F324 HW 1 MS

1. **delocalised electrons**
electrons are spread over more than two atoms **AW (1)**

π-bond
formed by overlap of p-orbitals/ diagram to show **(1)** 2

[2]

2. (a) any two of …
fibres / dyes / explosives / pharmaceuticals etc **(1)(1)** 2
*allow any specific examples as long as they do involve aromatic nitro or amine groups – eg **NOT** nylon, fertiliser etc*

(b) temp 50-60° **(1)**
concentrated (acids) **(1)** 2
allow abbreviations for concentrated

(c) $C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O$
reactants **(1)** products **(1)** 2
allow a balanced equation for multiple nitration at any positions

(d) (i) a pair of electrons … **(1)**
… (electrons) move / transferred /
a (covalent) bond breaks/forms **(1)** 2

(ii) it accepts a pair of electrons (from the benzene) **(1)** 1
***NOT** a 'lone' pair*

(iii) $H(^+)$ (on the ring) is replaced by $NO_2(^+)$ **(1)** 1
allow 'substitutes'
ignore + charges

(iv) it is not used up / reformed at the end **AW (1)** 1

(e) π-bonding electrons are <u>delocalised</u> **(1)**

six π-electrons in benzene **(1)**
four π-electrons in the intermediate **(1)**

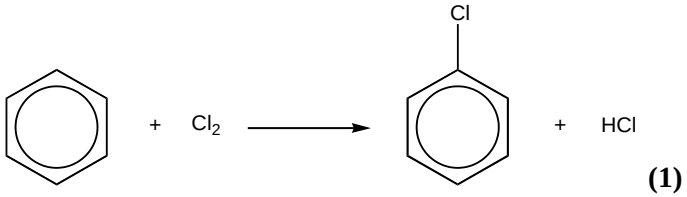
π-electrons are not over one carbon atom /
over **five** carbon atoms / p-orbitals in the intermediate **(1)**
this must be stated in words to compare benzene and the intermediate

π-electrons are over the **complete** ring / **all around** the ring
all six carbon atoms/ p-orbitals overlapping **(1)**

Quality of written communication
for at least two sentences/statements with legible text and
correct spelling, punctuation and grammar **(1)** 6

[17]

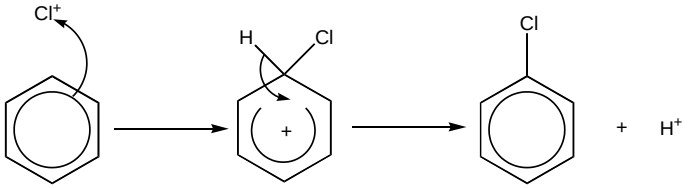
3. (a) (i)



(1) 1

(ii) Introduces a permanent dipole on Cl_2 / forms Cl^+/
$AlCl_3 + Cl_2 \rightarrow AlCl_4^- + Cl^+$/
$AlCl_3 + Cl_2 \rightarrow Cl^{\delta+} - AlCl_3^{\delta-}$ **(1)** 1

(iii)



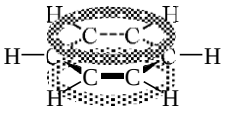
correct dipole / Cl^+ **(1)**
curly arrow from benzene ring to Cl^+ / $Cl^{\delta+}$ **(1)**
intermediate **(1)**
curly arrow from H to regenerate benzene ring in intermediate **(1)**
H^+ as other product **(1)** 4

(iv) electrophilic substitution **(1)**
with electrophilic spelt correctly 1

(b) In benzene, π electrons are delocalised/spread out **(1)**
In alkenes, π electrons are concentrated between 2 carbons **(1)**
Electrophiles attracted more to greater electron density in alkenes **(1)** 3

[10]

