



# Accreditation of degree programmes

[rsc.li/degreeaccreditation](https://rsc.li/degreeaccreditation)

## About us

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The Royal Society of Chemistry is an international organisation connecting chemical scientists with each other, with other scientists, and with society as a whole. We develop, recognise and celebrate professional capabilities, and we bring people together to spark new ideas and new partnerships. We support teachers to inspire future generations of scientists, and we speak up to influence the people making decisions that affect us all.

One of our Royal Charter objectives requires us:

*to establish, uphold and advance the standards of qualification, competence and conduct of those who practise chemistry as a profession*

More than 450 degree programmes at over 80 universities around the world are currently accredited by our well-established and respected accreditation system.

## About this document

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Through accreditation, we promote good practices in the university education of chemical scientists, and make sure that future practising scientists are knowledgeable and competent.

These guidelines describe what we look for in a degree programme that is submitted for accreditation. We outline the key requirements that set the threshold standards. These are designed to provide a flexible framework that allows for innovation and the wider development of contemporary education focusing on learning outcomes. We explain our accreditation process and give guidance on the information that you need to submit.

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## Part one: what is accreditation?

### Why is accreditation important?

Accreditation of degree programmes by professional and statutory bodies is a mark of assurance that particular standards are met. Accredited programmes address the needs of employers and students, and provide marketing advantages for universities.

Our accreditation is a peer review process founded on the judgement of professional chemists. This ultimately provides a credible and independently verifiable method for employers and students to differentiate between degree programmes.

Our accreditation service can be summarised in terms of its features, advantages and benefits for the HEI:

| Feature of service                                                     | Advantage                                                                                                                                                                                                                      | Benefit                                                                                                                                                                                                                                                                                         |
|------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Externally validated mark of excellence by a leading professional body | Allows differentiation of the institution, thereby enhancing its profile and credibility as a provider of quality chemistry education                                                                                          | <ul style="list-style-type: none"> <li>Enhanced prospects for student recruitment</li> <li>Enhanced prospects for government funding</li> <li>Increased engagement and networking with other leading universities</li> <li>Enhanced mobility and employability for graduate students</li> </ul> |
| An independent benchmark against respected quality standards           | Provides a peer review mechanism to assess, evaluate and enhance chemistry degree programmes. Our assessors are experts from leading universities worldwide which leads to continuous improvement and sharing of best practice | <ul style="list-style-type: none"> <li>University able to stay at the forefront of education standards</li> <li>Improved prospects for student recruitment and funding by government or corporates</li> </ul>                                                                                   |

## Pathways to accreditation

This document explains accreditation for Bachelor's level degrees as well as integrated Master's (MChem, MSci) and discrete Master's (MSc) levels.

We can assess any chemistry-based programme, and make a judgement based on output standards against our accreditation key requirements.

## How accreditation works

Our accreditation operates as a single, global, summative assessment process for all degree programmes based on the discipline of chemistry. It is a peer-reviewed process managed by our Committee for Accreditation and Validation (CAV), that is responsible for assessing applications, applying the published criteria and making judgements. Royal Society of Chemistry Trustees appoint CAV committee members from our membership. This ensures that reviewers have contemporary experience of university-level education and an understanding of the demands of employers and academia. We also employ professionally qualified staff whose role is to help and advise you and to manage the accreditation process. Together CAV members and our staff ensure the high quality of our accreditation.

Accreditation lasts for a period of five years, after which you are invited to submit your programmes for re-accreditation. Continued accreditation throughout the five year period is dependent on you telling us of any subsequent changes in the structure or content of your programmes. For major changes, we carry out a formal review of a programme's accreditation status.

Importantly, accreditation is more than a single mark of quality. It provides you with opportunities for wider engagement with us through our extensive range of activities for promoting and developing science. Because we share a common purpose: advancing excellence in the chemical sciences.

## Reference points

We do not set our standards in isolation. We use internationally recognised guidelines and frameworks and exploit our global networks to define a robust accreditation process with a relevant set of academic values. In developing accreditation criteria, we have used several reference points, both generic and subject specific. A key reference document is the chemistry Subject Benchmark Statement which was published in revised form by the UK's Quality Assurance Agency for Higher Education (QAA) in 2014.<sup>1</sup> We supported the QAA's benchmarking group that had representation not only from university departments in England, Scotland and Wales but also from the chemistry-based industries.

The statement covers Bachelor's and all types of Master's degree programmes. It is a distinctive document within a wider geographical context and represents the most contemporary statement on chemical education standards and is a valuable point of reference for the accreditation of degree programmes.

Your first step to accreditation is to make sure the specifications and outputs of your programmes are clearly aligned with published qualification frameworks and the QAA Chemistry Benchmark Statement. If your programmes are subject to an alternative local benchmark statement you should check with us before submission that any divergence is justifiable in the context of your own national qualifications framework.

