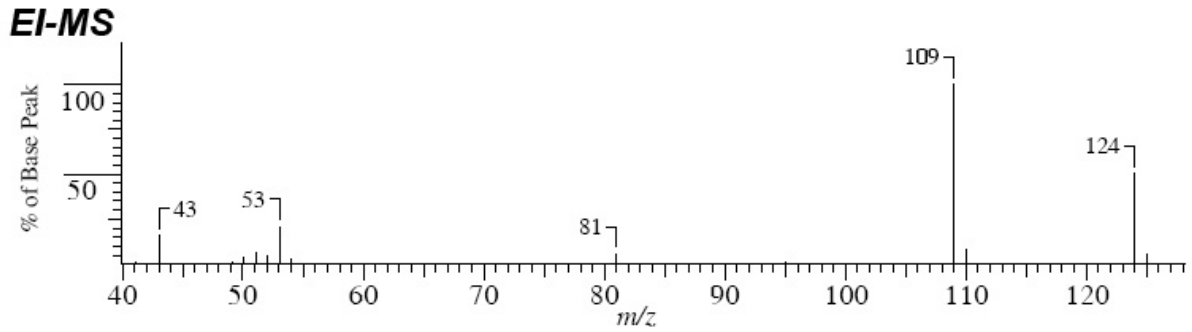
HOMEWORK-2 DUE FRI. OCT. 3

Use the data below to propose and defend a structure of a compound. Under each piece of data provide "conclusions". There is a final assignment page at the end.



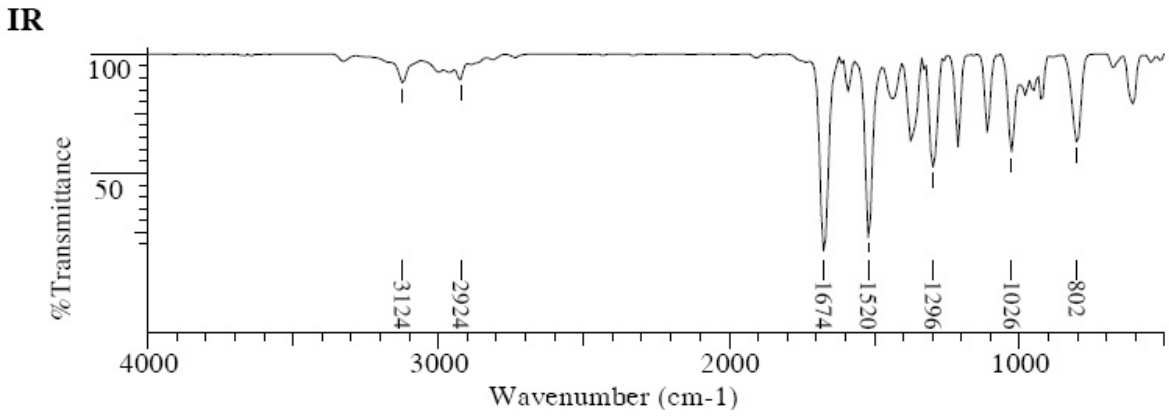
Conclusions:

Rule of 13: n=9, r=7 so a base formula of C_9H_{16}. In the ^{13}C NMR there are 7 C's so that makes our formula $C_7H_8O_2$. (we know that it is O and not N from the acetyl group (M-43) and IR (C=O).

m/z = 109 corresponds to the loss of a methyl group (M-15)

m/z = 81 corresponds to the loss of an acetyl group (M-43)

