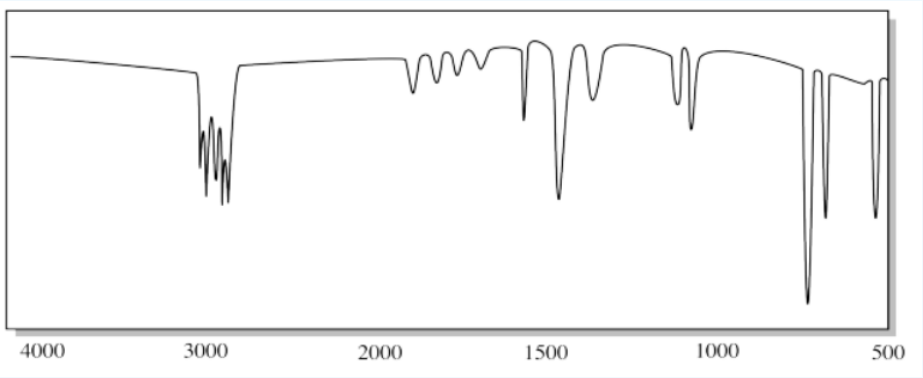
i)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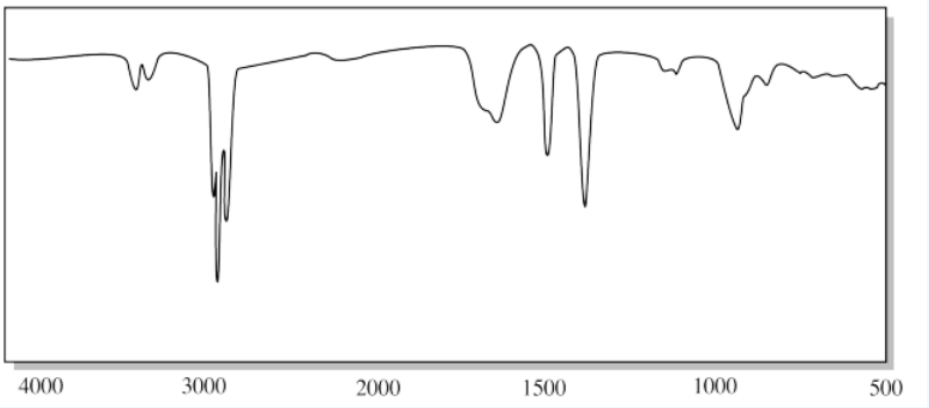
j)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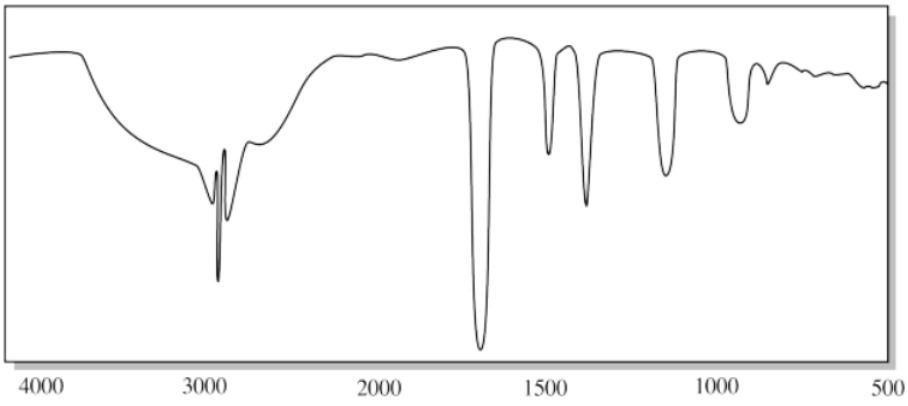
k)



Answer

a) The rounded OH peak near 3300 cm^{-1} and the strong C-O peak near 1100 cm^{-1} suggest an alcohol.

b) The sharp CH peaks below 3000 cm^{-1}, the weak CH_2 bending modes near 1500 cm^{-1} and the absence of any other features suggest an alkane.

c) The strong C=O peak near 1700 cm^{-1} and the strong C-O peak near 1100 cm^{-1} suggest an ester.

d) The strong C=O peak near 1700 cm^{-1} and the absence of additional features other than those associated with saturated hydrocarbons suggest a ketone.

