SQA Advanced Unit specification

General information for centres

Unit title: Thermodynamics and Kinetics: Theory and Laboratory Skills (SCQF level 8)

Unit code: HV15 48

Superclass: RD

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Source: Scottish Qualifications Authority

Version: 01

Unit purpose

This Unit is designed to enable learners to understand key aspects of thermodynamics and kinetics. Learners will also develop practical skills in techniques relevant to thermodynamics and kinetics. The Unit is suitable for learners studying at SQA Advanced Diploma level, and will provide the necessary underpinning knowledge and skills to enable progression to further study of physical chemistry at degree level or to seek employment in science based industries.

Outcomes

On successful completion of the Unit the learner will be able to:

1 Describe and apply the main principles, laws and formulae associated with chemical thermodynamics.
2 Describe and apply the main principles, laws and formulae associated with chemical kinetics.
3 Perform practical experiments related to thermodynamics and kinetics.

Credit points and level

1 SQA Credit at SCQF level 8: (8 SCQF credit points at SCQF level 8)

Recommended entry to the Unit

Entry is at the discretion of the centre, however it is recommended that learners should have completed the Units HV00 47 *Fundamental Chemistry: Theory and Laboratory Skills* and HV0M 47 *Physical Chemistry: Theory and Laboratory Skills* or equivalent.

Core Skills

Achievement of this Unit gives automatic certification of the following Core Skills component:

Complete Core Skill	None
Core Skill component	Using Number 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.

Context for delivery

If this Unit is delivered as part of a Group Award, it is recommended that it should be taught and assessed within the subject area of the Group Award to which it contributes.

The Assessment Support Pack (ASP) for this Unit provides assessment and marking guidelines that exemplify the national standard for achievement. It is a valid, reliable and practicable assessment. Centres wishing to develop their own assessments should refer to the ASP to ensure a comparable standard. A list of existing ASPs is available to download from SQA's website **(http://www.sqa.org.uk/sqa/46233.2769.html)**.

Equality and inclusion

This Unit specification has been designed to ensure that there are no unnecessary barriers to learning or assessment. The individual needs of learners should be taken into account when planning learning experiences, selecting assessment methods or considering alternative evidence.

Further advice can be found on our website **www.sqa.org.uk/assessmentarrangements**.

SQA Advanced Unit specification: Statement of standards

Unit title: Thermodynamics and Kinetics: Theory and Laboratory Skills (SCQF level 8)

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.

Where evidence for Outcomes is assessed on a sample basis, the whole of the content listed in the Knowledge and/or Skills section must be taught and available for assessment. Learners should not know in advance the items on which they will be assessed and different items should be sampled on each assessment occasion.

Outcome 1

Describe and apply the main principles, laws and formulae associated with chemical thermodynamics.

Knowledge and/or Skills

- Reaction enthalpies
- Temperature variation of reaction enthalpies
- Deductions from entropy data concerning the spontaneity of a process
- Chemical equilibrium
- Chemical equilibria calculations using thermodynamic data
- Clapeyron equation
- Clausius-Clapeyron equation
- Validity of Clausius-Clapeyron equation

Outcome 2

Describe and apply the main principles, laws and formulae associated with chemical kinetics.

Knowledge and/or Skills

- Reaction mechanisms in terms of elementary steps
- Order, rate constant and half-life of reactions
- Effect of temperature on reaction rate in terms of activation energy
- Arrhenius equation
- Catalytic activity with respect to activation energy effects and adsorption theories

Outcome 3

Perform practical experiments related to thermodynamics and kinetics.

Knowledge and/or Skills

- Thermodynamics and kinetic experiments
- Working safely, within current health and safety regulations
- Consistent and accurate results
- Recording observations and results
- Evaluation skills
- Result analysis and conclusions

Evidence Requirements for this Unit

Written and/or oral recorded evidence for Outcome 1 should be assessed using a closed-book assessment under supervised conditions. The assessment will use a sampling approach to the Knowledge and/or Skills as detailed below. It is recommended that the assessment be completed within 1 hour 30 minutes. Learners can only have access to the *SQA Databook for HN Chemistry* or any suitable replacement when sitting the assessment.

Written and/or oral recorded evidence for Outcome 2 should be assessed using a closed-book assessment under supervised conditions. The assessment will use a sampling approach to the Knowledge and/or Skills as detailed below. It is recommended that the assessment be completed within 1 hour 30 minutes. Learners can only have access to the *SQA Databook for HN Chemistry* or any suitable replacement when sitting the assessment.