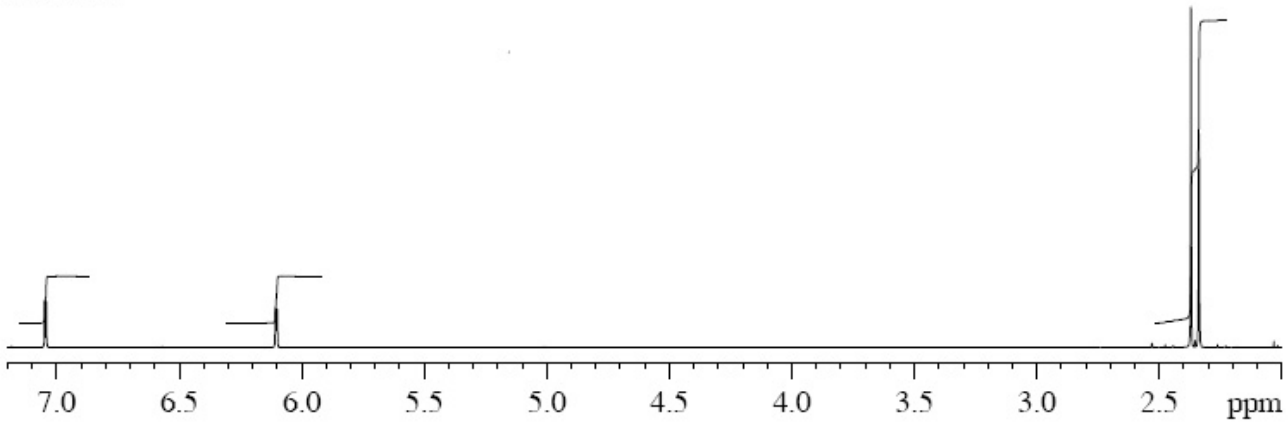
for $C_7H_8O_2$; U = 4



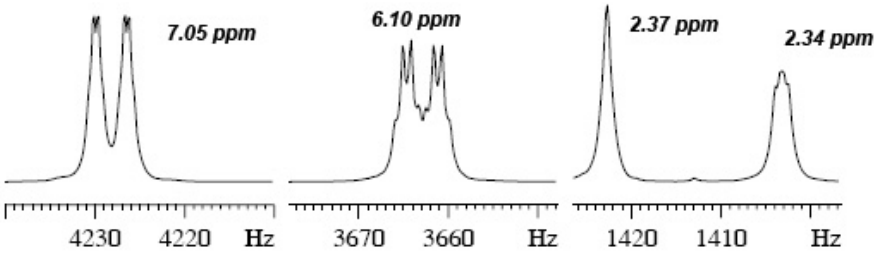
Conclusions:

3124 cm^{-1}: sp^2 hybridized C-H stretch
2924 cm^{-1}: sp^3 hybridized C-H stretch
1674 cm^{-1}: C=O stretch (the low wavenumber indicates that is conjugated!)
1026 cm^{-1}: C-O sigma bond stretch
Since we have a C=O stretch and U=4….we cannot have a benzene ring!

1H NMR



1HNMR Expansions



Conclusions:

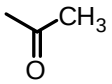
7.05 and 6.10 are coupled doublets (J = 4 Hz, in the aromatic region!)

The singlet at 2.37 suggests an isolated $–CH_3$ group.

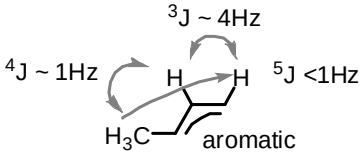
The app t at 2.34 suggests a $–CH_3$ group that is experiencing long range ($^{4\text{-}5}J$ coupling~ 1 Hz). This is consistent with the dq at 6.10 (J = 4, ~1 Hz)

