(16) **Today**

Chap 12 & 13: Practice Identifying Unknowns

Chap 21.1: Nomenclature
Chap 21.2: Nucleophilic Acyl Substitution

Next Class (17)

Chap 21.2: Nucleophilic Acyl Substitution
Chap 21.3: Reactions of Carboxylic Acids

(18) **Second Class from Today**

Chap 21.3: Reactions of Carboxylic Acids
Chap 21.4: Reactions of Acid Halides
Chap 21.6: Reactions of Esters

Third Class from Today (19)

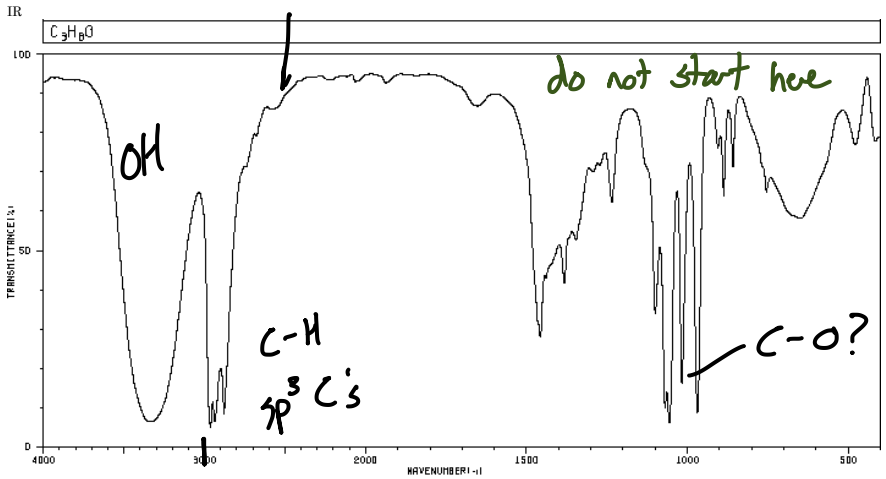
Chap 21.4: Reactions of Acid Halides
Chap 21.6: Reactions of Esters
Chap 21.7: Reactions of Amides

Please hand in reworked test 1.

Please remember, this assignment does not add points back onto your test score. This is a separate assignment that is worth 5% of your overall grade.

I do not need your test back, please just hand in the reworked answers.