<sup>1</sup> <https://www.qaa.ac.uk/quality-code/subject-benchmark-statements>

## Bachelor's accreditation

Bachelor's accredited programmes are expected to provide students with:

- a broad and balanced appreciation of key chemical concepts.
- a range of practical skills so that they can understand and assess risks and work safely in the laboratory.
- the ability to apply standard methodology to the solution of problems in chemistry.
- the knowledge and skills base which leads to graduate employment or to further study.

In terms of professional qualification, an accredited Bachelor's degree provides access to professional categories of Royal Society of Chemistry membership and partially meets the academic requirements for Chartered Chemist (CCChem).

## Master's accreditation

Master's accredited programmes are expected to provide students with:

- an in-depth understanding of specialised areas of chemical science.
- the ability to plan and carry out experiments independently and assess the significance of outcomes.
- the ability to adapt and apply methodology to the solution of unfamiliar types of problems.
- a critical awareness of advances at the forefront of the chemical science discipline.
- effective preparation for professional employment or doctoral studies in the chemical sciences.

In terms of professional qualification, Master's accreditation provides access to professional categories of Royal Society of Chemistry membership and fully satisfies the academic requirements for our Chartered Chemist (CCChem) award.

There are generally two types of Master's degree programmes: discrete and integrated.

### a) Discrete Master's programmes

These programmes normally follow on from the award of a Bachelor level qualification. This is the study pattern followed in most parts of the world. The chemical science qualification conferred is usually either MSc (Master of Science) or simply referred to as a Master's degree. In the UK there are also several MRes (Master of Research) qualifications in the chemical sciences.

### b) Integrated Master's programmes

These programmes take students from university entry to master's level, combining learning outcomes at Bachelor's and Master's levels. The qualification conferred is usually MChem (Master in Chemistry) or MSci (Master in Science). Normally there is no intermediate award of a Bachelor's qualification.

## Accreditation values

Accredited degree programmes stimulate students in the subject of chemistry and allow them to develop an appreciation of its application in different contexts. We don't want to inhibit creative curriculum development designed to meet evolving needs and regional demand, so we don't specify required content in detail. However, to become accredited, a degree programme must satisfy a range of criteria based on knowledge and understanding, intellectual abilities, and both practical and professional skills.

In general terms, an accredited degree programme provides:

- knowledge of chemical science that builds upon secondary education (study prior to university) and incorporates a critical understanding of theories and principles.
- essential skills for applying chemical knowledge and solving complex scientific problems with a strong emphasis on laboratory skills in synthesis and analysis.
- development of professional skills which allow transferability within the chemical sciences and across employment sectors.
- competence in dealing with challenging activities or projects while taking on responsibility for decision-making in variable contexts.

## Part two: output standards for Royal Society of Chemistry accredited programmes

The criteria for accreditation are broken down into a number of key requirements. To gain accreditation, universities must demonstrate that they provide students with all the relevant key requirements for the programme type listed.

| Key requirements (KR) for accreditation |                                                                                                                                                                                      | Bachelor's | Integrated Master's | Discrete Master's |
|-----------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|---------------------|-------------------|
| Breadth (knowledge)                     | KR1: Evidence of study of the main branches of chemistry is provided and developed at appropriate times during the course.                                                           | ✓          | ✓                   |                   |
|                                         | KR2: Programme outcomes should include a breadth of understanding of chemistry with the ability to solve problems at the threshold level of competence as exemplified in Appendix A. | ✓          | ✓                   |                   |
|                                         | KR3: Breadth of understanding of chemistry through prior learning must be assured through admissions processes.                                                                      |            |                     | ✓                 |
| Depth (knowledge)                       | KR4: Programmes should build on knowledge base to allow students to appreciate developments, in some areas, at the forefront of the discipline.                                      | ✓          |                     |                   |
|                                         | KR5: Programmes should ensure a depth of knowledge in specialist areas of chemical science demonstrated by an ability to solve problems at the level exemplified in Appendix B.      |            | ✓                   | ✓                 |
| Practical skills                        | KR6: Students must develop a range of practical skills.                                                                                                                              | ✓          | ✓                   | ✓                 |
| Project work                            | KR7: Programmes must incorporate some independent investigative methodology.                                                                                                         | ✓          |                     |                   |
|                                         | KR8: Programmes must provide research training to enable students to complete a substantial project, the outcome of which is potentially publishable.                                |            | ✓                   | ✓                 |

Further guidance on each of the key requirements can be found in the following pages.



