

# 58<sup>th</sup> INTERNATIONAL CHEMISTRY OLYMPIAD

## 2026

### UK Round One

### MARK SCHEME

Although we would encourage students to always quote answers to an appropriate number of significant figures, do not penalise students for significant figure errors. Allow where a student's answers differ slightly from the mark scheme due to the use of rounded/non-rounded data from an earlier part of the question.

In general, 'error carried forward' (referred to as ECF) can be applied. We have tried to indicate where this may happen in the mark scheme and where ECF is not allowed.

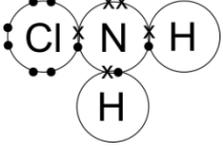
For answers with missing or incorrect units, penalise one mark for the first occurrence in **each** question and write **UNIT** next to it. Do not penalise for subsequent occurrences in the same question.

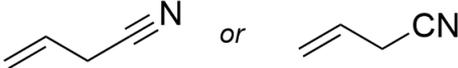
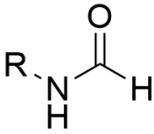
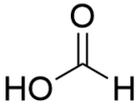
Organic structures are shown in their skeletal form, but also accept displayed formulae if the representation is unambiguous.

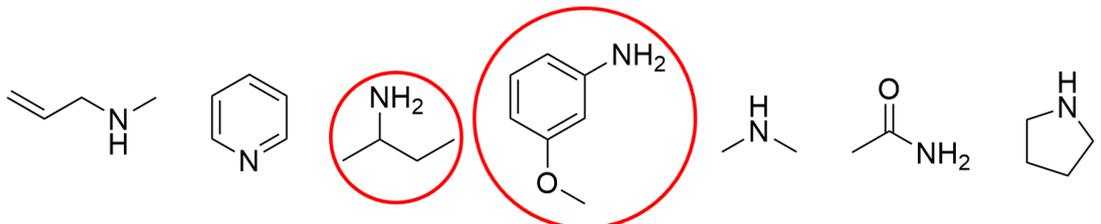
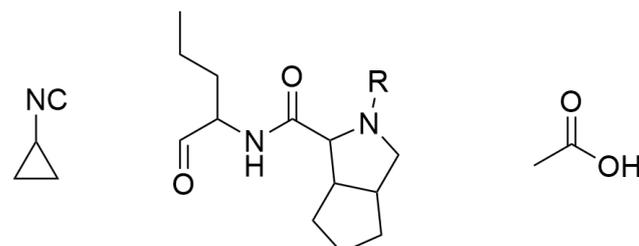
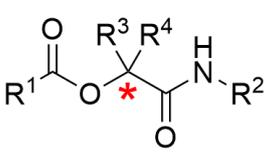
State symbols are not required for balanced equations and students should not be penalised if they are absent.

No half marks are to be awarded. One blank tick box has been included per mark available for each part. Please mark by placing a tick in each box if mark is scored.