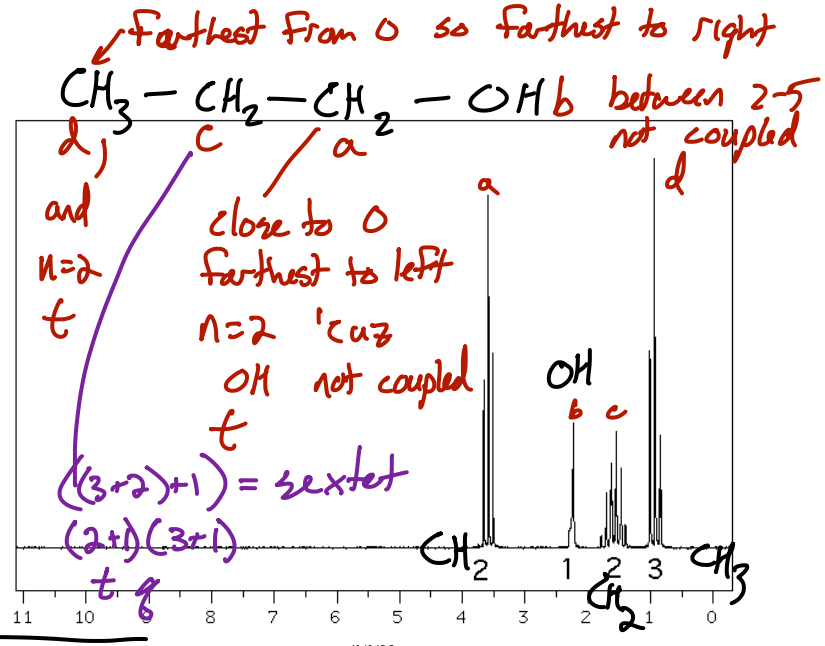
IR

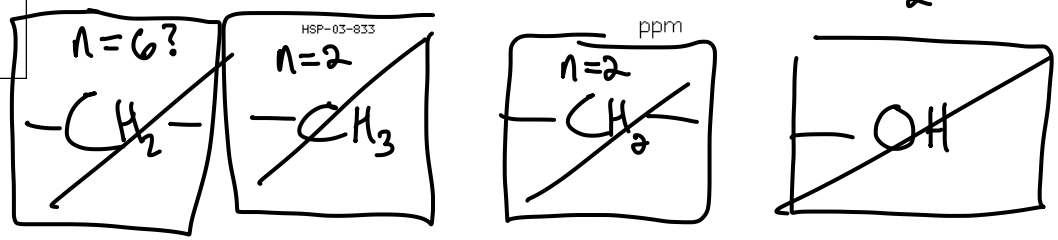


3333	6	1383	39	1017	16
2963	4	1346	50	969	8
2936	6	1293	66	905	72
2878	8	1236	60	888	62
1656	84	1100	32	858	68
1651	84	1069	9	755	82
1466	26	1066	8	479	74

^{1}H NMR

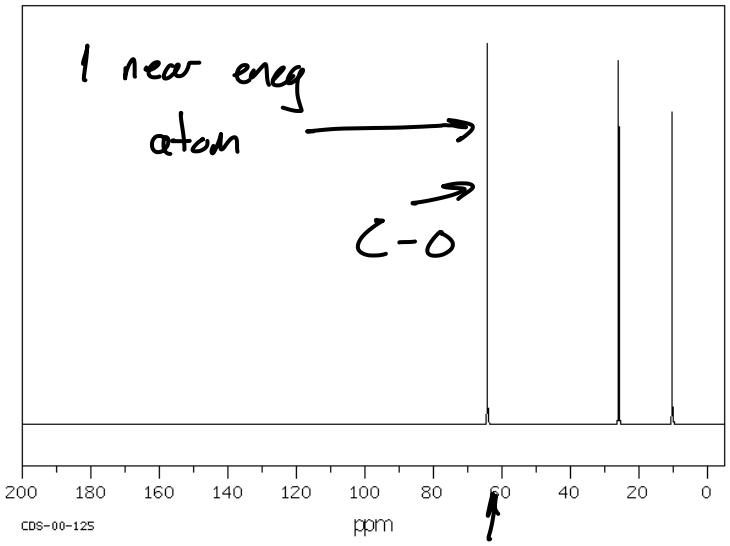
ppm	Int.
3.658	431
3.585	906
3.511	501
2.225	322
1.717	49
1.699	143
1.629	216
1.544	300
1.467	204
1.46	103
1.398	60
1.009	508
0.932	1000
0.846	289