Written and/or oral recorded evidence for Outcome 3 should be assessed by production of a full laboratory report, or by completion of an appropriate pro forma. An assessor's observation checklist could be used to record performance evidence of practical experiments.

Outcome 1

The assessment will sample six of the eight Knowledge and/or Skills items. Learners will not have prior knowledge of which items are being assessed. Those items which are not sampled must be covered in the alternative (re-sit) assessment.

Where an item is sampled, a learner's response will be judged satisfactory where the evidence shows that the learner can:

- Perform calculations to determine reaction enthalpies.
- Perform calculations involving reaction enthalpies under variation of temperature.
- Make deductions from entropy data concerning the spontaneity of a process.
- Describe factors affecting chemical equilibrium.
- Perform calculations related to chemical equilibria using thermodynamic data.
- Perform calculations using the Clapeyron equation.
- Perform calculations using the Clausius-Clapeyron equation.
- Identify the conditions necessary for the validity of the Clausius-Clapeyron equation.

Outcome 2

The assessment will sample four of the five Knowledge and/or Skills items. Learners will not have prior knowledge of which items are being assessed. Those items which are not sampled must be covered in the alternative (re-sit) assessment.

Where an item is sampled, a learner's response will be judged satisfactory where the evidence shows that the learner can:

- Describe reaction mechanisms in terms of elementary steps.
- Perform calculations of order, rate constant and half-life of reactions.
- Describe the effect of temperature on reaction rate in terms of activation energy.
- Perform calculations involving the Arrhenius equation.
- Describe catalytic activity with respect to activation energy effects and adsorption theories.

Outcome 3

Learners will perform a minimum of two practical experiments, the content of one of the practical experiments must be related to Outcome 1 with the content of the other practical experiment being related to Outcome 2. A learner's response will be judged satisfactory where the evidence shows that the learner can achieve all of the following:

- Follow instructions to perform experiments related to thermodynamics and kinetics.
- Work in a safe manner regarding current health and safety regulations.
- Achieve consistent and accurate results.
- Record experimental observations and results clearly and accurately.
- Evaluate validity of results in terms of sources of and values of experimental errors.
- Analyse results correctly and state valid conclusions.

An assessor observation checklist will be used to record the learner's performance of the practical work in line with given instructions and health and safety requirements.

Learners must report one of the two practical experiments by production of a full laboratory report. Learners may report the remaining practical experiment by production of a full laboratory report or by completion of an appropriate pro forma. Where a pro forma approach is deployed, the pro forma will not present information or assistance to the learners on how to correctly perform calculations, analyse experimental results or experimental errors. Learners will be expected to perform such activities independently on the basis of the experimental data.

Where a learner does not perform an assessed practical experiment to the required standard, they will be given the chance to either reattempt the same practical experiment, or to undertake a different practical experiment of similar complexity. Where a laboratory report or pro forma does not meet required standard, then the learner will be given a single opportunity to re-draft. If the required standard is still not attained, then an alternative practical experiment will be set.

SQA Advanced Unit Support Notes

Unit title: Thermodynamics and Kinetics: Theory and Laboratory Skills (SCQF Level 8)

Unit Support Notes are offered as guidance and are not mandatory.

While the exact time allocated to this Unit is at the discretion of the centre, the notional design length is 40 hours.

Guidance on the content and context for this Unit

This Unit is part of the framework for the SQA Advanced Diploma in Applied Sciences and the SQA Advanced Diploma in Applied Chemical Sciences but may be suitable for inclusion in other SQA Advanced science and engineering qualifications. It is designed to develop the theoretical and practical aspects of thermodynamics and kinetics introduced in the Units HV00 47 *Fundamental Chemistry: Theory and Laboratory Skills* and HV0M 47 *Physical Chemistry: Theory and Laboratory Skills*.

Outcome 1 — Describe and apply the main principles, laws and formulae associated with chemical thermodynamics

- Calculations involving the determination of reaction enthalpies from standard enthalpies of formation and bond enthalpies.
- Calculations involving reaction enthalpies under conditions of variation of temperature, including application of the Kirchoff equation.
- Making deductions from entropy data concerning the spontaneity of a process, including chemical reactions, expansion of a gas, temperature change and phase change.
- Description of factors affecting chemical equilibrium, including temperature, pressure, catalyst, concentration and activity.
- Calculations relating chemical equilibria to thermodynamic data, eg relationship of free energy to equilibrium constants, solubility product and chemical activity, variation of equilibrium constants with temperature, etc.
- Calculations using the Clapeyron equation to elucidate behaviour of substances at phase transitions.
- Calculations using Clausius-Clapeyron equation to elucidate behaviour of substances at liquid-vapour phase transitions.
- The conditions necessary for the validity of the Clausius-Clapeyron equation.