Question	1	2	3	4	5	Total
Marks Available	8	18	19	26	13	84

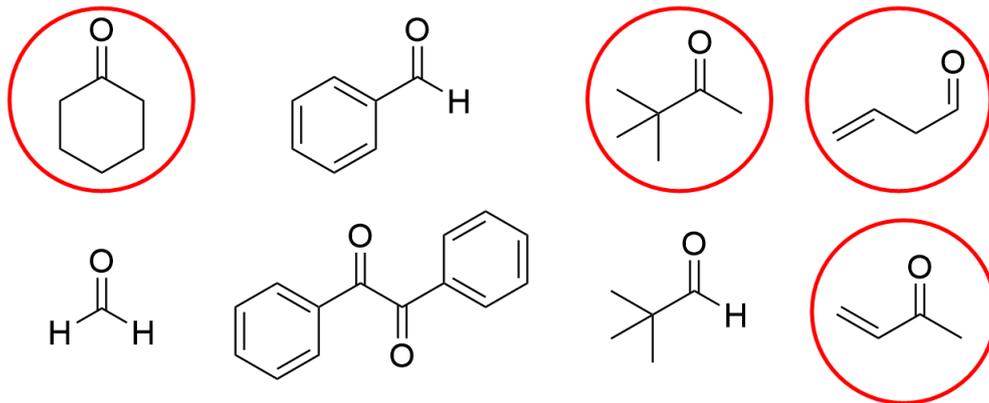
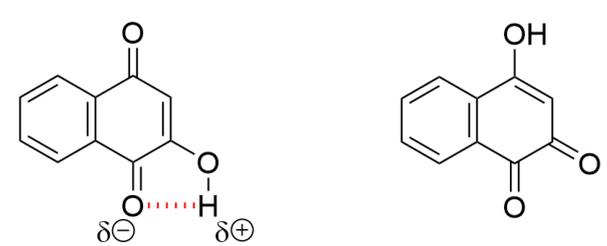
1.	This question is about pee in the pool	Mark			
(a)	<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 33%; text-align: center; padding: 5px;"><math>\text{Cl}_2</math> 0</td> <td style="width: 33%; text-align: center; padding: 5px;"><math>\text{HOCl}</math> +1 or 1</td> <td style="width: 33%; text-align: center; padding: 5px;"><math>\text{HCl}</math> -1 or -1</td> </tr> </table>	$\text{Cl}_2$ 0	$\text{HOCl}$ +1 or 1	$\text{HCl}$ -1 or -1	<input checked="" type="checkbox"/>
$\text{Cl}_2$ 0	$\text{HOCl}$ +1 or 1	$\text{HCl}$ -1 or -1			
<i>All three correct two marks. Two correct and one incorrect one mark. One correct only no marks. Accept if the + sign is missing for HOCl and they have just written "1".</i>		<input checked="" type="checkbox"/>			
(b)	$\text{Na}_2\text{CO}_3 + 2\text{HOCl} \rightarrow 2\text{NaOCl} + \text{H}_2\text{O} + \text{CO}_2$ <p><i>State symbols are not required. Accept multiples of this equation.</i></p> <p><i>Accept <math>\text{Na}_2\text{CO}_3 + 2\text{HOCl} \rightarrow 2\text{NaOCl} + \text{H}_2\text{CO}_3</math></i></p> <p><i>Do not accept any reactions where NaCl is given as a product.</i></p>	<input checked="" type="checkbox"/>			
(c)	<p>(i) <math>3\text{OCl}^- \rightarrow \text{ClO}_3^- + 2\text{Cl}^-</math></p> <p><i>State symbols are not required. Accept multiples of this equation.</i></p> <p><i>Do not accept non-ionic versions of this equation, e.g., <math>3\text{NaOCl} \rightarrow \text{NaClO}_3 + 2\text{NaCl}</math>, as students were specifically asked for the ionic equation.</i></p>	<input checked="" type="checkbox"/>			
<p>(ii) Trigonal pyramidal or pyramidal</p>		<input checked="" type="checkbox"/>			
(d)	$(\text{NH}_2)_2\text{CO} + \text{H}_2\text{O} \rightarrow 2\text{NH}_3 + \text{CO}_2$ <p><i>State symbols are not required. Accept multiples of this equation.</i></p>	<input checked="" type="checkbox"/>			
(e)	 <p><i>Dots and crosses can be the other way around.</i></p>	<input checked="" type="checkbox"/>			
(f)	$c = k \times p(\text{NCl}_3)$ $p(\text{NCl}_3) = \frac{5.0 \times 10^{-4} \text{ mol dm}^{-3}}{435 \text{ mol dm}^{-3} \text{ atm}^{-1}}$ $p(\text{NCl}_3) = 1.15 \times 10^{-6} \text{ atm}$	<input checked="" type="checkbox"/>			
<i>Total out of 8</i>		<b>8</b>			

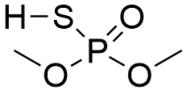
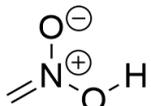
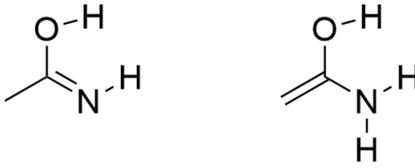
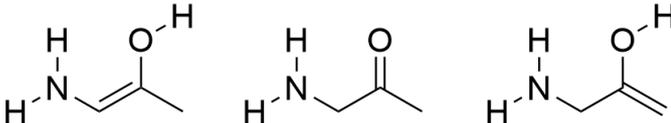
2.	This question is about isocyanides	Mark
(a)	$\text{R}-\ddot{\text{N}}=\text{C}:$ <p><i>Both lone pairs must be drawn in for the mark. Bond angles/geometry around the nitrogen is not important, if the number of bonds is correct.</i></p>	<input checked="" type="checkbox"/>
(b)	(i) <b>B</b>  <p><i>Accept if nitrile group is drawn out or written in abbreviated form.</i></p>	<input checked="" type="checkbox"/>
	(ii) AgBr or silver bromide	<input checked="" type="checkbox"/>
(c)	$n = 8 \times 10^{-8} \text{ mol dm}^{-3} \times 50 \times 10^3 \text{ m}^3$ $n = 4 \times 10^{-3} \text{ mol}$ $\text{molecules} = 4 \times 10^{-3} \text{ mol} \times 6.022 \times 10^{23} \text{ mol}^{-1}$ $= 2.4 \times 10^{21} \text{ molecules}$ <p><i>Students need to remember the conversion factor of 1000 between m<sup>3</sup> and dm<sup>3</sup>. Molecules does not have to be written as the "unit".</i></p>	<input checked="" type="checkbox"/>
(d)	(i) <b>C</b> 	<input checked="" type="checkbox"/>
	(ii) <b>D</b>  <p><i>Accept if the student has written formic acid, HCO<sub>2</sub>H, or HCOOH, as they understand the functional group present. If the student has written CH<sub>2</sub>O<sub>2</sub> or CH<sub>2</sub>O<sub>2</sub> then do not award the mark as there is no clear demonstration of their knowledge of the functional group.</i></p>	<input checked="" type="checkbox"/>
(e)	$\text{C}_3\text{H}_5\text{NH}_2 + 3\text{NaOH} + \text{CHCl}_3 \rightarrow \text{C}_3\text{H}_5\text{NC} + 3\text{NaCl} + 3\text{H}_2\text{O}$ <p><i>State symbols are not required. Accept multiples of this equation.</i></p>	<input checked="" type="checkbox"/>

