(16) **Today**

^{13}C NMR and Practice

Spring Break Begins at 4:30

Next Class (17)

Chap 12: Infrared Spectroscopy

Chap 20

(18) **Second Class from Today**

Chap 20

Third Class from Today (19)

Chap 20

Please rework Test 1 and hand in on March 19.

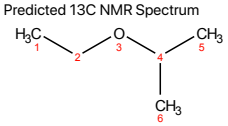
^1H little magnets 99+ %

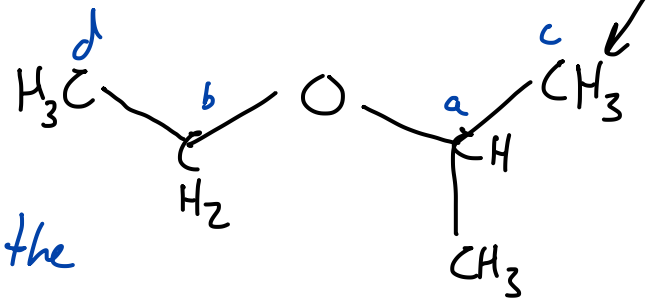
^{13}C also little magnets weaker magnets than ^1H

also ~1 % of C is ^{13}C

don't see ^{13}C resonance in ^1H NMR because the resonance frequencies are different

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

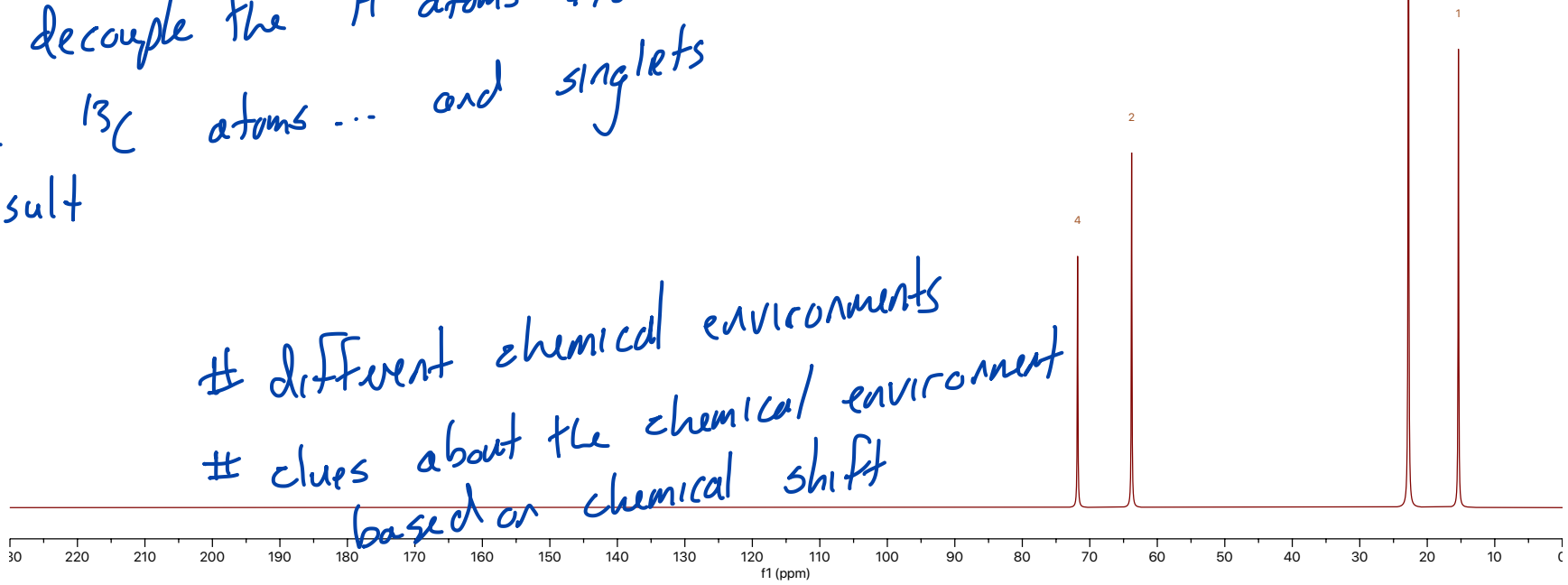




this C has 3 H's bound to it... so this should be a quartet, right? Because we make it not

these are singlets

blast the radio at the ^{1}H's so they keep flipping; thus, we decouple the ^{1}H atoms from the ^{13}C atoms... and singlets result



