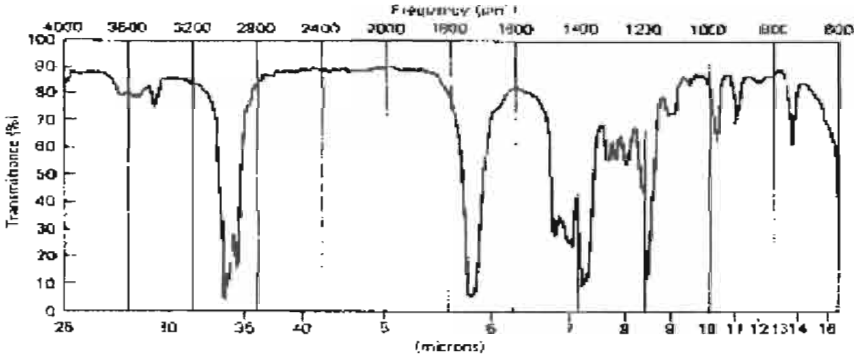
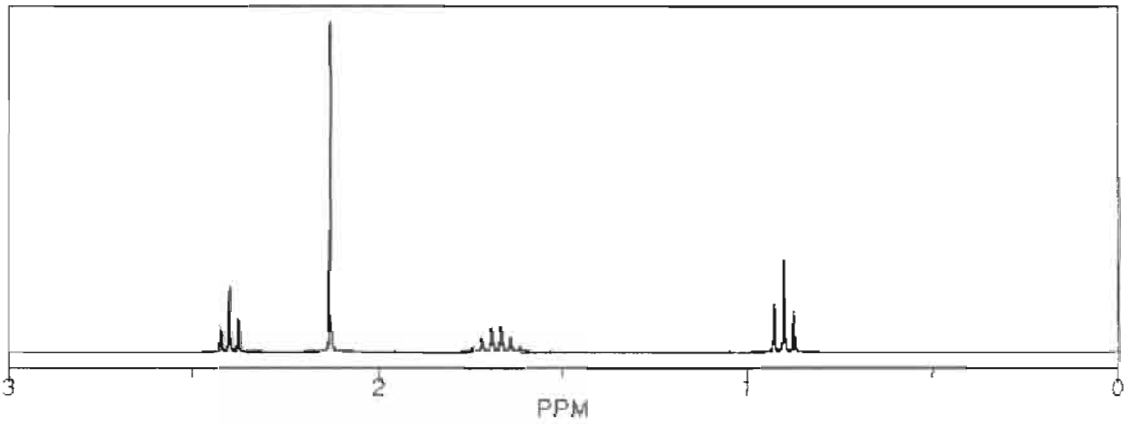
12, 13 & 14. Spectroscopy Problem Set