e) The CH peak above 3000 cm^{-1} and the strong oop bending modes below 1000 cm^{-1} suggest an alkene. The presence of two oop bending peaks may point to a terminal alkene ($C=CH_2$).

f) The sharp N-H peaks near 3200 cm^{-1} and the strong C=O peak near 1600 cm^{-1} suggest an amide. the presence of two N-H peaks rather than one points to a primary amide ($O=C-NH_2$).

g) The small, triangular "sharktooth" peak near 3200 cm^{-1} suggests an amine. With just one N-H peak, this is probably a primary amine ($R-NH_2$).

h) The strong C-O peak near 1100 cm^{-1} suggests an ether.

i) The C-H peaks above 3000 cm^{-1} and the oop bending modes below 1000 cm^{-1} certainly suggest double bonds. The progression of tooth-like "aromatic overtones" between 1600 and 2000 cm^{-1} strongly indicates a substituted benzene.

j) The small, triangular "sharktooth" peaks near 3200 cm^{-1} suggest an amine. With two N-H peaks, this is probably a secondary amine (R_2NH).

l) The broad, deep OH peak between 3300 cm^{-1} and 2600 cm^{-1} and the C=O peak near 1700 cm^{-1} suggests a carboxylic acid. The O-H peak of a carboxylic acid is often missed; it is moved to lower frequency by hydrogen bonding.

? Exercise 3.10.3

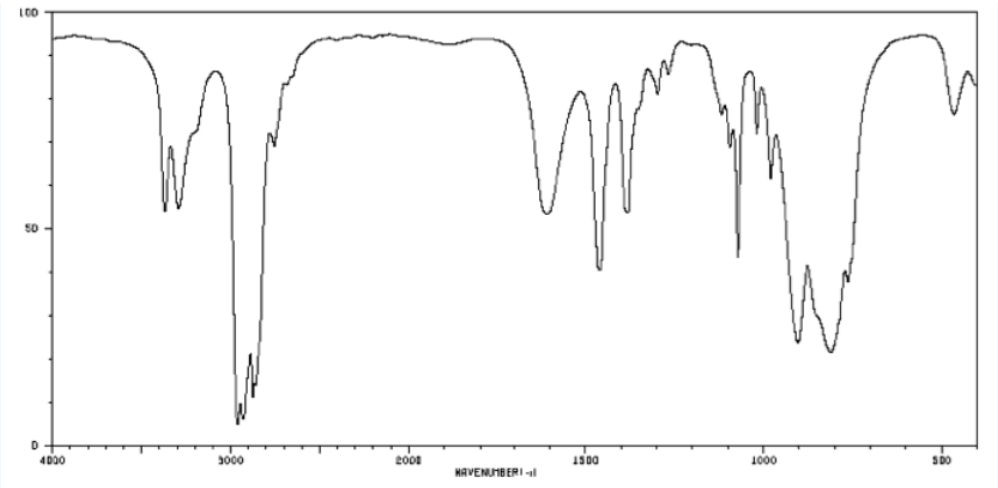
a) Identify at least three important peaks/bonds in each of the following IR spectra.

b) Identify the functional group present in each of these samples. See the Functional Group Section

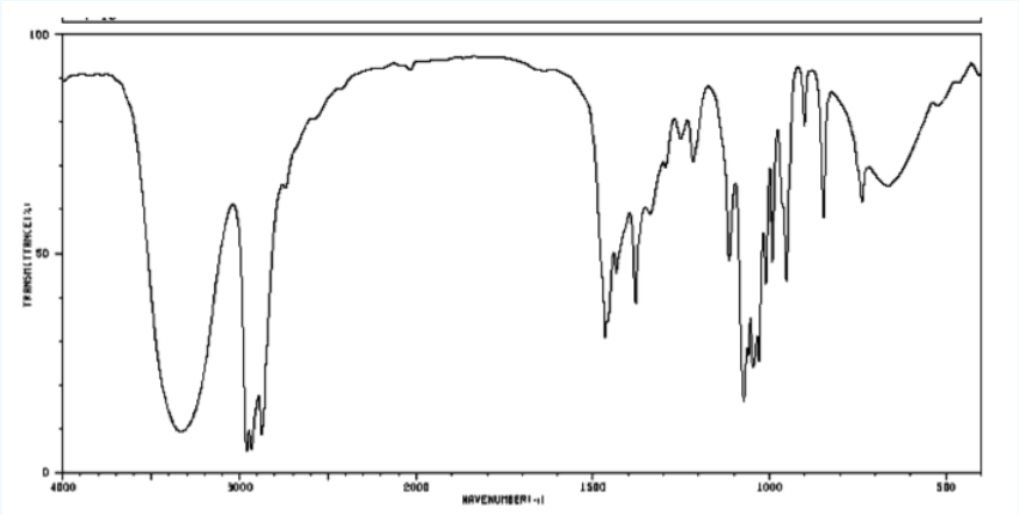
for help.

