

Today

Next Class

Spectroscopic Identification of an Unknown

Test on Mass Spectrometry, Infrared Spectroscopy (Chap 13), and NMR Spectroscopy (Chap 14)

Organic Lab in
Wilson 309
today

Topics for Mass Spectrometry: basic understand of how a mass spectrometer works, m & $m+1$ peaks, m & $m+2$ peaks, using $m+1$ peaks to determine the number of C atoms in an ion, using the "Rule of 13" to determine the formula of an ion, fragmentation reactions of alkyl halides

Monday

Chap 15.1 – 15.6

Old Tests that cover the same topics

Spring 19 test 1
Spring 12 Test 4
Spring 09 Test 3
Spring 07 Test 4
Spring 05 Test 4
Spring 03 Test 4

Spring 13 Quiz 4 and one question from Spring 13 Test 3
Spring 2011 Quiz 3, Test 3
Spring 08 Quiz 3, Test 3
Spring 06 Test 4
Spring 04 Test 4

Extra Zoom office hours on Thursday 10:00 - 11:00 and 1:00 - 2:00

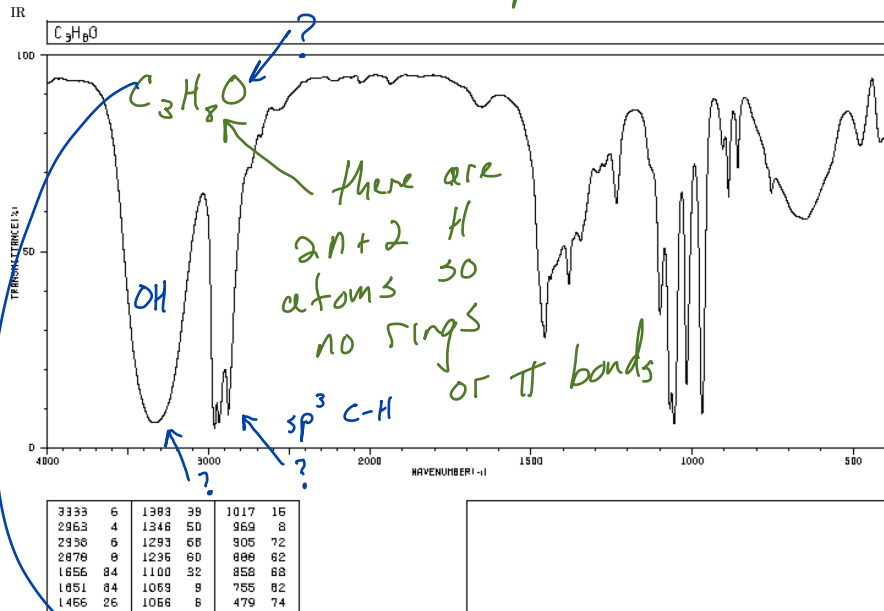
Spectral data obtained from

Spectral Database for Organic Compounds, SDDBS

National Institute of Advanced Industrial Science and
Technology (AIST), Japan

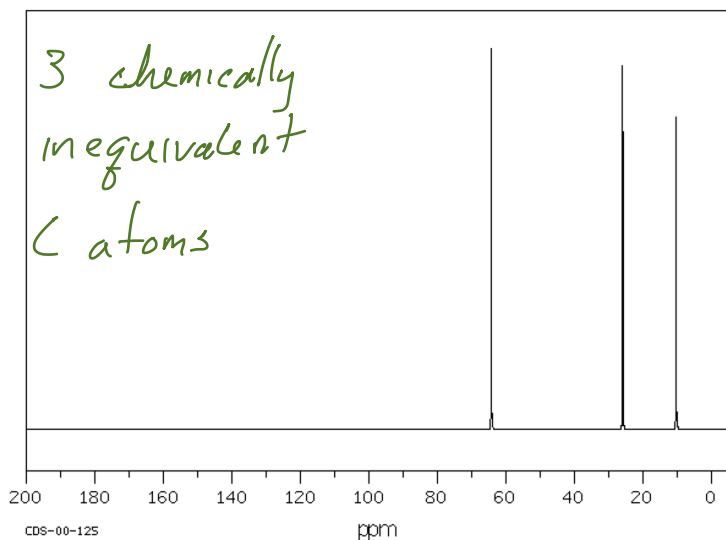
www.aist.go.jp/RIODB/SDDBS/cgi-bin/cre_index.cgi

What does the IR spectrum tell us?