| Key requirements (KR) for accreditation |                                                                                                                                                                                    | Bachelor's | Integrated Master's | Discrete Master's |
|-----------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|---------------------|-------------------|
| Placement                               | KR9: Any external placements must be subject to assessment against explicit and demanding criteria with universities retaining control and supervision of its students.            | ✓          | ✓                   | ✓                 |
| Professional skills                     | KR10: Programmes must develop a broad range of transferable key skills.                                                                                                            | ✓          | ✓                   |                   |
|                                         | KR11: Programmes must develop the professional skills for those intending to practice chemical science as a profession.                                                            |            | ✓                   | ✓                 |
| Assessment                              | KR12: Assessment should be varied, appropriate and rigorous, and require students to apply their knowledge and solve problems.                                                     | ✓          | ✓                   | ✓                 |
| Title                                   | KR13: The title of a programme should be indicative of content and address the assumptions an employer will make on the graduates' abilities based on the title.                   | ✓          | ✓                   | ✓                 |
| Quality assurance                       | KR14: Universities must have robust quality assurance mechanisms in place for all aspects of its programmes.                                                                       | ✓          | ✓                   | ✓                 |
|                                         | KR15: Resources devoted to a programme should provide students with a suitably supportive environment so enabling them to be successful in achieving the stated learning outcomes. | ✓          | ✓                   | ✓                 |
| Learning environment                    | KR16: The learning environment should provide staff and students with suitable academic development and wellbeing support mechanisms to meet the stated learning outcomes.         | ✓          | ✓                   | ✓                 |

## Guidance notes on key requirements

### Breadth (knowledge)

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                                                          |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|
| <b>KR1: Evidence of study of the main branches of the chemistry is provided and developed at appropriate times during the course.</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | Applicable to:<br><b>i) Bachelor's</b><br><b>ii) Integrated Master's</b> |
| <ul style="list-style-type: none"> <li>The chemical sciences represent a broad field of study. It is essential that those studying an accredited programme demonstrate knowledge of the key chemical concepts either as outlined within the QAA Chemistry Benchmark Statement or, where an alternative qualifications framework exists, in the context of an acceptable, local benchmark statement that has already been approved by the Committee for Accreditation and Validation.</li> <li>The nature of chemistry is such that there are no distinct boundaries between branches of the subject or indeed with other subjects. The traditional division into inorganic, organic and physical chemistry does not necessarily adequately reflect the growing importance of interdisciplinary areas such as analytical chemistry, biological chemistry, computational chemistry, environmental chemistry and others.</li> <li>These studies should lead on from secondary/high school science education and are likely to feature at an introductory stage of the degree programme.</li> <li>Students must develop an ability to evaluate and interpret key chemical principles.</li> <li>Programmes titled 'Chemistry' will provide a balanced programme across the discipline. Although specialism is allowed, if significant weighting is given to the specialism this must be reflected in the title.</li> <li>Typically programmes titled 'Chemistry and xxx' should have an even split in the studies, whereas Chemistry with xxx' or 'Xxx Chemistry' should devote ca. 25% of the course to the specialism.</li> <li>To be accredited suitably titled interdisciplinary chemical science degrees such as Pharmaceutical science, Nanotechnology, Chemical physics, Forensic science etc should include the core concepts as outlined above.</li> <li>Stakeholders expect that core chemical concepts form a fundamental part of Royal Society of Chemistry accreditation.</li> </ul> |                                                                          |
| <b>KR2: Programme outcomes should include a breadth of understanding of chemistry with the ability to solve problems at the threshold level of competence as exemplified in Appendix A.</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Applicable to:<br><b>i) Bachelor's</b><br><b>ii) Integrated Master's</b> |
| <ul style="list-style-type: none"> <li>Students completing an accredited programme must be able to demonstrate a systematic understanding of fundamental physicochemical principles and an ability to apply that knowledge to the solution of theoretical and practical problems.</li> <li>Students must also be enabled to gain knowledge of a range of inorganic and organic materials and be able to realise their understanding in the synthesis and isolation of such materials and the analysis of their properties.</li> <li>The required threshold level is exemplified by the standard of problem questions in Appendix A.</li> <li>For Bachelor's programmes, the threshold for breadth of study must be achieved within a programme's learning outcomes.</li> <li>For integrated Master's programmes, the threshold for breadth of study should be achieved at an intermediate stage of the programme. For a full time four year programme, this would typically be by the end of year 3. For a full time 5 year programme, this would typically be by the end of year 4.</li> <li>Programmes that are developed to provide a wide ranging and extensive knowledge of chemistry, for example those titled simply 'Chemistry', would normally be expected to offer the required level of breadth across the chemistry discipline.</li> <li>Programmes with more specialist objectives, eg those titled 'medicinal chemistry', can provide reduced coverage in the least relevant areas. This must be compensated for by an increased coverage in more relevant areas of chemical science.</li> <li>Problems in Appendix A are intended to be indicative of the standard which the Royal Society of Chemistry expects students to attain and are in no way intended to define curriculum content.</li> </ul>                                                                                                                                                                        |                                                                          |

**KR3: Breadth of understanding of chemistry through prior learning must be assured through admissions processes.**Applicable to:  
**Discrete Master's only**

