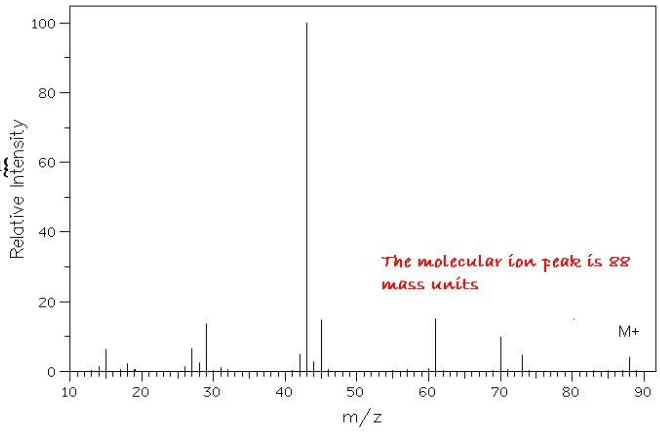
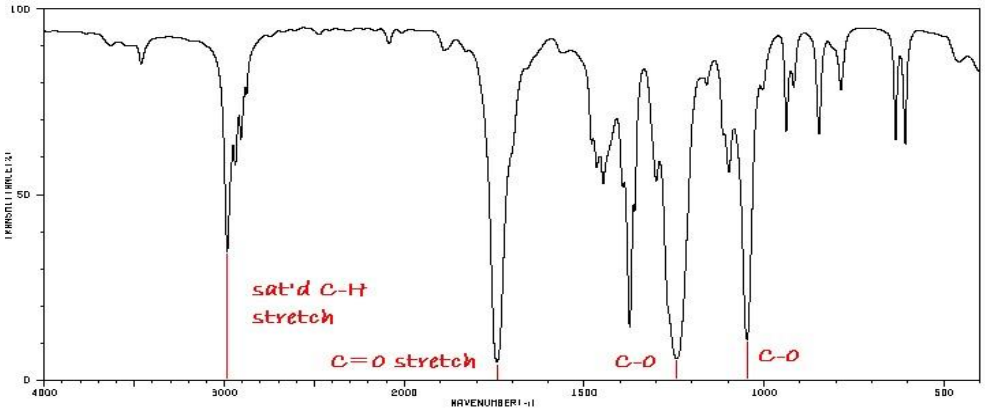
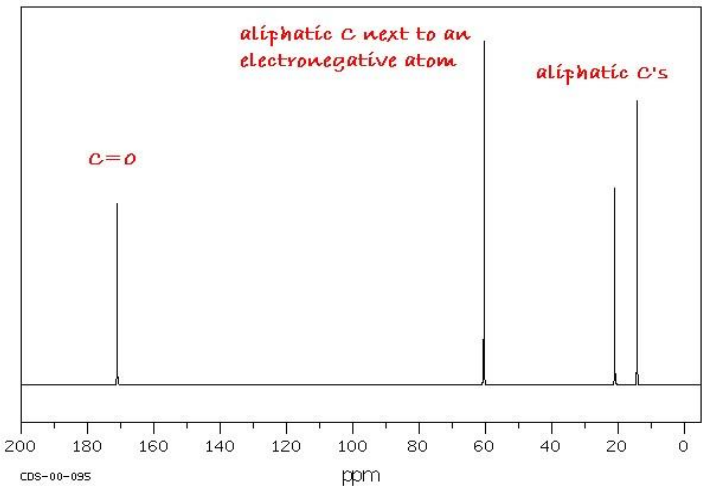
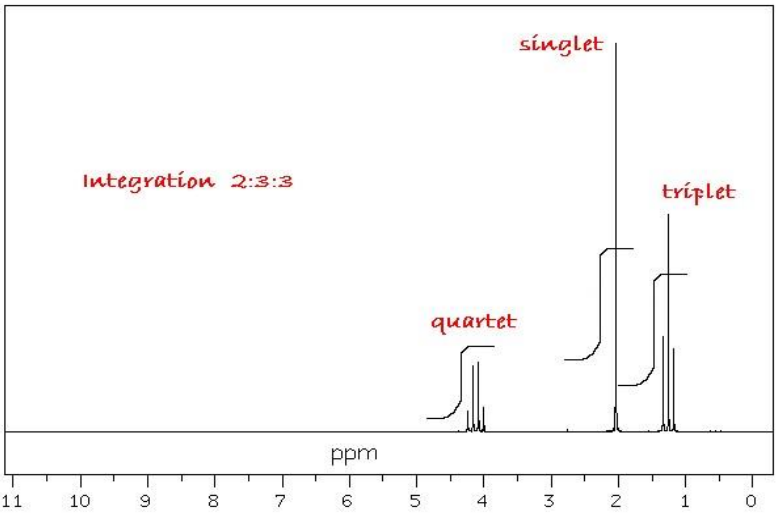
Example Spectra Problem The spectra here have been marked to indicate major absorptions. Other answers are entered on the next page.









Answer to Example Problem

The integral molecular weight of the unknown is 88. Because this is an even number, the compound has either no nitrogen atoms or an even number of N atoms. The highest m/z peaks do not show evidence of the presence of atoms such as Cl or Br (which would have two peaks in 75:25 and 50:50 ratios, respectively).

Elemental Analysis:

None was given

IR Analysis:

The absorption at 3000 cm^{-1} (and not to the left) shows only aliphatic (saturated) C–H groups. The carbonyl, C=O, absorbs strongly at 1740 cm^{-1}. The two intense peaks between 1000-1300 cm^{-1} indicate the carbonyl belongs to the ester group.

^{13}C-NMR analysis:

The NMR shows 4 different kinds of carbon atoms. The absorption at 172 ppm is typical of the carbonyl carbon. The upfield absorptions at 14 and 21 ppm are likely $–CH_3$ and/or $–CH_2–$ groups (although no C– H splitting patterns are given with this spectrum). The absorption at 61 ppm could be a C next to an electronegative atom.

^{1}H-NMR analysis:

The NMR shows three different kinds of CH groups. The integration of 2:3:3 suggests a methylene ($–CH_2–$) and two methyls ($–CH_3$). The CH group absorbing as a singlet cannot be next to a neighboring CH group (n+1=1 and so n=0). The upfield triplet must be next to a C bonded to 2H's (n+1=3) and the downfield quartet must be next to a C bonded to 3 H's (n+1=4). The triplet integrates for 3H's and so must be a $–CH_3$ group next to a methylene; the quartet integrates for 2 H's and so must be a $–CH_2–$ next to a methyl. Thus, there is an ethyl group present, $–CH_2CH_3$.

Combined Analysis:

The IR shows the only functional group present is an ester. There is no aromaticity or other unsaturation in the molecule (except for the C=O). This means that the absorption in the ^{13}C-NMR at 61 ppm cannot be due to a C=C group and the carbon causing the absorption is next to the oxygen atom of the ester. The presence of a C=O is confirmed in the ^{13}C-NMR. The ester group accounts for 44 amu of the 88 integral mass. The ethyl group is on one side of the ester functional group and accounts for 29 mass units. The remaining mass (88-44-29 = 15 and belongs to the singlet methyl group. The methyl is on the other side of the ester functional group. Because the quartet is so far downfield in the range for methylene ^{1}H-NMR absorption, the methylene must be bonded to the O of the ester.

Unknown Identity:	**Structure:**
Thus, the unknown is identified as <u>ethyl acetate</u>.