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

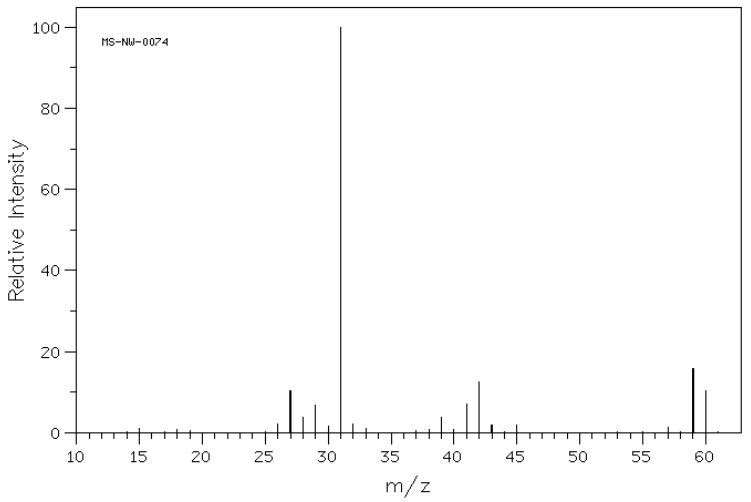
3 chemically distinct C atoms



MS

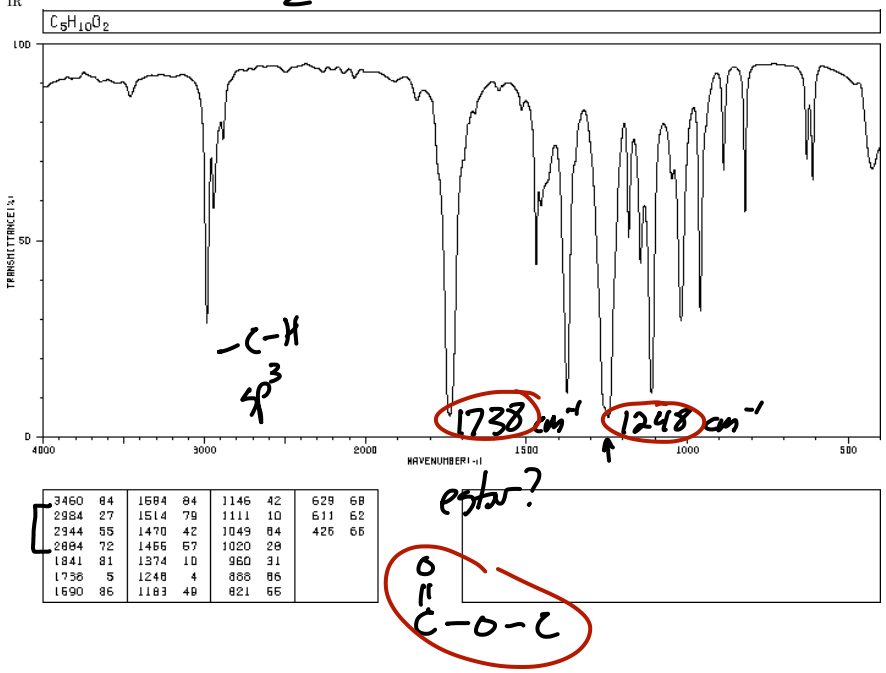
molecular ion = 60

m/z	relative intensity
15	1
26	2
27	10
28	3
29	6
30	1
31	100
32	2
33	1
39	3
41	7
42	12
43	2
45	1
57	1
59	15
60	10



$$\frac{2 \cdot 5 + 2 - 10}{2} = 1$$

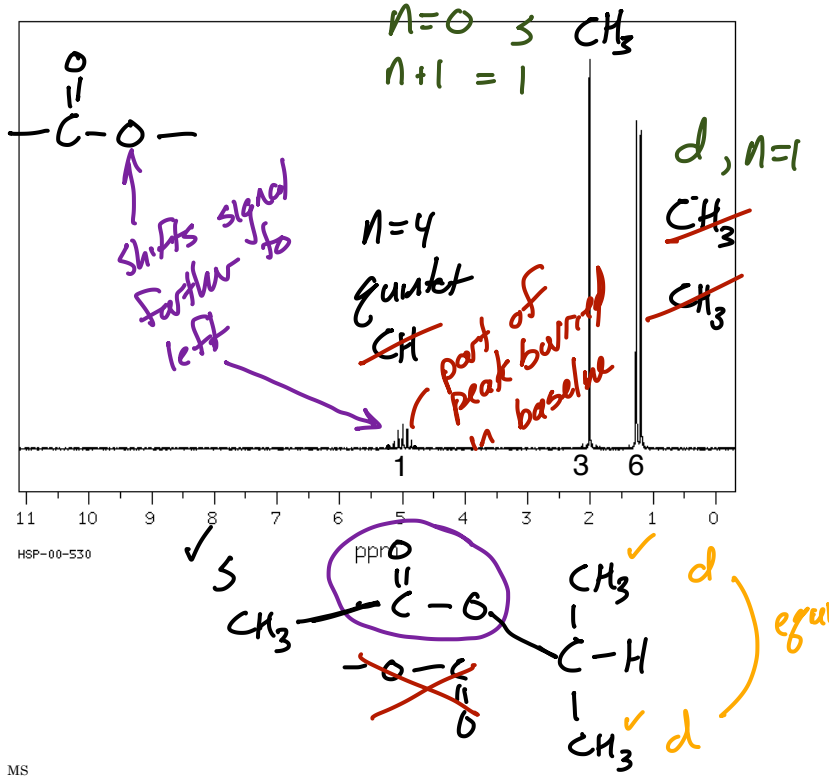
IR



3460	84	1684	84	1146	42	629	68
2984	27	1514	79	1111	10	611	62
2944	55	1470	42	1049	84	425	66
2884	72	1466	67	1020	28		
1841	81	1374	10	960	31		
1736	5	1248	4	886	86		
1690	86	1183	49	821	65		

