

ORGANIC CUMMULATIVE EXAM

March 6, 1999

Name _____

1. Give the structure of the compound $C_9H_{10}O$ the spectral data of which are given on the next page. Give your answer here and provide the rationale for you decision. Assign the NMR spectra on the following page.

MF C₉H₁₀O

MW 134

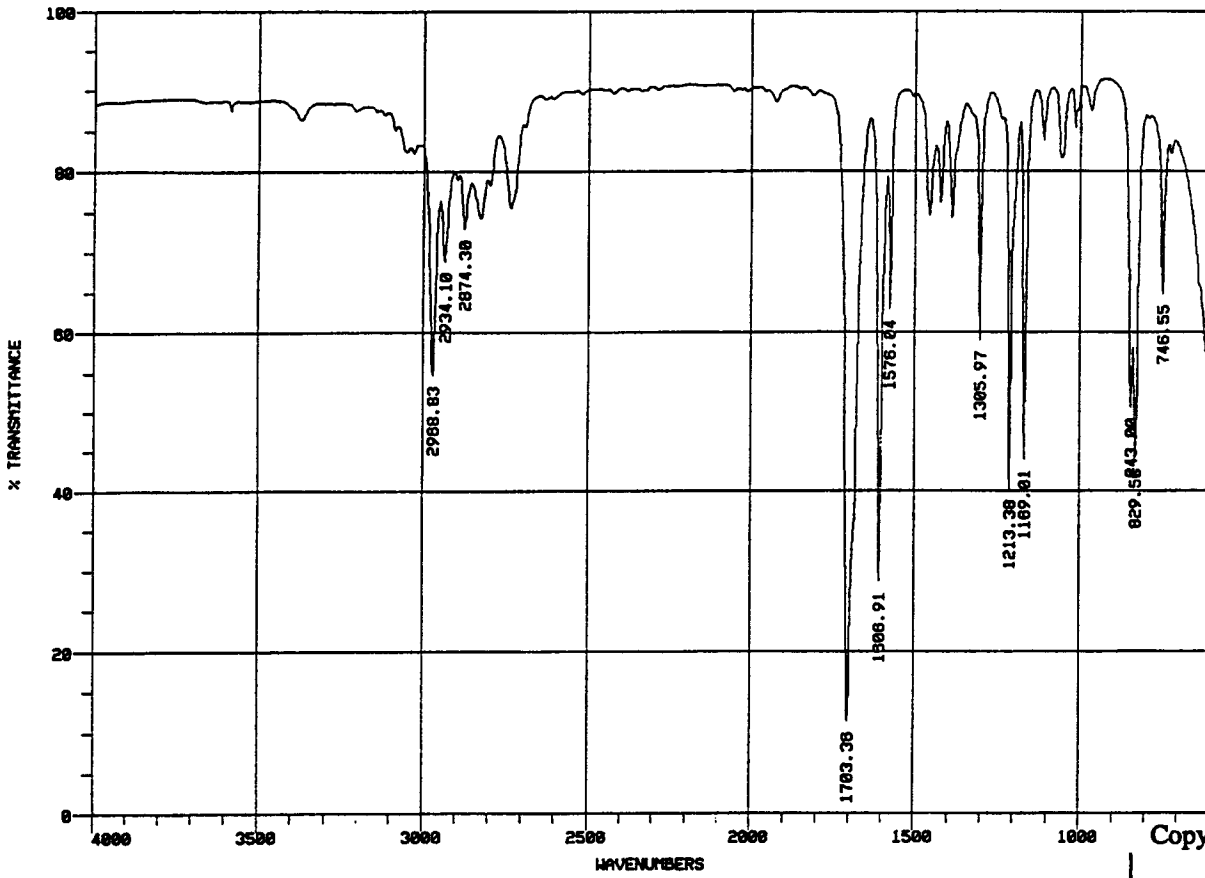
%C 80.6

%H 7.5

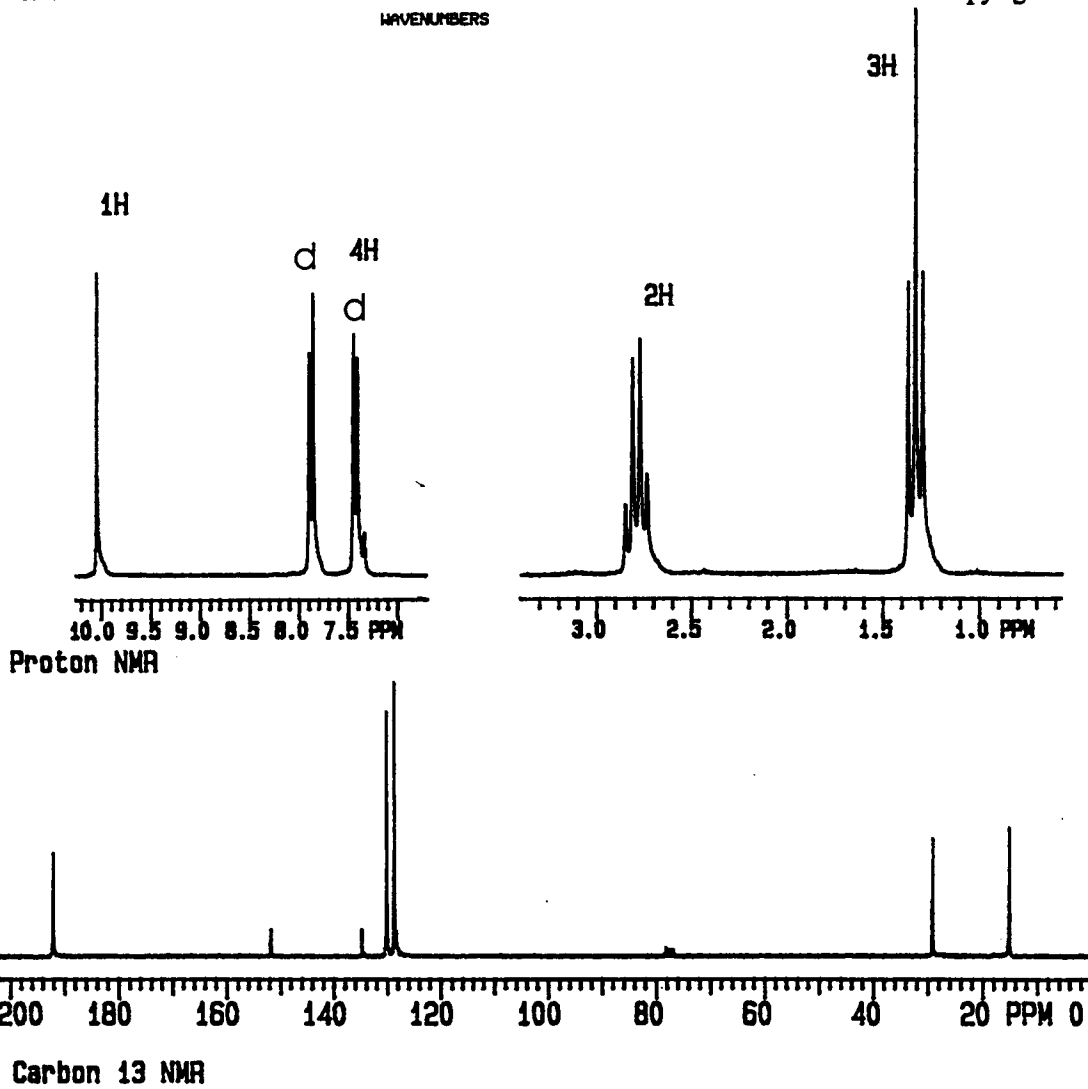
Mass Spec. Data

relative abund.