c) Draw a possible structure for each of these compounds (there may be many, many correct answers).

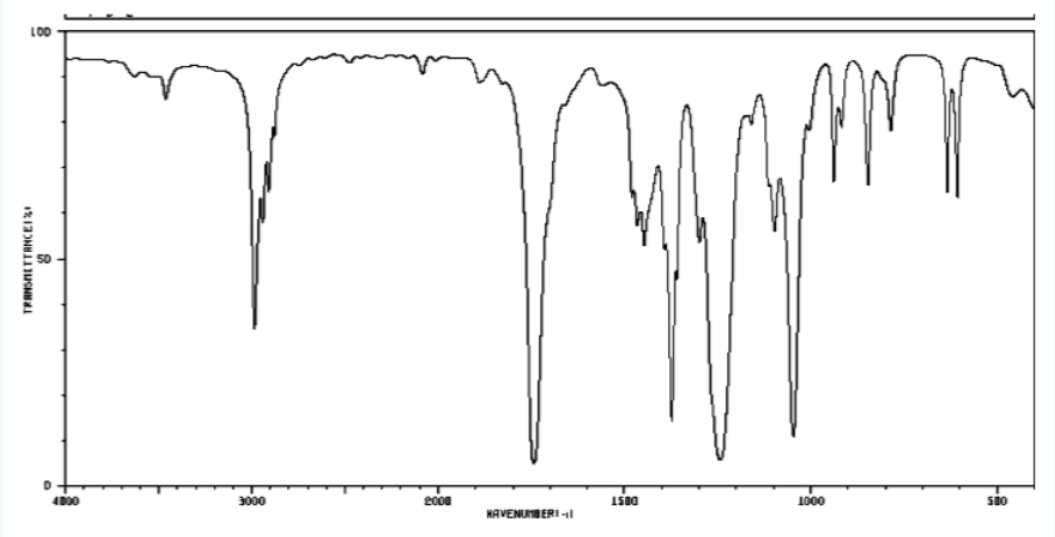
problem i)



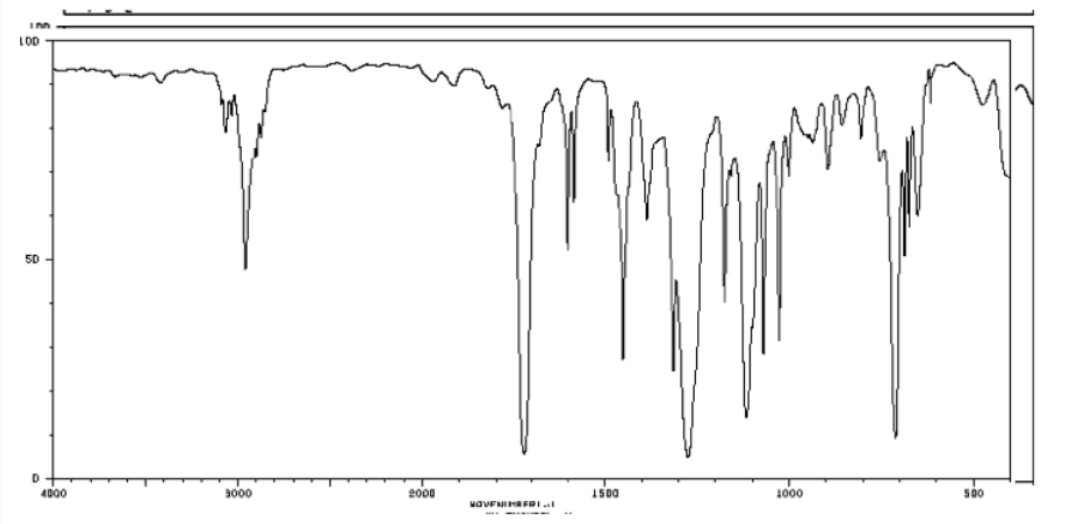
problem ii)