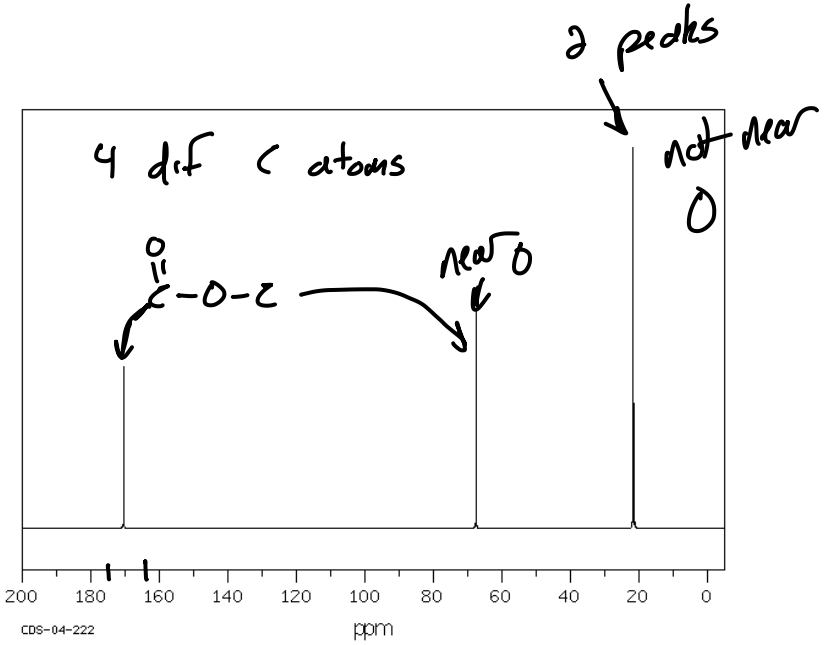
^{1}H NMR

ppm	Int.
5.134	17
5.063	47
4.993	64
4.923	50
4.853	19
2.017	1000
1.268	842
1.198	818