(f)	 <p>Two marks if two correct molecules circled and no incorrect molecules circled. One mark if two correct molecules circled and one incorrect molecule circled. One mark if one correct molecule circled only and nothing else. One mark if one correct molecule circled only and one incorrect molecule circled. No marks if two or more incorrect molecules circled.</p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/>
(g)	 <p>One mark for each correct structure. Ignore any stereochemistry drawn.</p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/> <input checked="" type="checkbox"/>
(h)	$n = 2 \text{ isocyanides} \times 3 \text{ ketones} \times 3 \text{ acids}$ $n = 18$ <p>One mark for the correct numerical answer. Working is not needed. No mark for reasoning if final number is not correct.</p>	<input checked="" type="checkbox"/>
(i)	 <p>No marks if any other atom has an asterisk.</p>	<input checked="" type="checkbox"/>
(j)	<p>The R<sup>3</sup> and R<sup>4</sup> substituents are different for both aldehydes and one of the two ketones. This means there are seven possibilities for the aldehyde/ketone partner.</p> $n = 2 \text{ isocyanides} \times 7 \text{ ketones or aldehydes} \times 3 \text{ acids}$ $n = 42$ <p>Two marks for the correct numerical answer. No partial credit. Working is not needed. No marks for reasoning if final number is not correct.</p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/>
(k)	<p>There are five chemically distinguishable isocyanide groups, two chemically distinguishable ketone groups, and five chemically distinguishable acid groups.</p> $n = 5 \text{ isocyanides} \times 2 \text{ ketones} \times 5 \text{ acids}$ $n = 50$ <p>Two marks for the correct numerical answer. No partial credit. Working is not needed. No marks for reasoning if final number is not correct.</p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/>

Total out of 18

18

3.	This question is about compounds in henna tattoos	Mark
(a)	$K_1 = \frac{[\text{B}]}{[\text{A}]} = \frac{0.003}{99.997} = 3.00 \times 10^{-5}$	<input checked="" type="checkbox"/>
(b)	$K_2 = \frac{[\text{D}]}{[\text{C}]} = 0.23$ $[\text{C}] + [\text{D}] = 100\%$ $[\text{C}] = 100\% - [\text{D}]$ $\frac{[\text{D}]}{100\% - [\text{D}]} = 0.23$ $[\text{D}] = 23\% - 0.23[\text{D}]$ $1.23[\text{D}] = 23\%$ $[\text{D}] = \frac{23\%}{1.23} = 18.7\%$ $[\text{C}] = 100\% - 18.7\% = 81.3\%$ <p><i>Two marks if both numbers are correct. One mark can be given if working is correct (i.e., use of simultaneous equations correctly) but final answer is incorrect due to a trivial error. One mark if student has only quoted one of C or D.</i></p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/>
(c)	 <p><i>Four correct circles and no incorrect circles, two marks.  Three correct circles and no incorrect circle, one mark.  Three correct circles and one incorrect circle, one mark.  Anything else, no marks.</i></p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/>
(d)	 <p><i>One mark for each correctly drawn tautomer. The final mark can be awarded if the hydrogen bond has been drawn in the correct place on the correct tautomer. The dipoles do not need to be drawn on the hydrogen bond for the mark.</i></p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/> <input checked="" type="checkbox"/>

(e)	<table border="1"> <thead> <tr> <th data-bbox="204 98 437 241">electrophilic aromatic substitution</th> <th data-bbox="437 98 667 241">nucleophilic aromatic substitution</th> <th data-bbox="667 98 900 241">reduction</th> <th data-bbox="900 98 1129 241">oxidation</th> <th data-bbox="1129 98 1362 241">hydrolysis</th> </tr> </thead> <tbody> <tr> <td data-bbox="204 241 437 309"></td> <td data-bbox="437 241 667 309"></td> <td data-bbox="667 241 900 309"></td> <td data-bbox="900 241 1129 309" style="text-align: center;">✓</td> <td data-bbox="1129 241 1362 309"></td> </tr> </tbody> </table>	electrophilic aromatic substitution	nucleophilic aromatic substitution	reduction	oxidation	hydrolysis				✓		<input checked="" type="checkbox"/>
electrophilic aromatic substitution	nucleophilic aromatic substitution	reduction	oxidation	hydrolysis								
			✓									
<i>No marks if more than one answer is ticked.</i>												
(f)	<p>(i)</p>  <p><i>One mark. Accept if student writes SH instead of drawing out the S–H bond.</i></p>	<input checked="" type="checkbox"/>										
	<p>(ii)</p>  <p><i>One mark. Accept if student writes OH instead of drawing out the O–H bond. Do not accept any version where there are no formal charges, or the nitrogen atom has five bonds.</i></p>	<input checked="" type="checkbox"/>										
(g)	<p>(i)</p>  <p><i>One mark if both correct only. Accept if student writes OH or NH instead of drawing out the O–H and N–H bond(s).</i></p>	<input checked="" type="checkbox"/>										
	<p>(ii)</p>  <p><i>Two marks if all three correct structures drawn. Can award one mark if two correct structures are drawn (with a maximum of one incorrect structure). Accept if student writes OH or NH instead of drawing out the O–H and N–H bond(s). Note stereochemistry is not graded, and so the C=C can be cis, trans, undefined or ambiguous as long as the bond connectivity is correct.</i></p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/>										
(h)	$\Delta_r H^\ominus = \sum \text{bonds broken} - \sum \text{bonds formed}$ $\Delta_r H^\ominus = ((743 + 348 + 412) - (463 + 360 + 612)) \text{ kJ mol}^{-1}$ $\Delta_r H^\ominus = +68 \text{ kJ mol}^{-1}$ <p><i>One mark. The positive sign does not have to be written, but if value written as negative then no marks should be awarded.</i></p>	<input checked="" type="checkbox"/>										

