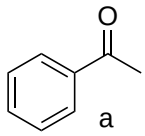
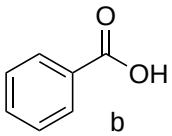
CEM 251, Problem Set 6: Spectroscopy

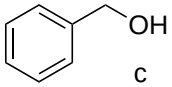
1. Match the following compounds with the IR spectra given.



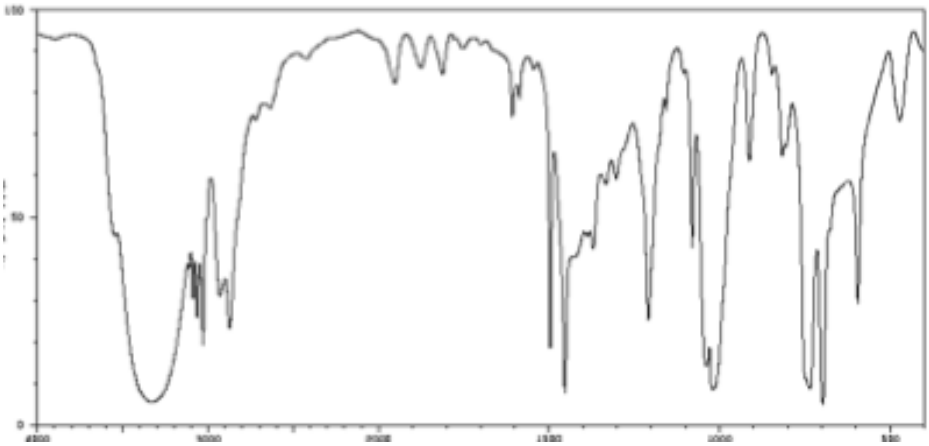
a



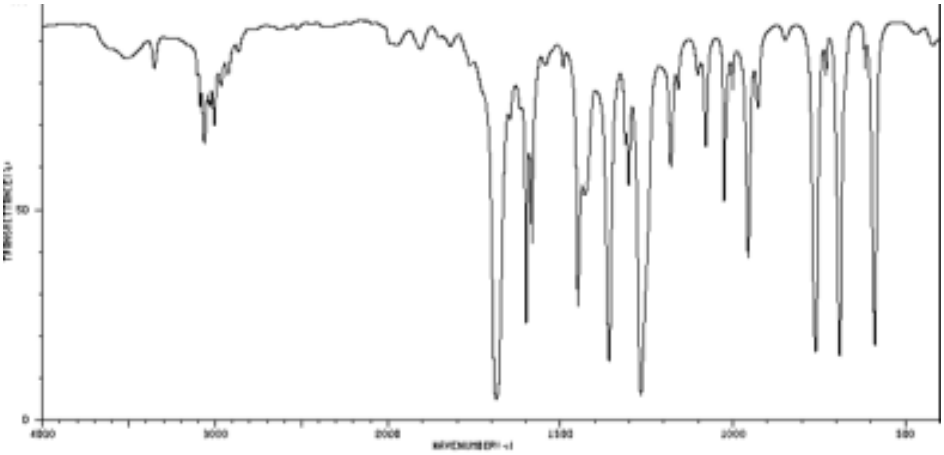
b



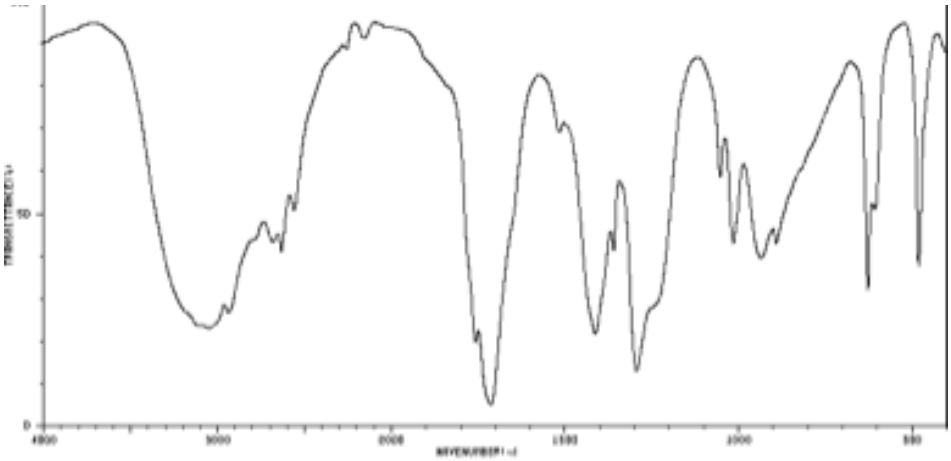
c



c



a