- There is an expectation that those embarking on discrete master's programmes have already developed a level of subject knowledge, abilities and skills in chemistry that enables them to pursue studies in chemical science at the Master's level and successfully achieve the prescribed learning outcomes.
- Typically those applying for discrete Master's programmes will have an undergraduate or equivalent qualification in chemistry or one which contained greater part chemistry. Through scrutiny of diploma supplements, interviews and/or any other means the university chooses, it must be established before admission that any prior qualification(s) has caused the student to develop subject knowledge and understanding at bachelor's level together with the appropriate abilities and skills described in the chemistry Subject Benchmark Statement.
- Admission processes can also be applied to those with an undergraduate or equivalent qualification in a related interdisciplinary area and/or those with suitable supplementary learning. In admitting such students, universities may wish to provide a programme of supplementary studies in order to strengthen areas of weakness.
- The accreditation process will seek to ensure that university admissions processes are robust and applied effectively.
- A discrete Master's degree which admits students from outside the chemical sciences can be accredited. However, only those students with prior learning in the chemical sciences will fully meet the academic requirements for CChem.

## Depth (knowledge)

**KR4: Programmes should build on the knowledge base to allow students to appreciate developments at the forefront of some areas of chemical sciences.**Applicable to:  
**Bachelor's only**

- Programmes must provide significant enhancement beyond the required level for breadth of study (defined by *KR1* and *KR2*) (see appendix A for appropriate example questions).
- Students should gain a detailed knowledge and critical understanding in one or more chemical science specialisms some of which are informed by or at the forefront of the subject.
- Specialisation should provide students with the knowledge base from which they can proceed to graduate employment or to further studies in the chemical sciences.
- Suitably titled specialist/interdisciplinary degrees such as Pharmaceutical science, Forensic science or Nanotechnology, should build on the core chemical science knowledge base and provide a distinct link between the specialism and the chemical sciences aspects at the forefront of the subject.

**KR5: Programmes should ensure a depth of knowledge in specialist areas of chemical science demonstrated by an ability to solve problems at the level exemplified in Appendix B.**

Applicable to:  
**all Master's programmes**

- A discrete Master's degree will contain an appropriate amount of taught material which should normally equate to 33-66% of overall content. There is an expectation that at least 83% of learning outcomes will be at Master's level, as outlined in the QAA MSc characteristics statement.
- Depth of study cross references to master's level in the chemistry Subject Benchmark Statement. (ref – *Advanced studies, Problem-solving*) and is exemplified by the provision of a number of problems of an advanced nature in appendix B. These are suitable for inclusion in unseen examinations, open-book examinations, and examinations where questions are issued in advance.
- Material at the level of appendix B problems would normally be included in the latter stages of a full time integrated Master's programme.
- Material at the level of appendix B problems would be a fundamental feature of a discrete Master's programme.
- There is an expectation that problems presented to students in assessments are unfamiliar, in that they have not been previously coached to tackle problems of a particular type.
- The range of problems that students will be expected to be able to solve will usually be narrower than in the case of those presented in appendix A. This allows institutions freedom to continue to develop specialist chemical science programmes. In all cases intellectual rigour demonstrated by depth of study will be necessary.
- Problems contained in appendix B are intended to be indicative of the standard which the Royal Society of Chemistry expects students to attain and are in no way intended to define curriculum content.

## Practical skills

### KR6: Students must develop a range of practical skills.

Applicable to:  
**all programmes**

- For Bachelor's programmes students should typically complete at least 300 timetabled hours (exclusive of project work). Allowances are permitted for fully integrated credit bearing industrial placements in a laboratory setting.
- For integrated Master's programmes, students should typically complete at least 400 timetabled hours (exclusive of the substantial project). Allowances are permitted for fully integrated credit bearing industrial placements in a laboratory setting.
- Practical work, while supporting theoretical aspects should be stimulating and challenging in its own right and provide the essential *Chemistry-related practical skills* described in the chemistry Subject Benchmark Statement.
- The practical component should be laboratory based and designed so that students are exposed to a variety of synthetic and measurement techniques.
- Practical work must be rigorously and appropriately assessed and contribute towards the final mark of the degree programme.
- Bachelor's level exit points from integrated Master's programmes are required to fully meet this key requirement.
- Health and safety training must be provided.
- Programmes with specialism would still be expected to meet the requisite practical hours. The nature of the practical content may reflect the nature of the specialism.
- Computational work, case studies and short investigative tasks can contribute to the total timetabled hours, along with supervised preparatory and write up sessions.
- The Royal Society of Chemistry will consider a lower value for programmes which incorporate a period of study in industry or for part time modes of study. In such cases a condition may be imposed on the accreditation status of the programme and applicants may be required to provide evidence of developing appropriate practical skills within a workplace context.
- For discrete Master's programmes, students must have prior learning of appropriate practical skills at Bachelor's level and programmes should seek to develop these further, for example, through project work.
- An institution can make reasonable adjustments such as: laboratory helper, help with fine manipulations, or directing laboratory work remotely for those unable to carry out laboratory work for reasons of disability. Accreditation is reflective of the overall programme rather than individual situations.