(i)

$$\Delta G^{\ominus} = \Delta H^{\ominus} - T\Delta S^{\ominus}$$

$$\Delta G^{\ominus} = -32,580 \text{ J mol}^{-1} - (298 \text{ K} \times -11.48 \text{ J K}^{-1}\text{mol}^{-1})$$

$$\Delta G^{\ominus} = -29,160 \text{ J mol}^{-1} = -29.16 \text{ kJ mol}^{-1}$$

$$\Delta G^{\ominus} = -RT \ln K_{gas}$$

$$K_{gas} = e^{-\frac{\Delta G^{\ominus}}{RT}}$$

$$K_{gas} = e^{-\left(\frac{-29,160 \text{ J mol}^{-1}}{8.314 \text{ J K}^{-1}\text{mol}^{-1} \times 298 \text{ K}}\right)}$$

$$K_{gas} = 1.29 \times 10^5$$

Two marks. One mark for correct calculation of  $\Delta G^{\ominus}$ , and one mark for correct calculation of  $K_{gas}$ .



(j)

$$\Delta_r G^{\ominus}_{water} = -\Delta_{sol} G^{\ominus}_{keto} + \Delta_r G^{\ominus}_{gas} + \Delta_{sol} G^{\ominus}_{enol}$$

$$\Delta_r G^{\ominus}_{water} = -(-126,000 \text{ J mol}^{-1}) + (-29,160 \text{ J mol}^{-1}) + (-109,200 \text{ J mol}^{-1})$$

$$\Delta_r G^{\ominus}_{water} = -12,360 \text{ J mol}^{-1} = -12.36 \text{ kJ mol}^{-1}$$

$$K_{water} = e^{-\frac{\Delta G^{\ominus}_{water}}{RT}}$$

$$K_{water} = e^{-\left(\frac{-12,360 \text{ J mol}^{-1}}{8.314 \text{ J K}^{-1}\text{mol}^{-1} \times 298 \text{ K}}\right)}$$

$$K_{water} = 147$$

Two marks. One mark for correct calculation of  $\Delta G^{\ominus}$ , and one mark for correct calculation of  $K_{gas}$ . ECF from (i) can be awarded. If  $K_{gas} = 3.05 \times 10^6$  is used:

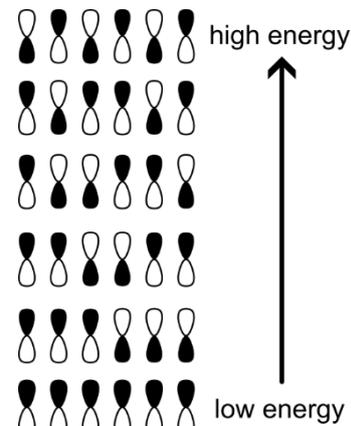
$$\Delta_r G^{\ominus}_{water} = -20,190 \text{ J mol}^{-1} = -20.19 \text{ kJ mol}^{-1}$$

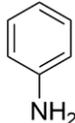
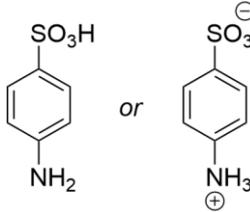
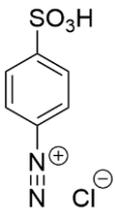
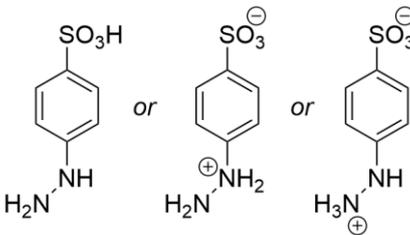
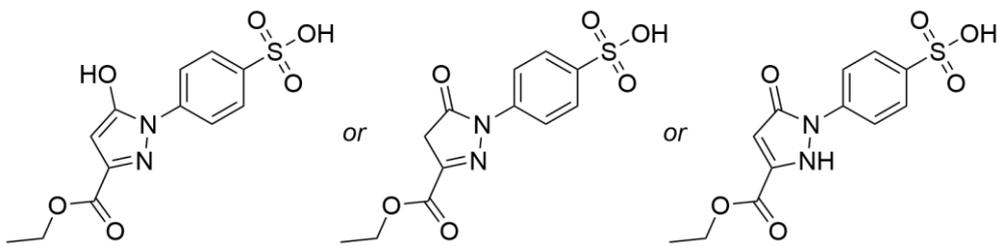
$$K_{water} = 3460$$



