National Unit specification: general information

Unit title: Physical Chemistry (SCQF level 7)

Unit code: H1FK 13

Course: Chemistry Advanced Higher

Superclass:	RD
Publication date:	April 2012
Source:	Scottish Qualifications Authority
Version:	01

Summary

This Unit develops a knowledge and understanding of Physical Chemistry within the contexts of chemical equilibria in aqueous solution, feasibility of chemical reactions and reaction kinetics. The Unit develops the candidate's knowledge and understanding of some of the major concepts used to explain chemical behaviour. The Unit also seeks to develop the candidate's problem solving abilities and practical skills.

Outcomes

1 Demonstrate and apply knowledge and understanding related to *Physical Chemistry*.
2 Demonstrate skills of scientific experimentation and investigation within the context of *Physical Chemistry*.

Recommended entry

Entry for this Unit is at the discretion of the centre. However candidates would normally be expected to have attained the skills and knowledge required by the following or equivalent:

♦ Higher Chemistry (Revised)
♦ Higher Chemistry

General information (cont)

Unit title: Physical Chemistry (SCQF level 7

Credit points and level

0.5 National Unit credit at SCQF level 7: (4 SCQF credit points at SCQF level 7*)

SCQF credit points are used to allocate credit to qualifications in the Scottish Credit and Qualifications Framework (SCQF). Each qualification in the Framework is allocated a number of SCQF credit points at an SCQF level. There are 12 SCQF levels, ranging from Access 1 to Doctorates.

Core Skills

Achievement of this Unit gives automatic certification of the following:

Complete Core Skill   None

Core Skill component   Critical Thinking at SCQF level 6
                                 Using Graphical Information at SCQF level 6

There are also opportunities to develop aspects of Core Skills which are highlighted in the Support Notes of this Unit specification.

National Unit specification: statement of standards

Unit title: Physical Chemistry (SCQF level 7

Acceptable performance in this Unit will be the satisfactory achievement of the standards set out in this part of the Unit specification. All sections of the statement of standards are mandatory and cannot be altered without reference to SQA.

Outcome 1

Demonstrate and apply knowledge and understanding related to *Physical Chemistry*.

Performance Criteria

(a) Make accurate statements about facts, concepts and relationships relating to *Physical Chemistry*.
(b) Use knowledge of *Physical Chemistry* to solve problems.
(c) Use knowledge of *Physical Chemistry* to explain observations and phenomena.

Outcome 2

Demonstrate skills of scientific experimentation and investigation in the context of *Physical Chemistry*.

Performance Criteria

(a) Use a range of data-handling skills in a scientific context.
(b) Use a range of skills related to the evaluation of scientific evidence.

Evidence Requirements for this Unit

Evidence is required to demonstrate that candidates have met the requirements of the Outcomes.

For each of the Unit Outcomes, written and/or recorded oral evidence of the appropriate level of achievement is required. This evidence must be produced under closed-book, supervised conditions within a time limit of 30 minutes.

The Instrument of Assessment must sample the content in each of the following areas:

♦ Chemical equilibrium
♦ Reaction feasibility
♦ Kinetics

An appropriate Instrument of assessment would be a closed-book, supervised test with a time limit of 30 minutes. Items in the test should cover all the Performance Criteria associated with both Outcomes 1 and 2, and could be set in familiar or unfamiliar contexts.

Further detail on the breadth and depth of content is provided within in the appendix to the specification.

National Unit specification: statement of standards (cont)

Unit title: Physical Chemistry (SCQF level 7

For Outcome 2, PC (a) candidates are required to demonstrate that they can use a range of data-handling skills. These skills include selecting, processing and presenting information. Information can be presented in a number of formats including: chemical formulae, balanced chemical equations, diagrams depicting laboratory apparatus, line graphs, scatter graphs, tables, diagrams and text.

For Outcome 2, PC (b), candidates are required to demonstrate that they can use a range of skills associated with the evaluation of scientific evidence. These skills include drawing valid conclusions and making predictions.