Outcome 2 — Describe and apply the main principles, laws and formulae associated with chemical kinetics

- Reaction mechanisms in terms of elementary steps and concept of rate determining step. Sequential step reactions and chain reactions. Overview of examples from organic chemistry — SN1, SN2 and halogenation of methane.
- Methods of determining reaction order. Investigation of concentration vs time data to elucidate if integrated rate equations for 1st and 2nd order kinetics apply. Half-life method applied to 1st order data, and initial rate method for ‘clock reactions’. Determination of rate constants and half-lives from experimental data.
- The effect of temperature on reaction rate in terms of activation energy, explained through application of Boltzmann distributions.
- Calculations involving the Arrhenius equation to determine activation energy from experimental data or to determine the effect of temperature change on rate constants.
- Catalytic activity explained in terms of activation and adsorption (concentration) theories.

Outcome 3 — Perform practical experiments related to thermodynamics and kinetics

Guidance on suitable practical experiments for assessment purposes is given elsewhere in this document. However, it is envisaged that learners will also participate in a range of other practical experiments which will both develop their laboratory skills and support the theory covered in Outcomes 1–2.

In carrying out such activities, learners should follow Good Laboratory Practice (GLP) and carry out or be familiar with the risk and Control of Substances Hazardous to Health (COSHH) assessments on all procedures undertaken. Opportunities should be taken to develop awareness of the sources of experimental error and of the accuracy of measurements, with quantification of errors where possible

Guidance on approaches to delivery of this Unit

There is no particular order in which Outcomes 1–2 would be best delivered. It is envisaged that laboratory work and demonstrations will feature across the delivery of each of the Outcomes, and that the assessed practical experiments for Outcome 3 will be undertaken in a similar timeframe to the underpinning theory.

It is envisaged that delivery of Outcome 1 could commence with a review/revision of reaction enthalpies and Hess's Law from SCQF level 7. Learners could then perform different approaches to determination of reaction enthalpies under standard conditions, from use of standard enthalpies of formation and bond dissociation enthalpies. Learners could then proceed to consider how to convert enthalpies determined under standard conditions to those at non-standard conditions, including by use of the Kirchoff equation.

The concept of equilibrium and factors that affect equilibrium and Le Chatelier's principle could then be revised, along with the concepts of entropy and Gibbs Free Energy from SCQF level 7. The entropy change associated with physical processes (temperature, volume, pressure changes) could then be covered and deductions on spontaneity made. Spontaneity of chemical reactions could then be revised and the relationships of equilibrium constants to Gibbs Free Energy and temperature should be examined. The concepts of chemical activity of electrolytes could be introduced, and used to explain 'salting in' and 'salting out' effects and should be applied to the calculation of K_{sp}'s. The final section in the Outcome moves learner's knowledge of phase equilibria into calculations using both the Clapeyron and Clausius-Clapeyron equations. The conditions under which the latter equation can be applied should be explained.

It is envisaged that Outcome 2 could commence with a revision of concepts of kinetics from SCQF level 7, including collision theory, factors affecting rates, potential energy profiles and activation energies. Learners could then proceed to be introduced to a range of reaction mechanisms, and the difference in the kinetics of sequential step and chain reactions. There is a natural link with areas which learners would cover in organic chemistry, including SN1 and SN2 reactions and the free radical halogenation of methane. There are only a very small number of mechanisms which learners would be expected to memorise, but they should be able to make deductions about other mechanisms from supplied kinetic data and vice versa. The integrated rate laws for 1st and 2nd order reactions could then be introduced, and then how reaction order can be determined from experiment by checking graphical fit of data versus integrated rate expressions or by half-life method (1st order only). The application of 'initial rate' method to 'clock reactions' should also be covered. The effect of temperature on rate could be discussed qualitatively in terms of potential energy profiles, activation energies and Boltzmann distributions, followed by quantitative treatments involving the Arrhenius

equation. Finally, the effects of catalysts on reaction rates could be covered in terms of both activation and adsorption theories.

It is envisaged that Outcome 3 will be delivered alongside the theoretical based Outcomes. A range of practical experiments could be utilised to both support understanding of the underlying theory and to prepare students for undertaking the assessed practical experiments. Aspects suitable for experimental investigation might include an investigation of colligative properties, determination of partition coefficients, investigation of liquid-vapour phase equilibria, determination of equilibrium constants, determination of reaction order, determination of activation energy for 'clock reactions', modelling exercises on entropy as a function of probability.

