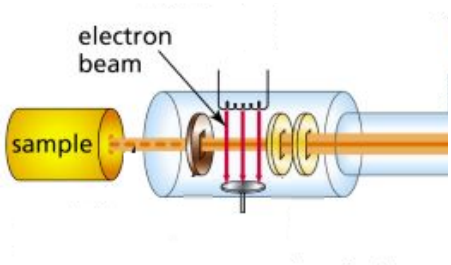
Name _____ Test 1 (2/22)
CHEM 0203 (Organic) Spring 2019

1. The molar mass of 2-bromo-2-methylpentane is 165.07 g/mol; its mass spectrum does not have a peak with an m/z of 165. The mass spectrum does, however, contain two peaks with similar intensity at m/z of 164 and 166. (a. 6 pts.) Explain the absence of the peak at 165 and (b. 6 pts.) the appearance of the two peaks at 164 and 166.

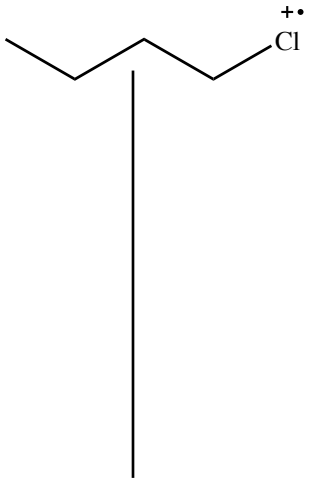
1. _____
2. _____
3. _____
4. _____
5. _____
6. _____
7. _____
8. _____
9. _____
10. _____
11. _____

2. (10 pts.) A portion of a cartoon representation of a mass spectrometer is shown below. Describe what the electron beam does.



3. In a mass spectrometer, radical, cationic alkyl halides fragment using homolytic and heterolytic mechanisms. (a. 12 pts.) Draw the fragments that would form from the most likely heterolytic and homolytic cleavage reactions, and (b. 6 pts.) circle the fragments that would be observed in the mass spectrum.

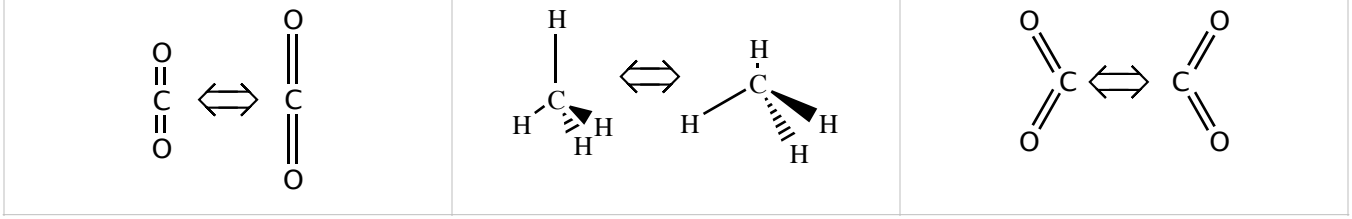
heterolytic cleavage products



homolytic cleavage products

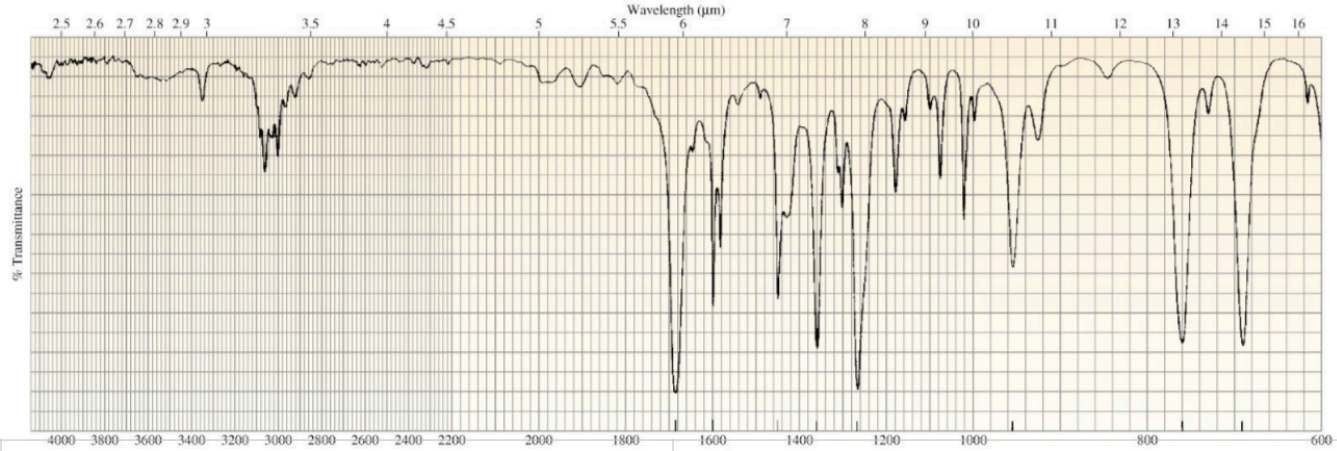
4. (10 pts.) For a molecular vibration to be IR active (seen in the infrared spectrum) what must the vibration do to the molecule.