1. Identify the unknown compound from the spectra presented.

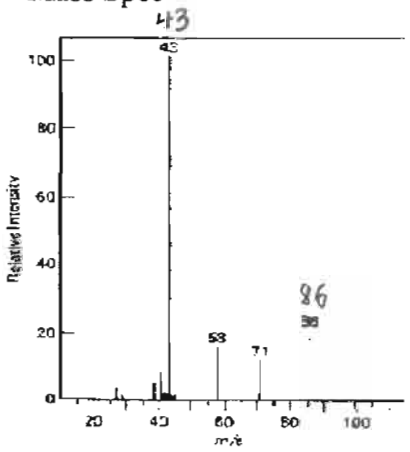
Infrared



Proton NMR



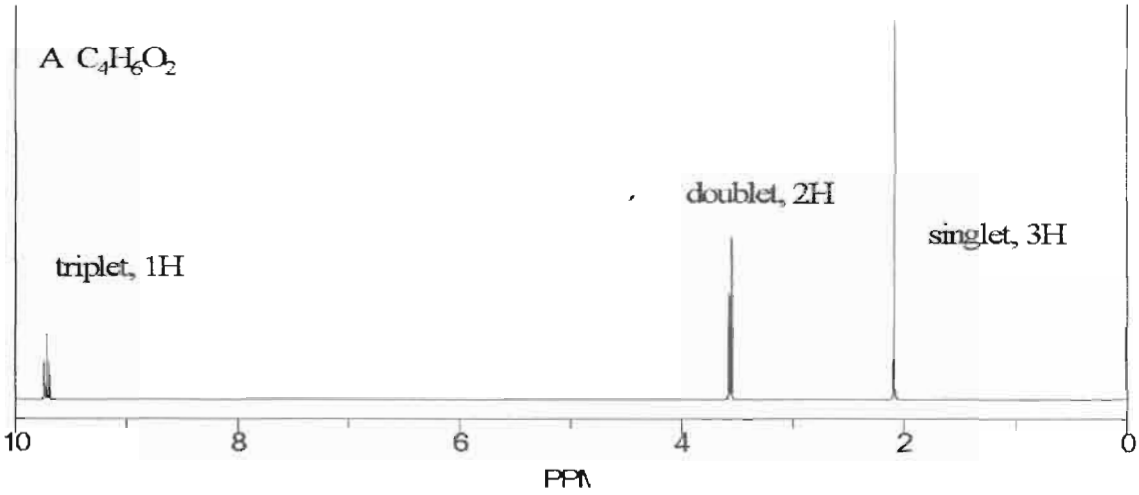
Mass Spec



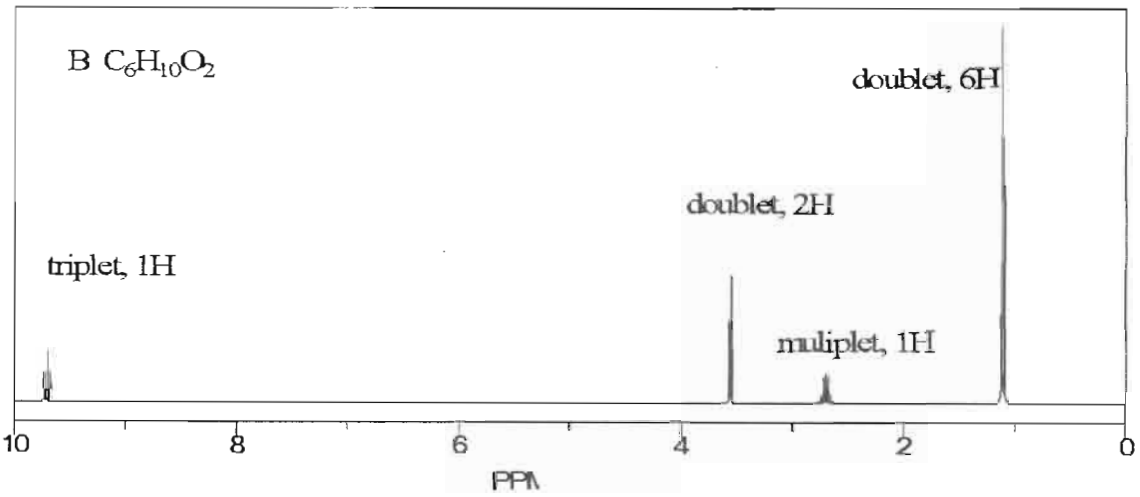
Relative intensities

86	(100%)
87	5.6%
88	0.35

2. A naturally occurring molecule, $C_{10}H_{16}$, was subjected to ozonolysis and yielded two compounds, A and B. A had the formula $C_4H_6O_2$ and the NMR spectrum presented below. A produces a bright mirror when treated with ammoniacal ammonia.