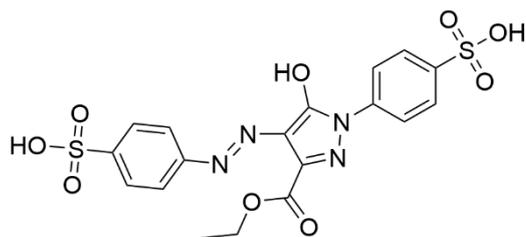
Total out of 19

**19**

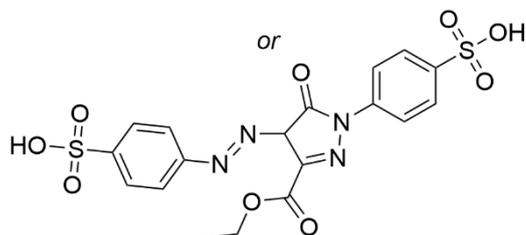
4.	This question is about rice, spice, and mice	Mark						
(a)	$C_{40}H_{56}$	<input checked="" type="checkbox"/>						
(b)	(i) 10	<input checked="" type="checkbox"/>						
	(ii) 11	<input checked="" type="checkbox"/>						
	<i>One mark each. No credit if written the wrong way around.</i>	<input checked="" type="checkbox"/>						
(c)	<table border="1" style="width: 100%; text-align: center;"> <tr> <td style="width: 25%;">lowest energy</td> <td style="width: 50%;"></td> <td style="width: 25%;">highest energy</td> </tr> <tr> <td><b>B</b></td> <td><b>A</b></td> <td><b>D</b></td> </tr> </table>	lowest energy		highest energy	<b>B</b>	<b>A</b>	<b>D</b>	<input checked="" type="checkbox"/>
lowest energy		highest energy						
<b>B</b>	<b>A</b>	<b>D</b>						
	<i>Two marks if all in correct place. One mark can be awarded if two are in the correct place.</i>	<input checked="" type="checkbox"/>						
(d)	 <p style="text-align: center;"><i>Each row of p orbitals is marked separately. All six rows shaded correctly three marks. Four or five rows shaded correctly two marks. Two or three rows shaded correctly one mark. No marks if one row or no whole rows are shaded correctly. No credit can be given for rows in the wrong place.</i></p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/> <input checked="" type="checkbox"/>						
(e)	(i) $\Delta E = 4(6.85 \times 10^{-19} \text{ J}) \sin\left(\frac{90^\circ}{6 + 1}\right) = 6.10 \times 10^{-19} \text{ J}$	<input checked="" type="checkbox"/>						
	(ii) $\lambda = \frac{hc}{\Delta E}$ $\lambda = \frac{(6.626 \times 10^{-34} \text{ J s})(2.998 \times 10^8 \text{ m s}^{-1})}{6.10 \times 10^{-19} \text{ J}} = 3.26 \times 10^{-7} \text{ m}$ $\lambda = 326 \text{ nm}$ <p style="text-align: center;"><i>No credit if answer not given in nm as this was asked in the question.</i></p>	<input checked="" type="checkbox"/>						
(f)	<table border="1" style="width: 100%; text-align: center;"> <tr> <td style="width: 50%;">yes</td> <td style="width: 50%;">no</td> </tr> <tr> <td></td> <td style="text-align: center;">✓</td> </tr> </table> <p style="text-align: center;"><i>Allow ECF from part (e)(ii). If answer to (e)(ii) is 380-720 nm then yes is ECF answer.</i></p>	yes	no		✓	<input checked="" type="checkbox"/>		
yes	no							
	✓							
(g)	<table border="1" style="width: 100%; text-align: center;"> <tr> <td style="width: 33%;">it decreases</td> <td style="width: 33%;">it stays the same</td> <td style="width: 33%;">it increases</td> </tr> <tr> <td></td> <td></td> <td style="text-align: center;">✓</td> </tr> </table>	it decreases	it stays the same	it increases			✓	<input checked="" type="checkbox"/>
it decreases	it stays the same	it increases						
		✓						

