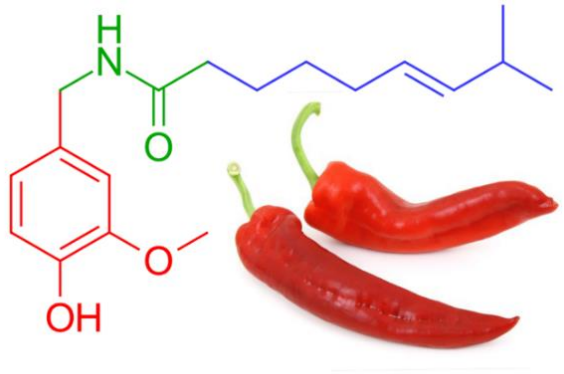
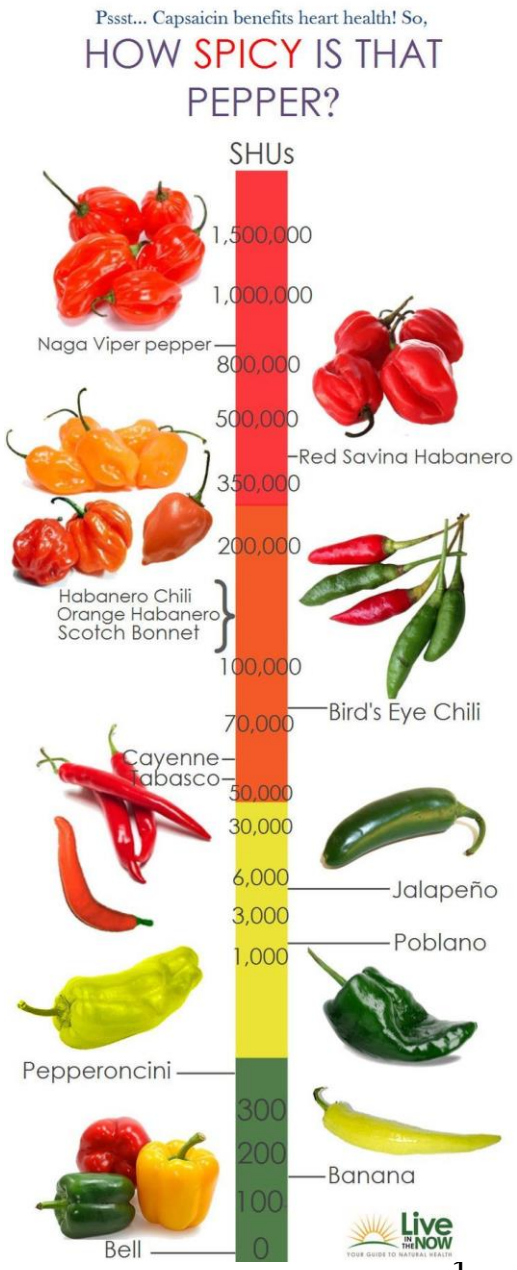
Benzene e composti aromatici

- **Benzene struttura e nomenclatura**
- **Composti aromatici di interesse**
- **Aromaticità — Regola di Hückel**





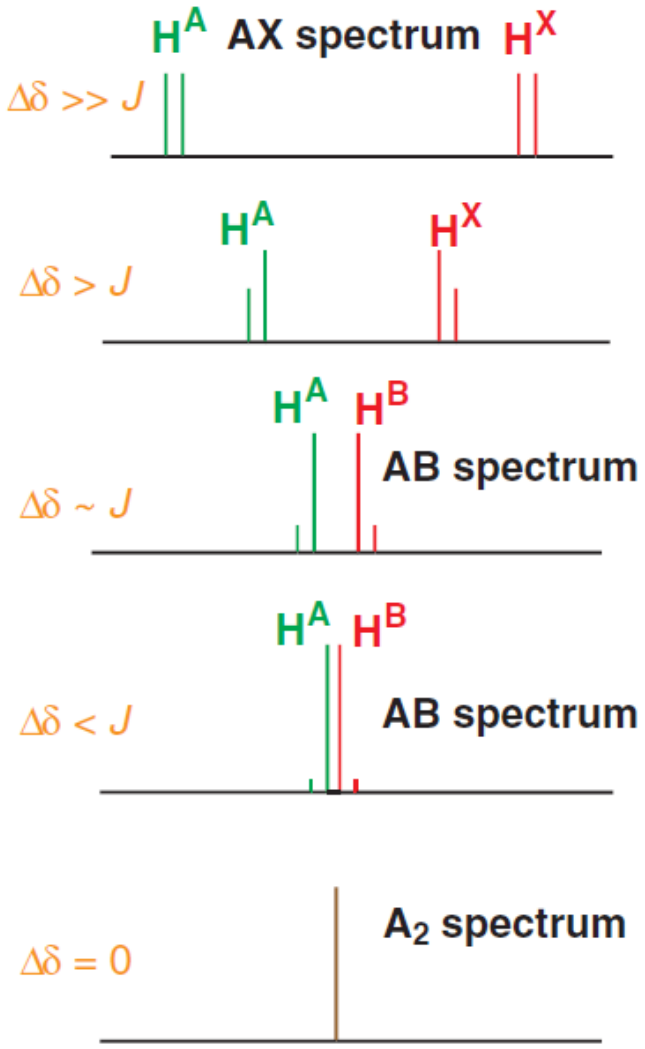
La **capsaicina** è responsabile del caratteristico sapore piccante dei peperoni jalapeño e habañero. Sebbene produca inizialmente una sensazione di bruciore al contatto con la bocca o la pelle, applicazioni ripetute desensibilizzano l'area al dolore. Per questo viene usato come principio attivo di numerose creme topiche per il trattamento del dolore cronico. La capsaicina è stata anche usata come deterrente negli spray al peperoncino e come additivo per rendere il becchime a prova di scoiattolo.