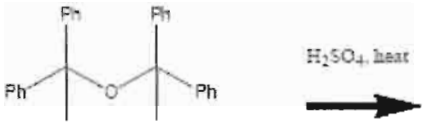


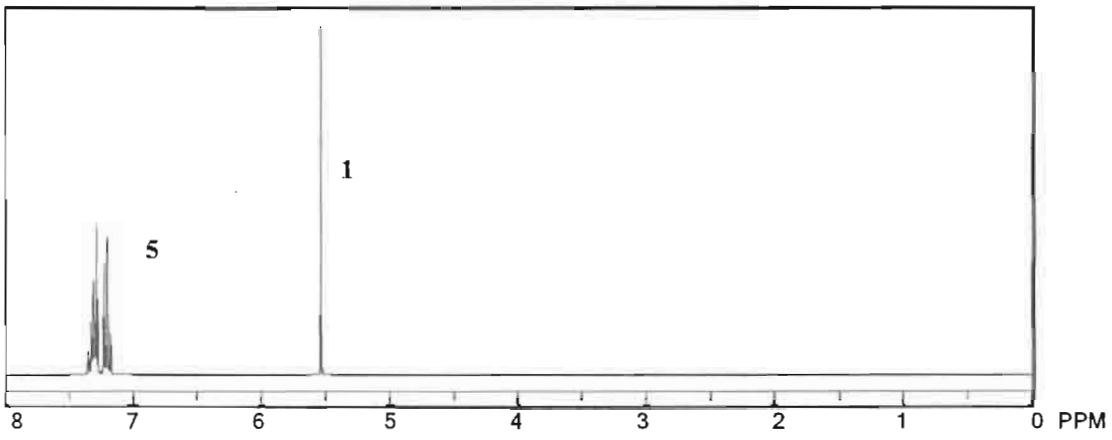
B has the formula $C_6H_{10}O_2$ and the NMR below.



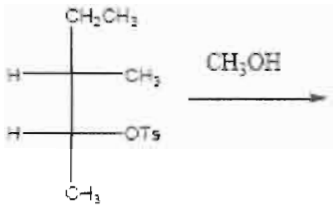
Present reasonable structures for all compounds X, A & B.

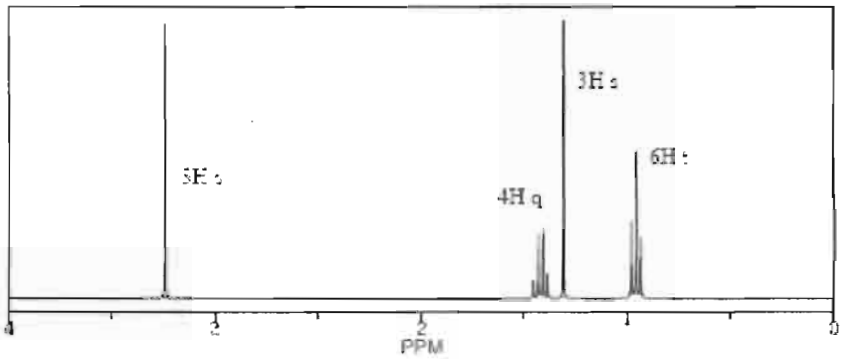
3. Use the proton NMR spectrum provided below to determine the identity of the product formed in the following reaction.