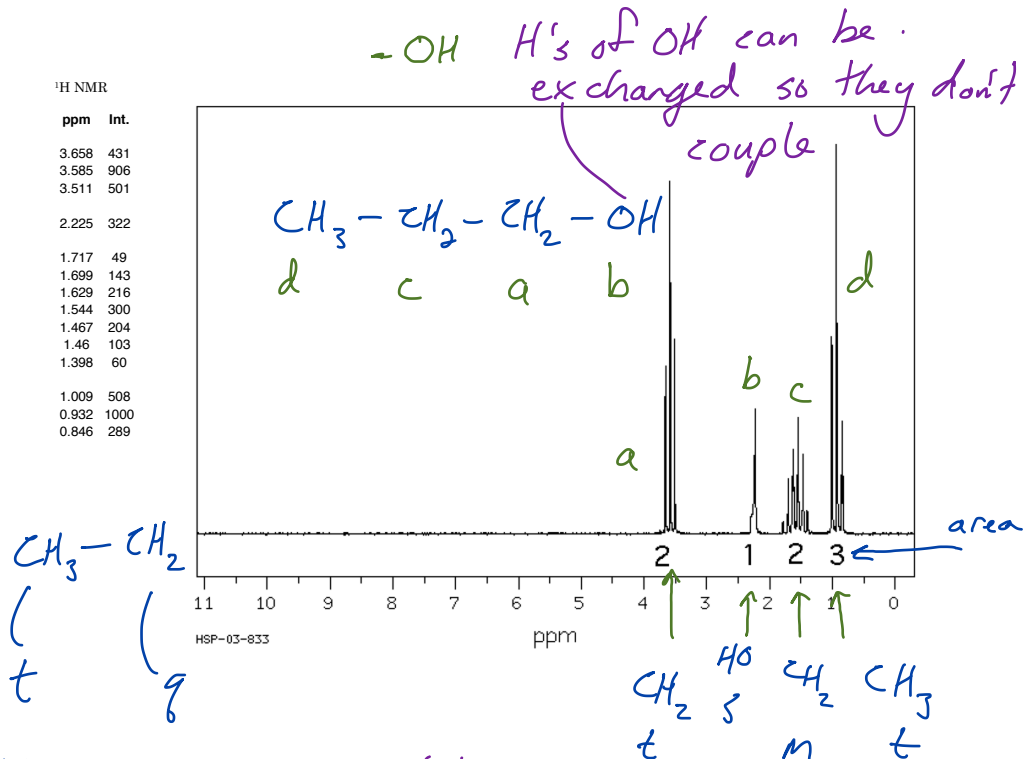
For n C atoms an acyclic molecule with no db's would have $2n+2$ H atoms

^{13}C NMR



1H NMR

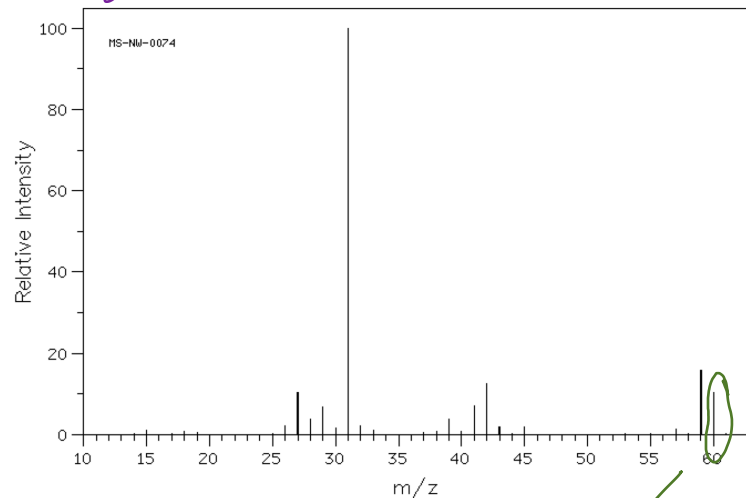
ppm	Int.
3.658	431
3.585	906
3.511	501
2.225	322
1.717	49
1.699	143
1.629	216
1.544	300
1.467	204
1.46	103
1.398	60
1.009	508
0.932	1000
0.846	289