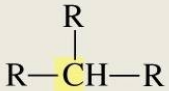
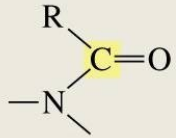
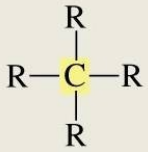
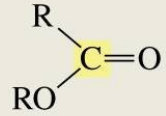
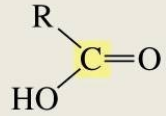
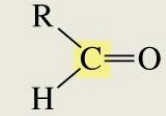
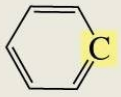
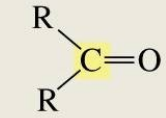
different chemical environments

clues about the chemical environment based on chemical shift

C atoms are in 4 different chemical environments

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

Table 14.4 Approximate Values of Chemical Shifts for ^{13}C NMR

Type of carbon	Approximate chemical shift (ppm)	Type of carbon	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0	C—I	0–40
R—CH_3	8–35	C—Br	25–65
R—CH_2—R	15–50	C—Cl C—N C—O	35–80 40–60 50–80
	20–60		165–175
	30–40		165–175
≡C	65–85		175–185
=C	100–150		190–200
	110–170		205–220

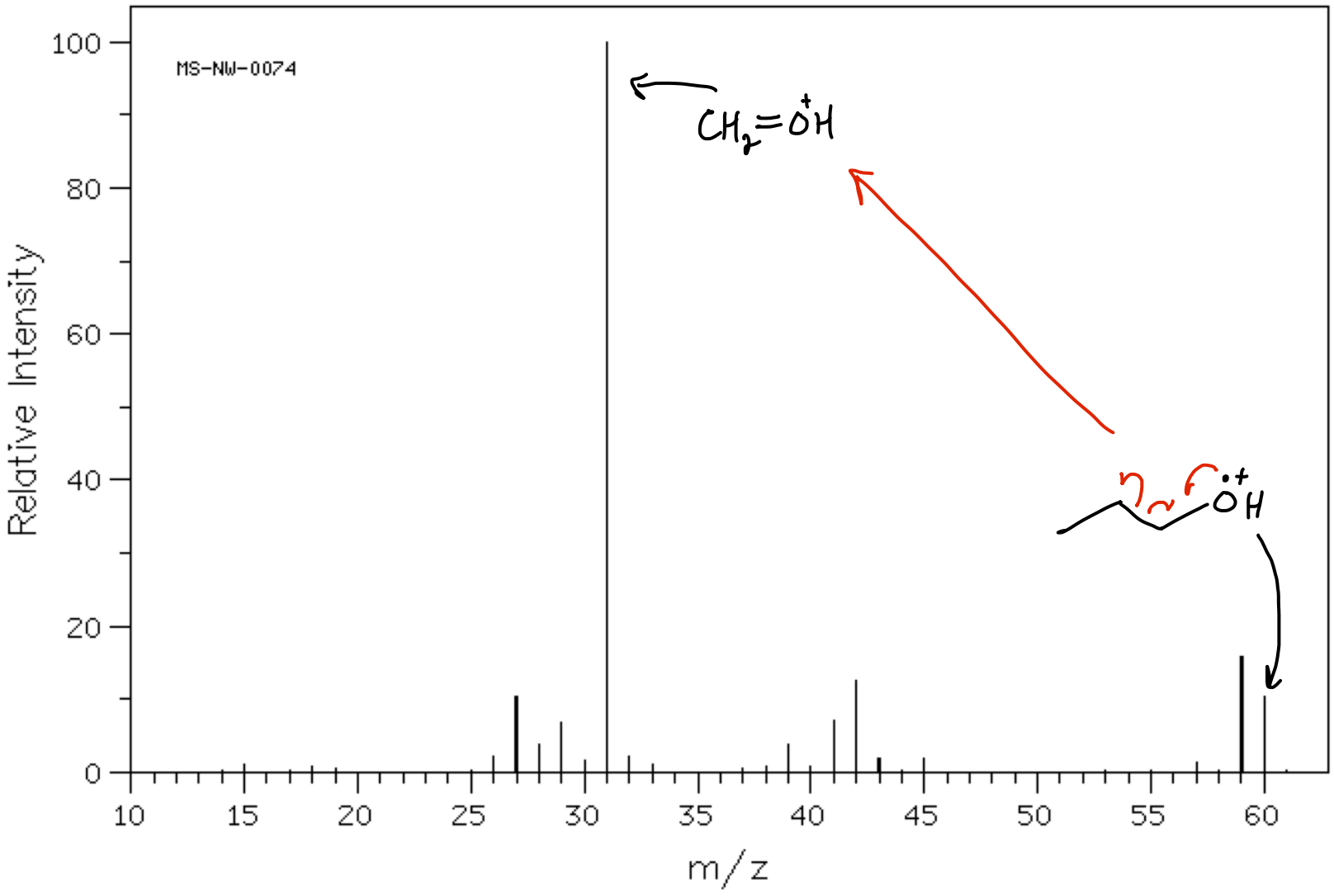
Practice

MS

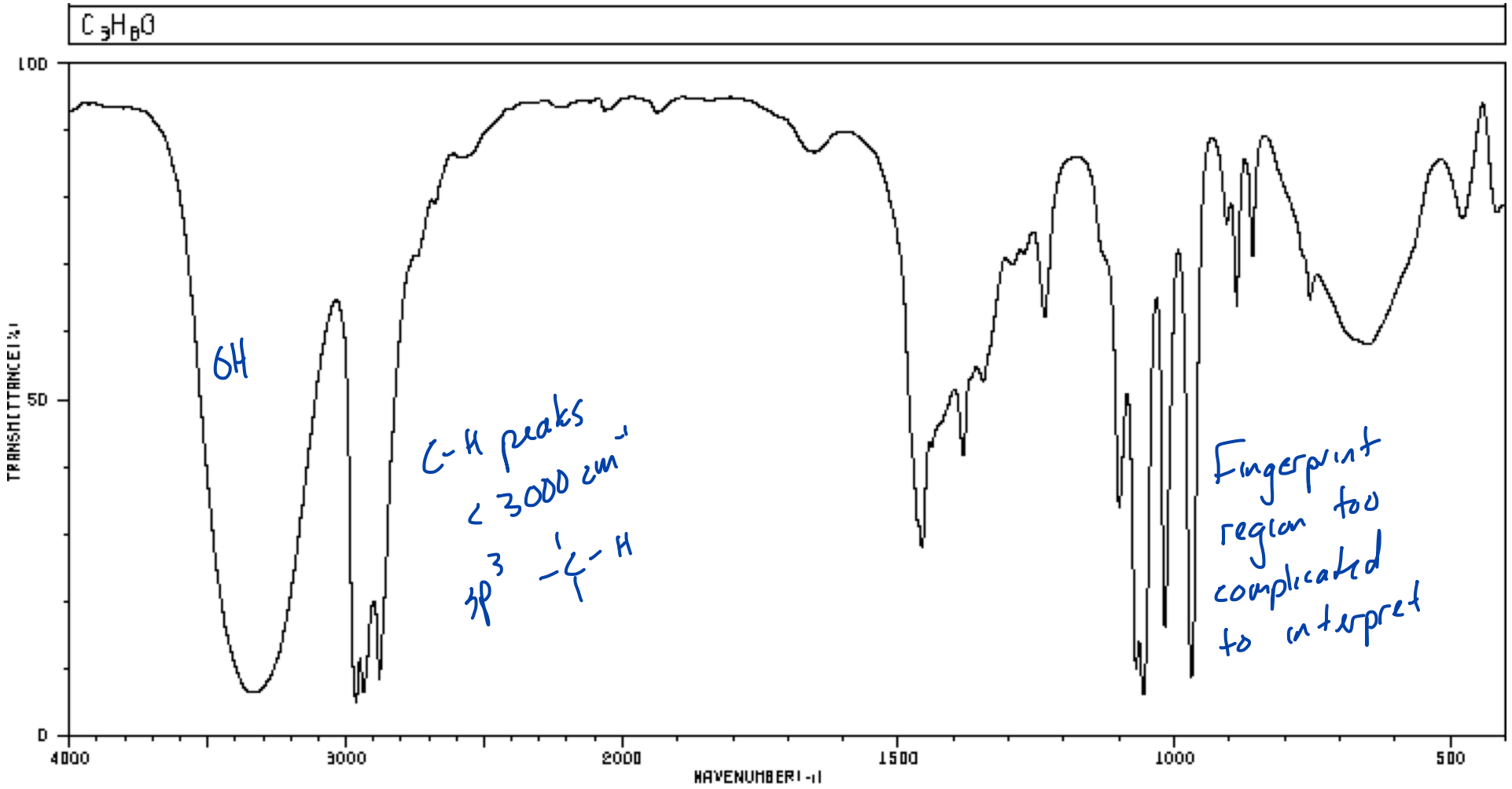