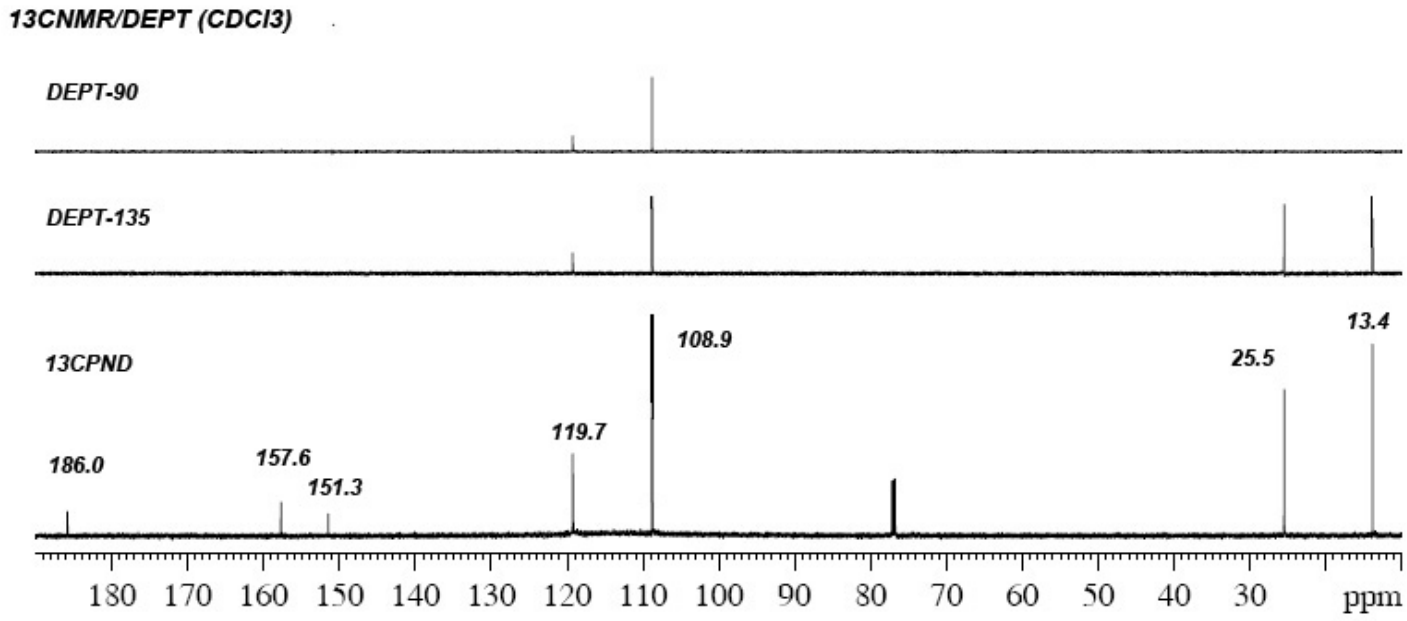
Both $–CH_3$ groups are downfield ~ 2.5 ppm suggesting that they are attached to an aromatic ring or α-to a carbonyl.

With the acetyl mass fragment we can be sure that we have a methyl ketone:



We can also suggest the following spin system:





Conclusions:

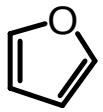
186 is consistent with a conjugated methyl ketone.

157.6 and 151.3 are consistent with oxygenated aromatic carbons.

119 and 108 are consistent with aromatic carbons.

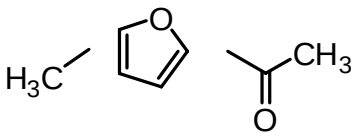
25 and 13 are consistent with methyl groups (also their absence in the DEPT-90.