4. **bonding in benzene**
overlap of p-orbitals / π bonds/electrons (or labelled) **(1)**



above and below the ring (or shown in a diagram) **(1)**
electrons are <u>delocalised</u> (or labelled) **(1)**
C–C bonds are: same length/strength / in between single and double / σ-bonded **AW (1)**

greater reactivity of phenol
(the ring is activated because …)
<u>lone</u> pair from O is delocalised into the ring **(1)**
so electron density (of the ring) is increased **(1)**
so electrophiles are more attracted (to the ring) / dipole in electrophile more easily induced **(1)**
*(**NOT** just more easily "attacked" or "susceptible")*

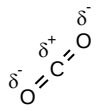
Quality of written communication mark for at least two complete sentences in which the meaning is clear with correct spelling, punctuation and grammar **(1)** 8

[8]

5. (a) (i) NaOH / Na **(1)** 1

(ii) $C_6H_5OH + NaOH \rightarrow C_6H_5O^-Na^+ + H_2O$ /
$C_6H_5OH + Na \rightarrow C_6H_5O^-Na^+ + ½H_2$ **(1)** 1

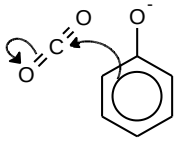
(b) (i)



(1) 1

allow a dipole on just one C=O bond

(ii)



(1)(1) 2

(iii) lone/electron pair from oxygen is delocalised into the ring /interacts with π-electrons **(1)**

increases π-electron density / negative charge (around the ring) **(1)**

attracts electrophiles more **(1)** 3

(c) M_r salicylic acid = 138 **(1)**

moles (in 1:1 reaction) = $3500 \times 10^6/138 = 2.536 \times 10^7$ **(1)**

mass of phenol needed = $2.536 \times 10^7 \times 94 = 2384$ tonnes **(1)**

allowing for 45% yield = $2384 \times {}^{100}/_{45}$ = **5298/5300** (tonnes) **(1)** 4

allow 5297.5–5300

allow ecf throughout

[12]

6. (a) Correct structure of 3-nitrophenol or any multiple nitrated phenol **(1)** 1

(b) M_r phenol (C_6H_6O) = 94.0 **(1)**

M_r 4-nitrophenol ($C_6H_5NO_3$) = 139.0 **(1)**

expected mass/moles of nitrophenol from 100 g = 148 g/1.06 mol (or ecf from wrong M_rs) **(1)**

at 27% yield gives 40 / 39.9 (g) (or ecf) **(1)** 4

last mark is for 0.27 × expected mass to 2 or 3 sf

(c) **conditions for nitration of benzene:**
HNO_3 is concentrated **(1)**

conc H_2SO_4 is present **(1)**

heating or stated temp above 50°C **(1)** 3

explanation for greater reactivity of phenol
lone pair from O atom is delocalised into the ring **(1)**

greater (π) electron density around the ring **(1)**

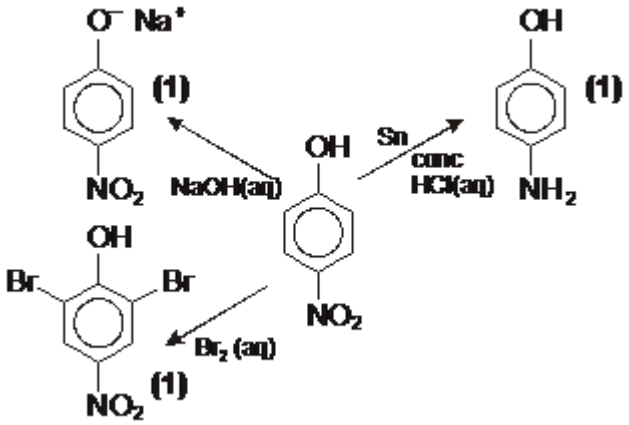
(the benzene ring in phenol) is activated **(1)**

attracts electrophiles/$^{+}NO_2$ more / makes it more susceptible to electrophiles **AW (1)** 4

quality of Written Communication mark for at least two legible sentences with correct spelling, punctuation and grammar 1

[13]

7.



3

allow bromination in any positions on the ring

[3]