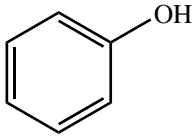
5. (12 pts.) Circle the drawings that represent IR active vibrations.

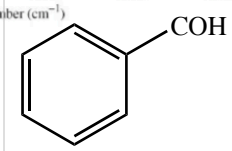


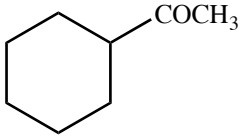
6. (12 pts.) Carbonyl stretching vibrations absorb IR light at higher energy than ether stretching vibrations. Briefly explain why the vibration of the C to O bond in the carbonyl absorbs at higher energy.

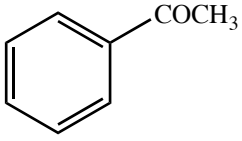
7. (a. 2 pts.) Circle the molecule that produced the following spectrum, (b. 9 pts.) briefly explain why structures were ruled out, and (c. 3 pts.) briefly explain why your choice is the correct one.



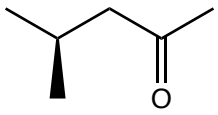


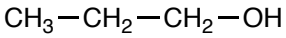


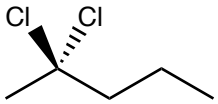




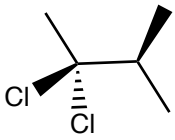
8. (12 pts.) Determine the number of signals/peaks that are expected in the ^{1}H NMR spectra of the following molecules.

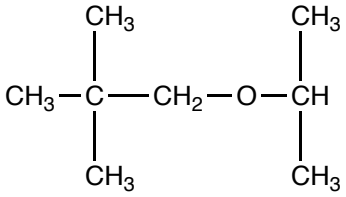


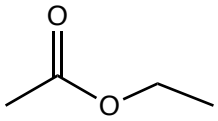




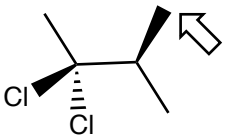
9. (12 pts.) Determine the relative positions of the peaks in the ^{1}H NMR spectrum and label the protons alphabetically starting with the protons that resonate at the highest frequency.

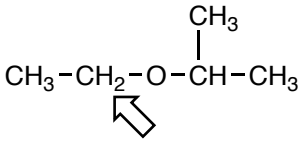


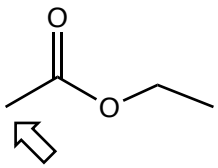




10. (12 pts.) Determine the multiplicity of the peak attributed to the indicated protons.