molecular ion = 60

mass of molecule to help determine formula

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

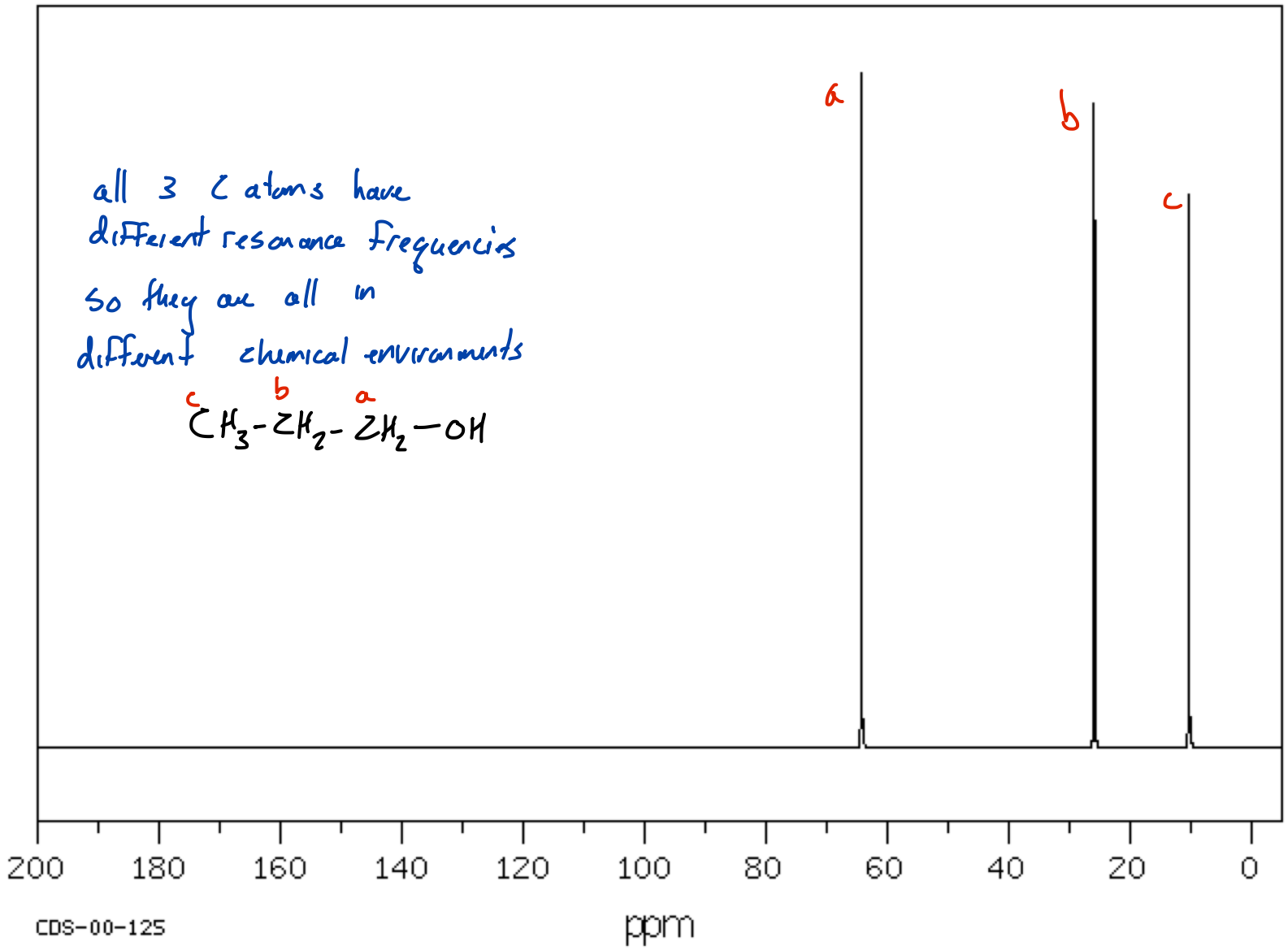


IR



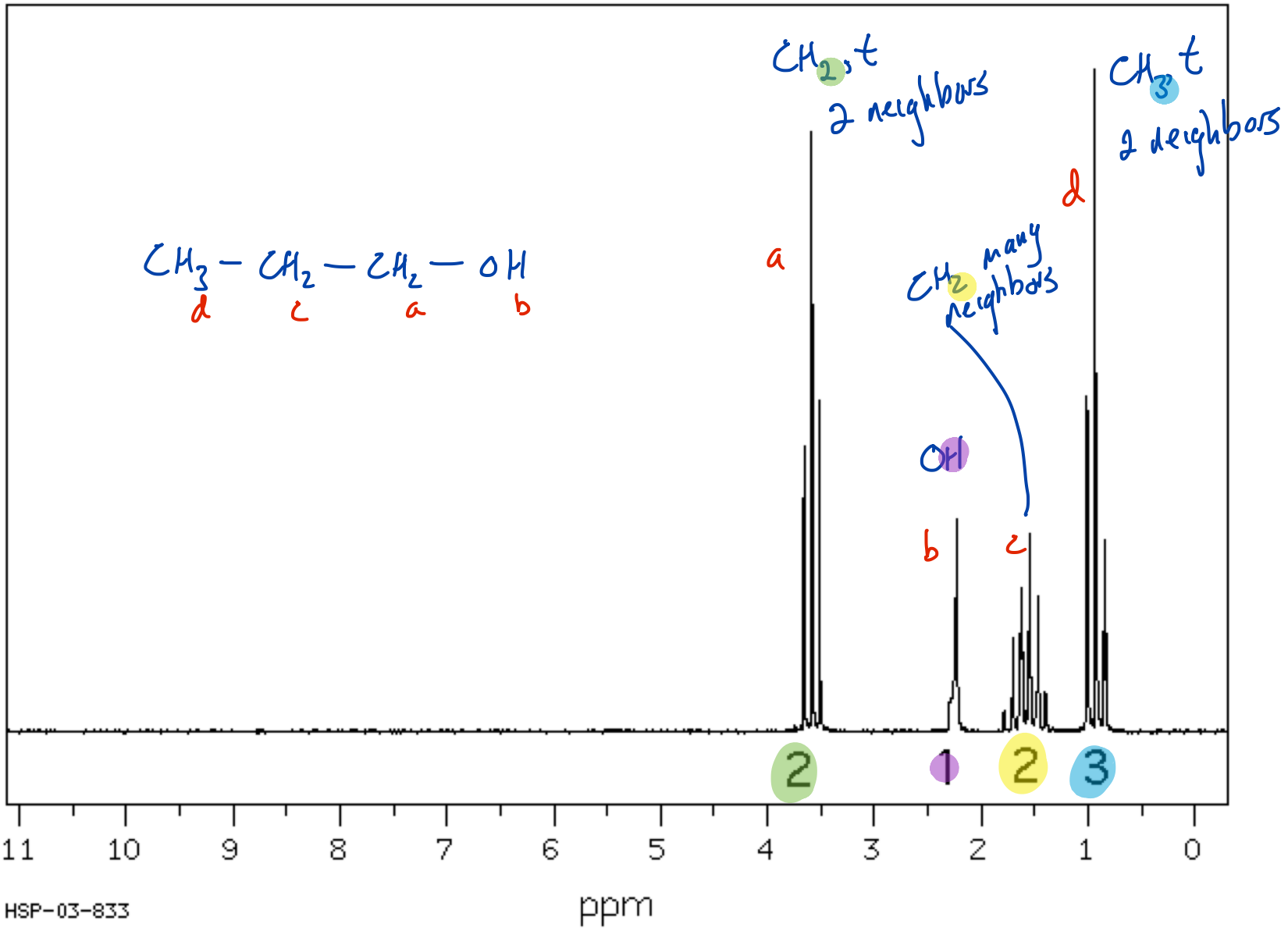
3333	6	1383	39	1017	16
2963	4	1346	50	969	8
2938	6	1293	66	905	72
2878	0	1236	60	888	62
1656	84	1100	32	858	68
1651	84	1069	9	755	82
1466	26	1066	6	479	74

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

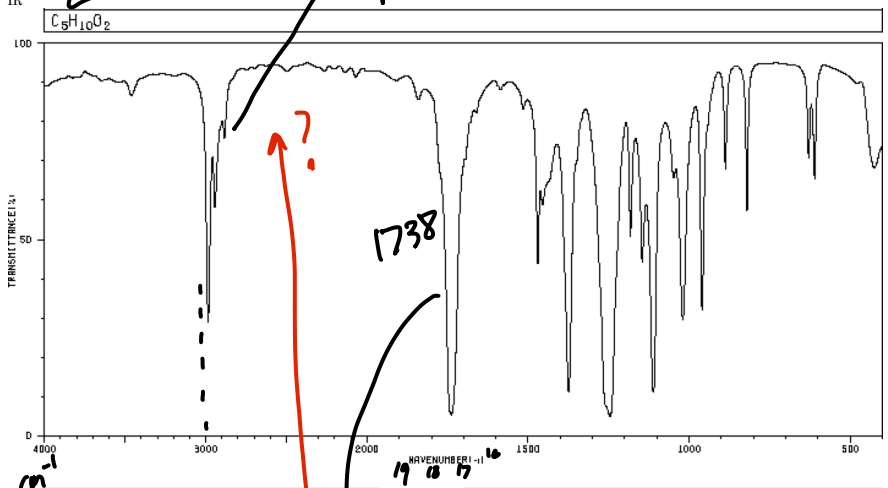

all 3 C atoms have