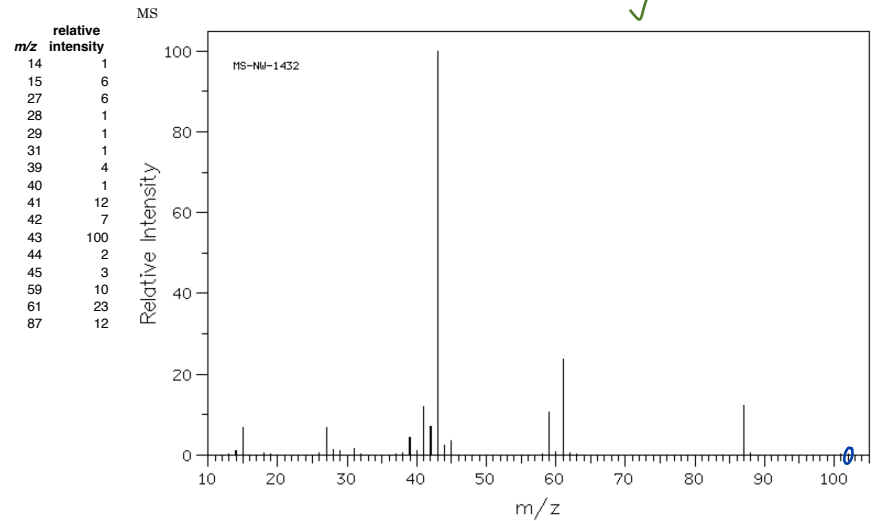
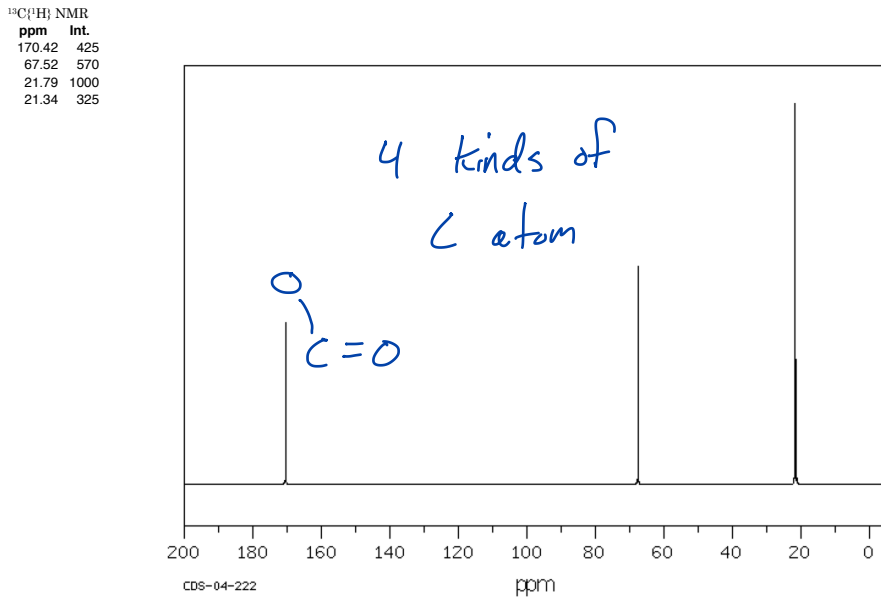