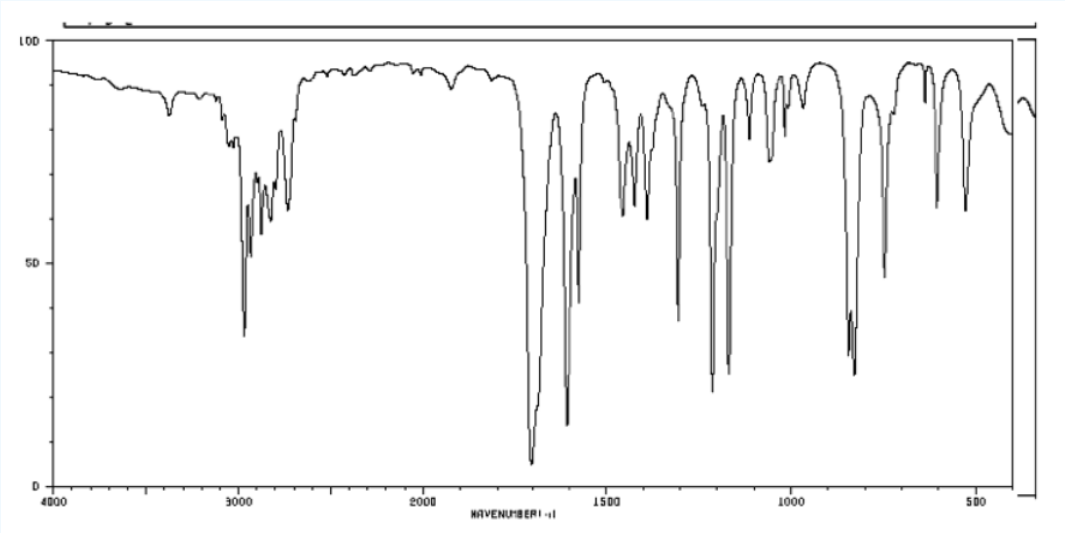
problem iii)



problem iv)



problem v)



Answer

i)

a)

3200 cm^{-1} (sharp): N-H

2900 cm^{-1} (sharp): $C_{sp}3$-H

1600 cm^{-1} (broad): probably NH_2 bending

b) A primary amine.

c)

ii)

a)

3400 cm^{-1} (strong, broad): O-H

2900 cm^{-1} (sharp): $C_{sp}3$-H

1050 cm^{-1} (strong): probably C-O

b) Alcohol.

c)

iii)

a)

2900 cm^{-1} (sharp): $C_{sp}3$-H

1700 cm^{-1} (strong): C=O

1200 and 1000 cm^{-1} (strong & medium): C-O

b) Ester

c)

iv)

a)

3050 cm^{-1} (sharp): $C_{sp}2$-H

1700 cm^{-1} (strong): C=O

1200 and 1000 cm^{-1} (strong & medium): C-O

b) Ester; probably contains an aromatic as well

c)

v)

a)

2750 and 2650 cm^{-1} (medium, sharp): C-H of an aldehyde

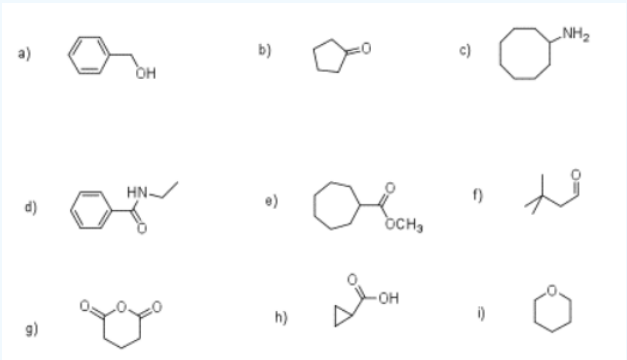
1700 cm^{-1} (strong): C=O

Below 1000 cm^{-1} (strong & medium): oop bends

b) Aldehyde; probably contains an aromatic as well

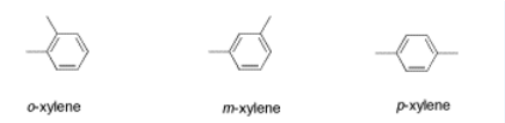
Exercise 3.10.4

Sketch an approximate IR spectrum for each of the following compounds:



Exercise 3.10.5

The oop bends are sometimes useful in distinguishing substitution pattrens around a benzene ring. Using the spectra of o-, m-, and p-xylene, formulate some guidelines about what the oop bends look like when substituents are one, two or three carbons away on a benzene ring.