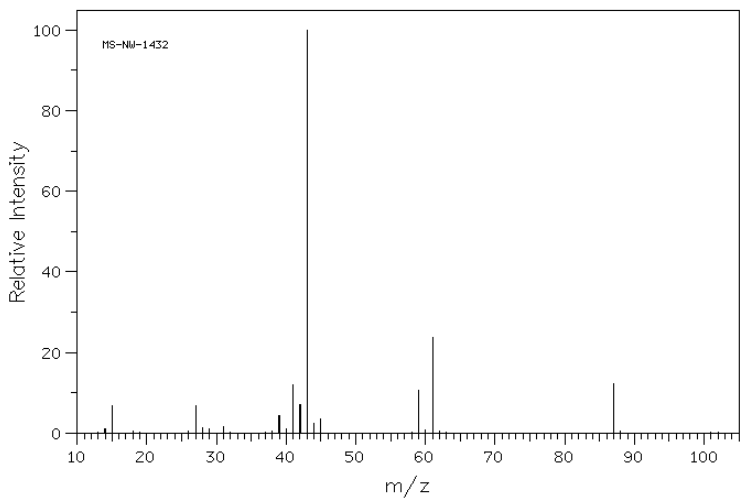
$^{13}C\{^1H\}$ NMR

ppm	Int.
170.42	425
67.52	570
21.79	1000
21.34	325

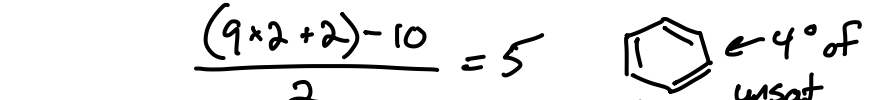


MS

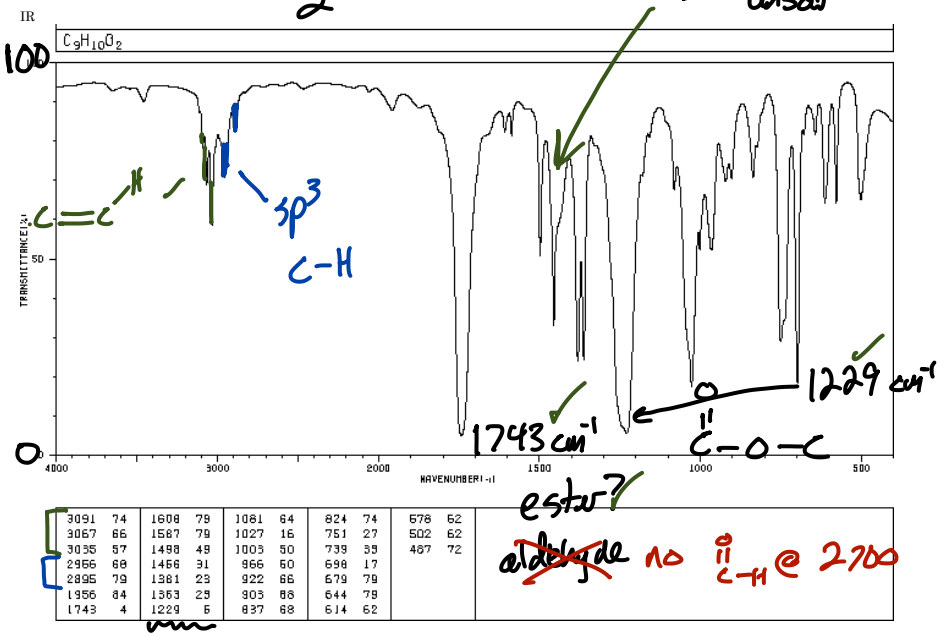
m/z	relative intensity
14	1
15	6
27	6
28	1
29	1
31	1
39	4
40	1
41	12
42	7
43	100
44	2
45	3
59	10
61	23
87	12



$\frac{(9\times2+2)-10}{2} = 5$



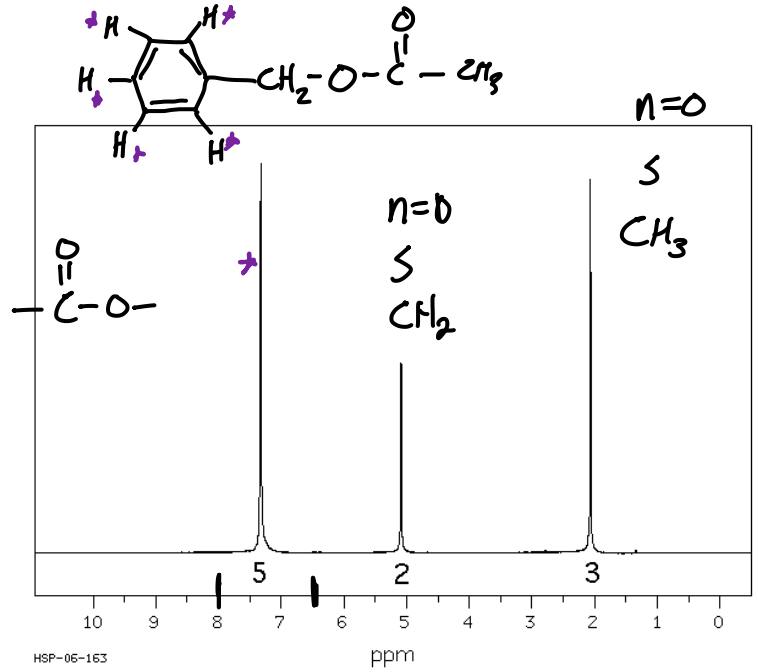
IR



3091	74	1608	79	1081	64	824	74	678	62
3067	66	1587	79	1027	16	751	27	502	62
3035	57	1498	49	1003	50	739	39	467	72
2966	68	1456	31	966	60	698	17		
2895	79	1381	23	922	66	679	79		
1956	84	1363	23	903	68	644	79		
1743	4	1229	6	837	68	614	62		