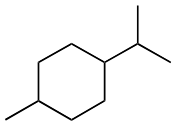
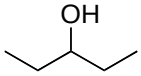
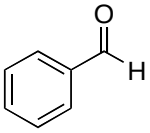
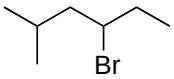
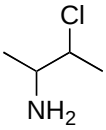


b

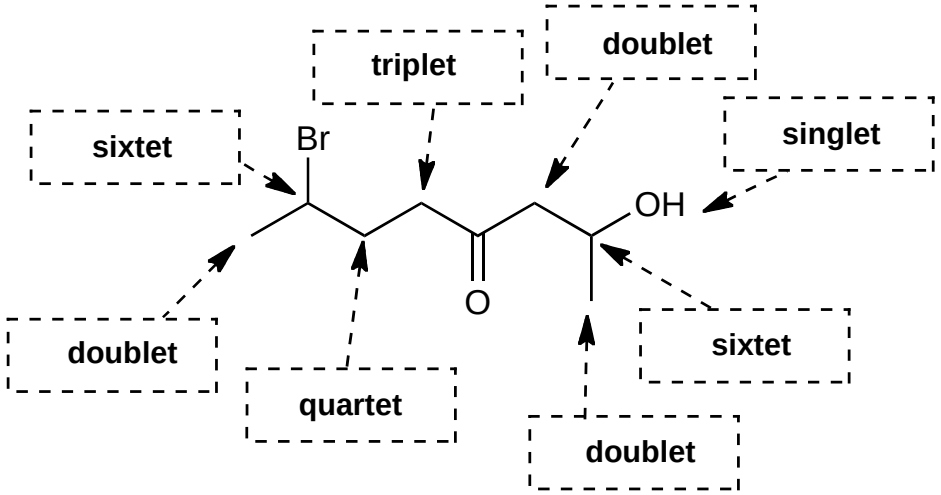
2. For the following molecular formulas calculate the number of RDBs (rings or double bonds, degrees of unsaturation).