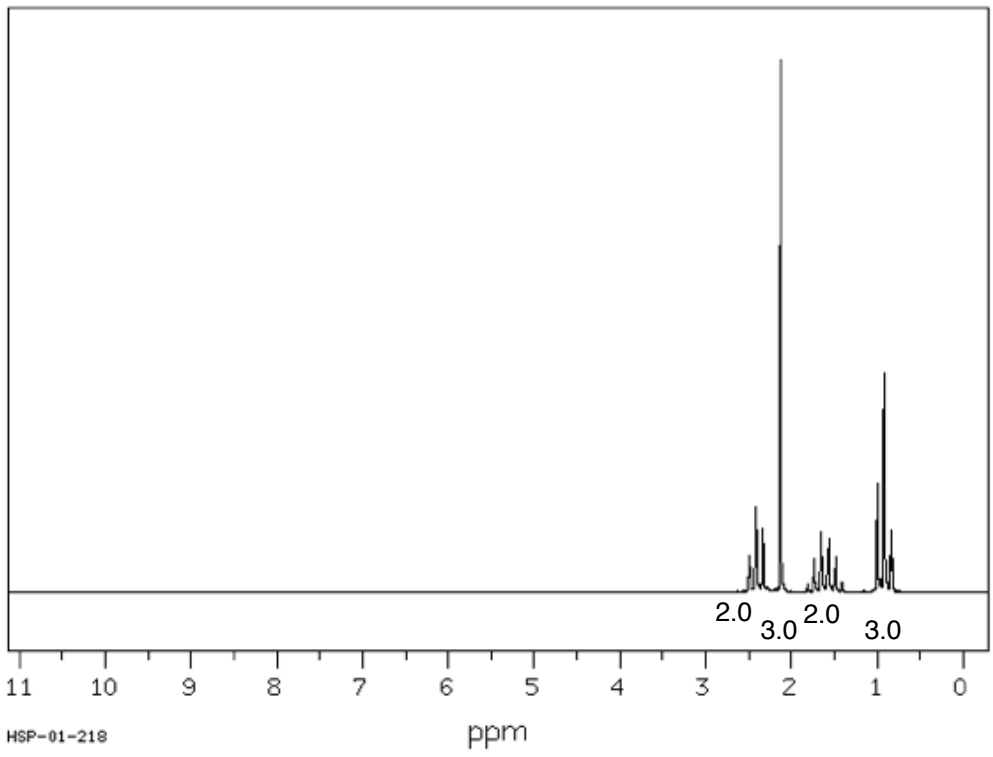




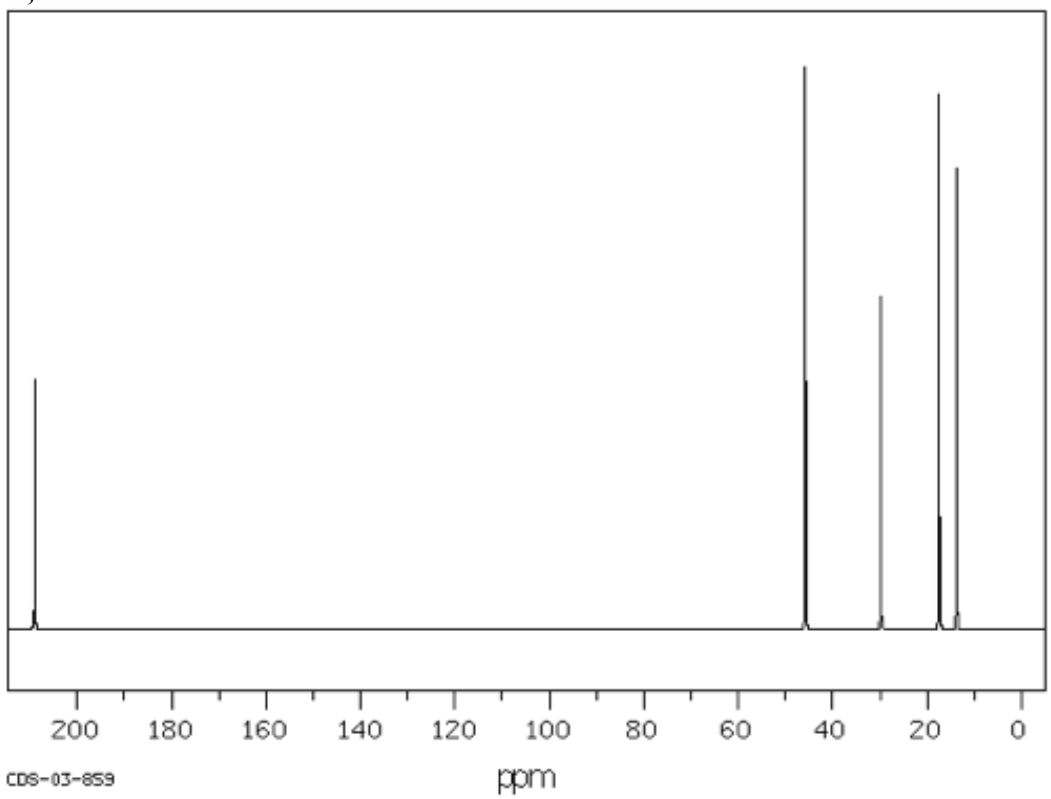
11. Based on the spectral data provided below and on the next page, (a. 10 pts.) determine the structure of the unknown $C_5H_{10}O$, (b. 4 pts.) identify the peaks for two functional groups in the IR spectrum, and (c. 4 pts.) unambiguously assign the peaks in the ^{1}H NMR spectrum; that is, label each peak in the ^{1}H NMR spectrum alphabetically starting with an "a" at the left end of the spectrum and label the protons on the structure with the corresponding letter.