different resonance frequencies
so they are all in
different chemical environments
c
b
a
CH3-CH2-CH2-OH
a
b
c
200
180
160
140
120
100
80
60
40
20
0
CDS-00-125
ppm

^{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



IR



3460	84	1684	84	1146	42	629	68
2984	27	1514	79	1111	10	611	62
2944	55	1470	42	1049	84	426	56
2884	72	1466	67	1020	20		
1841	81	1374	10	960	31		
1738	5	1248	4	888	86		
1690	86	1183	49	821	66		

C_5

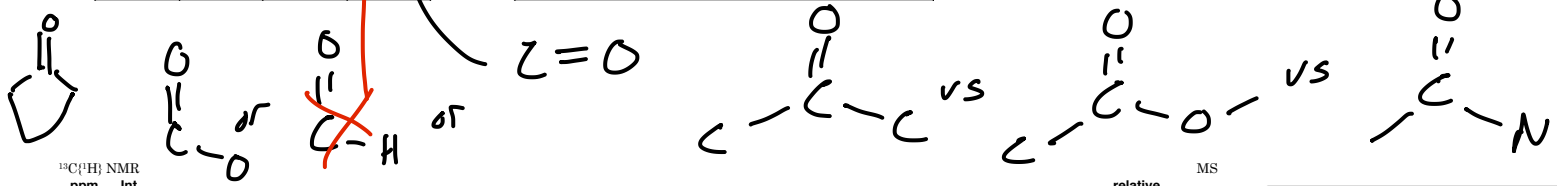
sp^3 C-H

?