(h)	$\Delta n = 1.45 - 1.33 = 0.12$ $c_t = \frac{0.12}{0.143 \text{ mol}^{-1} \text{ dm}^3} = 0.839 \text{ mol dm}^{-3}$ $n_t = c_t V = 0.839 \text{ mol dm}^{-3} \times 8.50 \times 10^{-3} \text{ dm}^3 = 7.13 \times 10^{-3} \text{ mol}$ $m_t = n_t \times M_r = 7.13 \times 10^{-3} \text{ mol} \times 534.4 \text{ g mol}^{-1} = 3.81 \text{ g}$ <p><i>Correct answer scores two marks. One mark can be awarded for correctly calculating the concentration of tartrazine, the second mark for correctly calculating the minimum mass of tartrazine.</i></p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/>	
(i)	<p><b>A</b></p>  <p><i>One mark.</i></p>	<p><b>B</b></p>  <p><i>One mark for correct structure. ECF can be awarded from A if structure of B matches formula.</i></p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/>
	<p><b>C</b></p>  <p><i>One mark for correct structure. Diazonium group does not have to be drawn out. ECF can be awarded from B if structure of C matches formula.</i></p>	<p><b>D</b></p>  <p><i>Two marks for correct structure. ECF can be awarded from C if structure of D matches formula.</i></p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/> <input checked="" type="checkbox"/>
	<p><b>E</b></p>  <p><i>Two marks for correct structure. Any of the three reasonable tautomeric forms above scores full credit. Allow if SO3H abbreviation used. ECF can be awarded from D.</i></p>	<input checked="" type="checkbox"/> <input checked="" type="checkbox"/>	

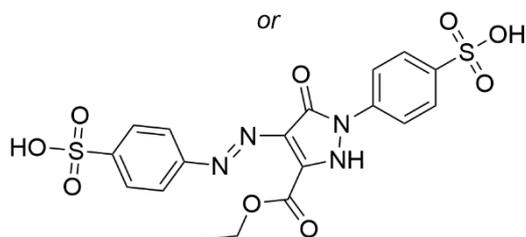
F



or



or



One mark for correct structure. Allow if  $\text{SO}_3\text{H}$  abbreviation used. No ECF can be awarded as student can work backwards from tartrazine.



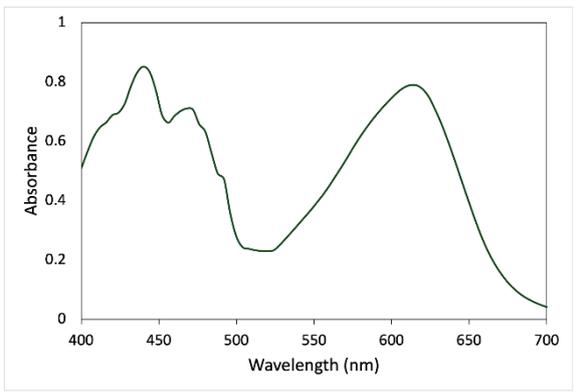
(i)

blue	yellow	orange	red
✓			

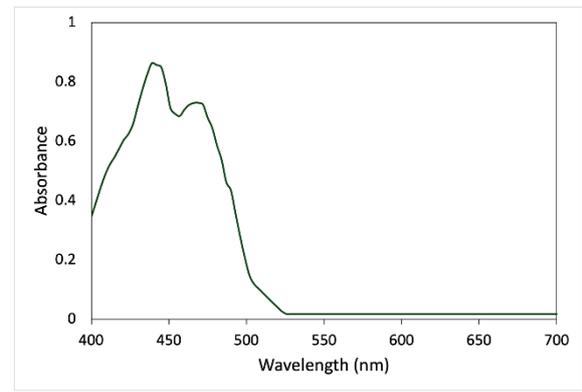


(k)

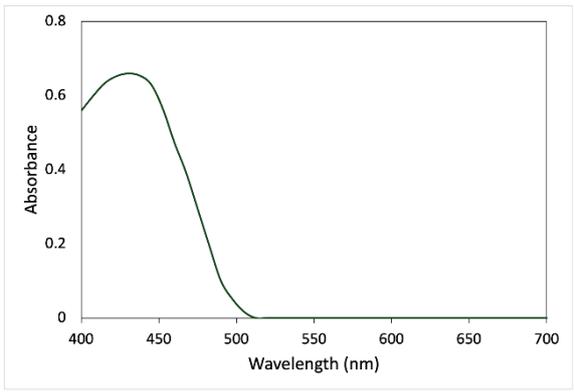
3



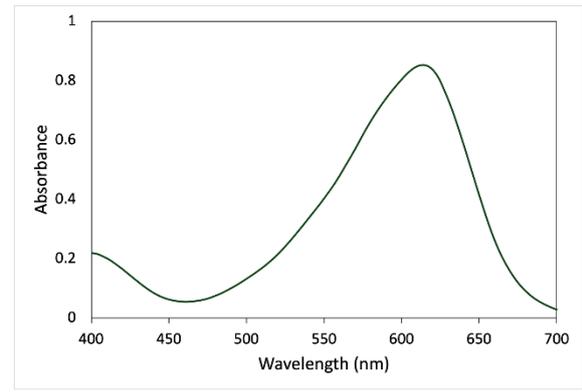
5



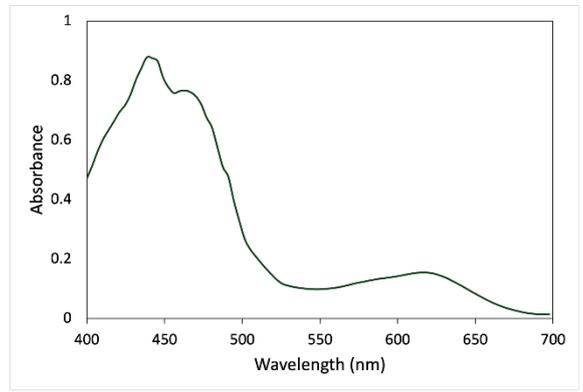
1



4



2



All five correct three marks. Three correct two marks. Two correct one mark.