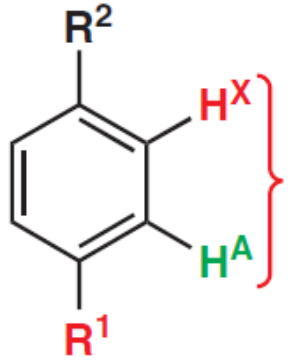
Squirrels just won't give up

https://www.treehugger.com/trying-find-squirrel-proof-birdseed-good-luck-4863352

Immagini slides da J.G. Smith, Organic Chemistry, V Ed, McGramHill Education

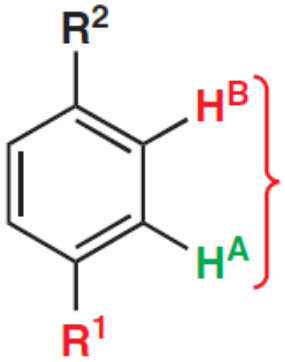
Benzene para disostituito - ^{1}H NMR





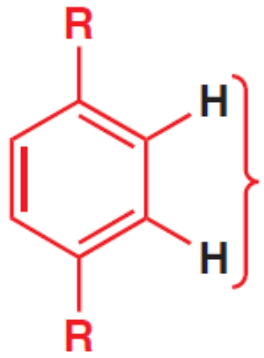
Two different Hs ($R^1 \neq R^2$) gives two doublets

two 2H doublets



if Hs are similar, coupling is seen but doublets are distorted

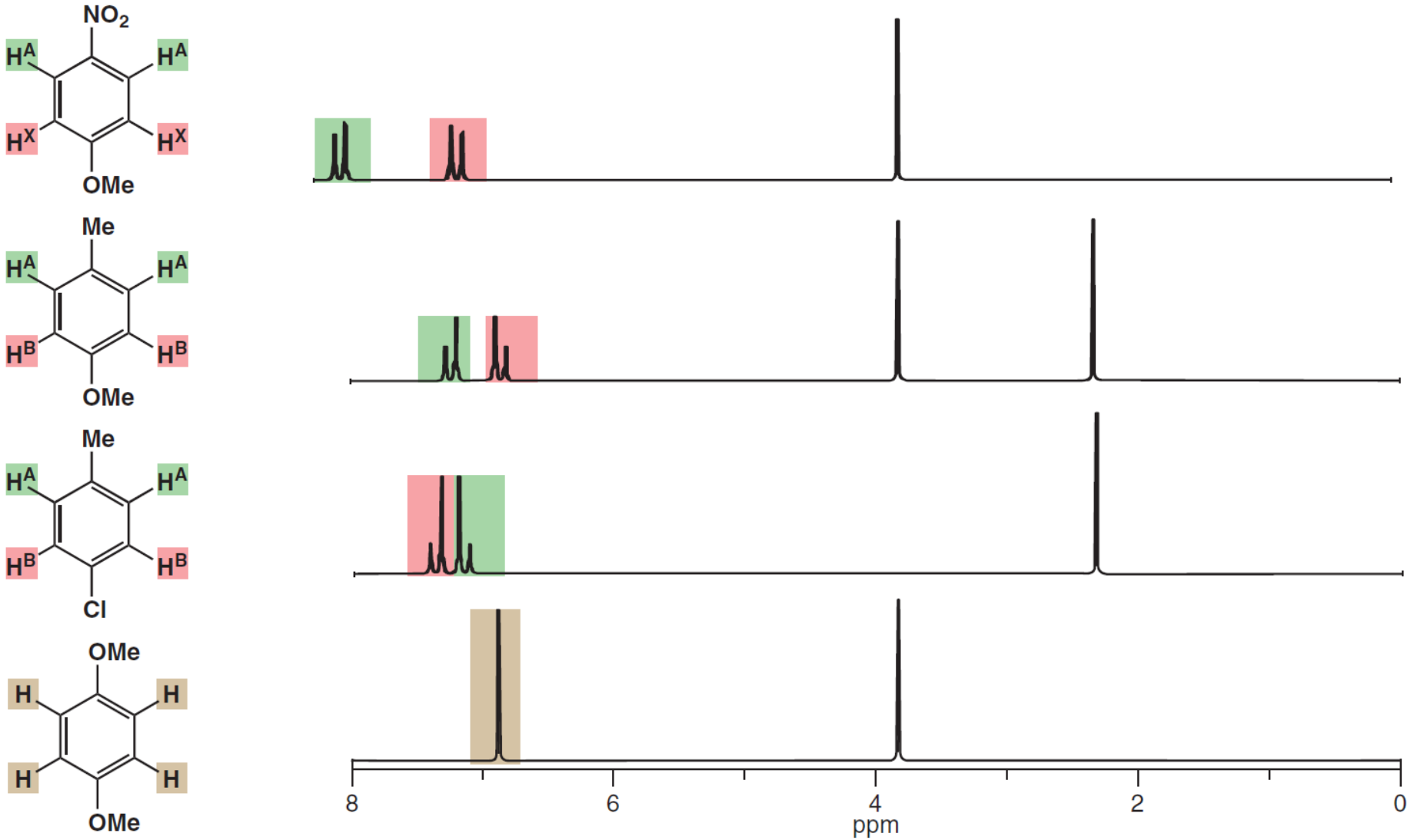
two distorted 2H doublets



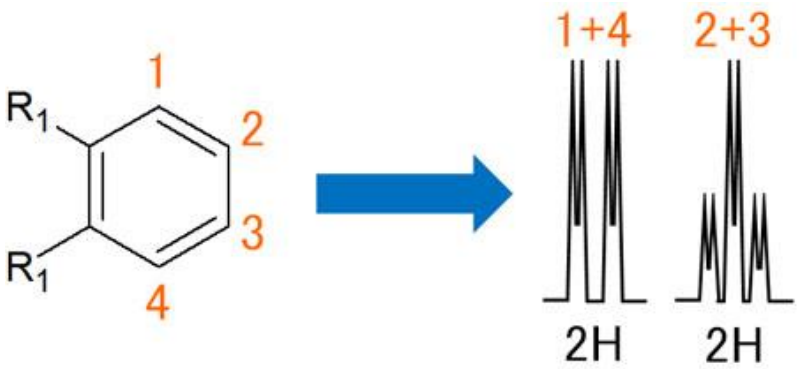
no coupling between these identical neighbours