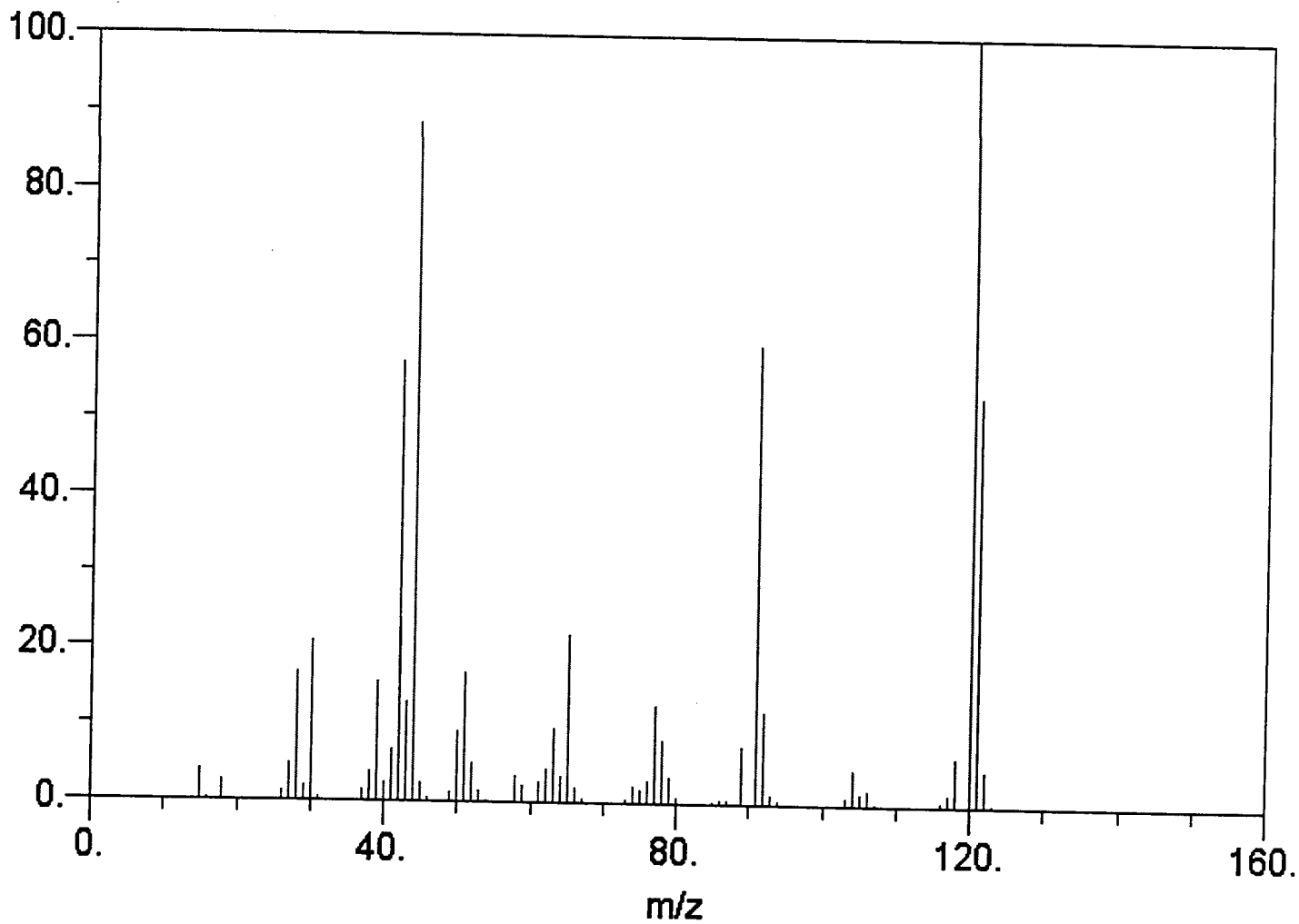
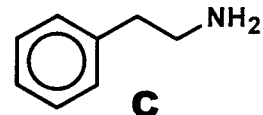
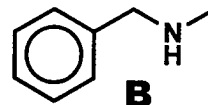
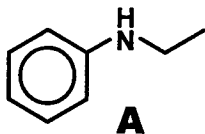
m/z	abund.
77	22
79	19
89	9
91	54
103	14
105	42
119	13
133	100
134	99
135	19

