Spectral Problems

The following slides contain a combination of IR, H-1 and C-13 NMR, and mass spectra. The first click will show the spectra and the second click will show the structure and name. Some of the spectra also will display a pop-up with comments on spectral features. Some of the problems show the molecular formula. Others give molecular weight and %composition from which you should be able to easily calculate the molecular formula. (See page 21-22 in your textbook if you need to review how to do this). The problems are ordered roughly from easy to difficult.

[redacted]

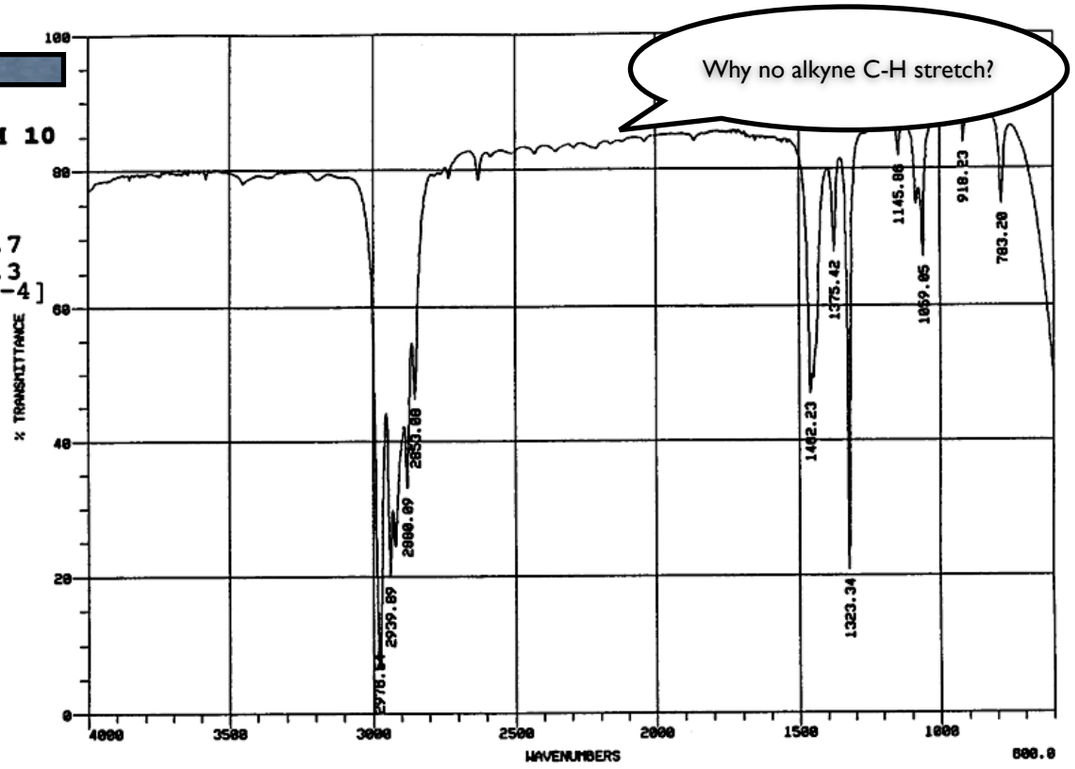
PROBLEM 10

MW 82

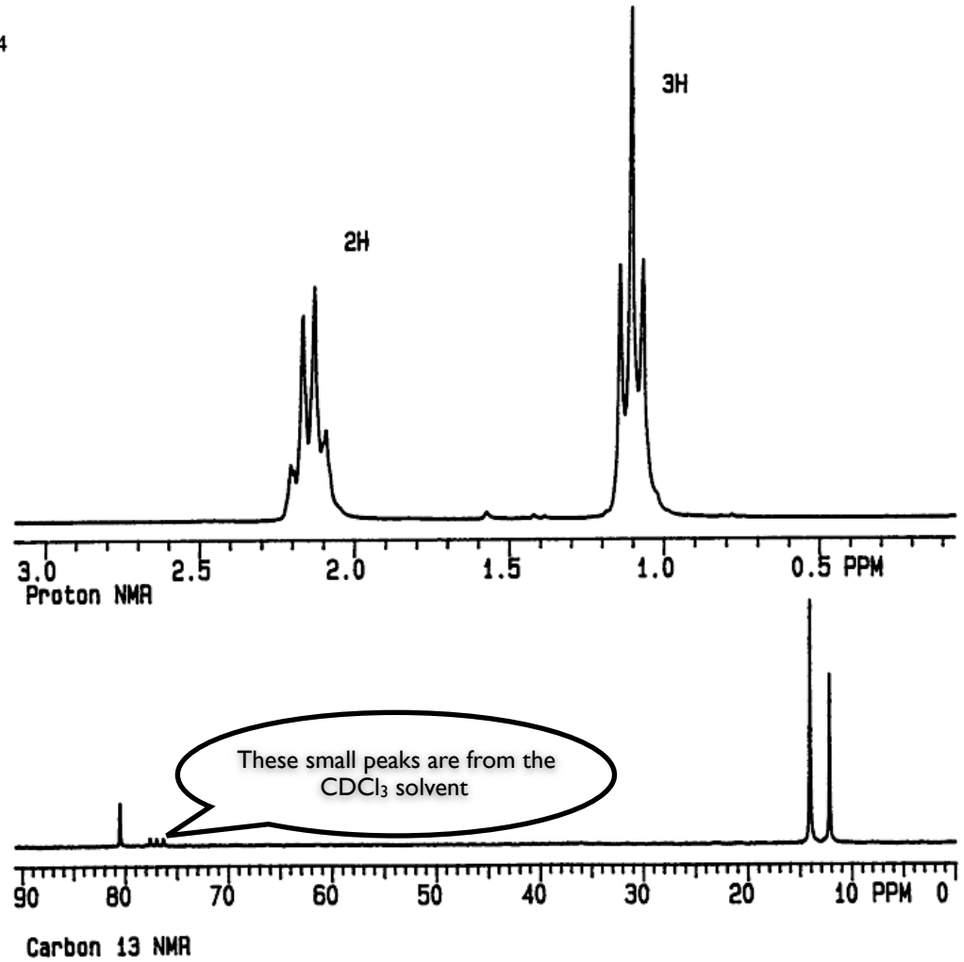
%C 87.7
%H 12.3
[928-49-4]

Mass Spec. Data

m/z	relative abund.
27	13
39	59
42	13
53	20
54	35
65	14
67	100
68	7
79	7
81	16
82	78
83	6



Why no alkyne C-H stretch?



3-hexyne

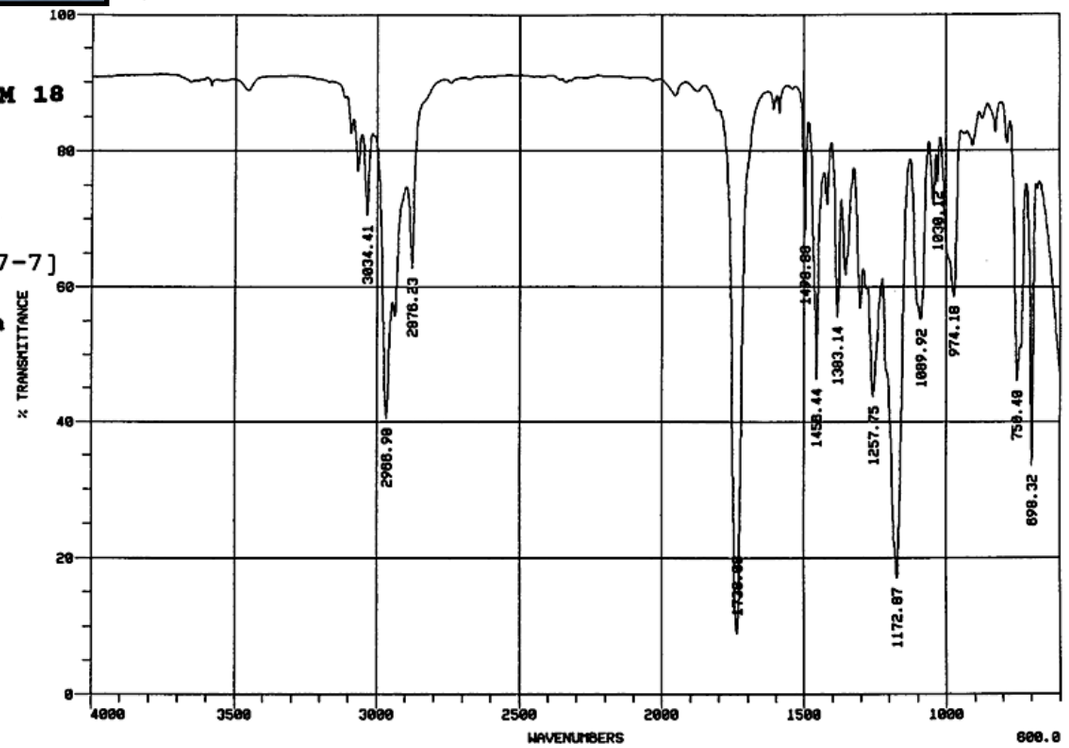
PROBLEM 18

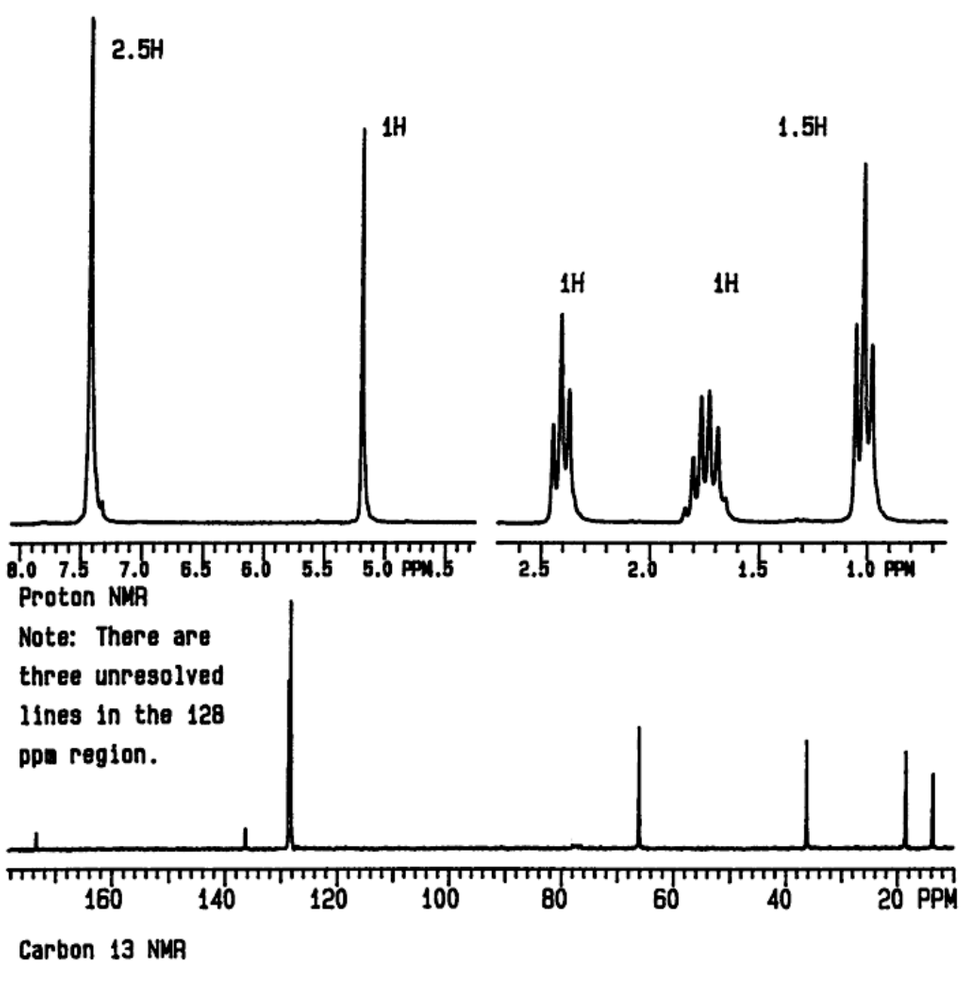
MW 178

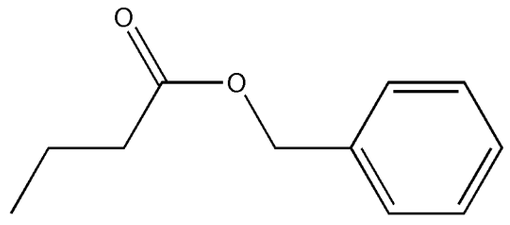
%C 74.1
%H 7.9
[103-37-7]

Mass Spec. Data

m/z	relative abund.
27	24
51	14
65	24
71	45
77	15
79	16
89	9
90	27
91	100
92	13
107	12
108	90
109	10
178	20







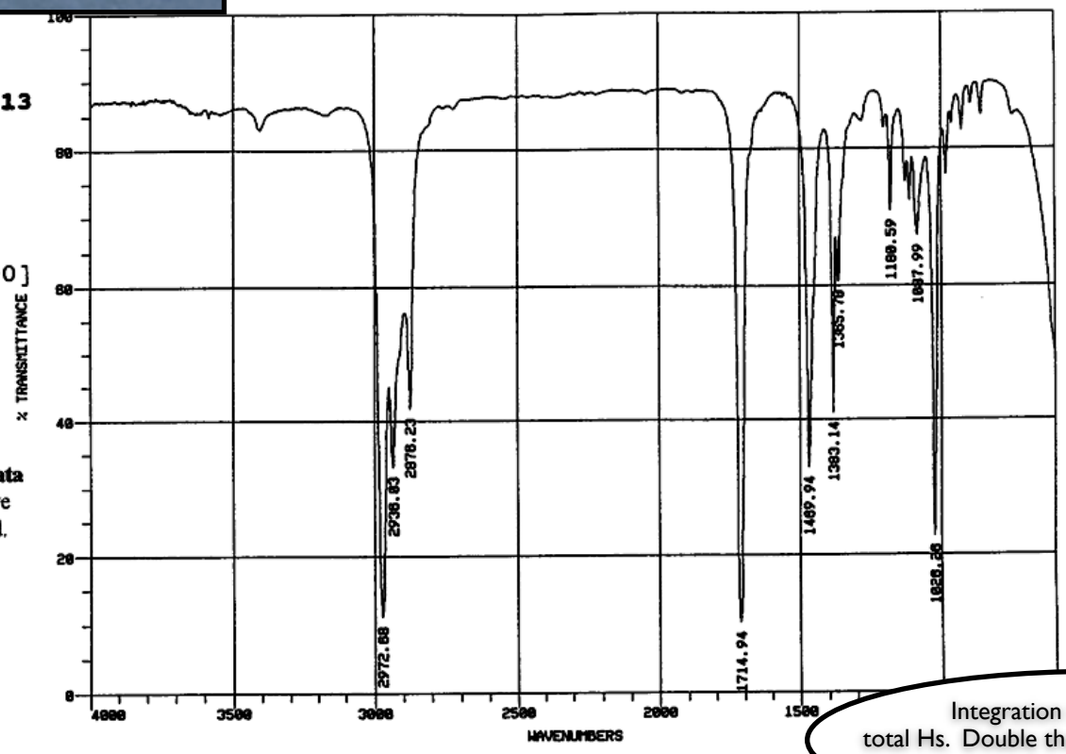
benzyl butanoate

PROBLEM 13

MW 114

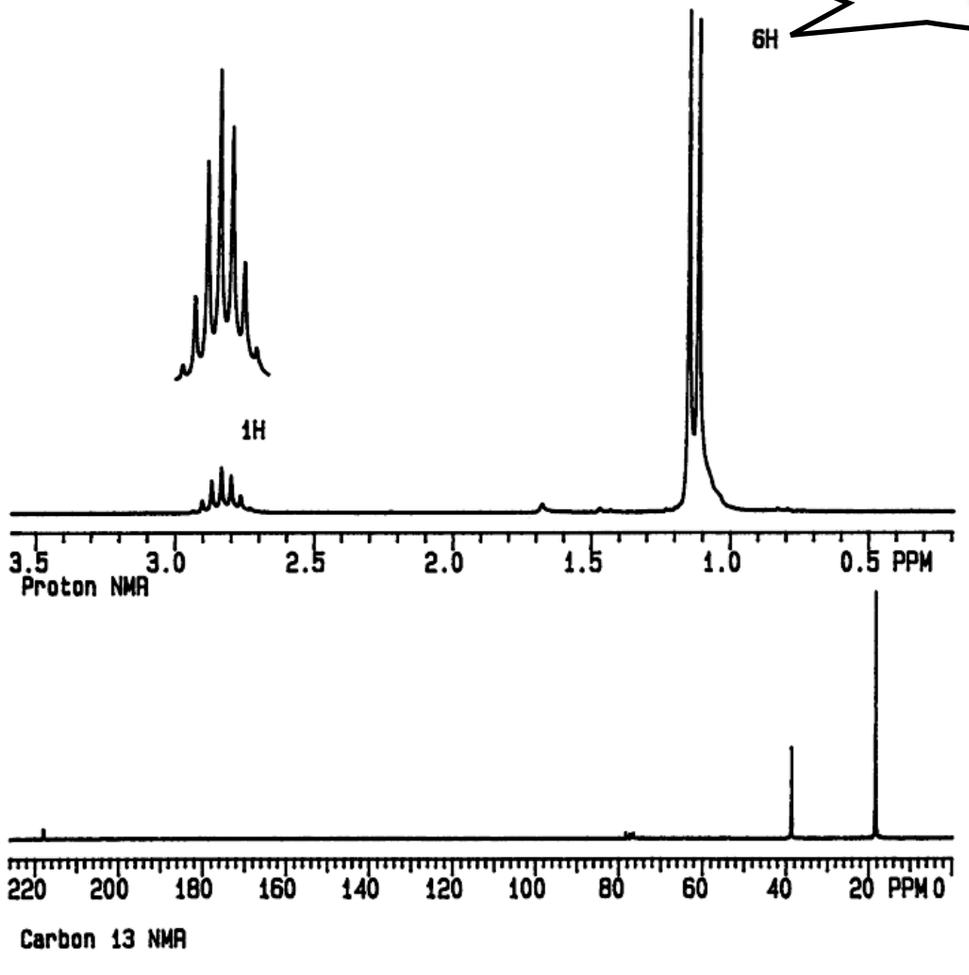
%C 73.6
%H 12.4

[565-80-0]

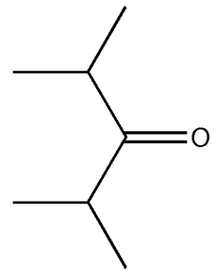


Mass Spec. Data

m/z	relative abund.
27	21
41	19
42	6
43	100
71	28
114	6



Integration is proportional to total Hs. Double the numbers here to get the actual number of Hs.



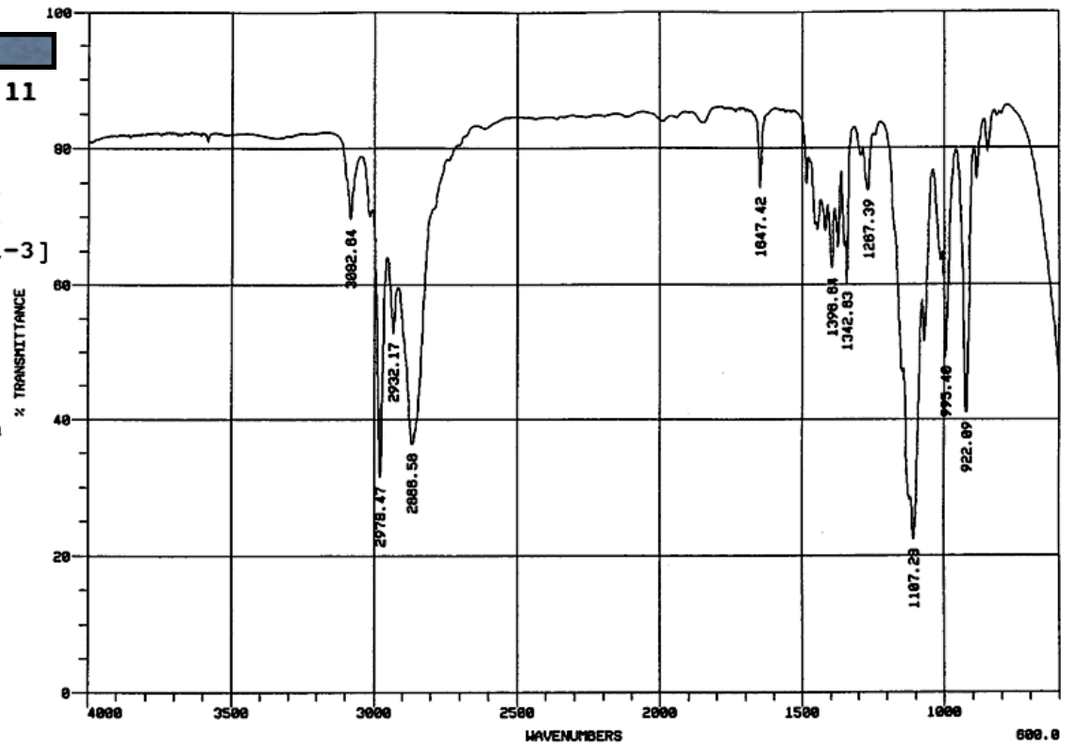
2,4-dimethyl-3-pentanone

[redacted]

PROBLEM 11

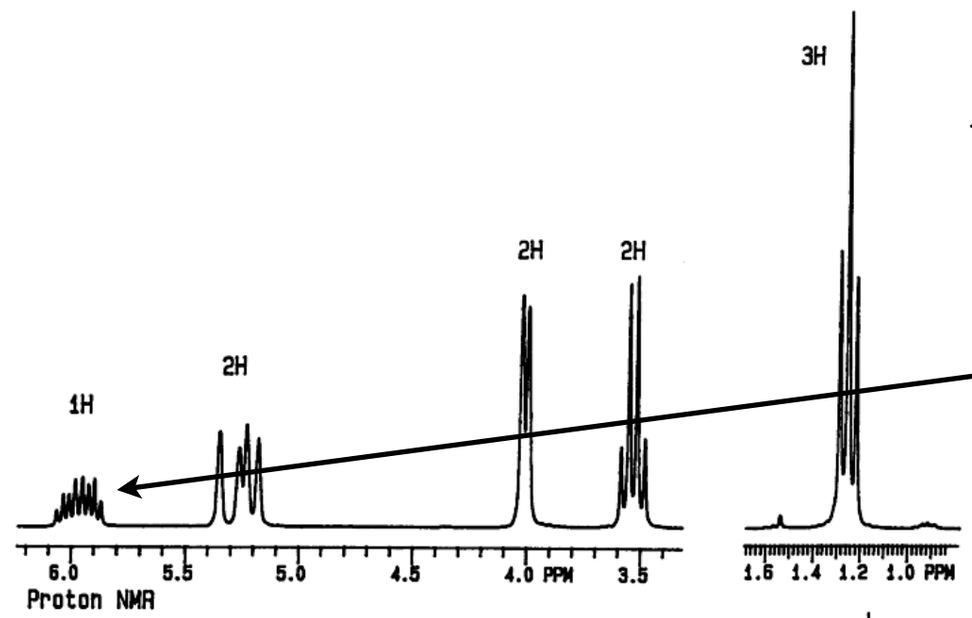
MW 86

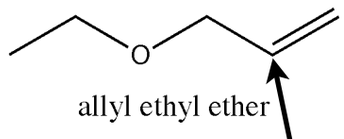
%C 69.7
%H 11.7
[557-31-3]



Mass Spec. Data

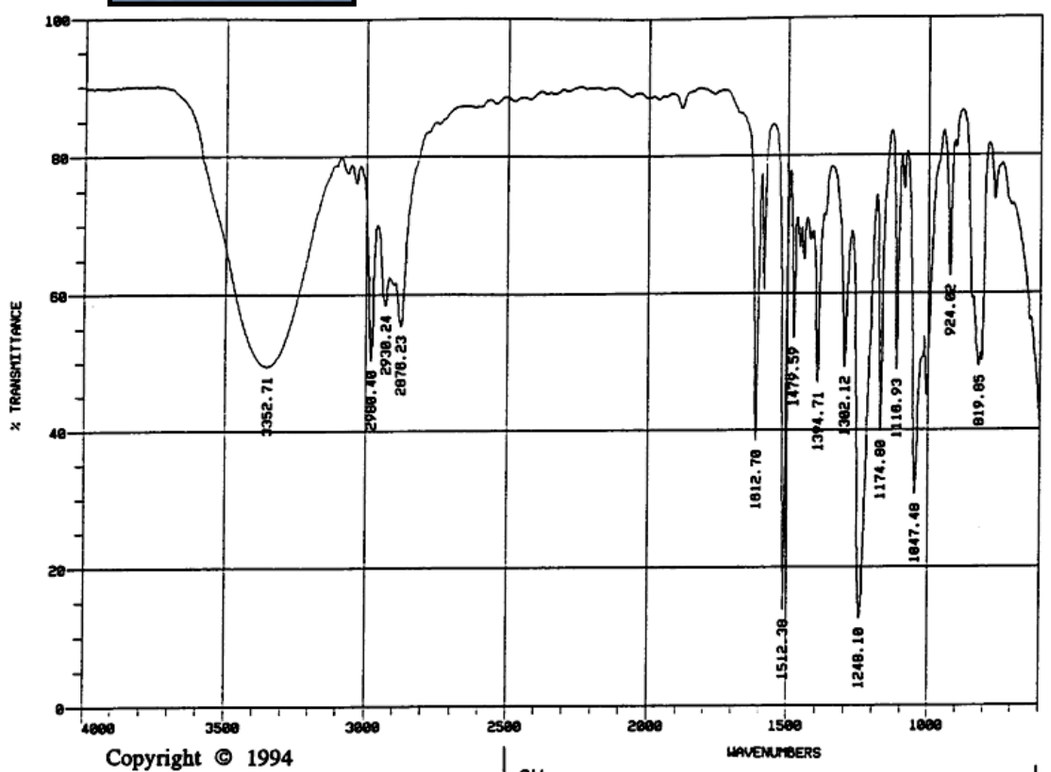
m/z	relative abund.
15	23
26	20
27	61
29	92
30	20
31	45
39	47
41	100
45	10
57	82
58	86
86	12





allyl ethyl ether

This proton is split by the methylene protons and differently by the cis- and trans- terminal protons, so the signal is a 12-uplet.