Total out of 26

26

## 5. This question is about minerals

Mark

- (a) Balancing charges for: Cu = +2; Al = +3; PO<sub>4</sub> = -3; H = -1  
 Charge of Cu, Al, PO<sub>4</sub> is (1 × +2) + (6 × +3) + (4 × -3) = +8  
 Charge remaining for OH<sup>-</sup> is -8.  
 Therefore number of OH<sup>-</sup>, x = 8

*One mark for correct answer. Working does not need to be shown.*



- (b) For dehydrated turquoise, formula = CuAl<sub>6</sub>(PO<sub>4</sub>)<sub>4</sub>(OH)<sub>x</sub>

	$M_r$	definite	variable
Al	26.98	6	
Cu	63.55	1	
P	30.97	4	
O	16.00	16	x
H	1.008	0	x
<b>Total</b>		<b>605.31</b>	<b>17.008x</b>

$$M_r(\text{turquoise}) = (605.31 + 17.008x) \text{ g mol}^{-1}$$

$$\%mass(\text{Cu}) = \frac{63.55 \text{ g mol}^{-1}}{M_r(\text{turquoise})}$$

For  $x = 8$

$$\%mass(\text{Cu}) = \frac{63.55 \text{ g mol}^{-1}}{(605.31 + (17.008 \times 8)) \text{ g mol}^{-1}}$$

$$\%mass(\text{Cu}) = 8.57\%$$

For  $x = 10$

$$\%mass(\text{Cu}) = \frac{63.55 \text{ g mol}^{-1}}{(605.31 + (17.008 \times 10)) \text{ g mol}^{-1}}$$

$$\%mass(\text{Cu}) = 8.20\%$$

*One mark for correct answer. Working does not need to be shown. ECF from part (a) can be awarded.*



- (c)

libethenite	turquoise
<b>F</b>	<b>B</b>

$$M_r(\text{libethenite}) = 239.078 \text{ g mol}^{-1}$$

$$\%mass(\text{Cu, libethenite}) = \frac{2 \times 63.55 \text{ g mol}^{-1}}{239.078 \text{ g mol}^{-1}}$$

$$\%mass(\text{Cu, libethenite}) = 53.2\%$$

Therefore, sample **F** (53%) is in the range of libethenite.

*One mark for libethenite. Working does not need to be shown.*



$$M_r(\text{turquoise}) = (605.31 + 17.008x + 18.016y) \text{ g mol}^{-1}$$

For  $x = 8, y = 2$ :

$$\%mass(\text{Cu, turquoise}) = \frac{63.55 \text{ g mol}^{-1}}{(605.31 + 17.008 \times 8 + 18.016 \times 2) \text{ g mol}^{-1}}$$

$$\%mass(\text{Cu, turquoise}) = 8.17\%$$

For  $x = 8, y = 8$ :

$$\%mass(\text{Cu, turquoise}) = \frac{63.55 \text{ g mol}^{-1}}{(605.31 + 17.008 \times 8 + 18.016 \times 8) \text{ g mol}^{-1}}$$

$$\%mass(\text{Cu, turquoise}) = 7.18\%$$

Therefore, sample **B** (7%) is in the range of turquoise.

*One mark for turquoise. Working does not need to be shown.*

*The highest reasonable ECF for turquoise is  $x = 1, y = 2$ .*

$$\%mass(\text{Cu, turquoise}) = \frac{63.55 \text{ g mol}^{-1}}{(605.31 + 17.008 \times 1 + 18.016 \times 2) \text{ g mol}^{-1}}$$

$$\%mass(\text{Cu, turquoise}) = 9.65\%$$

*As this is still closer to sample **B** than sample **C**, this means sample **B** is the only acceptable ECF answer for turquoise in this question.*



(d) The P–O bond length,  $r_{PO}$ , is half of the opposite vertex-to-vertex distance of the cube.