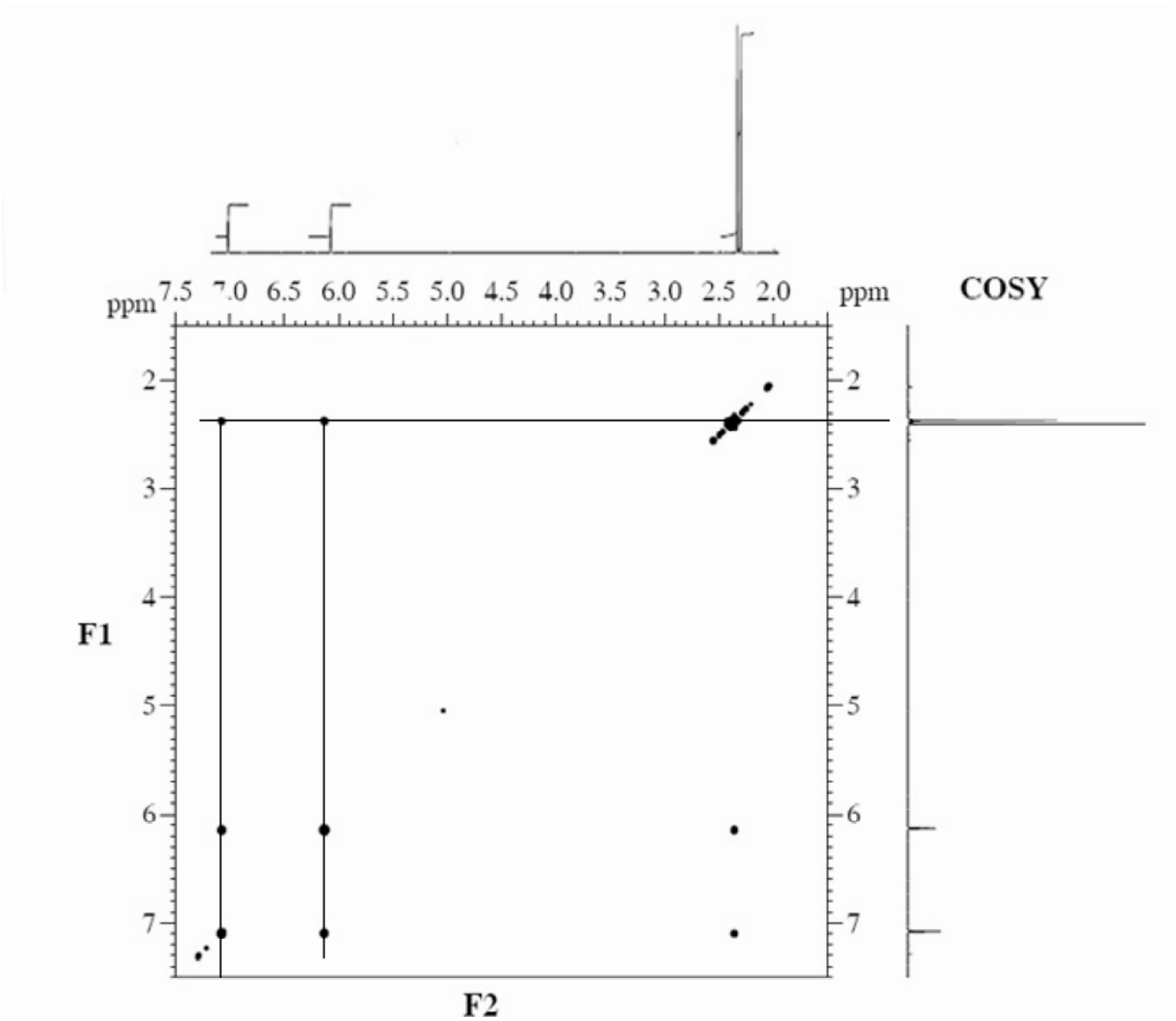
So we have an aromatic system with 4 carbons….2 of which may be oxygenated! Highly suggestive of a furan



Now we have the aromatic nucleus and two substituents:

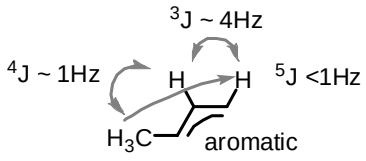
Note the Furan and Carbonyl are also consistent with U = 4!