## Project work

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------|
| <b>KR7: Programmes must incorporate some independent investigative methodology.</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | Applicable to:<br><b>Bachelor's only</b>         |
| <ul style="list-style-type: none"> <li>• These are open ended activities which require students to manage their own learning.</li> <li>• Activities should require students to apply information that they have learned earlier in the programme in order to consolidate and extend their knowledge and understanding of chemistry.</li> <li>• One or more activities can be incorporated and could include:               <ul style="list-style-type: none"> <li>– research project</li> <li>– literature investigation</li> <li>– collaborative project work</li> <li>– external placement</li> <li>– open ended practicals of an investigative nature (not included in KR6)</li> </ul> </li> <li>• These activities would typically account for 25% of the student workload in the final year.</li> <li>• Bachelor's level exit points from integrated Master's programmes are required to fully meet this key requirement.</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                  |
| <b>KR8: Programmes must provide research training to enable students to complete a substantial project, the outcome of which is potentially publishable.</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | Applicable to:<br><b>all Master's programmes</b> |
| <ul style="list-style-type: none"> <li>• For integrated Master's programmes, the substantial project should normally account for not less than one half of student workload in the final year.</li> <li>• For discrete Master's programmes, the substantial project should normally account for not less than one third of the entire programme.</li> <li>• Project work is an important element in the education of a professional chemist since it facilitates the development of essential high-level career skills.</li> <li>• Programmes should provide suitable research training to enable students to successfully complete a substantial research project.</li> <li>• The project, which can include those in computational and theoretical chemistry or in chemical pedagogy, would normally be completed in the final stage of a programme. It must be of an investigative nature and contain a substantial amount of advanced chemistry, drawing on the chemical and related literature.</li> <li>• Projects should require some originality and be of a quality that is potentially publishable, i.e. work that has not been reported previously in the literature.</li> <li>• The project should be an individual project, although team projects can be considered, and may be undertaken either in an academic institution or in industry.</li> <li>• Assessment criteria for projects should be transparent and clearly explained to students before the project work commences.</li> <li>• Project work must be assessed rigorously and contribute significantly to the final classification or grade.</li> </ul> |                                                  |

## External placements

**KR9: External placements must be subject to assessment against explicit and demanding criteria with universities retaining control and supervision of its students.**

Applicable to:  
**all relevant  
programmes**

- Many chemical science programmes incorporate a placement either in industry or at university in a different country. For purposes of accreditation, placements need to be carefully selected on the basis of an agreed programme of work acceptable to both the home university and the external partner.
- Placements should be subject to assessment against explicit and demanding criteria and make an appropriate contribution to the final degree classification or grade.
- Industrial placements will usually involve both a major work-related assignment and elements of guided study when incorporated in integrated master's programmes.
- The guided study component would normally be broadly based in chemistry with content and level of learning outcomes comparable with respective studies at the university.
- Typically for a placement lasting one academic year, guided study would form around one quarter of learning activity/credit. Industrial partners should be made aware of the need for guided study and allow students to be released from work to complete their studies.
- Universities are encouraged to make best use of technology to ensure that students are provided with quality distance learning materials and can readily access support from the university.
- Placements at a university in a different country can follow a similar format to placements in industry although alternatively and possibly more commonly, students will study courses provided by the partner university. Such courses must be of a comparable level of outcome to those at the home university.
- Students returning to their home university after a placement must be suitably prepared to continue their chemical science studies at the appropriate level.
- The Royal Society of Chemistry recognises that some universities offer placement opportunities that extend the length of study normally associated with a degree programme. While these may be credit rated, they tend not to contribute to the final classification or grade of the degree awarded. Such programmes allow students to focus more on the placement experience and do not necessarily lend themselves towards a guided study component.

## Professional skills

### KR10: Programmes must develop a broad range of transferable key skills.

Applicable to:  
i) Bachelor's  
ii) Integrated Master's

- Transferable skills development is an essential feature of all degree programmes.
- Requisite transferable skills cross reference to generic skills outlined in the QAA chemistry Subject Benchmark Statement at Bachelor's level (see appendix C for an example of a skills matrix). These should incorporate:
  - communication skills
  - scientific writing, data presentation, referencing literature
  - problem solving skills relating to qualitative and quantitative information
  - numeracy and mathematical skills
  - ethical responsibilities
  - sourcing of information
  - information technology and data processing
  - teamworking
  - time management and organisational skills
  - personal development awareness
  - business skills
- Programmes should promote a sense of proper scientific conduct and ethical responsibility.
- Collectively students' generic skills should provide a basis to undertake further training of a professional nature.
- Students' competence in the application of transferable skills must be assessed and appropriately weighted.

### KR11: Programmes must develop the professional skills for those intending to practice chemical science as a profession.