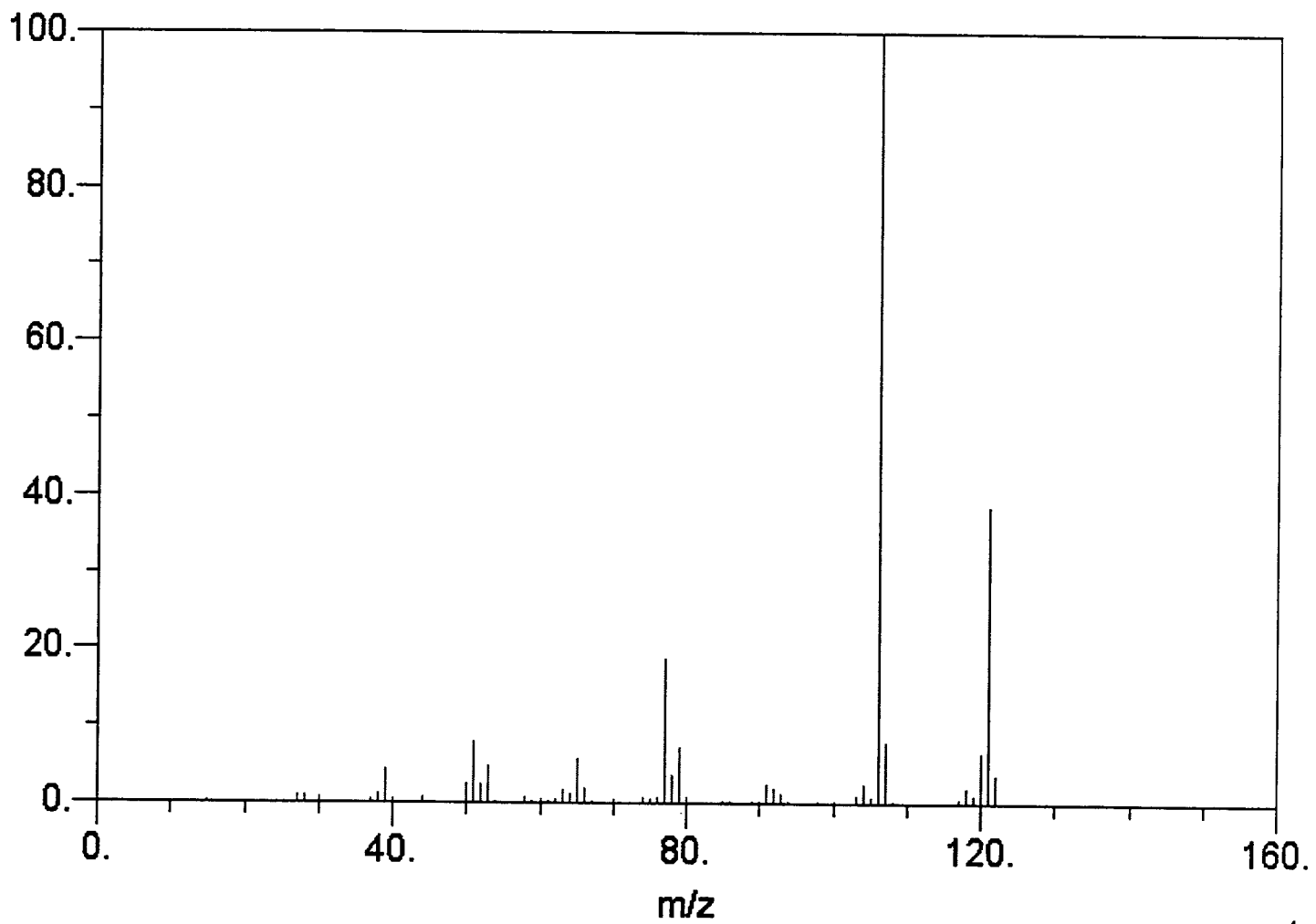