1738

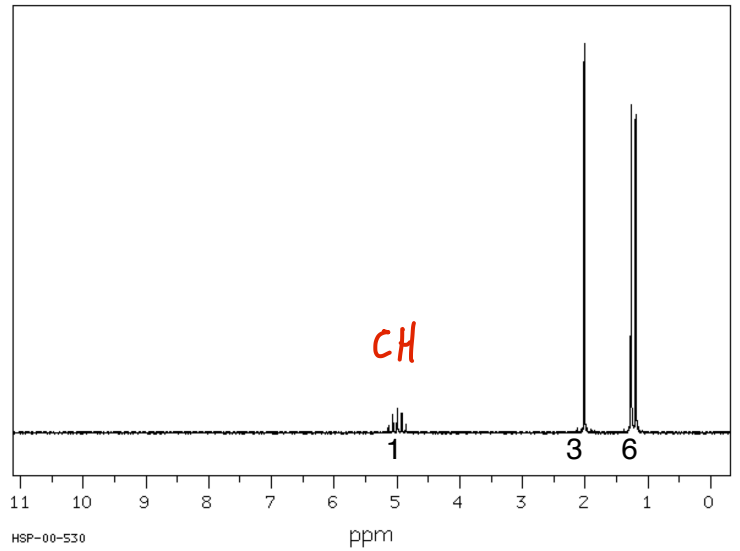
C=O

~3000 cm^{-1}



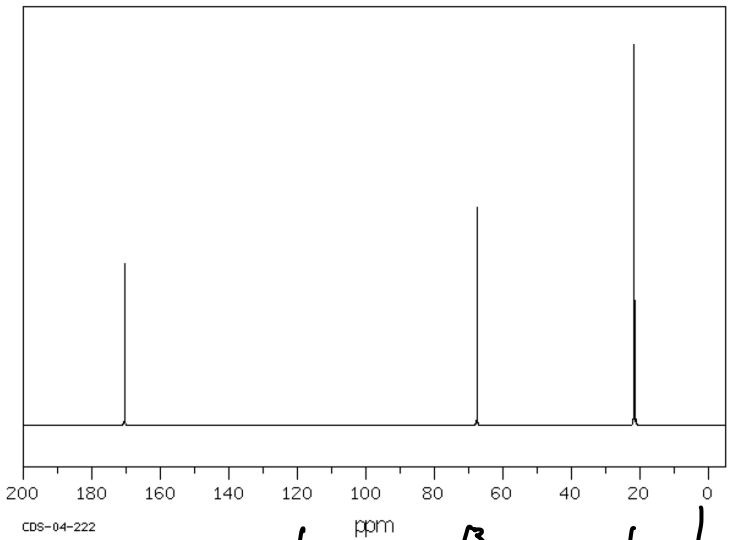
^{1}H NMR

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

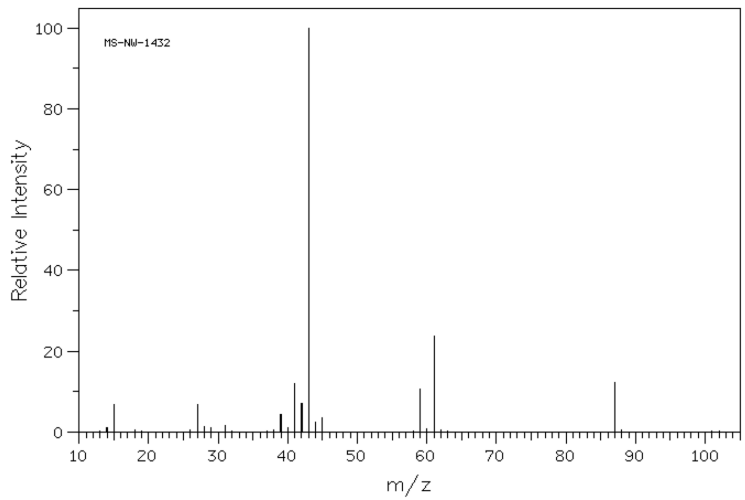
ppm	Int.
170.42	425
67.52	570
21.79	1000
21.34	325