Guidance on approaches to assessment of this Unit

Evidence can be generated using different types of assessment. The following are suggestions only. There may be other methods that would be more suitable to learners.

Outcomes 1 could be assessed by a closed-book assessment with an appropriate cut-off score that covers the sampling requirements as detailed in the Evidence Requirements. Assessment should be carried out in supervised conditions, and it is recommended that the assessment be completed within 1 hour 30 minutes. Learners can only have access to the *SQA Databook for HN Chemistry* or any suitable replacement when sitting the assessment.

Outcomes 2 could be assessed by a closed-book assessment with an appropriate cut-off score that covers the sampling requirements as detailed in the Evidence Requirements. Assessment should be carried out in supervised conditions, and it is recommended that the assessment be completed within 1 hour 30 minutes. Learners can only have access to the *SQA Databook for HN Chemistry* or any suitable replacement when sitting the assessment.

Where evidence of Outcomes 1 and 2 is assessed by sampling, the whole of the content listed in the Knowledge and/or Skills must be taught and available for assessment. Learners should not know in advance the items on which they will be assessed, and different items should be sampled on each assessment occasion. Any items not sampled in the first assessment, must be included in the alternative (re-sit) assessment.

In Outcome 3 learners are required to undertake two assessed practical experiments, the content of one of the practical experiments must be related to Outcome 1 with the content of the other practical experiment being related to Outcome 2. Examples of suitable experiments are given below. However, this list is not prescriptive, and other practical experiments of similar complexity may be used by the centre.

Suitable practical experiments in thermodynamics are:

- Determine the vapour pressure of water over a range of temperatures and hence obtain a value for its latent heat.
- Determine the equilibrium constant for the esterification of ethanoic acid over a range of temperatures and use this to obtain a value for ΔG.
- Determination of the dissociation constants of ethanoic and trichloroethanoic acids and comparison of the ΔG values.
- Construction of a phase equilibrium plot for a ternary liquid mixture, eg chloroform, water, ethanoic acid.
- Use of Clausius-Clapeyron equation to investigate Raoult's law by measuring the boiling points of liquid mixtures, eg propanol/pentane vs pentane/heptane.

Suitable practical experiments in kinetics are:

- Hydrolysis of methyl methanoate in dilute NaOH solution.
- Determination of the energy of activation for the reaction of bromide and bromate ions.
- Kinetics of SN1 reaction, eg hydrolysis of 2-chloro-2-methylpropane.
- Kinetics of SN2 reaction, eg hydrolysis of iodoethane.

Assessed practical experiments will usually be performed individually. However, there may be some experiments that are suitable to be undertaken in pairs or small groups. If this is the case then the assessor should ensure that all participants are actively involved and are able to adequately demonstrate the required skills.

An exemplar instrument of assessment with marking guidelines has been produced to indicate the national standard of achievement at SCQF level 8.

Centres are reminded that prior verification of centre-devised assessments would help to ensure that the national standard is being met. Where learners experience a range of assessment methods, this helps them to develop different skills that should be transferable to work or further and higher education.

Opportunities for 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 learner evidence and that conditions of assessment as specified in the Evidence Requirements are met, regardless of the mode of gathering evidence. The most up-to-date guidance on the use of e-assessment to support SQA's qualifications is available at **www.sqa.org.uk/e-assessment**.

Opportunities for developing Core and other essential skills

This Unit has the *Using Number* component of *Numeracy* embedded in it. This means that when learners achieve the Unit, their Core Skills profile will also be updated to show they have achieved *Using Number* at SCQF level 6.

There may also be opportunities to gather evidence towards Core Skills in *Problem Solving* at SCQF level 6, and *Information and Communication Technology (ICT)* at SCQF level 4.

Numeracy — Using Number at SCQF level 6

Learners will be required to decide on the steps and operations to solve complex problems, carrying out sustained and complex calculations, eg performing calculations related to quantitative electrolysis, or of electromotive force under non-standard conditions.

Problem Solving — Reviewing and Evaluating at SCQF level 6

Following assessed practical experiments learners will be required to review and evaluate the effectiveness of the exercise with a thorough interpretation of random and systematic sources of error. They will be required to reach sound conclusions on the basis of the data collected and the inherent errors.

Information and Communication Technology (ICT) — Providing/Creating Information at SCQF level 4

Learners will make effective and appropriate use of ICT packages to produce laboratory reports or pro formas in an appropriate format. Packages used will likely include word processing, spreadsheets, and specialist chemical structure software.