The standard to be applied and the breadth of coverage are illustrated in the National Assessment Bank items available for this Unit. If a centre wishes to design its own assessments for this Unit they should be of a comparable standard.

National Unit specification: support notes

Unit title: Physical Chemistry (SCQF level 7

This part of the Unit specification is offered as guidance. The support notes are not mandatory.

While the exact time allocated to this Unit is at the discretion of the centre, the notional design length is 20 hours.

Guidance on the content and context for this Unit

The recommended content together with suggestions for possible contexts and activities to support and enrich learning and teaching are detailed in the Course specification.

This Unit allows candidates to develop knowledge and understanding of Physical Chemistry within the contexts of chemical equilibrium, feasibility of chemical reactions and reaction kinetics. The Unit should develop the candidate's knowledge and understanding of some of the major concepts used to explain chemical behaviour. The Unit also seeks to develop the candidate's problem solving abilities and practical skills.

This Unit offers a diverse and rich vein of contexts and opportunities for practical work as highlighted in the 'Possible contexts and activities' column of the content tables. Opportunities exist for candidates to learn as part of a group through practical work undertaken in partnership or in teams. By developing a greater understanding of some of the mathematical relationships in chemistry, candidates are better able to understand more about rates of chemical reactions and why chemical reactions take place in a particular direction.

Guidance on learning and teaching approaches for this Unit

General advice on approaches to learning and teaching is contained in the Course specification.

Guidance on approaches to assessment for this Unit

Outcomes 1 and 2

It is recommended that a holistic approach is taken for assessment of these Outcomes. Outcomes 1 and 2 can be assessed by an integrated end of Unit test with questions covering all the Performance Criteria. Within one question, assessment of knowledge and understanding and skills of experimentation and investigation can occur. Each question can address a number of assessment standards from either Outcome 1 or 2.

Appropriate assessment items are available from the National Assessment Bank.

National Unit specification: support notes (cont)

Unit title: Physical Chemistry (SCQF level 7

Opportunities for the use of e-assessment

E-assessment may be appropriate for some assessments in this Unit. By e-assessment we mean assessment which is supported by Information and Communication Technology (ICT), such as e-testing or the use of e-portfolios or social software. Centres which wish to use e-assessment must ensure that the national standard is applied to all candidate evidence and that conditions of assessment as specified in the Evidence Requirements are met, regardless of the mode of gathering evidence. Further advice is available in *SQA Guidelines on Online Assessment for Further Education (AA1641, March 2003), SQA Guidelines on e-assessment for Schools (BD2625, June 2005)*.

Opportunities for developing Core Skills

This Unit provides opportunities to develop *Communication, Numeracy, Information and Communication Technology (ICT)* and *Problem Solving* skills in addition to providing contexts and activities within which the skills associated with *Working with Others* can be developed.

Outcome 1, PC (b) and (c) develop a candidate's ability to communicate effectively key concepts and to explain clearly chemical phenomena in written media.

Within this Unit candidates will need to extract and process information presented in both tabular and graphical formats developing the Core Skill of *Numeracy*. Candidates will gain experience in a range of calculations building competence in number.

The appendix to this Unit specification contains an extensive list of 'Possible Contexts and Activities' which include a large number of web based activities, computer simulations and modelling opportunities which all serve to develop higher levels of competence in the key ICT skill s including; accessing information and providing/creating information.

The Unit appendix contains an extensive range of practical laboratory exercises which provide candidates with the opportunity to Work Co-operatively with Others.

Problem Solving skills are central to the sciences and are assessed through Outcome 1, PCs (b) and (c) and also through Outcome 2, PCs (a) and (b).

This Unit has the Using Graphical Information component of Numeracy, and the Critical Thinking component of Problem Solving, embedded in it. This means that when candidates achieve the Unit, their Core Skills profile will also be updated to show that they have achieved Using Graphical Information and Planning and Organising at SCQF level 6.

