Marks 8

- Shown overleaf are the mass (MS), infrared (IR), ^{1}H and ^{13}C NMR spectra for a compound of empirical formula $C_{10}H_{11}ClO$. Use this information to deduce a structure for this compound. (NMR chemical shift ranges can be found on the next page.) Show your working below.

Working

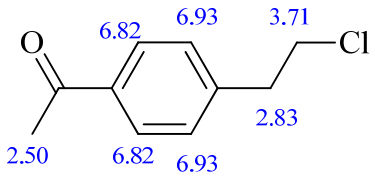
Peak at *m/z* = 43 in MS typical of $COCH_3$, confirmed by peak at 1700 cm^{-1} in IR and singlet at 2.5 in ^{1}H NMR.

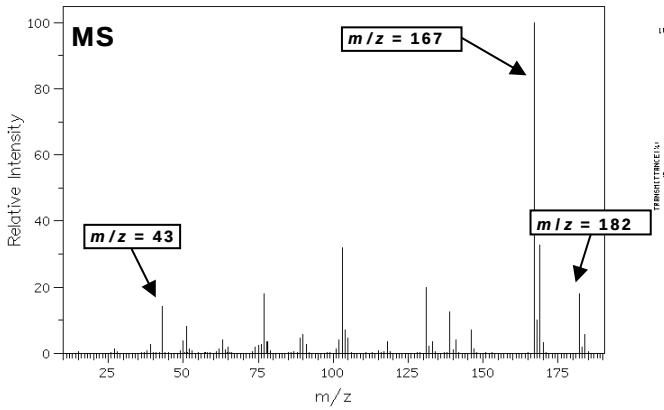
Doublets in ^{1}H NMR just below 7 are characteristic of a 1,4-disubstituted benzene ring.

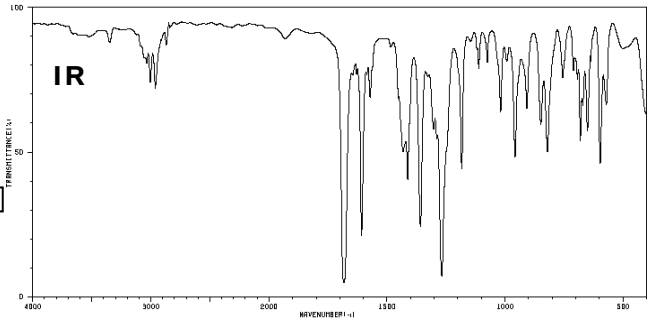
Triplets at 2.8 and 3.7 in ^{1}H NMR suggest 2 adjacent CH_2 groups.

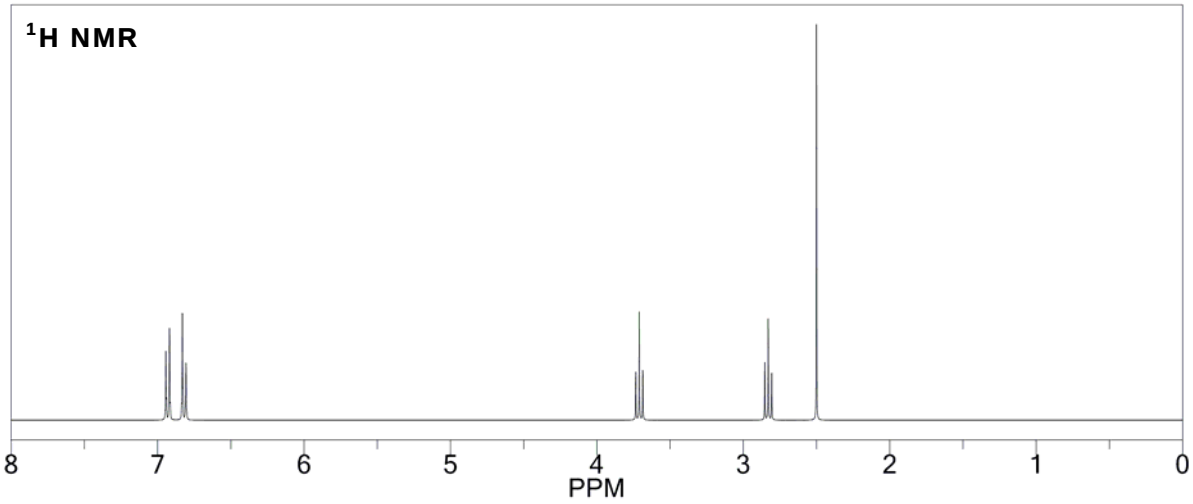
Hence structure below, supported by chemical data shift.