^{1}H NMR

ppm	Int.
7.327	1000
5.086	488
2.065	960

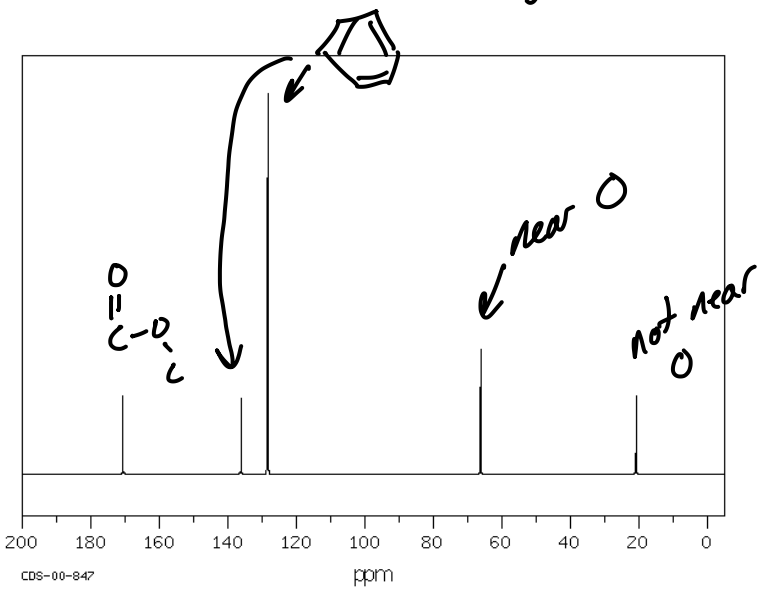


6 diff C atoms ... symmetry

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

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

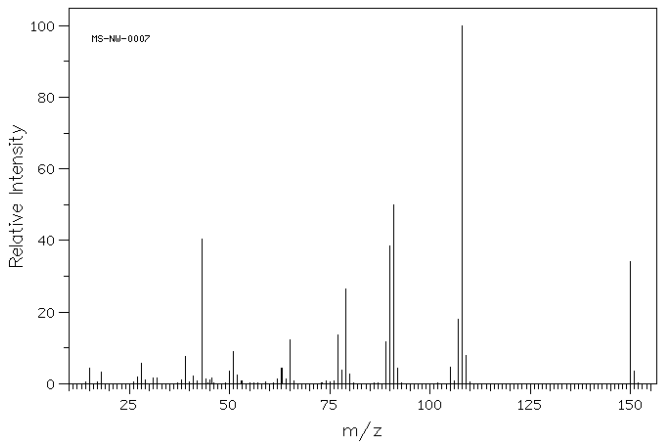
ppm	Int.
170.7	204
136.14	199
128.56	776
128.24	1000
66.24	328
20.82	204



molecular ion = 150

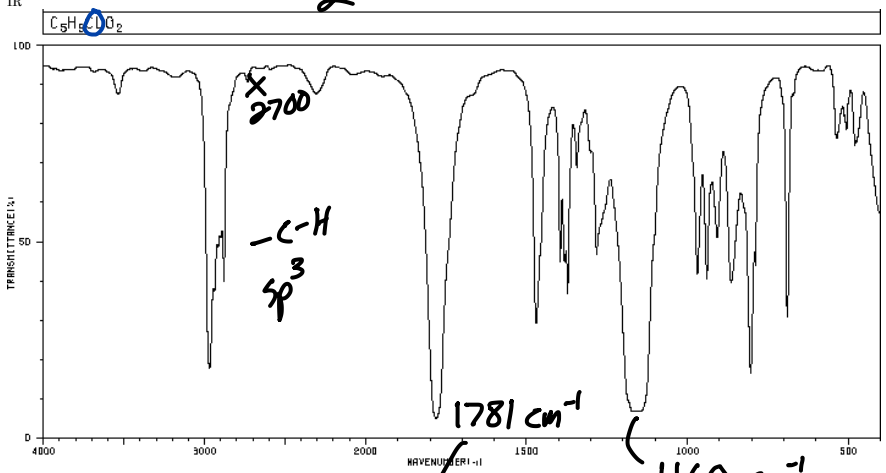
m/z	relative intensity	m/z	relative intensity
15	4	90	38
18	3	91	50
27	1	92	4
28	5	105	4
29	1	107	18
31	1	108	100
32	1	109	7
38	1	150	34
39	7	151	3
41	2		
43	40		
44	1		
45	1		
45.5	1		
50	3		
51	9		
52	2		
62	1		
63	4		
64	1		
65	12		
77	13		
78	3		
79	26		
80	2		
89	11		