Disabled candidates and/or those with additional support needs

The additional support needs of individual candidates should be taken into account when planning learning experiences, selecting assessment instruments, or considering whether any reasonable adjustments may be required. Further advice can be found on our website **www.sqa.org.uk/assessmentarrangements**

History of changes to Unit

Version	Description of change	Date

The left hand column below details the content in which candidates should develop knowledge and understanding. The middle column contains notes, which give further details of the breadth and depth of content expected. The right-hand column gives possible contexts and activities which could be used to develop knowledge, understanding and skills. Further details on many of the activities mentioned in the final column can be obtained from **National Qualifications Online**, part of the Education Scotland online service. Where such online support exists the ⌨ symbol appears in the text.

Physical Chemistry 20 hour Unit		
Content	**Notes**	**Possible contexts and activities**
1 Chemical Equilibrium		Try to ensure links to organic chemistry through pK_a values and buffers are constantly reinforced as well as links within the unit itself. Nclark.net and beckerdemos contain lots of good ideas for this Unit and other levels of Chemistry. These contain links to a variety of simulations, experiments and tutorials. ⌨
1(a) Equilibrium Constants	A chemical reaction is in equilibrium when the composition of the reactants and products remains constant indefinitely. The equilibrium constant (K) characterises the equilibrium composition of the reaction mixture. For the general reaction, $$aA + bB \rightleftharpoons cC + dD$$ $$K = \frac{[C]^c [D]^d}{[A]^a [B]^b}$$ where [A], [B], [C] and [D] are the equilibrium concentrations of A, B, C and D respectively and a, b, c and d are the stoichiometric coefficients in the balanced reaction equation. Equilibrium constants are independent of the concentrations or pressures of species in a given reaction. The numerical value of the equilibrium constant depends on the reaction temperature. For endothermic reactions a rise in temperature causes an increase in K, ie, the yield of the product is increased.	Strictly speaking, equilibrium constants are defined in terms of the activities of the reactants and products, but a good working approximation is achieved by using the concentration of solutions, in mol l^{-1}, in place of activities. Because the concentrations of pure solids or pure liquids are constant, by convention they can be given the value 1 in the equilibrium equation. chm.davidson.edu has an equilibrium simulation showing the effect of temperature changes ⌨ Partition coefficients could be included as a specific example of an equilibrium constant.

Content	Notes	Possible contexts and activities
1 Chemical Equilibrium (cont)		
	For exothermic reactions a rise in temperature causes a decrease in K, ie, the yield of the product is decreased. The presence of a catalyst does not affect the value of the equilibrium constant. Equilibrium constants have no units.	
1(b) Ionic product of water 🖥	In water and aqueous solutions there is an equilibrium between the water molecules and hydrogen and hydroxide ions. This ionisation of water can be represented by: $H_2O(\ell) + H_2O(\ell) \rightleftharpoons H_3O^+(aq) + OH^-(aq)$. Water is amphoteric. The dissociation constant for the ionisation of water is known as the ionic product and is represented by K_w. The value of the ionic product varies with temperature. At 25 ^{o}C the value of K_w is approximately 1×10^{-14}. A shorthand representation of $H_3O^+(aq)$ is $H^+(aq)$. Stoichiometric equations and equilibrium expressions can be written using $H^+(aq)$ instead of $H_3O^+(aq)$ where the meaning is clear. The relationship between pH and the hydrogen ion concentration is given by $pH = -\log_{10} [H^+]$	Point out that the equilibrium does not involve free protons but $H_3O^+(aq)$. Use K_w to calculate pH of water and it can be used to show that the pH of water varies with temperature. chemguide.co.uk website gives good information on the ionic product of water including variation of K_w at different temperatures. Unfortunately K_w has been given units. 🖥
1(c) The pH scale linked to H^+ ion concentration	$pH = -\log_{10}[H^+]$ and conversely $[H^+]=10^{-pH}$. In water and aqueous solutions with a pH value of 7 the concentrations of $H^+(aq)$ and $OH^-(aq)$ are both 10^{-7} mol l^{-1} at 25 ^{o}C. If the concentration of $H^+(aq)$ or the concentration of $OH^-(aq)$ is known, the concentration of the other ion can be calculated using K_w or by using $pH + pOH = 14$.	Calculations of $[H^+]$ for different pH values. quia.com has a fun quiz on calculating pH based on Who Wants to be a Millionaire. 🖥
1(d) Bronsted-Lowry acids/bases	The Bronsted-Lowry definitions of acid and base state that an acid is a proton donor and a base is a proton acceptor. For every acid there is a conjugate base, formed by the loss of a proton. For every base there is a conjugate acid, formed by the gain of a proton.	Video by Mark Rosengarten video defines Bronsted/Lowry acids and bases 🖥 Videos by Papapodcasts go further covering conjugate acids and bases 🖥