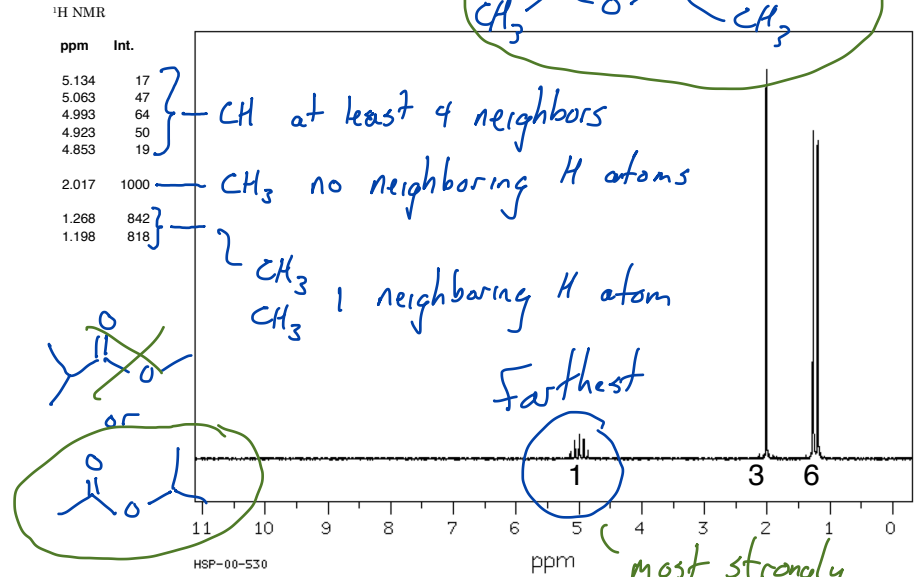
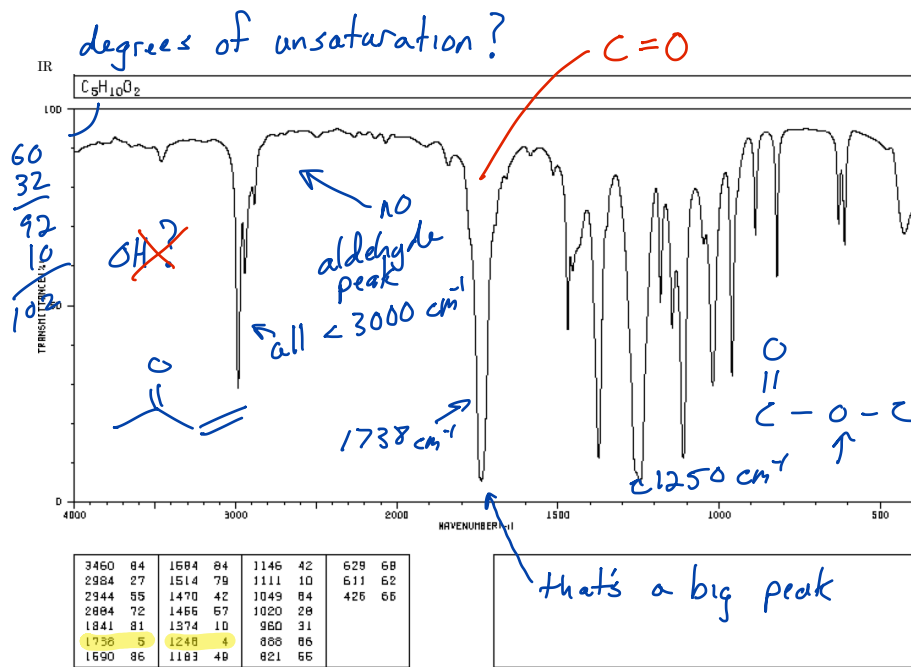
MS