^{1}H NMR

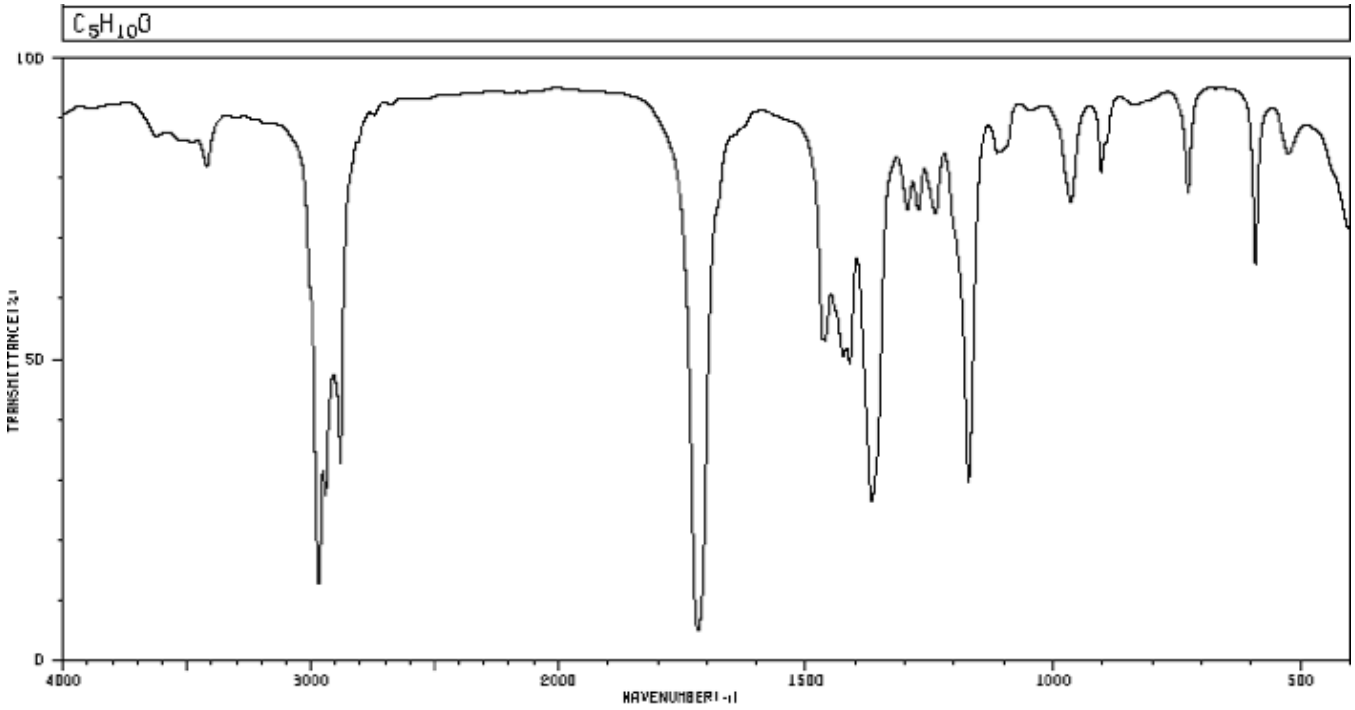
ppm	height
2.492	70
2.412	160
2.329	118
2.129	1000
1.738	36
1.727	62
1.650	114
1.560	99
1.483	67
1.472	37
0.998	206
0.921	413
0.835	118