Content	Notes	Possible contexts and activities
1(e) Strong and weak acids and bases	In aqueous solution, strong acids/bases are completely dissociated into ions but weak acids/bases are only partially dissociated. Examples of strong acids include hydrochloric acid, sulfuric acid and nitric acid. Ethanoic, carbonic and sulfurous acids are examples of weak acids. Solutions of metal hydroxides are strong bases. Ammonia and amines are examples of weak bases. The weakly acidic nature of solutions of carboxylic acids, sulfur dioxide and carbon dioxide can be explained by reference to equations showing the equilibria. The weakly alkaline nature of a solution of ammonia or amines can be explained by reference to an equation showing the equilibrium. The acid dissociation constant is represented by K_a or by pK_a where $pK_a = -\log_{10}K_a$ Although equimolar solutions of weak and strong acids/bases differ in pH, conductivity, and reaction rates they do not differ in stoichiometry of reactions.	mhhe.com has a video of a simple animation showing the difference between the strong acid, HCl, and the weak acid HF in terms of ionisation. 💻 Other Papapodcasts' videos cover strong/ weak acids and strong/weak bases. 💻 Investigation of pH of strong & weak acids and bases using pH meter or indicators. Investigate pH of differing metal/non-metal hydroxide solutions. Possible look at titration curves for strong/weak acids and bases. Short videos of these are available. 💻 Chem.iastate.edu website shows a simple simulation using a pH meter to test pH of various acids and alkalis of differing concentrations. 💻 Library.thinkquest.org has information on strong and weak acids and on the acid dissociation constant 💻
1(f) The pH of salt solutions	A soluble salt of a strong acid and a strong base dissolves in water to produce a neutral solution. A soluble salt of a weak acid and a strong base dissolves in water to produce an alkaline solution. A soluble salt of a strong acid and a weak base dissolves in water to produce an acidic solution. Soaps are salts of weak acids and strong bases. The acidity, alkalinity or neutrality of the above kinds of salt solution can be explained by reference to the appropriate equilibria.	Calculate acidity/basicity of a given salt solution and confirm by measurement of pH. Test pH of various salt solutions including sodium carbonate, sodium sulfite, sodium stearate, ammonium chloride, ammonium nitrate etc. The Chem.iastate.edu website also shows a simple simulation using a pH meter to test pH of various salt solutions of differing concentrations. 💻
1(g) Calculation of pH for a weak acid	The approximate pH of a weak acid can be calculated using $pH = \frac{1}{2} pK_a - \frac{1}{2} \log_{10}c$ where c is the nominal concentration of the acid in the solution.	Calculate pH of a $0 \cdot 1$ mol l^{-1} solution of a weak acid and confirm by measurement. Dilute it tenfold to show pH rises by $0 \cdot 5$ rather than by 1 as it would when diluting a strong acid such as $0 \cdot 1$ mol l^{-1} HCl. Good opportunity for candidates to practise diluting accurately.

Content	Notes	Possible contexts and activities
1(h) Buffer solutions	A buffer solution is one in which the pH remains approximately constant when small amounts of acid or base are added. An acid buffer consists of a solution of a weak acid and one of its salts. In an acid buffer solution the weak acid can supply hydrogen ions when these are removed by the addition of a small amount of base. The salt of the weak acid provides the conjugate base, which can absorb excess hydrogen ions produced by the addition of a small amount of acid. A basic buffer consists of a solution of a weak base and one of its salts. In a basic buffer solution the weak base removes excess hydrogen ions and the conjugate acid provided by the salt supplies hydrogen ions when these are removed. An approximate pH of an acid buffer solution can be calculated from its composition and from the acid dissociation constant, $pH = pK_a - \log_{10} \dfrac{[\text{acid}]}{[\text{salt}]}$	Prepare buffer solution, measure pH and compare with calculated value. Opportunity to use pH meter and use buffer solution to calibrate it. pH of blood important. Small change in pH causes major problems. Mhhe.com shows an animation of how a buffer solution resists change in pH when a strong acid or a strong base are added. Need to explain to candidates that acetic acid and acetate are the same as ethanoic and ethanoate. 🖥 The chem.iastate.edu website has another animation of a buffer solution in which candidates can prepare a buffer solution, test its pH, add acid or alkali and test the pH again. Can also use this to compare measured pH value of buffer against the calculated value. 🖥 Chemcollective.org has an interesting but difficult quiz. Unfortunately answers are not provided. 🖥 Michele.usc.edu has an animation showing the difference in pH changes when adding an acid or alkali to a buffer solution compared with adding acid or alkali to water. 🖥
1(i) Indicators	Indicators are weak acids for which the dissociation can be represented as: $HIn(aq) + H_2O(\ell) \rightleftharpoons H_3O^+(aq) + In^-(aq)$ The acid indicator dissociation constant is represented as K_{In} and is given by the following expression: $$K_{In} = \frac{[H_3O^+]\,[In^-]}{[HIn]}$$ In aqueous solution the colour of the acid indicator is distinctly different from that of its conjugate base. The colour of the indicator is determined by the ratio of $[HIn]$ to $[In^-]$. The theoretical point at which colour change occurs is when $[H^+] = K_{In}$.	Determine pH range over which indicator colour changes. (possibly using natural indicator extracted from a plant) Select and use appropriate indicators for titration of: weak acid and strong base strong acid and weak base. Use indicator for weak acid/weak base titration to show that a single indicator is not appropriate chemguide.co.uk shows titration curves for different combinations of acids and alkalis 🖥 jchemed.chem.wisc.edu has animations (series of slides) showing colour change in phenolphthalein in various titrations. 🖥

Content	Notes	Possible contexts and activities
1(i) Indicators (cont)	The colour change is assumed to be distinguishable when [HIn] and [In$^-$] differ by a factor of 10. The pH range over which a colour change occurs can be estimated by the expression: pH = pK_{In} ± 1	
2 Reaction feasibility		
2(a) Enthalpy of formation	The standard enthalpy of formation, ΔH^o_f, is the enthalpy change when one mole of a substance is formed from its elements in their standard states. The standard enthalpy of a reaction can be calculated from the standard enthalpies of formation of the reactants and products. $\Delta H^o = \Sigma \Delta H^o_f$ (products) - $\Sigma \Delta H^o_f$ (reactants). Knowledge of standard conditions is important.	
2(b) Entropy	The entropy (S) of a system is a measure of the degree of disorder of the system. The greater the degree of disorder, the greater the entropy. Entropy increases as temperature increases. Changes of state involve changes in entropy.	Investigate simple exothermic and endothermic reactions. Discuss in terms of entropy changes.
2(c) Second and Third Laws of Thermodynamics	One version of the Second Law of Thermodynamics states that the total entropy of a reaction system and its surroundings always increases for a spontaneous process. Heat energy released by the reaction system into the surroundings increases the entropy of the surroundings, whereas heat absorbed by the reaction system from the surroundings decreases the entropy of the surroundings. One version of the Third Law of Thermodynamics states that the entropy of a perfect crystal at 0 K is zero. The standard entropy of a substance is the entropy value for the standard state of the substance.	Some information on the laws of thermodynamics can be found on the bbc.co.uk website 🖳