Applicable to:  
all Master's  
programmes

- Professional skills development is an essential feature of all Master's programmes and relates directly to employability as a professional chemist.
- Requisite professional skills cross reference to generic skills outlined in the chemistry Subject Benchmark Statement at Master's level (see appendix C for an example of a skills matrix). These incorporate independent learning ability, self-direction and originality, and the ability to exercise initiative and personal responsibility along with:
  - problem solving including demonstration of self-direction and originality
  - critical thinking skills within data analysis and experiment design
  - learning skills required for professional development
  - communication and interaction with other disciplinary areas
  - decision making in unpredictable situations
- Programmes should provide the independent learning ability for continuing professional development and progression to Chartered Chemist through subsequent work practice.
- Students' competence in the application of professional skills should be assessed.



## Assessment

**KR12: Assessment should be varied, appropriate and rigorous, and require students to apply their knowledge and solve problems.**

Applicable to:  
**all programmes**

- Universities are encouraged to use of a wide range of assessment techniques matched to particular aspects of the programme which have been carefully designed and applied to ensure validity and reliability as discriminators.
- Programmes should seek to ensure students are encouraged to:
  - complete various forms of in-course assessment with particular, but not exclusive, evaluation of practical competence
  - apply their understanding of earlier fundamental principles at advanced stages of the programme
  - complete assessments in a diverse range of topics
  - demonstrate their problem solving abilities
  - critically analyse information, construct synopses, and devise solutions
  - deal with topics expansively using reason and argument
- An appropriate proportion of marks linked to key concepts should be assigned on the basis of formal examination conducted under controlled conditions. Such examinations can be open or closed book.
- Progression to subsequent stages of a programme should only be possible when a minimum competence has been demonstrated in pre-requisite areas.
- Universities must demonstrate that assessment of project work is rigorous and conducted against clear criteria.
- For Master's programmes, assessment of the project work is central to determining whether or not a programme has provided the subject knowledge, abilities and skills associated with Master's level learning outcomes and hence the basis for professional practice in the chemical sciences.
- The final grading of an award should be substantially weighted to student performance in the final stages of their programme, but should not rely exclusively on it.
- Links between all assessment and learning outcomes should be evident, and associated quality assurance should be robust.

## Programme title

**KR13: The title of a programme should be indicative of content and address the assumptions an employer will make on the graduates' abilities based on the title.**

Applicable to:  
**all programmes**

- When selecting programmes, students will often equate their career aspirations to the title. Similarly an employer of chemists will have preconceptions about graduates from a programme based on title. The title of a programme should be indicative of the content and it should follow that the subject knowledge, abilities and skills provided to successful students are directly relevant to the title.
- The Royal Society of Chemistry's general expectations are:
  - Programmes titled simply 'Chemistry' provide a balanced programme across the discipline. The substantial project can be any chemistry topic
  - Programmes with titles such as 'Chemistry with medicinal chemistry' or 'Chemistry with analytical chemistry' imply a balanced programme with a specialism in a particular area of chemical science
    - Bachelor's programmes should provide study in the specialism in the final year of study (see KR4)
    - Master's programmes must contain taught material from the implied specialism at Master's level and require students to conduct their substantial project in an area of chemical science related to specialism (see KR5 and KR8)
  - Programmes which combine studies in chemistry with that in another discipline such as 'Chemistry with French' and 'Chemistry with mathematics' denote a major/minor split
    - » Generally the minor subject would typically account for at least a quarter of the programme
    - » For Master's programmes, chemistry studies should be taken to Master's level and form the substantial project
- Broader chemical science degrees may be eligible for accreditation but must meet all key requirements. Stakeholders/employers expect a Royal Society of Chemistry accredited degree to retain a core breadth and depth of chemistry and practical aspects.

## Quality assurance

**KR14: Universities must have robust quality assurance mechanisms in place for all aspects of its programmes.**

Applicable to:  
**all programmes**

- A clear quality assurance framework should be in place and actively applied to ensure that outcome standards are appropriate, consistent and fair.
- QA processes must assure that:
  - programmes are adequately supported by learning resources
  - agreed specifications are followed
  - assessments are set at the appropriate standard
  - assessment processes are impartial and robust
  - successful students achieve the stated learning outcomes and are graded accordingly
  - students can progress fairly and effectively
  - content and assessments are regularly reviewed
  - feedback is obtained and considered from students
  - future stakeholder/employer input is sought on a regular basis through forums such as industrial advisory boards

**KR15: Resources devoted to a programme should provide students with a suitably supportive environment so enabling them to be successful in achieving the stated learning outcomes.**

Applicable to:  
**all programmes**

- Universities are expected to provide evidence that students on an accredited programme are adequately supported by appropriate learning resources and support such as computing and communication facilities (access to software, internet and email) and suitable library provision, including appropriate accessibility to key textbooks, major online chemical databases and the primary chemical literature, such as a range of peer-reviewed journals.
- Lecture theatres and classrooms should have demonstration facilities, projection capabilities and internet access. Laboratories should adhere to strict safety guidelines and should house appropriate instrumentation for teaching and research, which should be up to date, high quality and properly maintained.
- Ultimately, adequate support is judged by whether or not the resources devoted to a programme provide students with a suitably supportive environment so enabling them to be successful in achieving the stated learning outcomes.