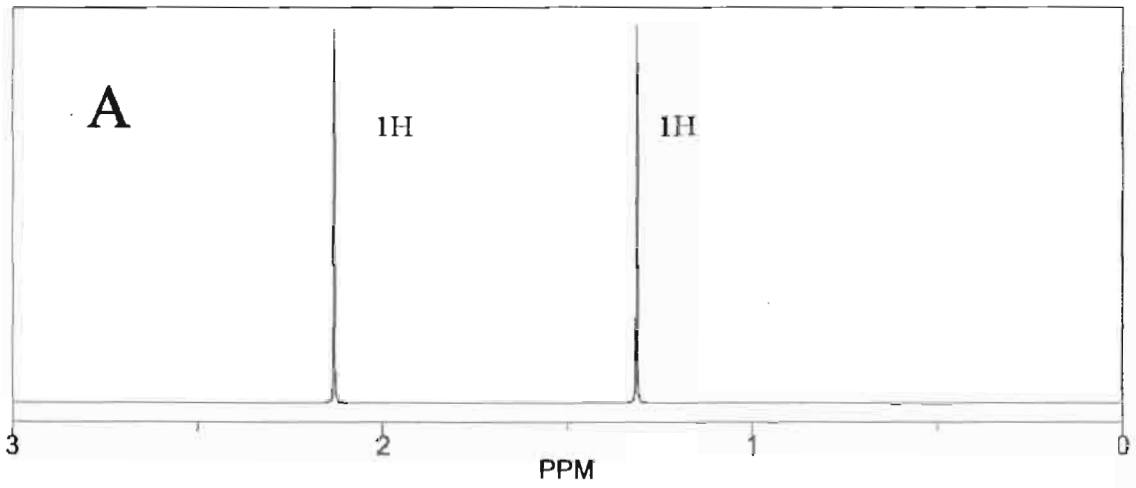


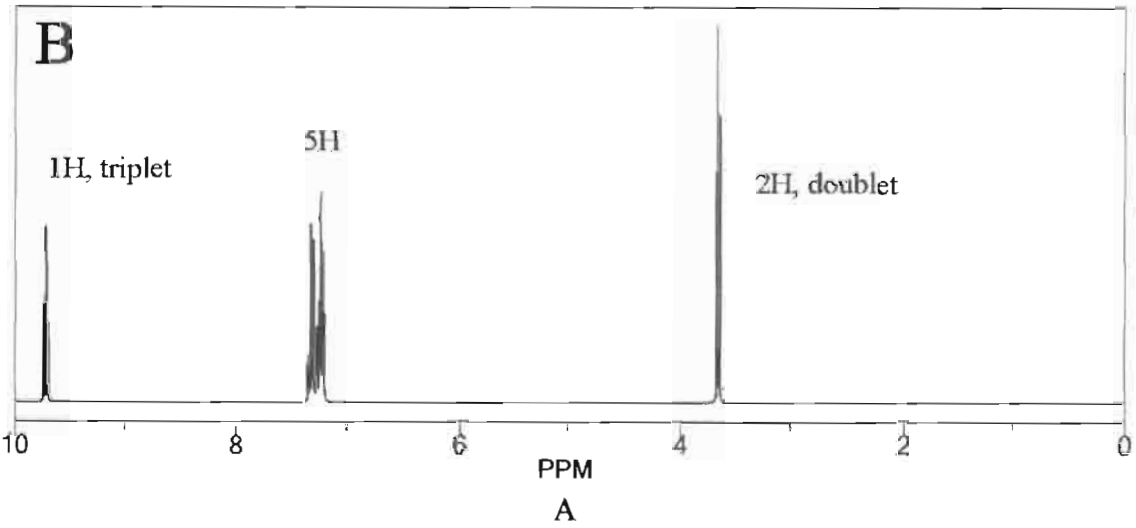
4. Use the proton NMR spectrum provided below to determine the identity of the product formed in the following reaction.





5. An unknown compound, X, has the formula $C_{23}H_{28}$. When X is subjected to ozonolysis two compounds are isolated: A and B. A has the formula $C_7H_{12}O_2$. A yields a positive iodoform and a negative Tollens. B is negative to iodoform and positive to Tollens. The NMR spectra of both A and B are presented below. Propose structures for X, A and B.





A

B

6. Compound A has a molecular formula $C_6H_{14}O$. It readily undergoes dehydration. Compound A has the following peaks in the proton NMR spectrum: δ 0.90 (t, 6H), 1.12 (s, 3H), 1.38 (s, 1H) and 1.48 (q, 4H). The 13C NMR spectrum shows signals at 72.98, 33.72, 25.85 and 8.16. Deduce a structure for the unknown compound.

7. Use the IR and proton NMR spectra shown below to determine the identity of compound B which has a molecular formula of $C_8H_{10}O$.