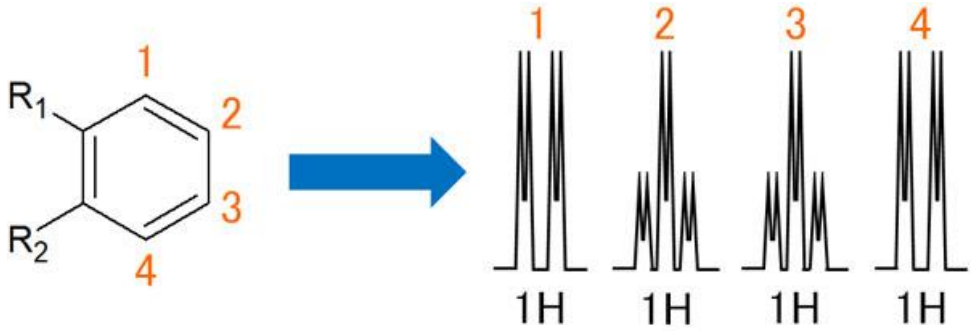
one 4H singlet

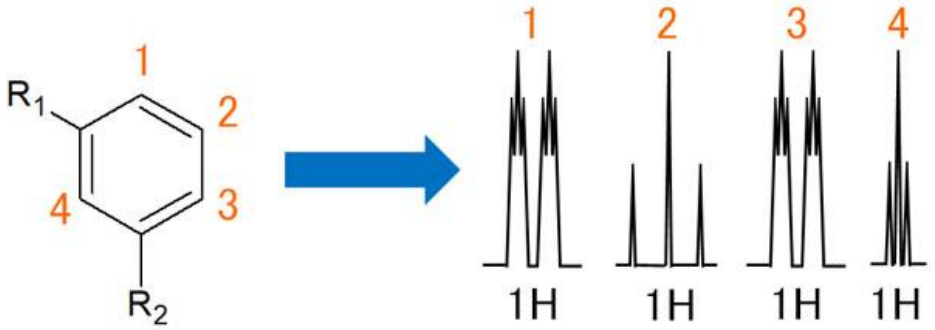
Benzene e derivati - ^{1}H NMR



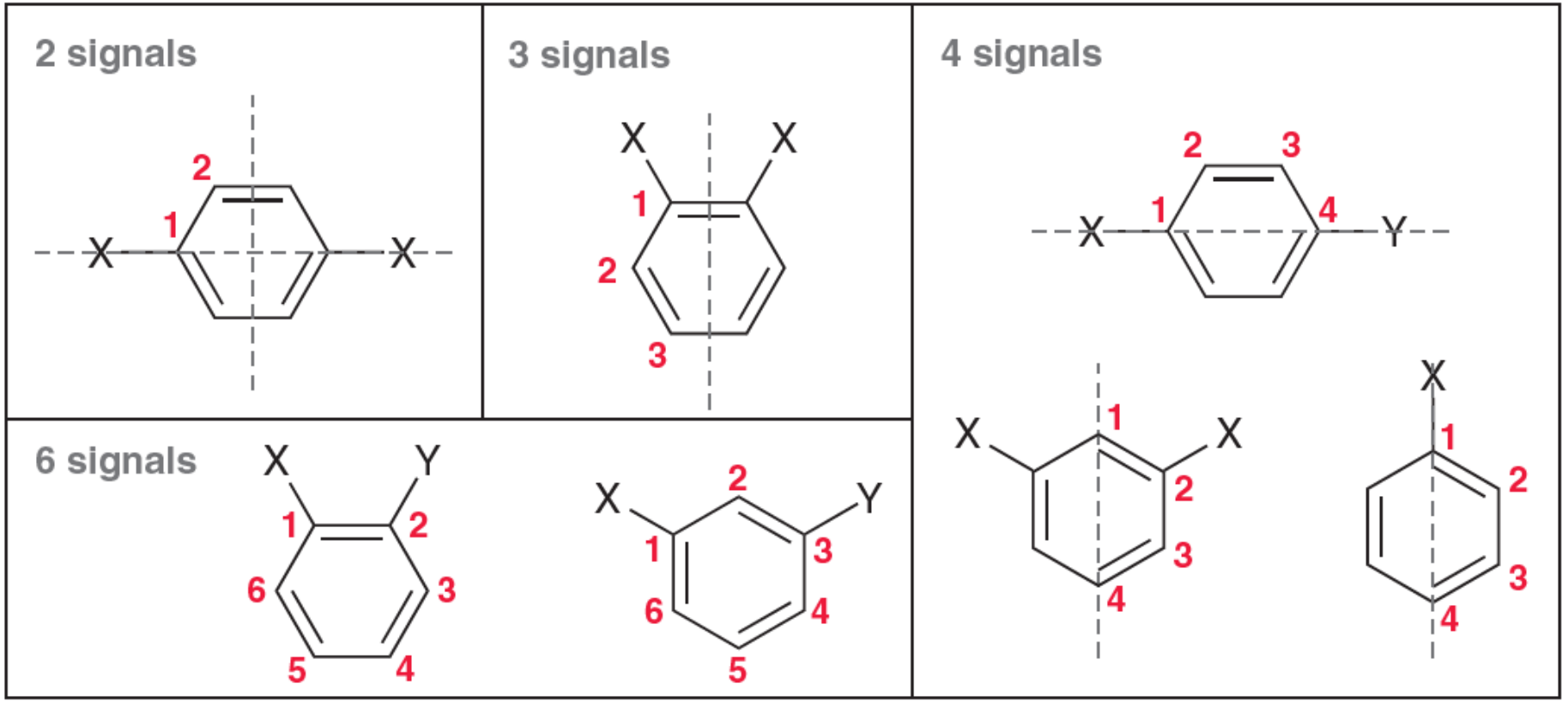
Benzene derivati disostituiti orto - ^{1}H NMR



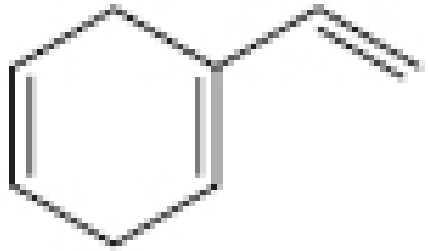


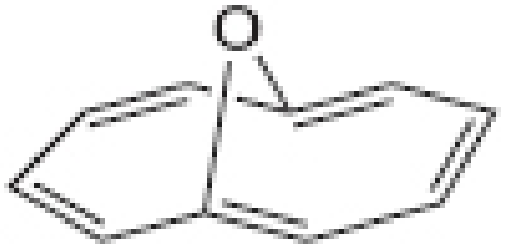


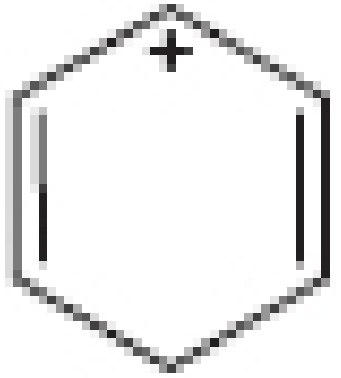
Benzene e derivati - ^{13}C NMR



Label each compound as aromatic, antiaromatic, or not aromatic.
Assume all completely conjugated rings are planar.

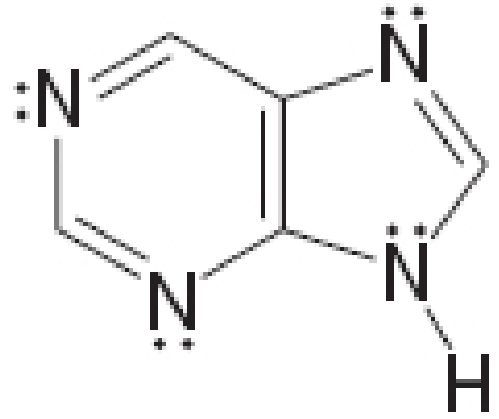






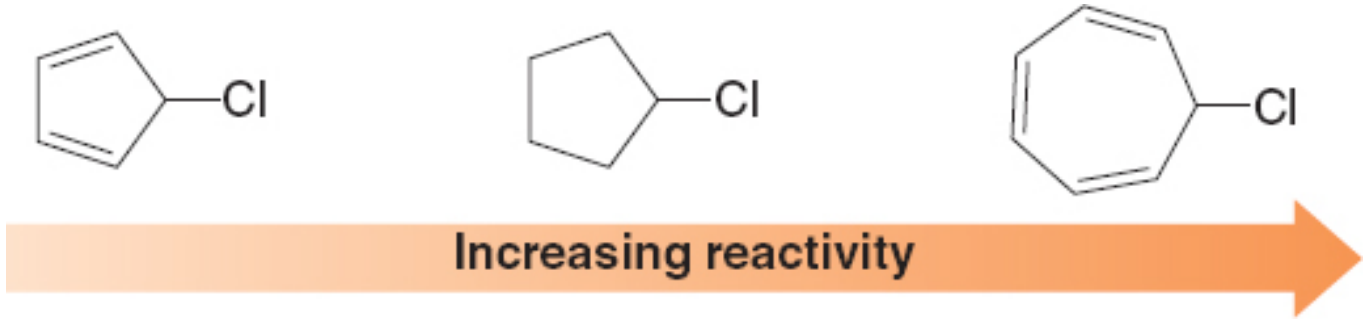
The purine heterocycle occurs commonly in the structure of DNA

a. How is each N atom hybridized?
b. In what type of orbital does each lone pair on a N atom reside?
c. How many π electrons does purine contain?
d. Is purine aromatic?.

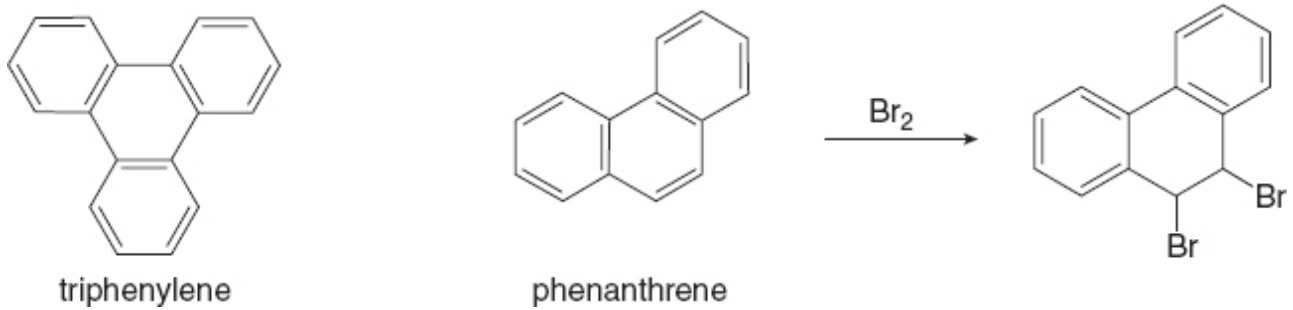


purine

Explain the observed rate of reactivity of the following 2° alkyl halides in an S_N1 reaction



Explain why triphenylene resembles benzene in that it does not undergo addition reactions with Br_2, but phenanthrene reacts with Br_2 to yield the addition product drawn. (Hint: Draw resonance structures for both triphenylene and phenanthrene, and use them to determine how delocalized each π bond is.)



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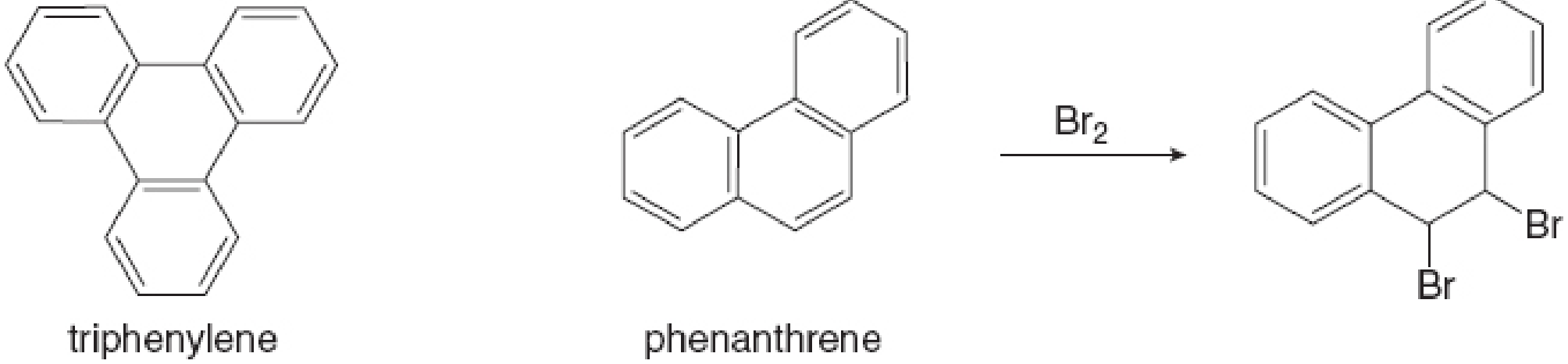

triphenylene

phenanthrene

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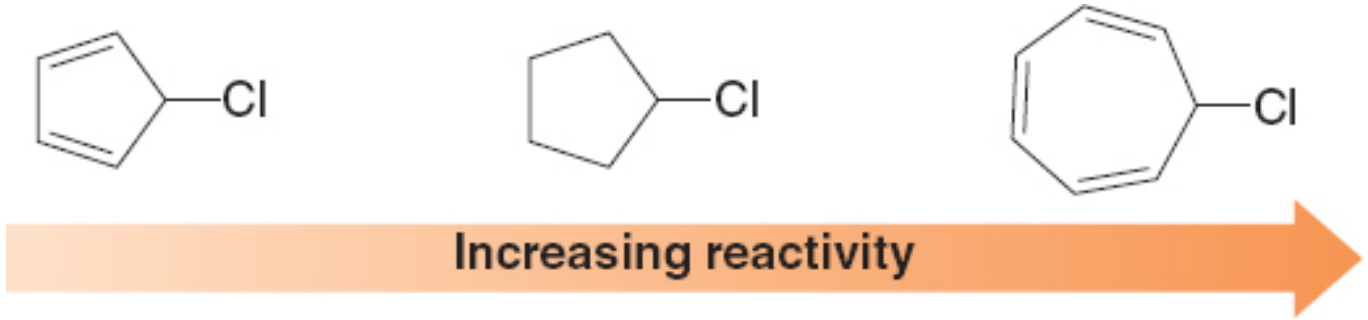

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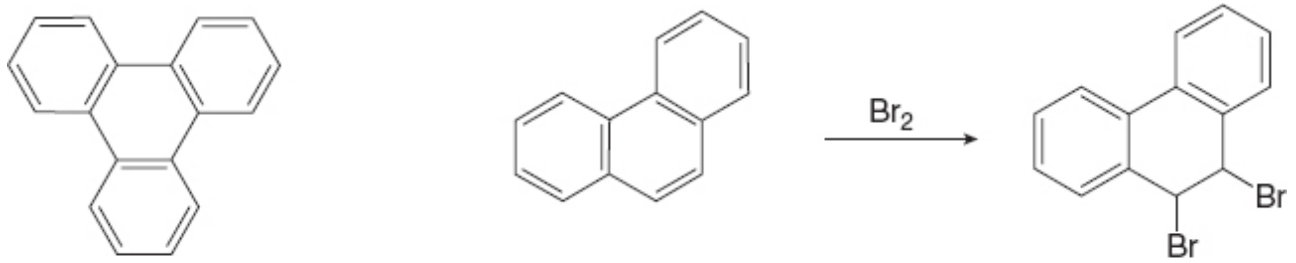
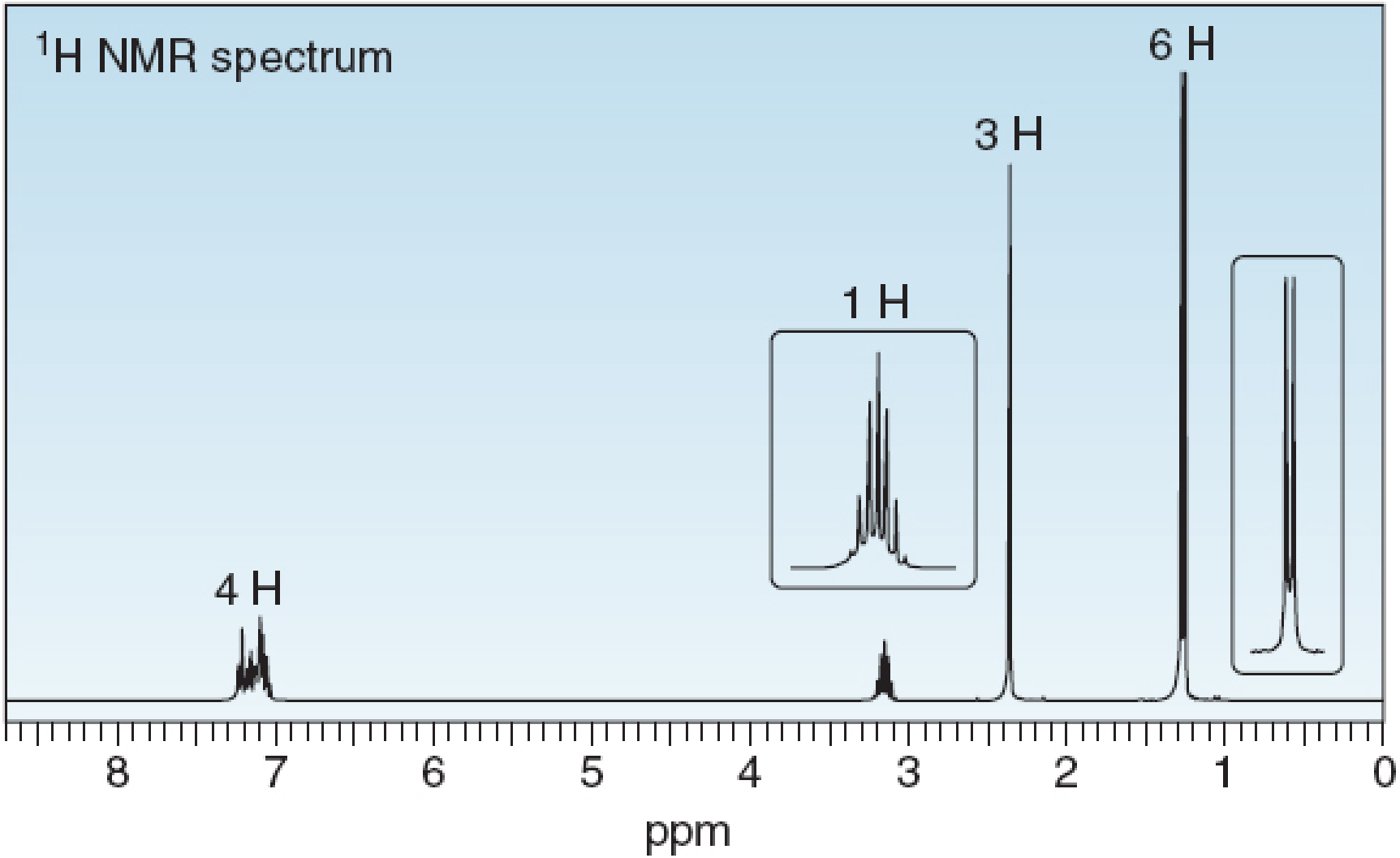


Explain why tetrahydrofuran has a higher boiling point and is much more water soluble than furan, even though both compounds are cyclic ethers containing four carbons.

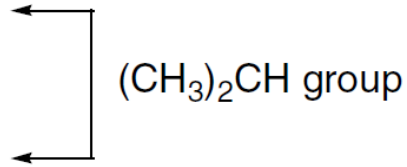
Propose a structure consistent with each set of data: $C_{10}H_{14}$: IR absorptions at 3150–2850, 1600, and 1500 cm−1



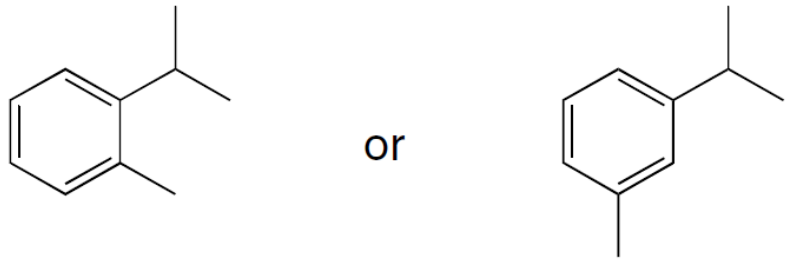
a. $C_{10}H_{14}$: IR absorptions at 3150–2850 (sp^2 and sp^3 hybridized C–H), 1600, and 1500 (due to a benzene ring) cm^{-1}

^1H NMR data:

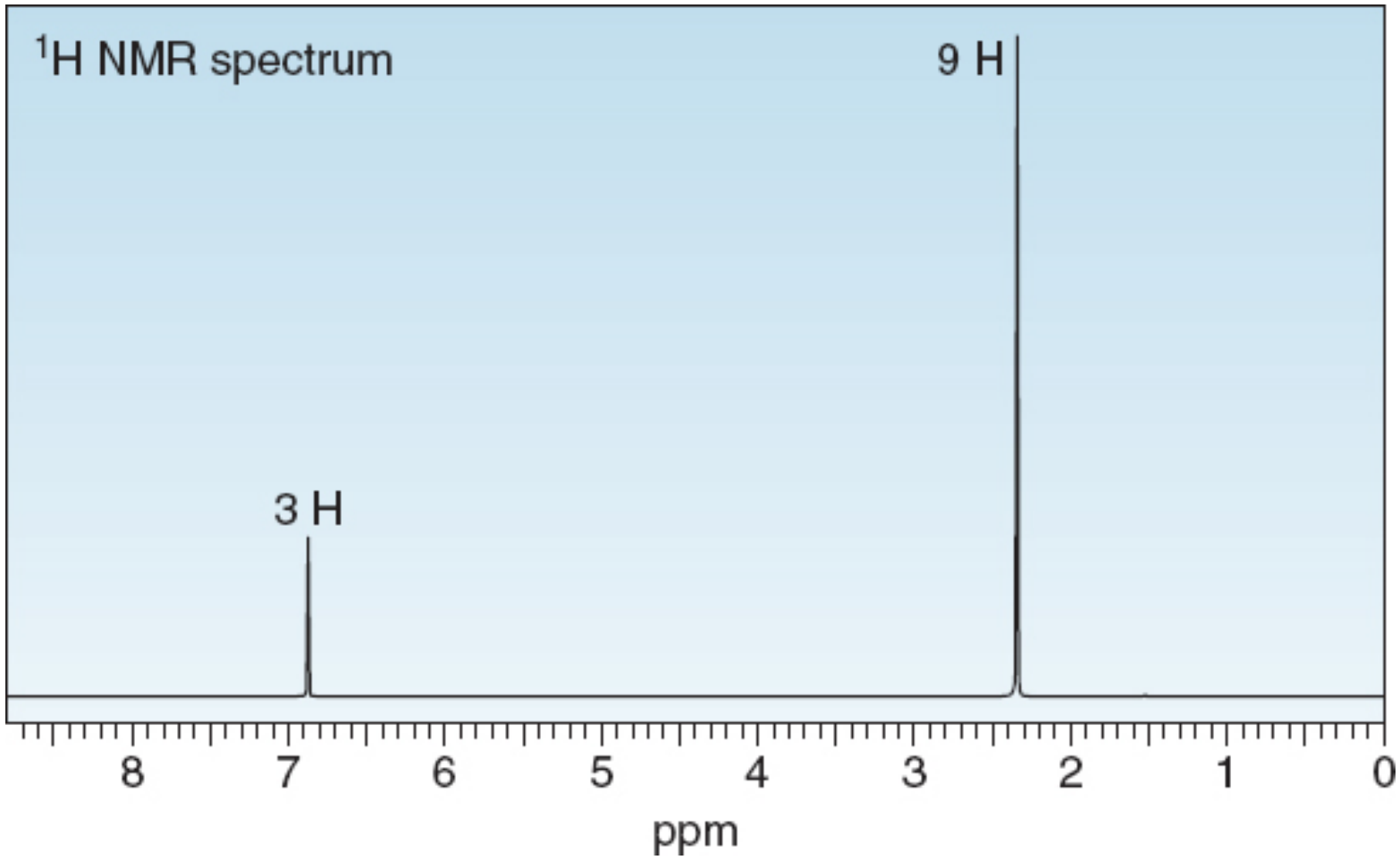
Absorption	**ppm**	**# of H's**	**Explanation**
doublet	1.2	6	6 H's adjacent to 1 H
singlet	2.3	3	CH_3
septet	3.1	1	1 H adjacent to 6 H's
multiplet	7–7.4	4	a disubstituted benzene ring



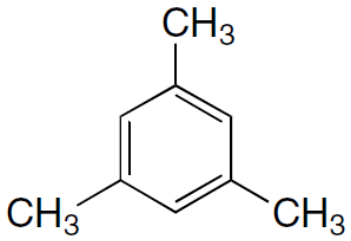
You can't tell from these data where the two groups are on the benzene ring. They are not para, since the para arrangement usually gives two sets of distinct peaks (resembling two doublets) so there are two possible structures—ortho and meta isomers.



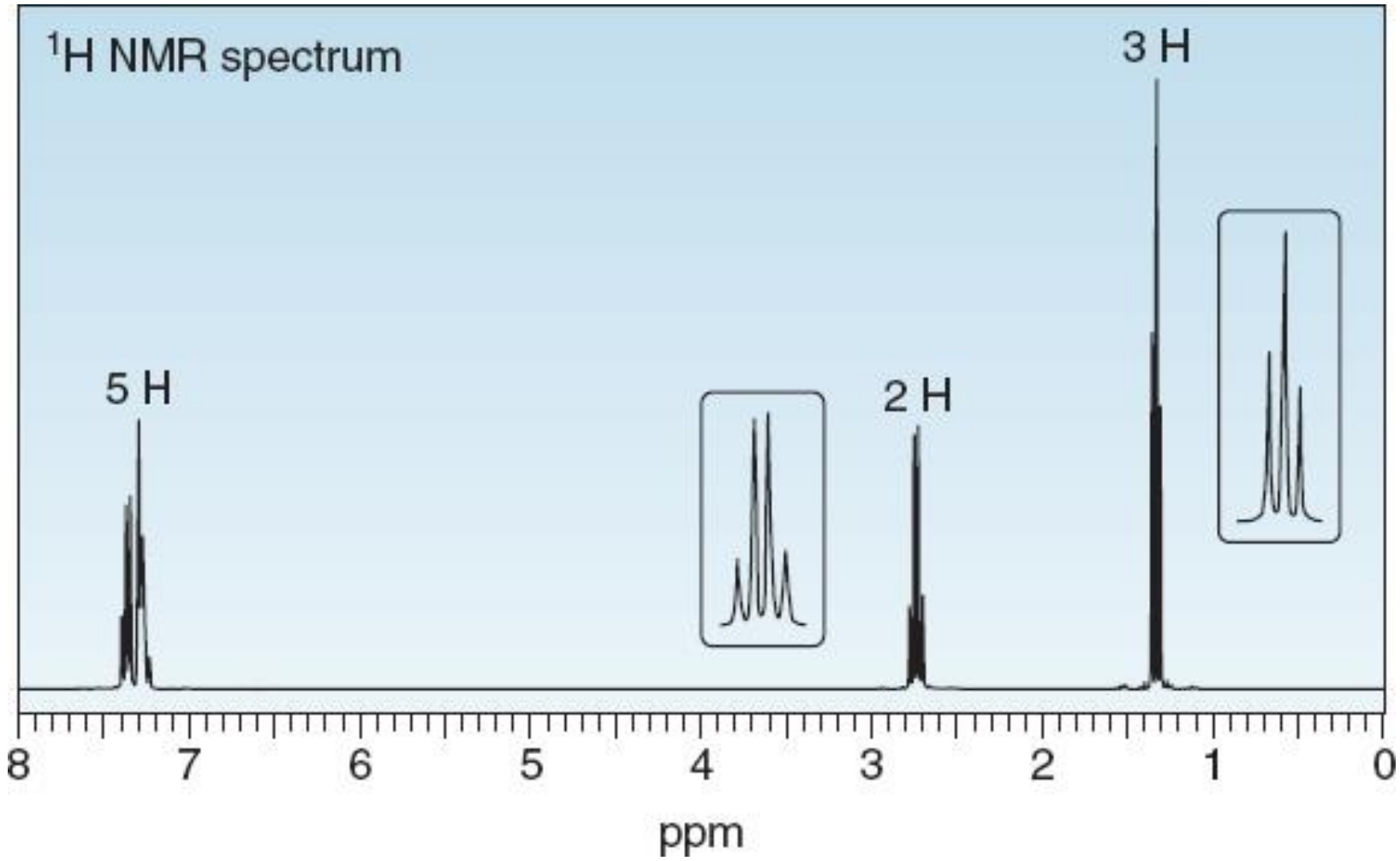
C_9H_{12}: ^{13}C NMR signals at 21, 127, and 138 ppm



b. C_9H_{12}: ^{13}C NMR signals at 21, 127, and 138 ppm → means three different types of C's.
^{1}H NMR shows 2 types of H's: 9 H's probably means 3 CH_3 groups; the other 3 H's are very deshielded so they are bonded to a benzene ring.
Only one possible structure fits:



C_8H_{10}: IR absorptions at 3108–2875, 1606, and 1496 cm^{-1}

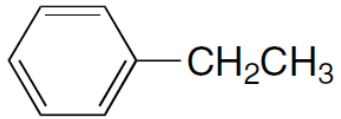


c. C_8H_{10}: IR absorptions at 3108–2875 (sp^2 and sp^3 hybridized C–H), 1606, and 1496 (due to a benzene ring) cm^{-1}

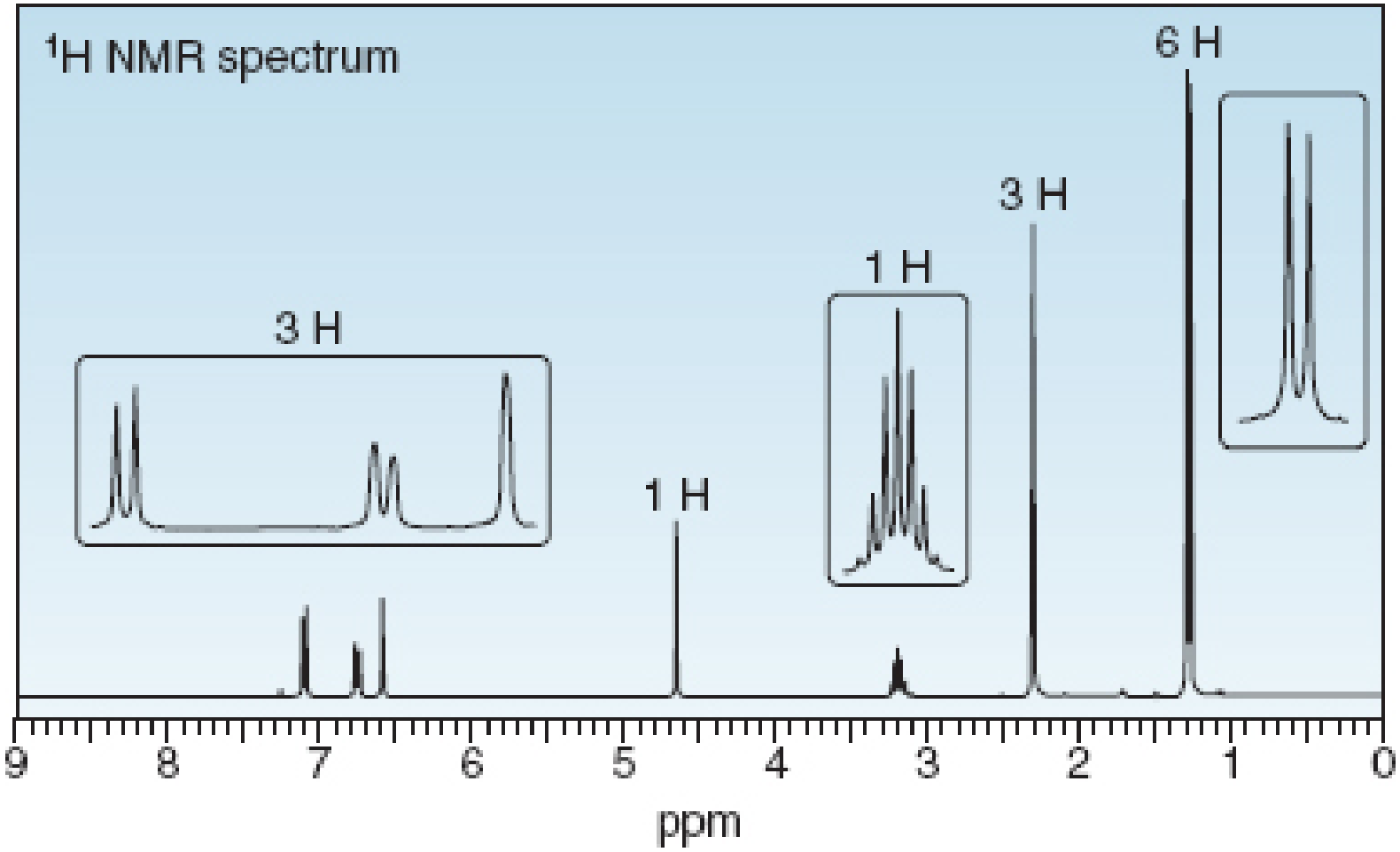
^1H NMR data:

Absorption	**ppm**	**# of H's**	**Explanation**
triplet	1.3	3	3 H's adjacent to 2 H's
quartet	2.7	2	2 H's adjacent to 3 H's
multiplet	7.3	5	a monosubstituted benzene ring

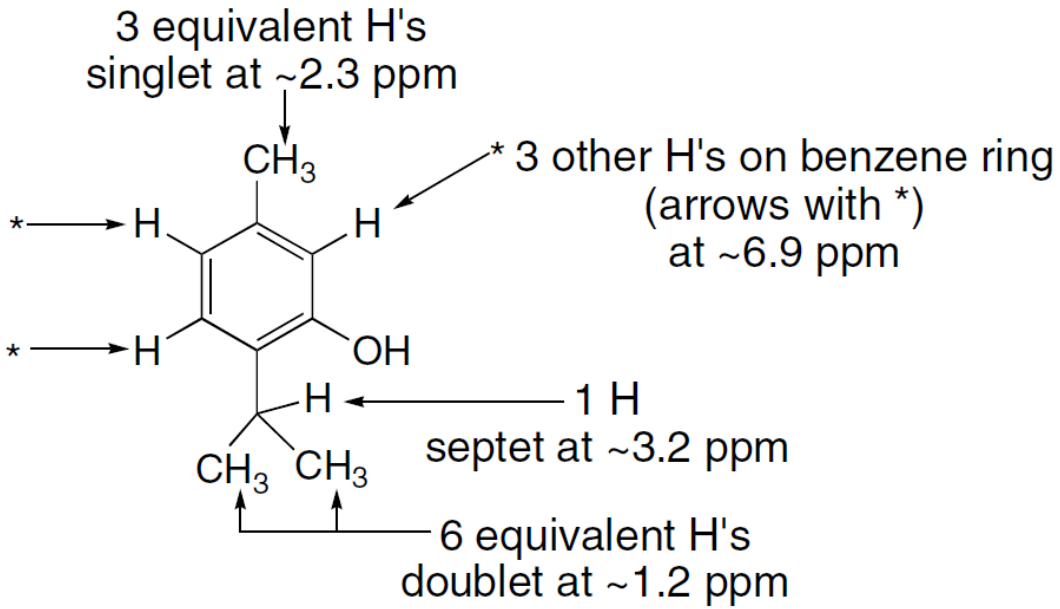
Structure:



molecular formula $C_{10}H_{14}O$: IR absorptions at 3500–3200, 3150–2850, 1621, and 1585 cm^{-1}. The ^1H NMR spectrum of thymol is given below.

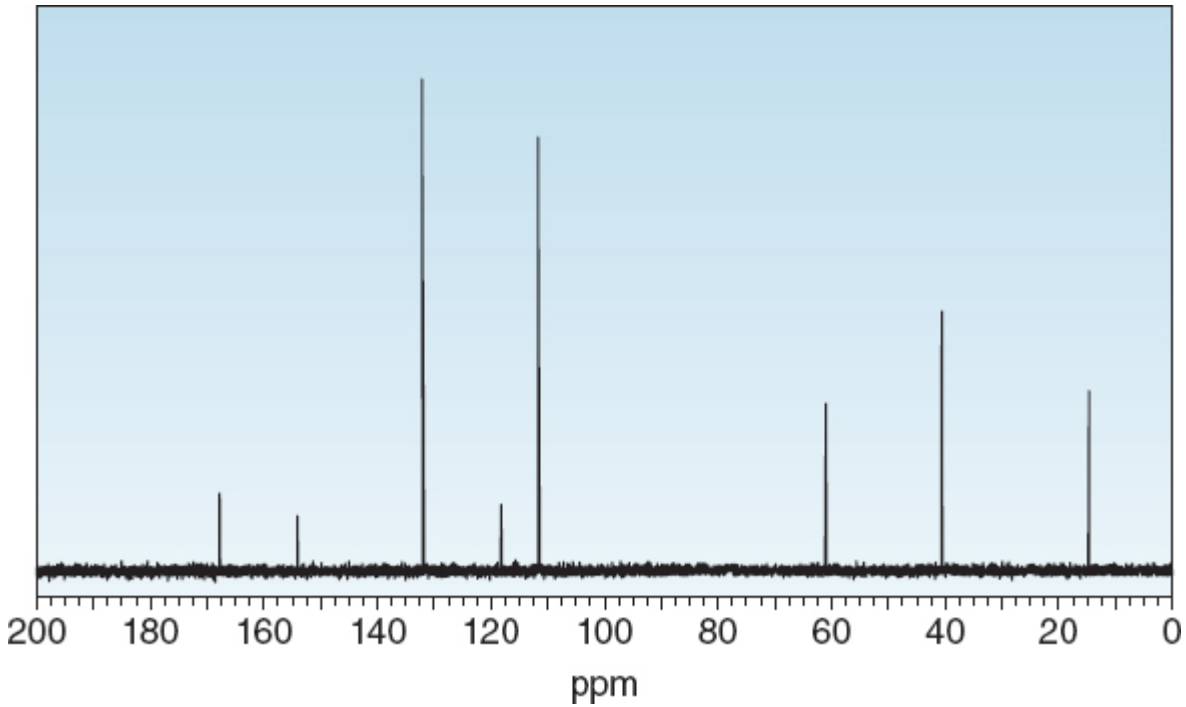


thymol

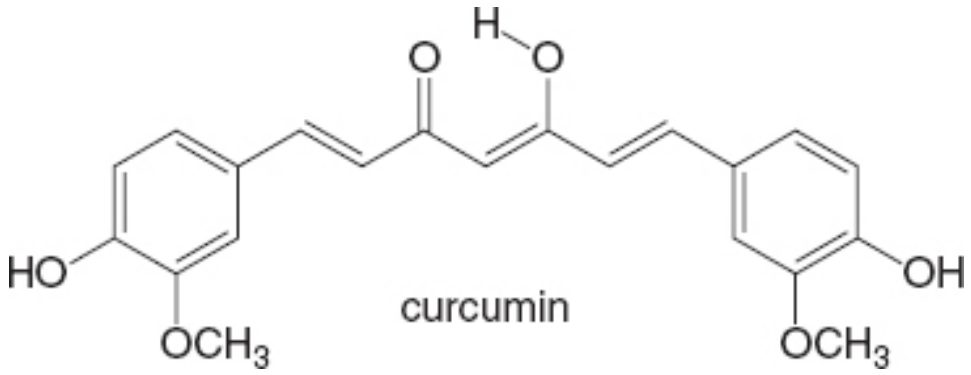


IR absorptions:
3500–3200 cm^{-1} (O–H)
3150–2850 cm^{-1} (C–H bonds)
1621 and 1585 cm^{-1} (benzene ring)

You have a sample of a compound of molecular formula C11H15NO2, which has a benzene ring substituted by two groups, (CH3)2N and CO2CH2CH3, and exhibits the given 13C NMR. What disubstituted benzene isomer corresponds to these 13C data?



Answer the following questions about curcumin, a yellow pigment isolated from turmeric, a tropical perennial in the ginger family and a principal ingredient in curry powder.



curcumin

a. we learned that most enols, compounds that contain a hydroxy group bonded to a C C, are unstable and tautomerize to carbonyl groups. Draw the keto form of the enol of curcumin, and explain why the enol is more stable than many other enols.
b. Explain why the enol O H proton is more acidic than an alcohol O H proton.
c. Why is curcumin colored?
d. Explain why curcumin is an antioxidant.