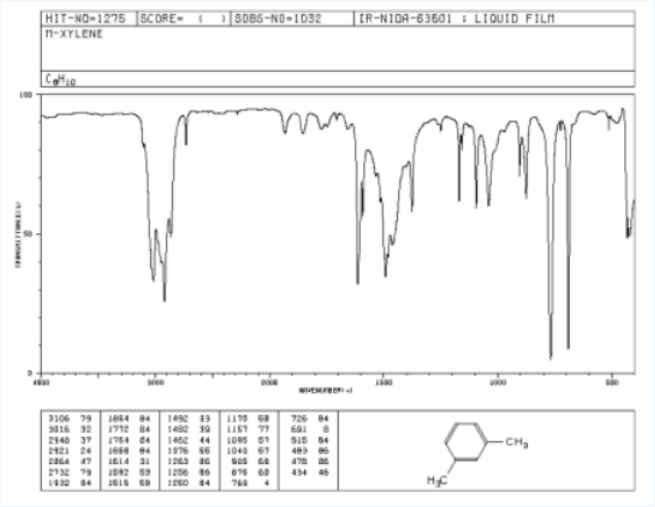


Figure 3.10.1: IR spectrum of m-xylene.

Source: SDBSWeb : http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology of Japan, 14 July 2008)

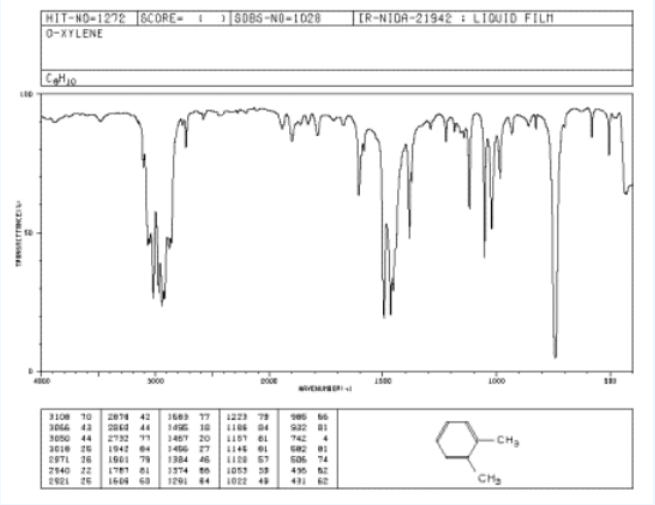


Figure 3.10.2: IR spectrum of o-xylene.

Source: SDBSWeb : http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology of Japan, 14 July 2008)

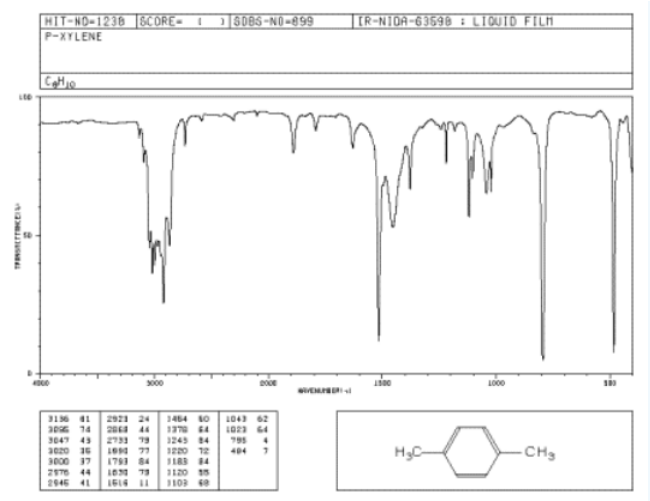


Figure 3.10.3 IR spectrum of p-xylene.

Source: SDBSWeb : http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology of Japan, 14 July 2008