**KR16: The learning environment should provide staff and students with suitable academic development and wellbeing support mechanisms to meet the stated learning outcomes.**

Applicable to:  
**all programmes**

- Royal Society of Chemistry accredited degree programmes must be delivered by an appropriate level of fully-qualified, full and/or part-time staff (academic, administrative and technical) who are knowledgeable and suitably skilled in the areas they are teaching and able to set assessments to an appropriate standard.
- An environment of health and safety should be employed throughout the programme. This should be championed by staff and support staff as to set an example.
- Appropriate professional development opportunities should be available to staff.
- The institution should promote and adopt a supportive, inclusive and diverse learning and teaching environment, and foster opportunities to widen participation.
- Suitable care for student wellbeing should be available to support students to ensure the optimal student experience.

## Part three: how to achieve accreditation

### Consultation

The first phase to achieving accreditation is to discuss your degree programmes with our professionally qualified staff. They can provide informed advice on your programme's potential for accreditation and help you to identify and collate information for your accreditation submission. Contact [accreditation@rsc.org](mailto:accreditation@rsc.org) to start this conversation.

### Application

You must provide comprehensive information on your degree programmes so we can make a proper judgement on the programmes' quality. Preparing a submission can be the rate-determining step in the accreditation process, so you should devote time and effort to completing the self-assessment form and organising the supplementary evidence, which should include:

- ☐ self evaluation form
- ☐ detailed syllabus and module specifications
- ☐ exam papers and model answers for most recent year
- ☐ laboratory scripts/handbooks/experimental details for all practicals
- ☐ selection of research projects across the breadth of the subject
- ☐ list of research project titles from the previous year
- ☐ examples of problem solving coursework\*
- ☐ external quality assurance reports
- ☐ admission policy documentation, for discrete masters courses only.

Our staff can help with this process and provide guidance on how to prepare your accreditation submission. We can receive all the documentation electronically. Please ensure the documents are filed in a logical manner and keep file paths and names as short as possible, such as shown on the right.

- ▲  RSC accreditation application
  -  Application forms
- ▲  Coursework examples
  -  Year 1
  -  Year 2
  -  Year 3
  -  Year 4
- ▲  Exams and model answers
  -  Year 1
  -  Year 2
  -  Year 3
  -  Year 4
  -  Placement info
- ▲  Practical schedules
  -  Year 1
  -  Year 2
  -  Year 3
  -  Year 4
-  Project titles and marking criteria
-  QA or external examiners reports and responses
- ▲  Syllabus and module details
  -  Year 1
  -  Year 2
  -  Year 3
  -  Year 4

\*Coursework or continuous assessment outside of formal examinations.

## Review

Once you've collected all the information, submit your application. We distribute the documentation to members of the Committee for Accreditation and Validation (CAV) for detailed initial consideration against the key requirements. The feedback of this initial review will form the basis of the site visit (see below).

## Department visit

The department visit is a key feature of the accreditation process and is designed to help the committee make its judgement. It provides a valuable opportunity for us to discuss the features of the programmes with your staff and with students and to check out the infrastructure and resources devoted to delivery.

We would expect senior staff from your department to be available to meet the assessors at some point. A meeting with some current students over lunch to discuss their learning experiences is an essential feature of the visit and we will also need to meet with QA representatives from your university.

The visit is across one day, and involves a team of trained peer assessors (2-3 committee members who are experts in the field of HE teaching) and a member of our professionally qualified staff.

Once we have received comments from the assessors we will contact you with a proposed agenda and any further documentation we would like to see during the visit. These will be sent approximately one week before the visit.

A typical one-day itinerary is shown overleaf. This is simply an example: the scale and duration of a visit will vary.

Any issues can be resolved and clarifications made. If anything has been left out of the documentation, this can be discussed in person. Ultimately having a department visit allows the accreditation committee to speed up its decision making processes.

## Example of a department visit agenda

### 9.30 Arrival and greeting with head of department

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This initial meeting allows introductions to be made and gives the department an opportunity to outline their overarching aims and objectives.

### 10.00 Private meeting of visiting team and review of additional materials

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This meeting enables the Royal Society of Chemistry's visiting team to review the preliminary comments (i.e. identifying the specific areas for clarification or discussion) and to agree its primary objectives for the visit. Any material that has been requested prior to the campus visit should be made available to the team including the requested project reports.

### 10.30 Tour of facilities

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The tour allows the visiting team to determine whether the learning resources available to support the programme are appropriate. The tour must include teaching laboratories and may include the library, IT facilities and any other specialist teaching areas or learning resources.

### 11.30 Meeting with QA department or departmental representatives responsible for this (international universities only)

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This meeting focuses on the quality assurance the institution has in place and will involve discussions around how quality assurance is maintained in their programme.