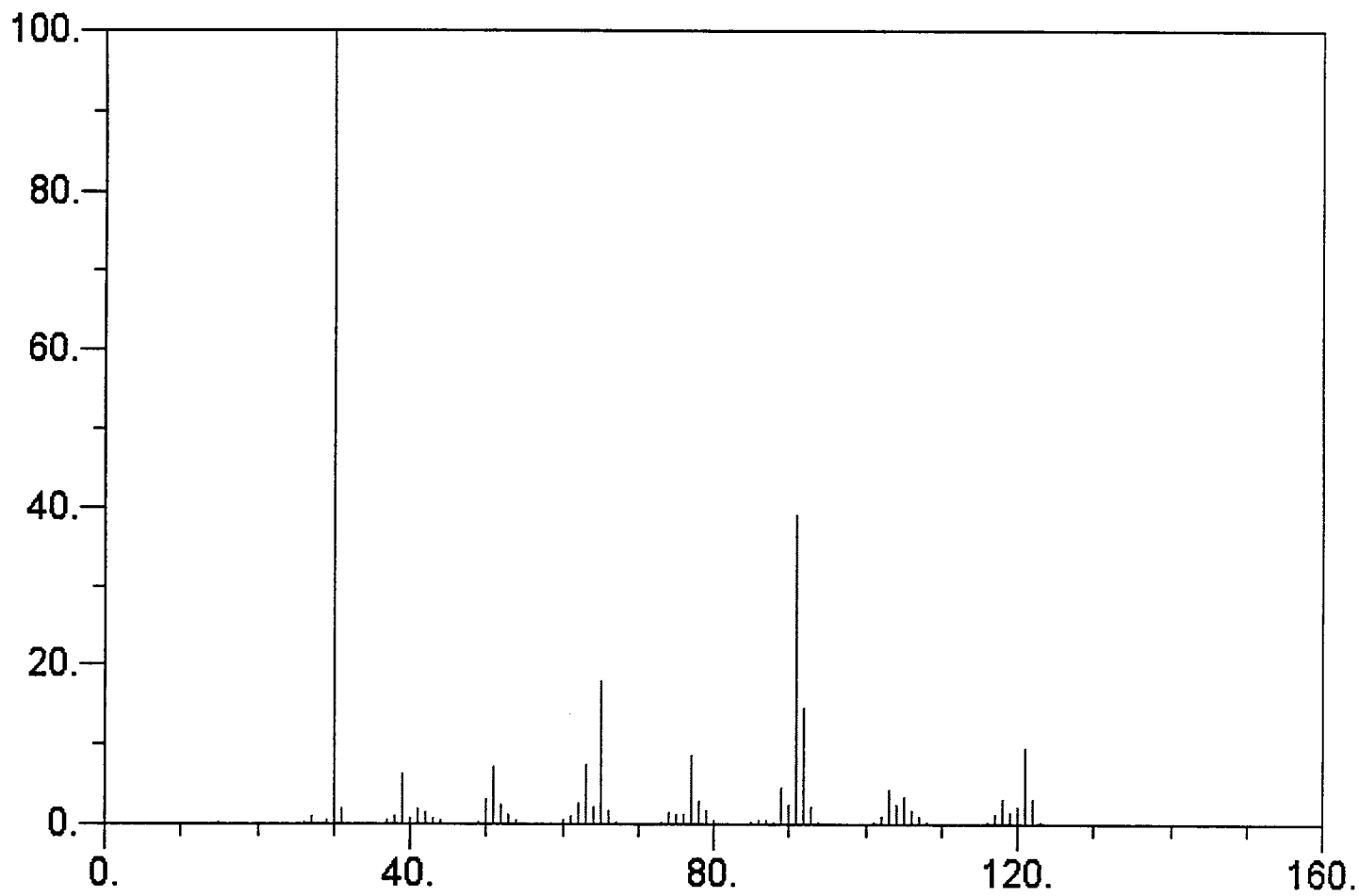