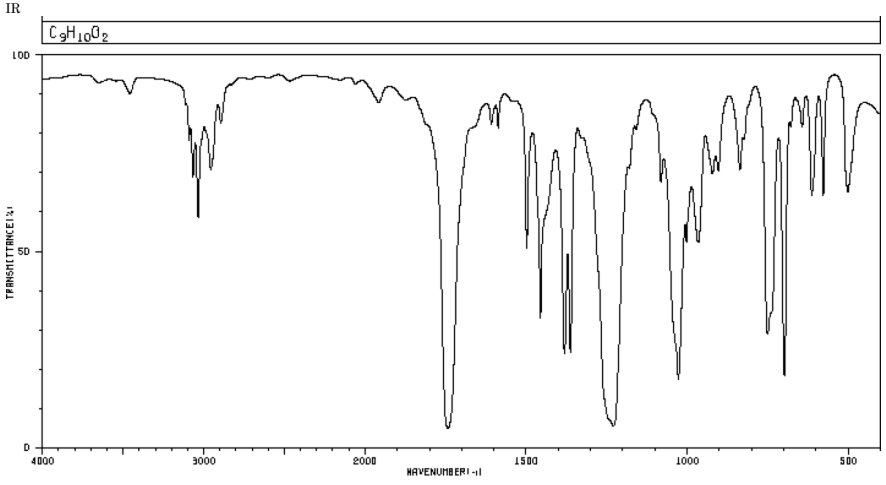
only 3 ^{13}C peaks!

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



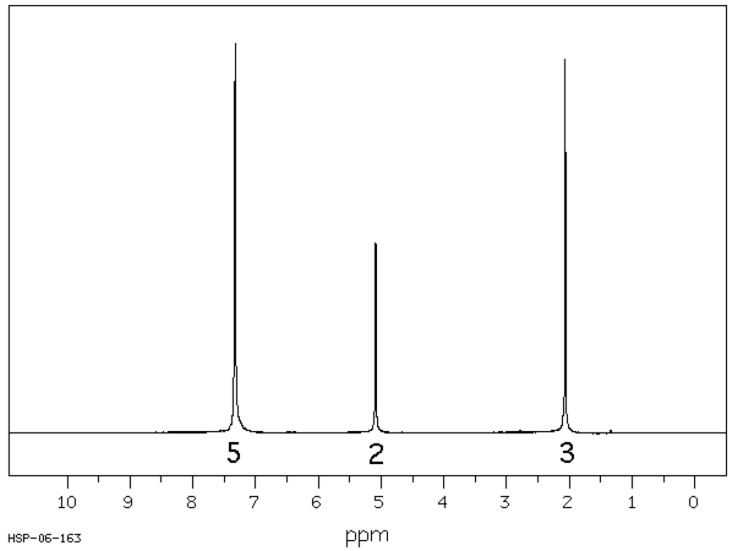
IR



3091	74	1608	79	1081	64	824	74	578	62
3067	86	1587	79	1027	16	751	27	502	62
3035	57	1498	49	1003	50	739	35	467	72
2956	68	1456	31	966	60	698	17		
2895	79	1381	23	922	86	679	79		
1956	84	1363	29	905	86	644	79		
1743	4	1229	6	837	68	614	62		

^{1}H NMR

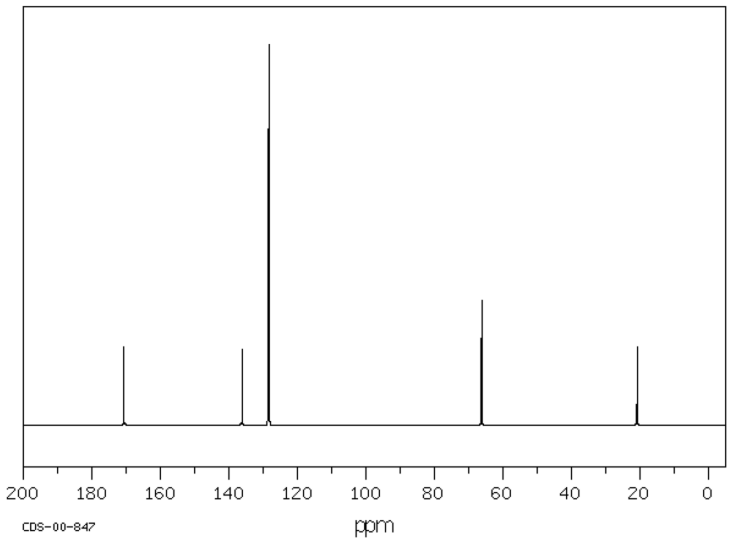
ppm	Int.
7.327	1000
5.086	488
2.065	960



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

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

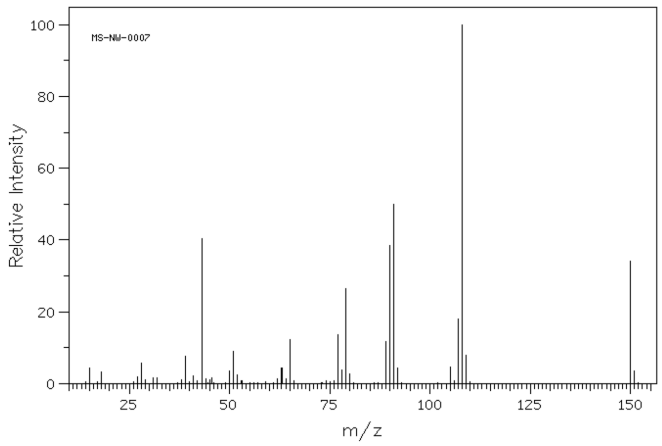
ppm	Int.
170.7	204
136.14	199
128.56	776
128.24	1000
66.24	328
20.82	204