	#RDBs
C_8H_7N	5
$C_7H_{11}BrO$	2
$C_8H_{15}NO$	2
$C_{10}H_{14}$	4
C_6H_8O	3
$C_{10}H_{22}NCl$	0

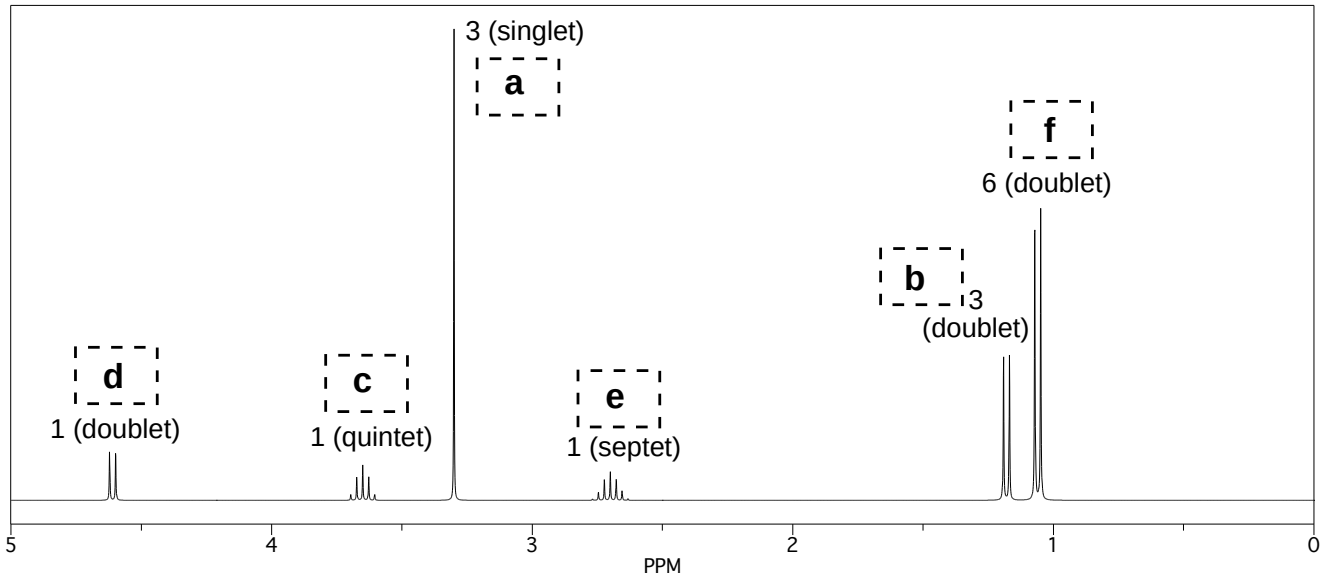
3. For the following molecules, how many different signals (peaks) would you expect to see in the ^{1}H NMR spectrum?

	# of 1H NMR peaks
	7
	4
	4
	6
	5

4. What should be the multiplicity of the 1H NMR peaks of each of the following groups of protons:



5. Which group of protons of the following molecule corresponds to which peak on the NMR spectrum shown?



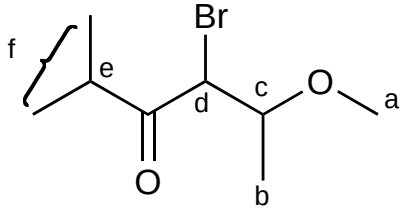
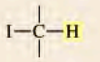
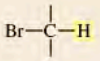
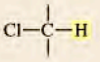
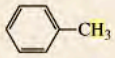
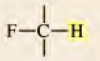
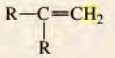
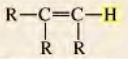
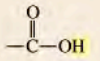


TABLE 13.1 Approximate Values of Chemical Shifts for ^1H NMR[a]

Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0		6.5–8
$-CH_3$	0.9		
$-CH_2-$	1.3		9.0–10
	1.4		2.5–4
	1.7		2.5–4
	2.1		3–4
	2.3		4–4.5
$-C\equiv C-H$	2.4	RNH_2	variable, 1.5–4
$R-O-CH_3$	3.3	ROH	variable, 2–5
	4.7	ArOH	variable, 4–7
	5.3		variable, 10–12

[a]The values are approximate because they are affected by neighboring substituents.

Table of IR Absorptions

Functional Group	*Characteristic Absorption(s)* (cm^{-1})
Alkyl C-H Stretch	2950 - 2850 (m or s)
Alkenyl C-H Stretch	3100 - 3010 (m)
Alkenyl C=C Stretch	1680 - 1620 (v)
Alkynyl C-H Stretch	~3300 (s)
Alkynyl C≡C Stretch	2260 - 2100 (v)
Aromatic C-H Stretch	~3030 (v)
Aromatic C-H Bending	860 - 680 (s)
Aromatic C=C Bending	1700 - 1500 (m,m)
Alcohol/Phenol O-H Stretch	3550 - 3200 (broad, s)
Carboxylic Acid O-H Stretch	3000 - 2500 (broad, v)
Amine N-H Stretch	3500 - 3300 (m)
Nitrile C≡N Stretch	2260 - 2220 (m)
Aldehyde C=O Stretch	1740 - 1690 (s)
Ketone C=O Stretch	1750 - 1680 (s)
Ester C=O Stretch	1750 - 1735 (s)
Carboxylic Acid C=O Stretch	1780 - 1710 (s)
Amide C=O Stretch	1690 - 1630 (s)
Amide N-H Stretch	3700 - 3500 (m)