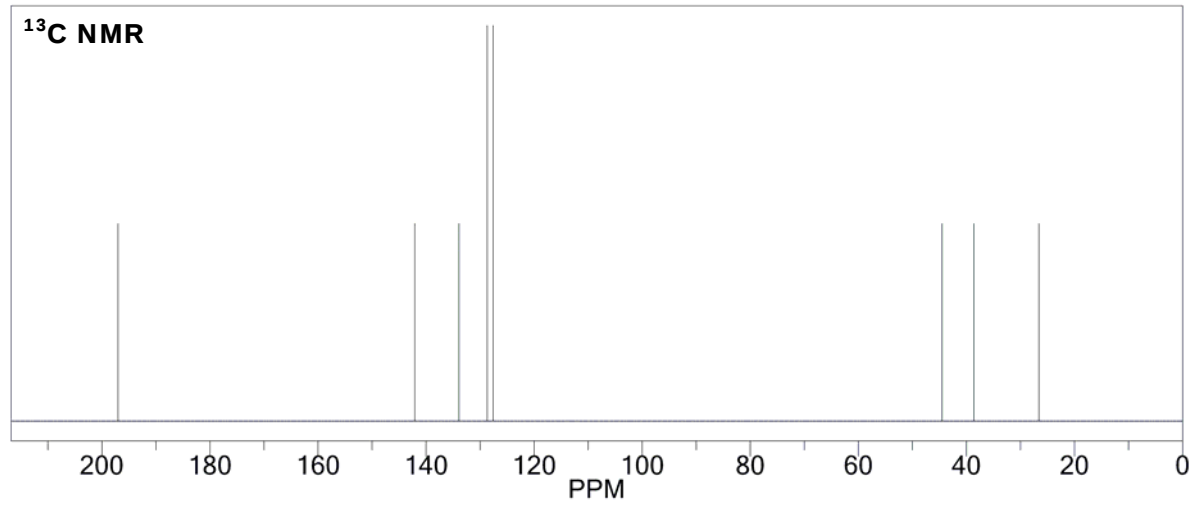
Structure



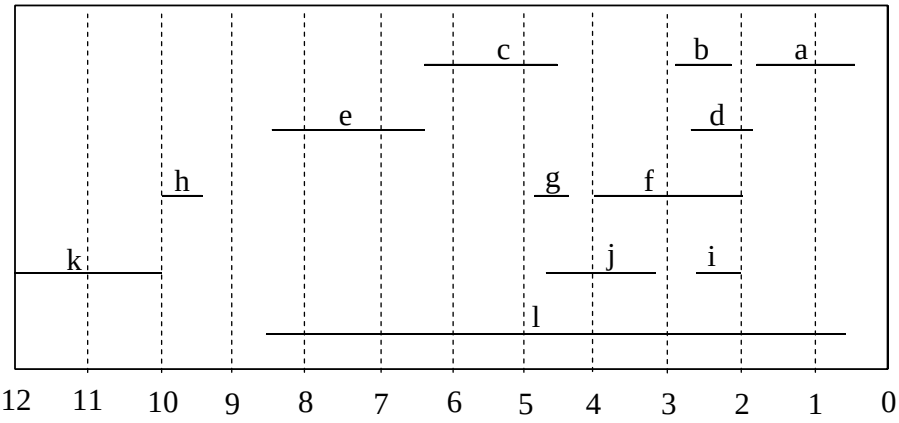

MS
m/z = 167
m/z = 43
m/z = 182
Relative Intensity
m/z


IR


1H NMR
PPM

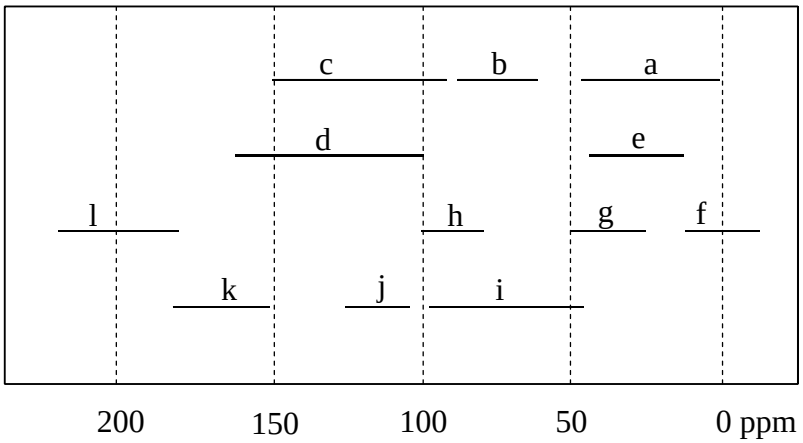

13C NMR
PPM

^{1}H NMR Chemical Shifts



a R−H
b Ph−C−H
c C=C−H
d C≡C−H
e Ph−H
f X−C−H (X = Cl, Br or I)
g F−C−H
h —C(=O)−H
i C(=O)−C−H
j O−C−H
k C(=O)−O−H
l ROH, PhOH, RNH

^{13}C NMR Chemical Shifts



a alkanes
b alkynes
c alkenes
d aromatics
e C-Br
f C-I
g C-Cl
h C-F
i C-O
j C≡N
k acids, esters, amides
l aldehydes, ketones