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2. Below and on the following page you will find three mass spectra. These are of a set of isomeric amines having the structures **A**, **B**, and **C**. In the space below show which structure goes with which mass spectrum and indicate reasoning behind your decision. In each case give the structure of the ion giving the base peak.





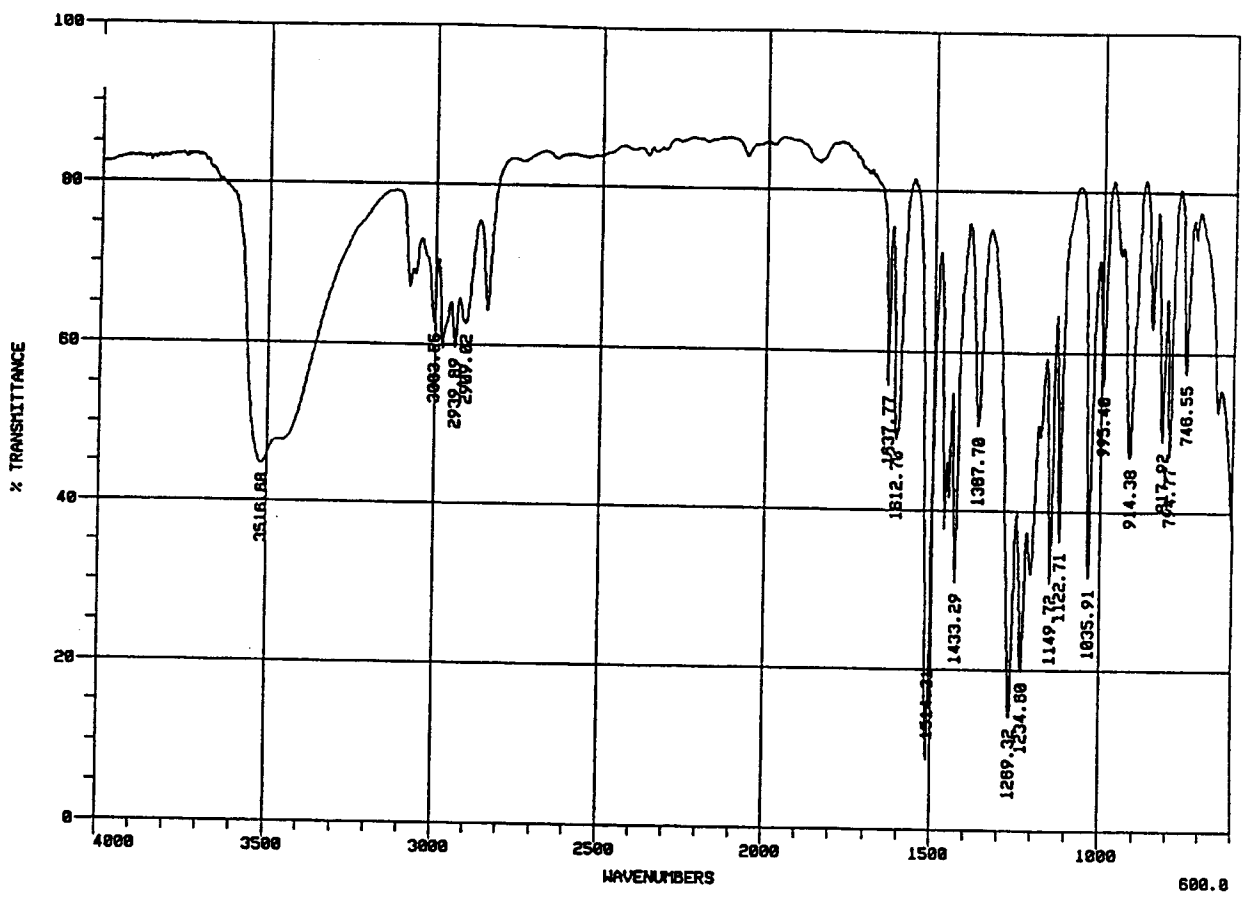
3. The spectra of the compound $C_{10}H_{12}O_2$ are given on the next page. When the 1H NMR spectrum was measured at 500 MHz the peaks between δ 6.5-7.0 clearly resolved into two sets of doublets with the same J and a singlet. A NOESY spectrum provided additional information. The singlet showed a cross peaks with the peaks at δ 3.9, 6.0, and 3.4. The newly resolved doublet at δ 6.7 showed a cross peak with the peaks at δ 3.4. The peak at δ 5.6 exchanged with D_2O . Note that not all of the multiplicities are resolved. Give the structure of the compound, provide your rationale and assign the NMR spectra.