Sustainability

Sustainability can be embedded in delivery of the Unit in a variety of ways. For example, by encouraging minimum usage, correct disposal procedures and possibly recycling (eg of solvents) during practical experiments.

History of changes to Unit

Version	Description of change	Date

SQA acknowledges the valuable contribution that Scotland's colleges have made to the development of SQA Advanced Qualifications.

FURTHER INFORMATION: Call SQA's Customer Contact Centre on 44 (0) 141 500 5030 or 0345 279 1000. Alternatively, complete our Centre Feedback Form.

General information for learners

Unit title: Thermodynamics and Kinetics: Theory and Laboratory Skills (SCQF level 8)

This section will help you decide whether this is the Unit for you by explaining what the Unit is about, what you should know or be able to do before you start, what you will need to do during the Unit and opportunities for further learning and employment.

This is a 1-credit Unit at SCQF level 8, which you are likely to be studying as part of the second year of an SQA Advanced Diploma science programme. Before progressing to this Unit it would be beneficial to have completed the Units HV00 47 *Fundamental Chemistry: Theory and Laboratory Skills* and HV0M 47 *Physical Chemistry: Theory and Laboratory Skills*, where you will have learned underpinning aspects of physical chemistry and developed your practical skills. There will be a strong emphasis on the importance of experimental data in understanding chemical principles, and on the applications of chemical knowledge in practical situations.

On completion of this Unit you should be able:

1 Describe and apply the main principles, laws and formulae associated with chemical thermodynamics.
2 Describe and apply the main principles, laws and formulae associated with chemical kinetics.
3 Perform practical experiments related to thermodynamics and kinetics

Outcome 1

In this Outcome you will build on the understanding of enthalpies and Hess's Law from SCQF level 7. You will learn of different approaches to the determination of reaction enthalpies under standard conditions, from use of standard enthalpies of formation and bond dissociation enthalpies. You will then proceed to consider how to convert enthalpies determined under standard conditions to non-standard conditions, including by use of the Kirchoff equation.

You will revisit the concepts of equilibrium and factors that affect equilibrium, along with the concepts of entropy and Gibbs Free Energy from SCQF level 7. You will learn of the entropy change associated with physical processes (temperature, volume, pressure changes) and the implications of this for spontaneity. The spontaneity of chemical reactions will then be recapped and the relationships of equilibrium constants to Gibbs Free Energy and temperature will be examined. You will be introduced to the concept of chemical activity of electrolytes, and this will be used to explain 'salting in' and 'salting out' effects and will be applied to the calculation of K_{sp}'s. You will then build your knowledge of phase equilibria, including performing calculations using both the Clapeyron and Clausius-Clapeyron equations. The conditions under which the latter equation can be applied will be examined.

Outcome 2

This Outcome will commence with a revision of concepts of kinetics from SCQF level 7, including collision theory, factors affecting rates, potential energy profiles and activation energies. You will then be introduced to a range of reaction mechanisms, and the difference in the kinetics of sequential step and chain reactions. There is a natural link with areas which you would cover in organic chemistry, including SN1 and SN2 reactions and the free radical halogenation of methane. You will not be expected to memorise a large number of reaction

mechanisms, but you will be expected to make deductions about mechanisms from supplied kinetic data and vice versa. You will be introduced to the integrated rate laws for 1st and 2nd order reactions, and how reaction order can be determined from experiment. The effect of temperature on rate will be discussed qualitatively in terms of potential energy profiles, activation energies and Boltzmann distributions, and by quantitative treatments involving the Arrhenius equation. Finally, you will examine the effects of catalysts on reaction rates in terms of both activation and adsorption theories.

Outcome 3

In this Outcome you will undertake practical experiments, based on the content of Outcomes 1 and 2.

During this practical work, you will also be expected to develop good laboratory practices as well as improve your skills of manipulation, observation and measurement. You will also be encouraged to develop safe working practices and to strive constantly to improve the accuracy and reliability of your results. The reporting and analysis of experimental data is an important aspect of the practical sessions.

Assessment

For Outcomes 1 and 2 you will take closed-book, end of Outcome assessments.

Outcome 3 will be assessed after you have learned the necessary practical skills, and will take the form of two practical experiments, for which you will report your results either in full laboratory reports, or by completion of pro forma reports.

Core Skills

This Unit has the Core Skill component of *Using Number* at SCQF level 6 embedded in it. You may also have opportunities to develop the Core Skills of *Problem Solving* at SCQF level 6, and *Information and Communication Technology (ICT)* at SCQF level 4.