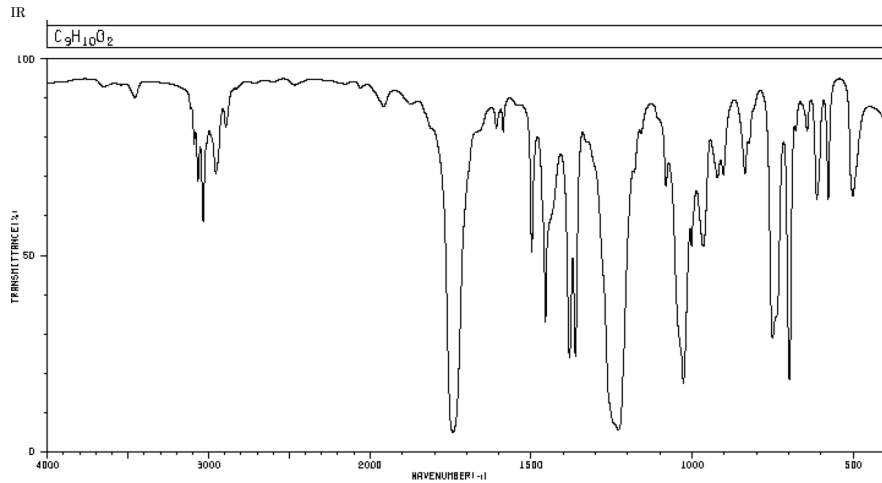
molecular ion = 60

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



molecule has a mass of 60 g/mol

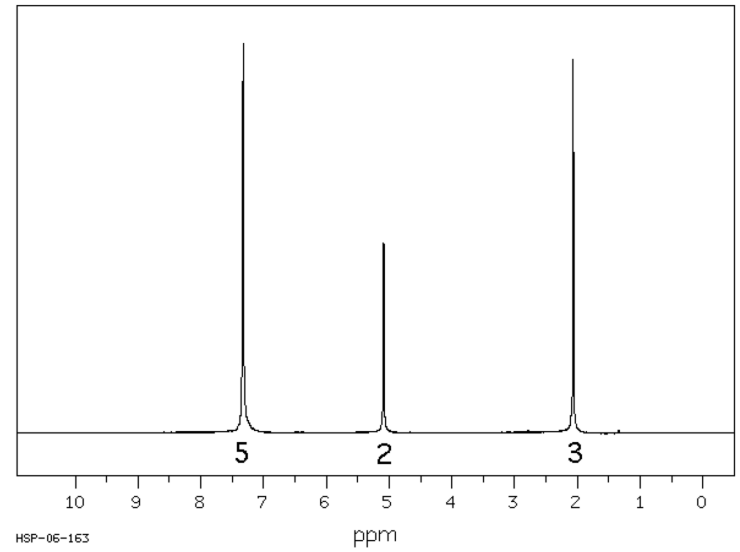




3091	74	1608	79	1081	64	824	74	678	62
3067	66	1587	79	1027	16	751	27	502	62
3035	57	1498	48	1003	50	739	33	487	72
2966	68	1468	31	966	60	698	17		
2895	79	1381	23	922	66	679	79		
1956	84	1363	23	903	88	644	79		
1743	4	1229	6	837	68	614	62		

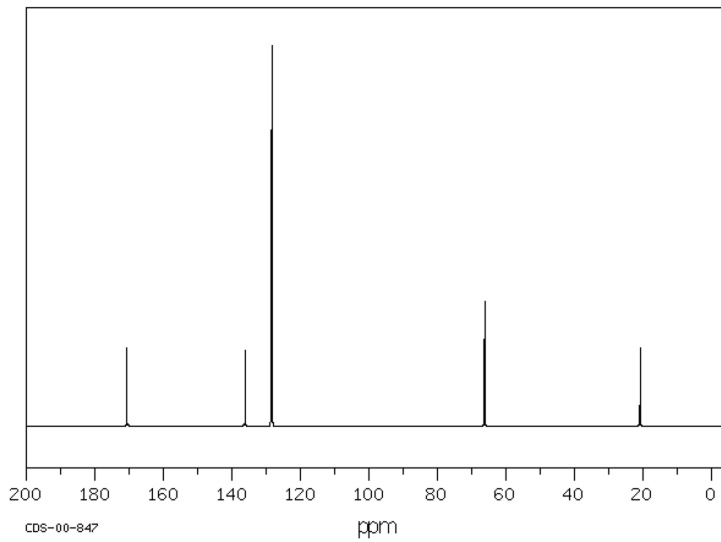
¹H NMR

ppm	Int.
7.327	1000
5.086	488
2.065	960



¹³C{¹H} NMR

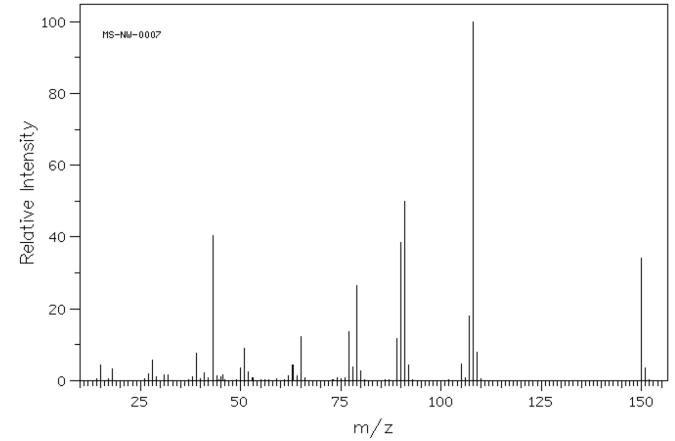
ppm	Int.
170.7	204
136.14	199
128.56	776
128.24	1000
66.24	328
20.82	204