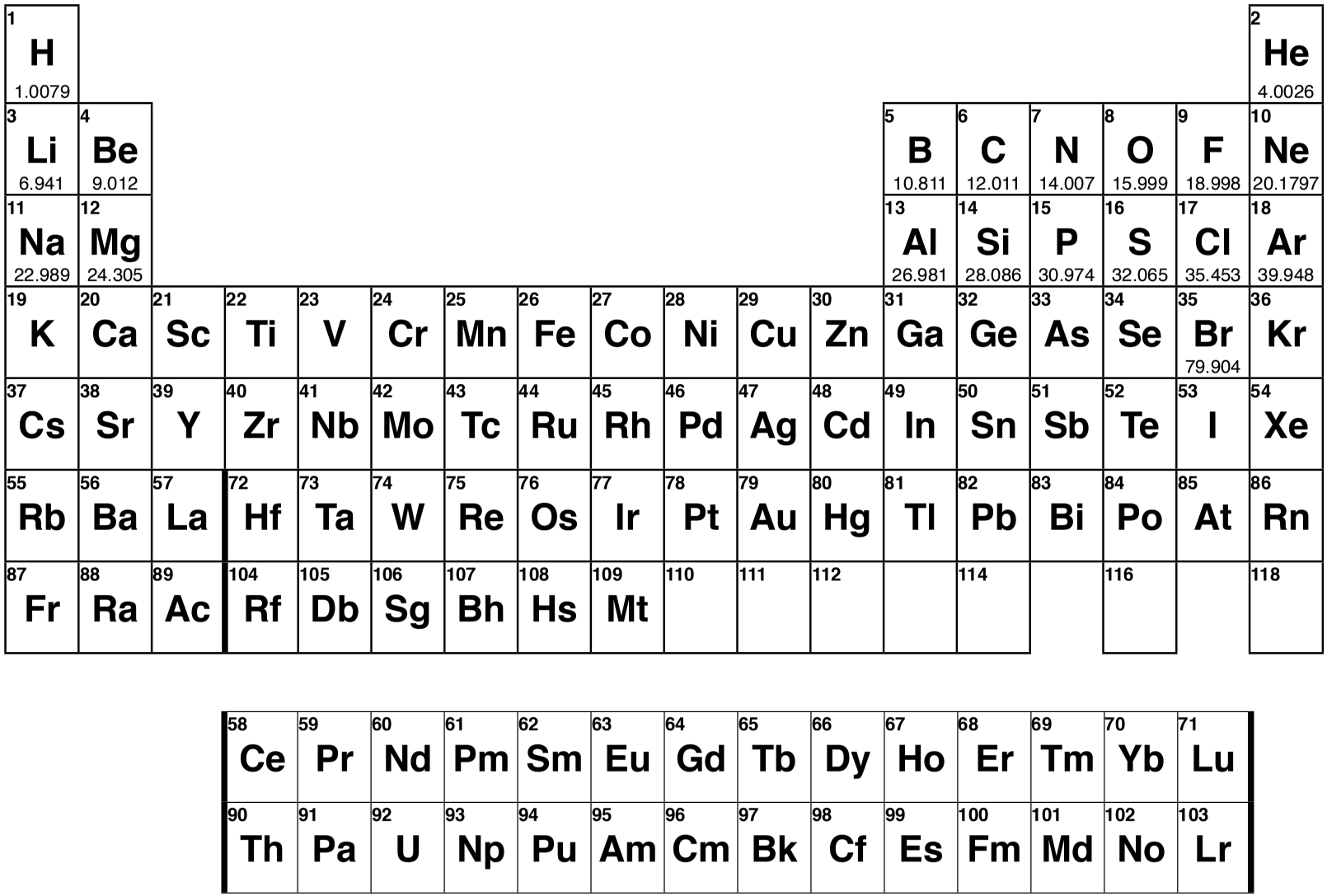
$^{13}C\{^{1}H\}$ NMR



IR



3419	79	1426	49	1114	81	692	64
2966	12	1412	47	1105	81	526	81
2939	26	1367	25	1100	81		
2879	31	1296	72	964	72		
1717	4	1274	72	903	79		
1467	50	1237	72	894	81		
1461	50	1172	28	727	74		


1 H 1.0079
2 He 4.0026
3 Li 6.941
4 Be 9.012
5 B 10.811
6 C 12.011
7 N 14.007
8 O 15.999
9 F 18.998
10 Ne 20.1797
11 Na 22.989
12 Mg 24.305
13 Al 26.981
14 Si 28.086
15 P 30.974
16 S 32.065
17 Cl 35.453
18 Ar 39.948
19 K
20 Ca
21 Sc
22 Ti
23 V
24 Cr
25 Mn
26 Fe
27 Co
28 Ni
29 Cu
30 Zn
31 Ga
32 Ge
33 As
34 Se
35 Br 79.904
36 Kr
37 Cs
38 Sr
39 Y
40 Zr
41 Nb
42 Mo
43 Tc
44 Ru
45 Rh
46 Pd
47 Ag
48 Cd
49 In
50 Sn
51 Sb
52 Te
53 I
54 Xe
55 Rb
56 Ba
57 La
72 Hf
73 Ta
74 W
75 Re
76 Os
77 Ir
78 Pt
79 Au
80 Hg
81 Tl
82 Pb
83 Bi
84 Po
85 At
86 Rn
87 Fr
88 Ra
89 Ac
104 Rf
105 Db
106 Sg
107 Bh
108 Hs
109 Mt
110
111
112
114
116
118
58 Ce
59 Pr
60 Nd
61 Pm
62 Sm
63 Eu
64 Gd
65 Tb
66 Dy
67 Ho
68 Er
69 Tm
70 Yb
71 Lu
90 Th
91 Pa
92 U
93 Np
94 Pu
95 Am
96 Cm
97 Bk
98 Cf
99 Es
100 Fm
101 Md
102 No
103 Lr