MS



$$\frac{(5\cdot 2+2-1)-9}{2} = 1$$

IR



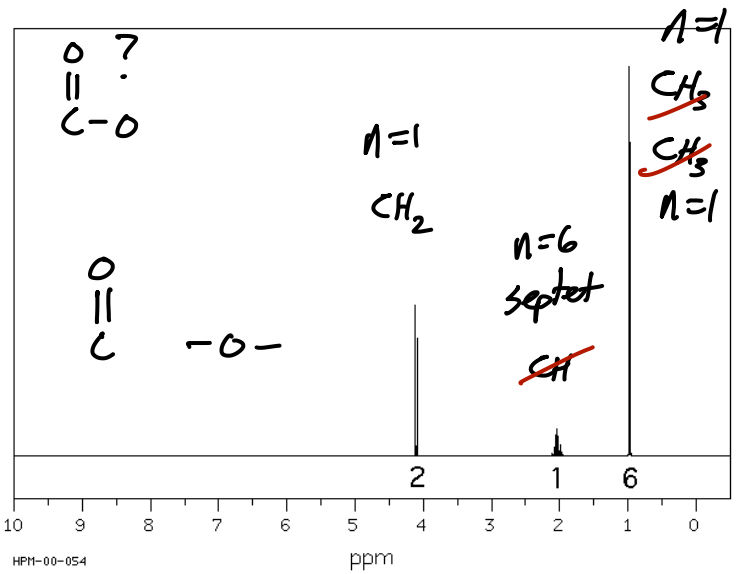
3636	84	1396	43	969	39	637	74
2969	17	1382	43	940	38	525	77
2936	36	1372	35	907	49	512	79
2879	30	1344	66	864	30	506	74
2309	84	1282	44	804	16	481	72
1781	4	1159	6	789	42		
1470	28	1163	6	690	29		

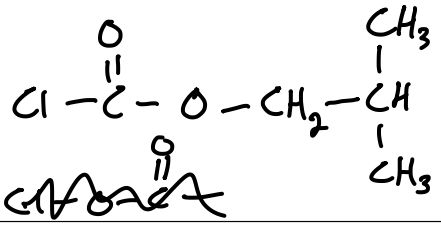
^{1}H NMR

ppm	Int.
4.118	335
4.096	343
2.113	10
2.091	32
2.069	62
2.046	79
2.024	65
2.002	35
1.98	11
0.992	1000
0.97	957

2

2



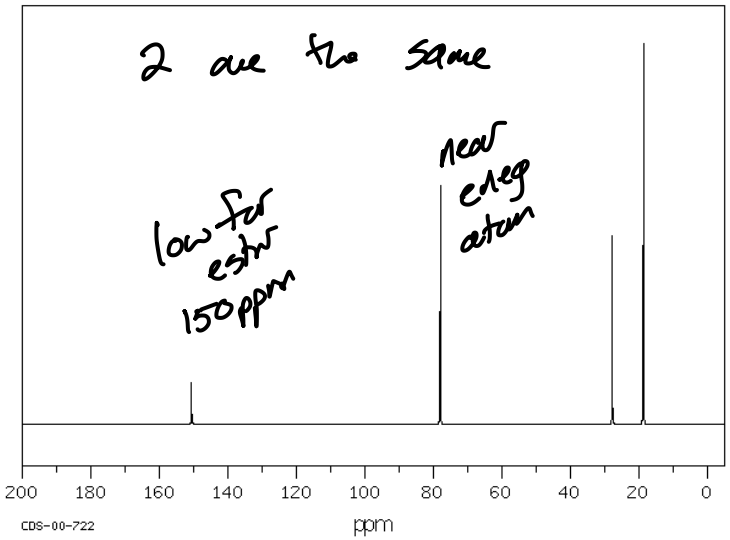


$^{13}C\{^1H\}$ NMR

4 dif C atom

CH_2 CH_3 CH

2 are the same



molecular ion = 136

MS

m/z	relative intensity
15	1
26	1
27	21
28	4
29	21
31	4
36	1
38	1
39	15
40	3
41	71
42	16
43	100
44	6
53	1
55	8
56	76
57	33
58	1
59	1
63	37
65	12
93	1
94	8
95	4
96	2
97	1