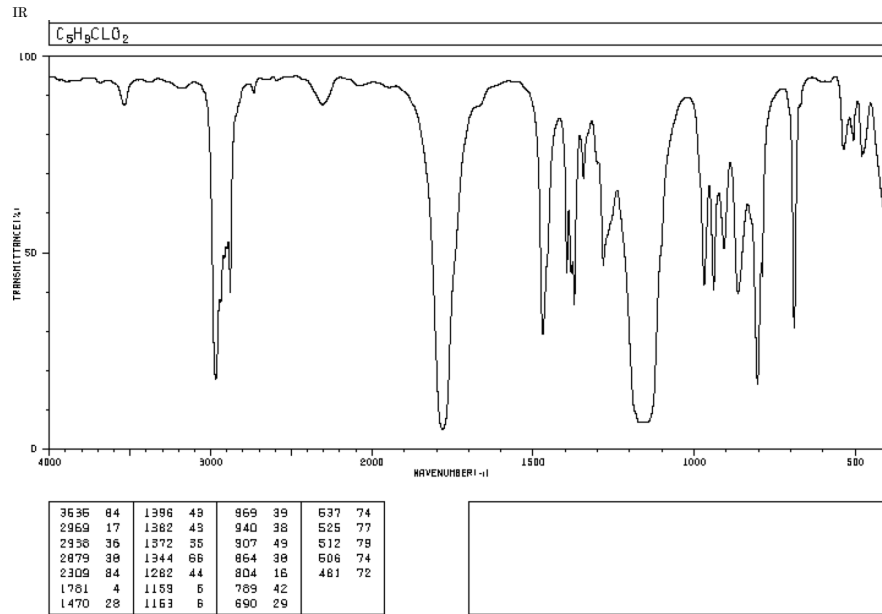


molecular ion = 150

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		

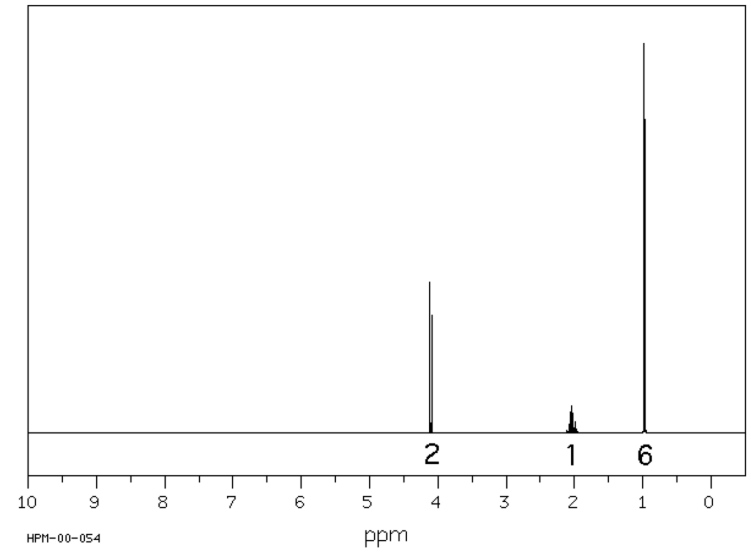
MS



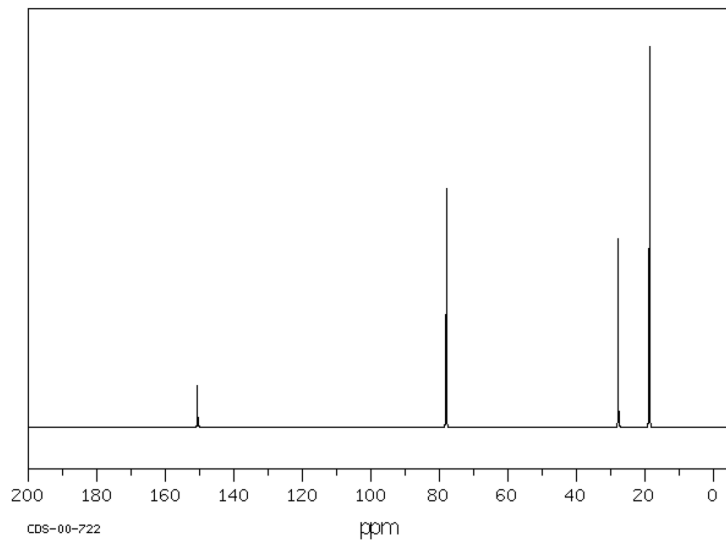


¹H NMR

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



¹³C{¹H} NMR



molecular ion = 136

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

MS