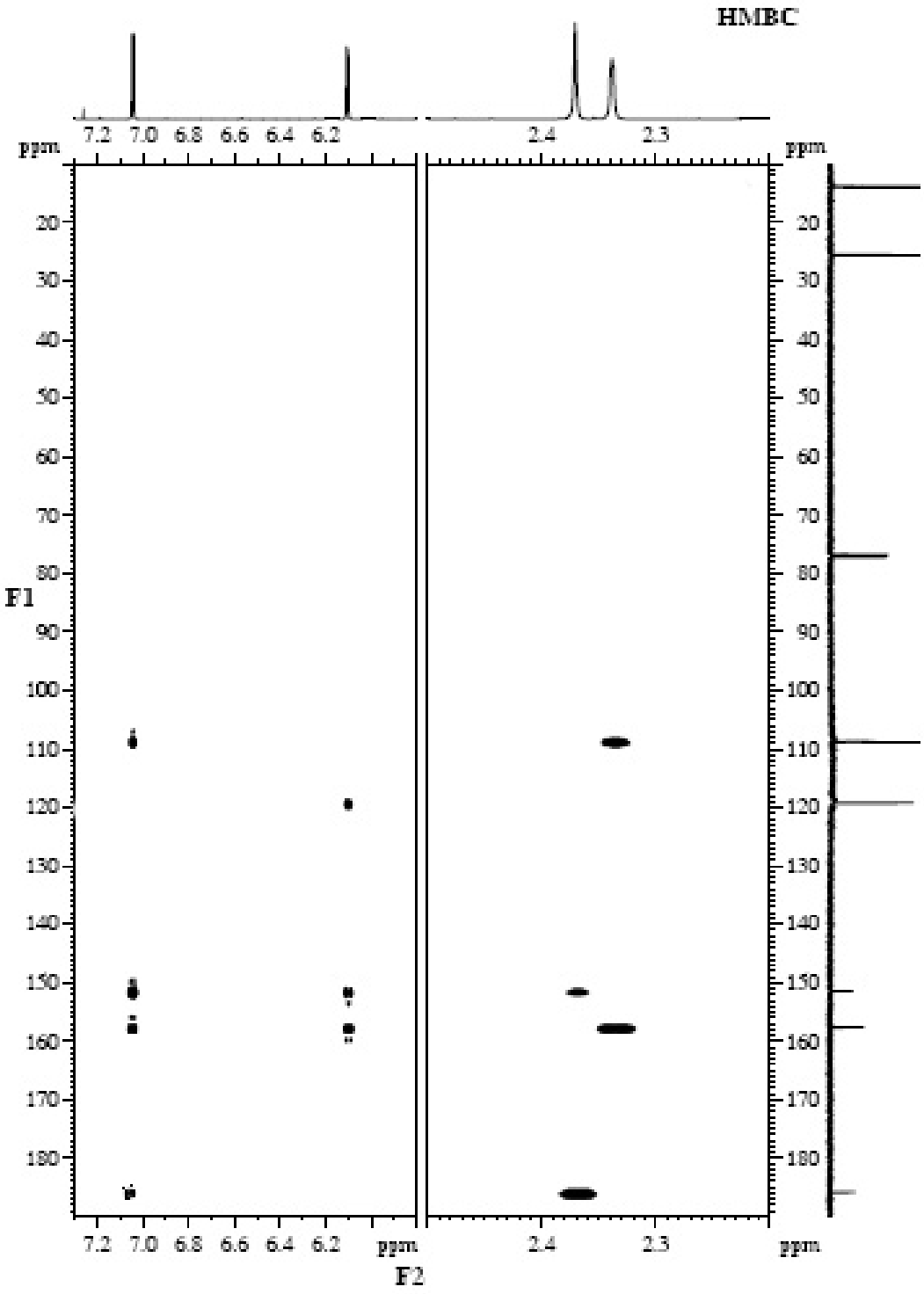




Conclusions:

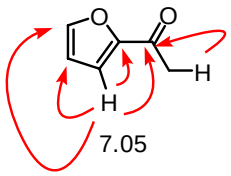
Reconfirms our ^{1}H arguments that we have the following spin system





Conclusions:

The proton at 7.05 must be ortho to the acetyl and ortho to the C-H bond…thus the furan must be 1,4-disubstituted.



Final Structural Assignment: