

(d) A π -bonding orbital for CO is shown in Figure 4.

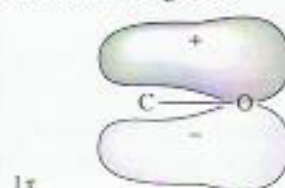


Figure 4 A π -bonding orbital for CO.

(e) Use must be made of the equation given in the *Data Sheet*:

$$\frac{\mu}{\text{C m}} = (1.602 \times 10^{-19} / \text{C}) \times q \times (n\text{\AA}) \times 10^{-30}$$

Hence the dipole moment for CO is

$$1.602 \times 10^{-19} \times 0.5 \times 1.14 \times 10^{-10} \text{ C m} = 9.13 \times 10^{-30} \text{ C m}$$

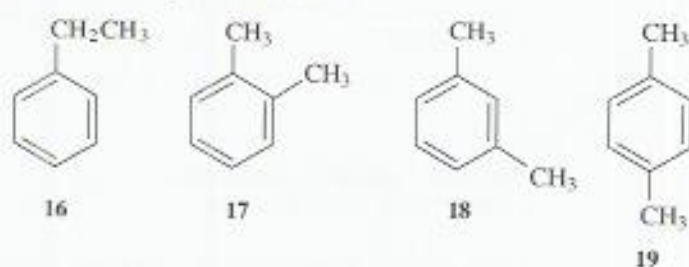
This could be improved by using a larger basis set, and by using DFT rather than Hartree-Fock.

Question 18

(a) The molecular formula of Compound **11** is C_8H_{10} . The corresponding saturated C_8 hydrocarbon is C_8H_{18} .

The number of double-bond equivalents in Compound **11** is therefore $(18 - 10)/2 = 4$. These correspond to the three $\text{C}=\text{C}$ double bonds of the benzene ring, and the ring itself.

Possible structures for Compound **11** are:



(b) A Friedel-Crafts alkylation reaction requires an *aromatic* substrate. Alternatively, it could be argued that the presence of four double-bond equivalents in Compound **11** suggests aromaticity.

Infrared spectra

Compound 11	$\text{C}-\text{H}$ stretch above 3000 cm^{-1}	$\text{C}=\text{C}-\text{H}$ aromatic
	$\text{C}-\text{H}$ stretch below 3000 cm^{-1}	aliphatic
	$\text{C}=\text{C}$ stretches near 1600 and 1500 cm^{-1}	aromatic ring vibrations

Conclusion Compound **11** contains an aromatic ring with aliphatic substitution.

NMR spectra

Compound **10** can only be $\text{CH}_3\text{CH}_2\text{CH}_2\text{Cl}$ or $(\text{CH}_3)_2\text{CHCl}$. The latter has two equivalent methyl groups, which would give rise to *one* quartet in the aliphatic region of the ^{13}C NMR (as observed). It also contains a CH group, which would give rise to a doublet in the aliphatic region. This too is seen in the ^{13}C NMR spectrum of Compound **10**, so the compound *must* be $(\text{CH}_3)_2\text{CHCl}$.

Compound 11	q at 16 p.p.m.	CH_3	aliphatic
	t at 29 p.p.m.	CH_2	aliphatic
	d at 126 p.p.m.	CH	alkene/aromatic
	d at 128 p.p.m.	CH	alkene/aromatic
	d at 129 p.p.m.	CH	alkene/aromatic
	s at 144 p.p.m.	C	alkene/aromatic