MW 164

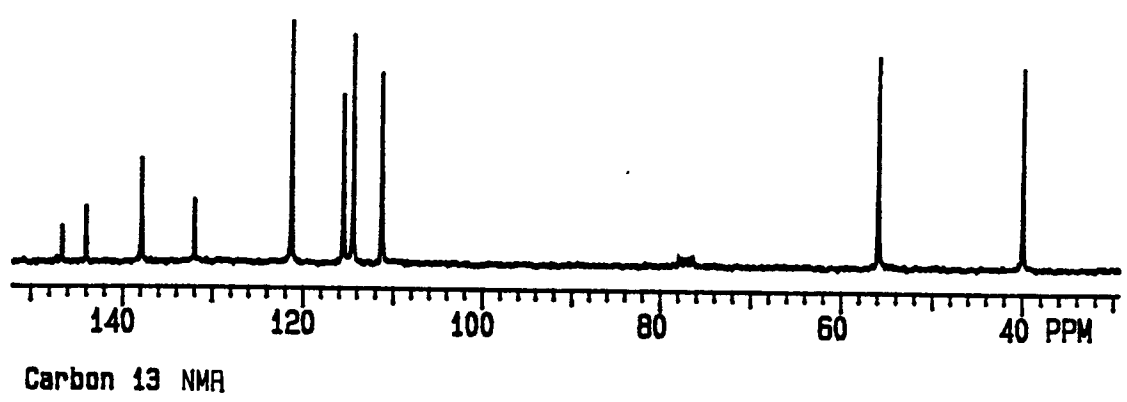
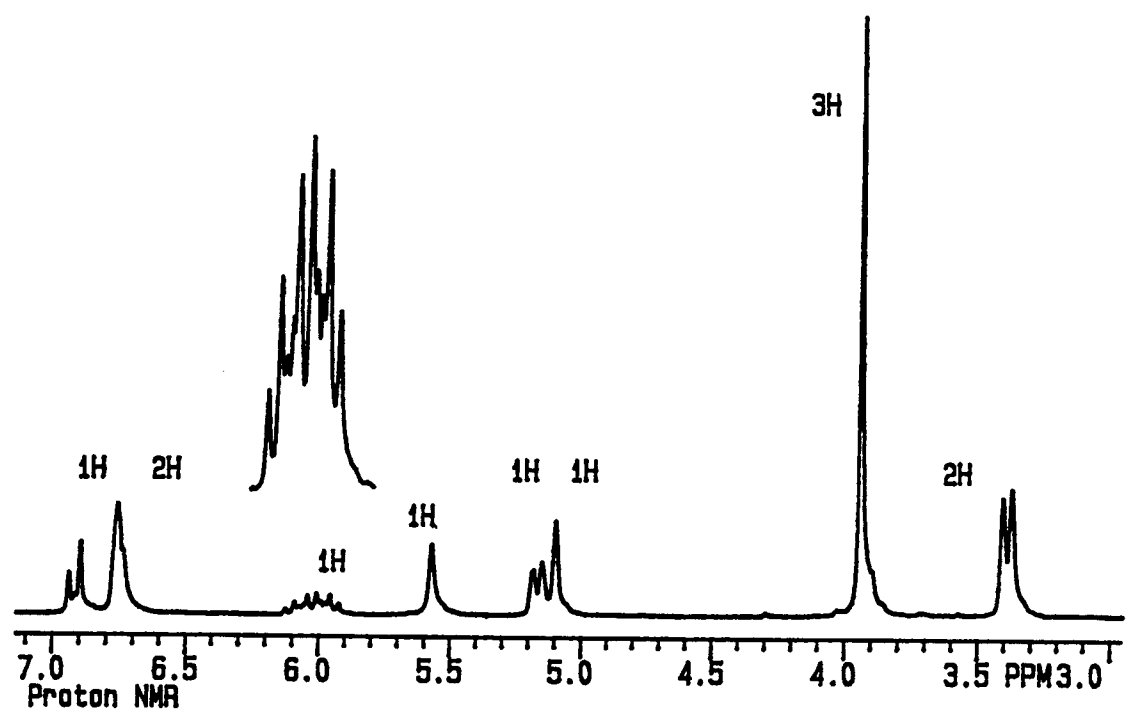
$C_{10}H_{12}O_2$

Mass Spec. Data

m/z	relative abund.
77	24
103	23
104	14
121	16
131	27
132	14
133	19
137	22
149	36
164	100
165	12



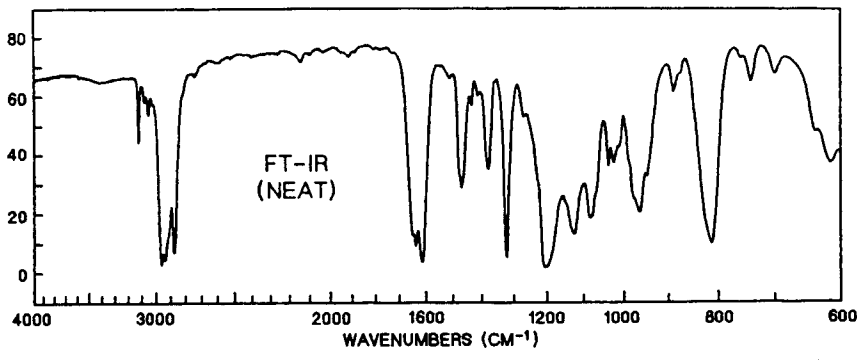
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4. The spectra given on the next page, including the COSY given on the last page, are for a compound having the formula $C_6H_{12}O$.

a. Is the base peak an odd or even electron ion?

b. Give the structure of the compound showing your rationale. Use the COSY spectrum to provide a complete assignment for the 1H NMR spectrum.



Exact M.S. (EI) = 100.0888
 UVλ_{max} = BLANK