Content	Notes	Possible contexts and activities
2(d) Calculating changes in entropy	The change in standard entropy for a reaction system can be calculated from the standard entropies of the reactants and products. $\Delta S^o = \Sigma S^o$ (products) - ΣS^o (reactants).	Experiment/demo of endothermic reaction of $Ba(OH)_2$ with NH_4Cl. Leek.high.staffs.sch.uk gives examples of practical work which can be carried out on spontaneous endothermic reactions. 🖥
2(e) Free energy	The change in free energy for a reaction is related to the enthalpy and entropy changes; $\Delta G = \Delta H - T\Delta S$. If the change in free energy (ΔG) between reactants and products is negative, a reaction may occur. This is because the equilibrium composition favours the products over the reactants. The standard free energy change for a reaction can be calculated from the standard free energies of formation of the reactants and products using the relationship, $\Delta G^o = \sum \Delta G_f^o$ (products) - $\sum \Delta G_f^o$ (reactants).	Chemconnections.org has a little applet showing graph of ΔG v temperature. Candidates can change values of ΔH^o and ΔS^o. 🖥
2(f) Applications of the concept of free energy	The feasibility of a chemical reaction under standard conditions can be predicted from the calculated value of the change in standard free energy (ΔG^o). The temperatures at which a reaction may be feasible can be estimated from $\Delta G^o = \Delta H^o - T\Delta S^o$ by considering the range of values of T for which $\Delta G^o < 0$.	Former AH PPA, verification of a thermodynamic prediction could be carried out here as an example of a theoretical prediction working out fairly closely to the observed experimental value. Suggest a larger quantity of $NaHCO_3(s)$ be used to ensure bulb of thermometer is completely covered but this will produce a volume of CO_2 greater than 100 cm^3 so needs to be monitored carefully and heating stopped and syringe removed from the barrel before 100 cm^3 reached. Ellingham diagrams can be used to show how ΔG^o varies with temperature and they were useful in predicting temperatures at which reductions of metal oxides became feasible.

Content	Notes	Possible contexts and activities
2(g) Equilibrium and free energy	Under non-standard conditions any reaction is feasible if ΔG is negative. At equilibrium $\Delta G = 0$. A reaction will proceed spontaneously in the forward direction until the composition is reached where $\Delta G = 0$.	
3 Kinetics		
3(a) Orders of reaction	The rate of a chemical reaction normally depends on the concentrations of the reactants. For a first order reaction the rate of reaction is proportional to the concentration of one reactant and the rate can be expressed as: rate = k[A] where k is the rate constant and [A] is the concentration of reactant A in mol l^{-1}. The order of a reaction with respect to any one reactant is the power to which the concentration of that reactant is raised in the rate equation. The overall order of a reaction is the sum of the powers to which the concentrations of the reactants are raised in the rate equation. The order of a reaction can only be determined from experimental data. The rate constant can be determined from initial rate data for a series of reactions in which the initial concentrations of reactants are varied. Integral orders of reaction from zero order to third order should be covered.	Propanone/iodine reaction PPA from current AH. Decolourisation of blue food dye. See SSERC bulletin No. 225. Within the body, drug molecules are converted into a number of different molecules that are more easily excreted into the urine. These molecules are called metabolites and the whole process is called metabolism. The metabolism of the drug will begin as soon as it is administered and in many cases the process follows first order kinetics, ie the rate of metabolism is proportional to the concentration of the drug. The RSC have a case study from The Horseracing Forensic Laboratory (HFL). There is a candidate worksheet and additional notes and answers for teachers. 🖥 Saskschools.ca has an example on reaction rates in which candidates can calculate the order of reaction and work out the rate law. 🖥
3(b) Reaction mechanisms	Reaction mechanisms usually occur by a series of steps. The rate of reaction is dependent on the slowest step which is called the 'rate determining step'. Experimentally determined rate equations can provide evidence for a proposed reaction mechanism.	S_N1 and S_N2 reaction mechanisms can be discussed here but will also be covered in the Organic Chemistry Unit. Saskschools.ca has lots of information on reaction mechanisms including examples. 🖥