For cube edge length,  $l$

$$l^2 + l^2 + l^2 = (2r_{PO})^2$$

$$3l^2 = 4r_{PO}^2$$

$$l = \frac{2r_{PO}}{\sqrt{3}}$$

The edge of the tetrahedron,  $a$ , is the O to O distance along the diagonal of the face of the cube

$$l^2 + l^2 = a^2$$

$$a = \sqrt{2}l$$

$$a = \frac{2\sqrt{2}r_{PO}}{\sqrt{3}}$$

$$a = \frac{2\sqrt{2} \times 1.54 \times 10^{-10} \text{ m}}{\sqrt{3}}$$

$$a = 2.515 \times 10^{-10} \text{ m}$$

$$V_{\text{tet}} = \frac{1}{6\sqrt{2}} (2.515 \times 10^{-10} \text{ m})^3$$

$$V_{\text{tet}} = 1.87 \times 10^{-30} \text{ m}^3$$

$$V_{\text{tet}} = 1.87 \text{ \AA}^3$$

*Correct answer scores both marks. One mark can be awarded for the correct algebraic expression for  $a = \frac{2\sqrt{2}r_{PO}}{\sqrt{3}}$ .*



(e) (i)

$$\begin{aligned} \text{filled volume} &= 8V_{PO_4} + 8V_{AlO_6} + 16V_{H_2O} \\ &= (8 \times 1.87 + 8 \times 9.00 + 16 \times 20) \text{ \AA}^3 \\ &= 406.96 \text{ \AA}^3 \end{aligned}$$

This occupies 50% of unit cell, so need to divide by 0.5 to get total volume.

$$\begin{aligned} \text{total volume} &= \frac{406.96 \text{ \AA}^3}{0.5} \\ &= 814 \text{ \AA}^3 \end{aligned}$$

*Correct answer scores both marks. One mark can be awarded for correct calculation of the filled volume. Allow ECF from part (d). If value of  $V_{tet} = 1.50 \text{ \AA}^3$  has been used, then ECF answer is:*

$$\begin{aligned} \text{filled volume} &= 404 \text{ \AA}^3 \\ \text{total volume} &= 808 \text{ \AA}^3 \end{aligned}$$



(ii) There are eight formula units in a unit cell.

$$\begin{aligned} M_r(\text{unit cell}) &= 8 \times (26.98 + 30.97 + 6(16.00) + 4(1.008)) \text{ g mol}^{-1} \\ &= 1263.856 \text{ g mol}^{-1} \end{aligned}$$

$$\begin{aligned} \text{mass}(\text{unit cell}) &= \frac{1263.856 \text{ g mol}^{-1}}{6.022 \times 10^{23} \text{ mol}^{-1}} \\ &= 2.099 \times 10^{-21} \text{ g} \end{aligned}$$

$$\begin{aligned} \text{density} &= \frac{2.099 \times 10^{-21} \text{ g}}{814 \times 10^{-24} \text{ cm}^3} \\ &= 2.58 \text{ g cm}^{-3} \end{aligned}$$

*One mark. Do not allow if density is given in different units. Allow ECF from part (e)(i). If value of total volume =  $808 \text{ \AA}^3$  has been used, then ECF answer is:*

$$\text{density} = 2.60 \text{ g cm}^{-3}$$

*If value of total volume =  $969 \text{ \AA}^3$  has been used, then ECF answer is:*

$$\text{density} = 2.17 \text{ g cm}^{-3}$$



(f) (i)

$$V_{\text{CuO}_6} = \left(\frac{r_{\text{CuO}}}{r_{\text{AlO}}}\right)^3 V_{\text{AlO}_6}$$
$$= \left(\frac{2.29 \text{ \AA}}{1.89 \text{ \AA}}\right)^3 \times 9.00 \text{ \AA}^3$$
$$= 16.01 \text{ \AA}^3$$

$$\text{filled volume} = 4V_{\text{PO}_4} + V_{\text{CuO}_6} + 6V_{\text{AlO}_6} + 14V_{\text{H}_2\text{O}/\text{OH}^-}$$
$$= (4 \times 1.87 + 16.01 + 6 \times 9.00 + 14 \times 20) \text{ \AA}^3$$
$$= 357.49 \text{ \AA}^3$$

This occupies 70% of unit cell, so need to divide by 0.7 to get total volume.

$$\text{total volume} = \frac{357.49 \text{ \AA}^3}{0.7}$$
$$= 511 \text{ \AA}^3$$

*Correct answer scores all three marks. First mark can be awarded for correct volume of the CuO<sub>6</sub> octahedron. Second mark for correct calculation of the filled volume. Third mark for final answer. Allow ECF from parts (a) and (d).*



(ii)  $M_r(\text{unit cell}) = (63.55 + 6(26.98) + 4(30.97) + 30(16.00) + 20(1.008)) \text{ g mol}^{-1}$

$$M_r(\text{unit cell}) = 849.47 \text{ g mol}^{-1}$$

$$\text{mass}(\text{unit cell}) = \frac{849.47 \text{ g mol}^{-1}}{6.022 \times 10^{23} \text{ mol}^{-1}}$$

$$= 1.411 \times 10^{-21} \text{ g}$$

$$\text{density} = \frac{1.411 \times 10^{-21} \text{ g}}{511 \times 10^{-24} \text{ cm}^3}$$

$$= 2.76 \text{ g cm}^{-3}$$

*One mark. Do not allow if density is given in different units. Allow ECF from part (f)(i). If value of total volume = 444 \AA<sup>3</sup> has been used, then ECF answer is:*

$$\text{density} = 3.18 \text{ g cm}^{-3}$$



Total out of 13

**13**