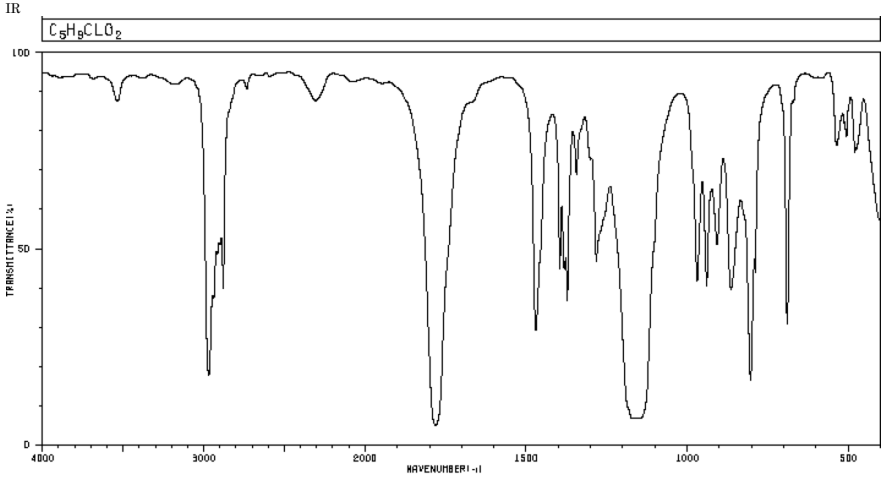
molecular ion = 150

MS

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		



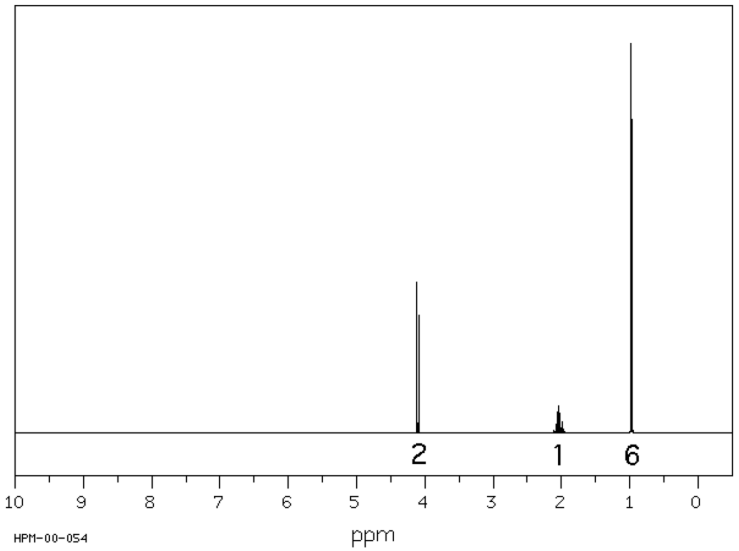
IR



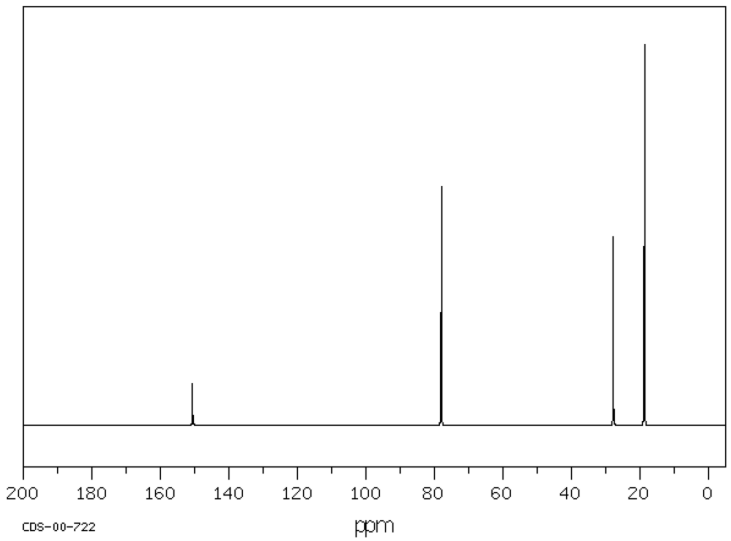
3636	84	1396	43	969	39	637	74
2969	17	1382	43	940	38	525	77
2936	36	1372	35	907	49	512	79
2879	30	1344	66	864	30	506	74
2309	84	1282	44	804	16	481	72
1781	4	1159	6	789	42		
1470	28	1153	6	690	29		

^{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



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



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