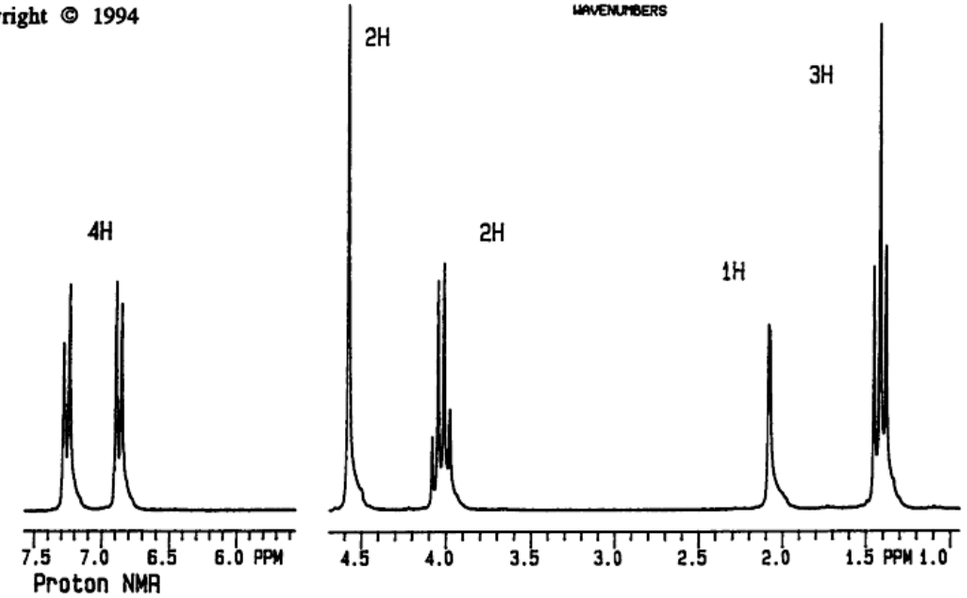


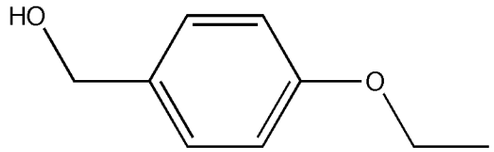
MF $C_9H_{12}O_2$

MW 152

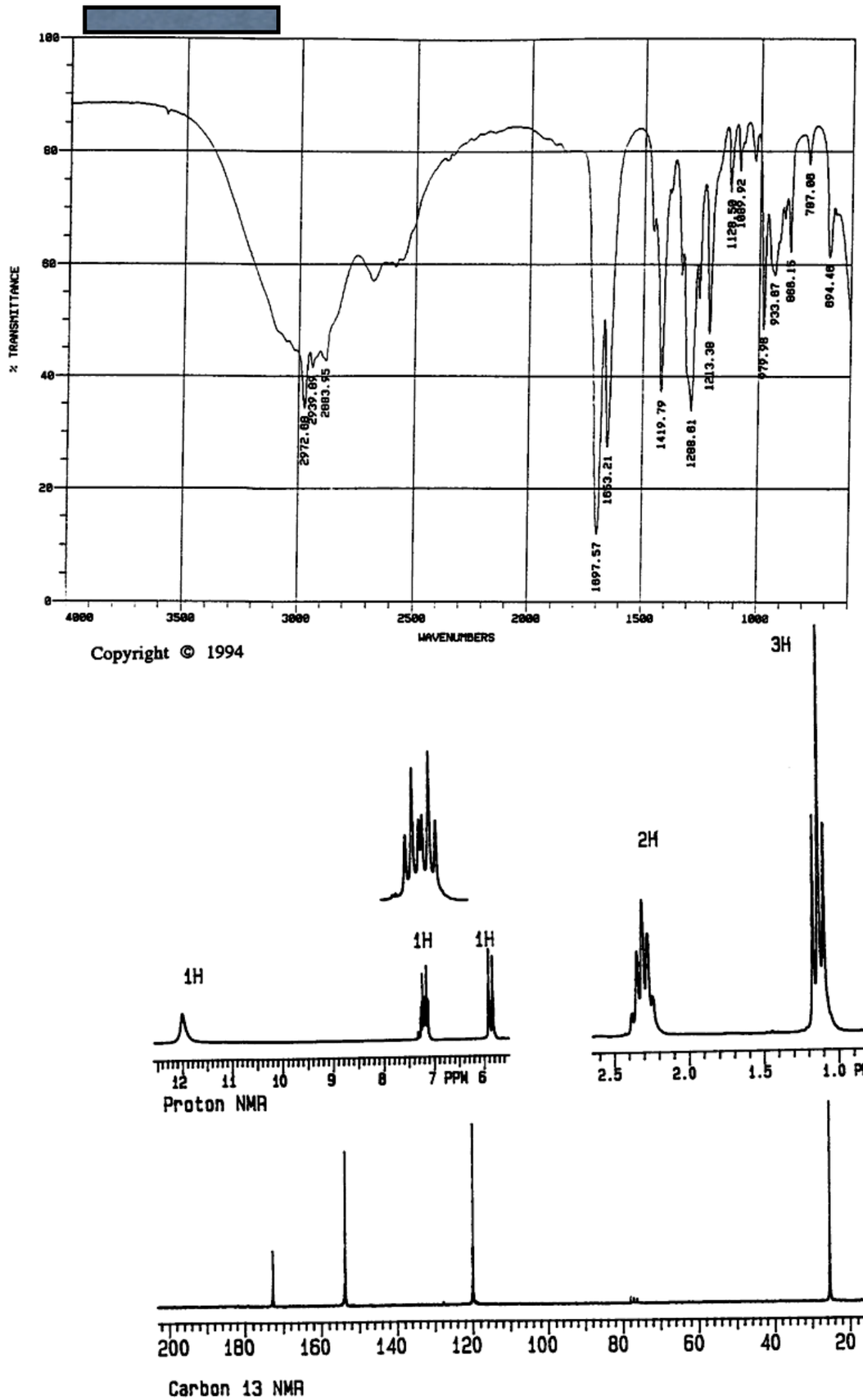
%C 71.0

%H 7.9





4-ethoxy benzyl alcohol

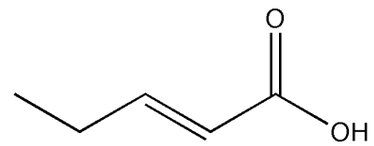


MF $C_5H_8O_2$

MW 100

%C 60.0

% H 8.0



trans-2-pentenoic acid