### 12.30 Lunch meeting with students

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This meeting allows the team to listen to the views of students and to gauge their experience of studying at the university. Ideally the meeting would include around 8-10 students from various year groups. If more than this number wish to attend, they are welcome to do so.

### 13.30 Meeting with programme team (head of department, head of teaching, heads of sections or programme leaders)

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This meeting focuses on the specific areas for clarification or discussion. It involves a wide ranging discussion on particular aspects of the programmes and is likely to drill down to more specific detail.

### 15.00 Private meeting of visiting team

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This meeting enables the visiting team to review the day, to ensure that its objectives have been satisfied, and to prepare some provisional feedback.

### 15.30 Feedback meeting – outline of next steps

---

Some informal feedback is given on the department visit. However no decision can be given on accreditation at this stage. The remaining stages of the process, together with a timescale for an accreditation outcome, are outlined.

### 16.00 Seminar from the visiting assessors (international universities only)

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An opportunity for students and staff at the university to hear from the visiting assessors about their research as well as learn more about what the Royal Society of Chemistry has to offer.

We prefer to keep the department visit relatively informal so that any aspects of the programme can be discussed openly. We don't publish visit reports, but use them to inform CAV.

## Judgement

After the department visit has taken place, your submission is formally considered at the next available meeting of CAV. Meetings are usually in March, June and December of each year.

The committee's final decision is based on its review of the submitted documentation and the department visit report. If the committee are confident that you have satisfied all the key requirements, accreditation is granted.

After the meeting you will receive a letter outlining the terms of accreditation together with a feedback document. The feedback document may contain up to five general components.

### 1. Evident strengths

We value good practices in teaching and learning and are keen to make sure that people involved in such activities are acknowledged for their commitment to students' learning experiences. If appropriate we will promote and share good practice through our networks and published materials.

### 2. Prerequisites

These prerequisites are necessary before we grant accreditation. If you have followed all previous consultation during the submission process, it is unlikely any prerequisites will be on the feedback form.

### 3. Requirements

In some instances, we will specify a condition for accreditation. It would normally need a change to your programme. You must make this change to maintain your programmes accredited status. We normally give a timescale for these changes, which is typically 12 months.

### 4. Recommendations

These are continuous enhancement features which you should make during the accreditation period (five years). They may involve more significant changes and you may need to review your specifications, procedures and practices.

We expect that, when programmes are submitted for re-accreditation after five years, the committee's recommendations will have been addressed.

### 5. Suggestions

Committee members often identify features that might be enhanced through alternative approaches. These are given to you as constructive suggestions. We hope that they will stimulate initiatives for programme development. You are not obliged to act on suggestions to keep your accreditation.

## Confirmation

Universities with accredited degree programmes receive an embossed certificate of accreditation, which you should display prominently to your students and other stakeholders. You should consider publicising your achievement in internal publications, websites, marketing material and local media. We can help with media communications if needed.

You can use our accredited degree logo on your course marketing information, such as websites and advertising material, or even on your degree certificates. Our logo is an internationally recognised mark of a high quality organisation. When using the logo, you must follow the guidelines at all times, which will be sent alongside the logo.

We publish a list of accredited degree programmes on our website which allows students to find where quality chemical education exists with minimal effort. The list includes web links to university websites, helping potential students to make direct contact with admissions tutors.

## Working together

Royal Society of Chemistry accreditation should be seen as a part of a wider engagement with an organisation which is committed to the promotion and advancement of the chemical sciences.

### Membership

We are keen to engage with those studying chemistry whether on accredited degree programmes or as research postgraduates. We actively promote Royal Society of Chemistry membership to students at discounted subscription rates. Students will be made aware of the professionalism of being associated with us, of how to develop into a fully competent professional chemical scientist and achieve Chartered Chemist (CChem) status.

In addition to a wide range of membership benefits, we have developed a network of student chemical societies and aim to encourage communication and enhance interactions for aspiring chemical scientists. For example, we advise and support student chemical societies in staging events for students at their university. We also provide a range of travel grants for students wishing to further their knowledge of chemistry.

Academic staff are encouraged to join us. Through their contribution to the profession, many leading faculty members will be eligible to become Fellows (FRSC) which is our senior membership category. Others can join as Members (MRSC) and may wish to become chartered. Irrespective of membership category, a wide range of membership benefits are available.

### Influence policy

Association with us provides access to specialist networks and an ability to influence policy in education, science and professional practice. In education, we constantly work to promote good practice in teaching and stimulate the interest of young people in studying chemical science. In science, we are committed to shaping the future direction of the chemical sciences. In professional practice, we set and provide guidance on standards of professional conduct and make sure that practising chemical scientists maintain a contemporary interest in their chosen profession.

### Publishing

We are one of the world's leading scientific publishers, offering an exceptional range of peer-reviewed journals, magazines, books, databases and publishing services to the chemical science community. Universities with accredited programmes will already have some association with us. Enhancement of this relationship is our goal and we hope that faculty members will publish their best work in our high impact journals.



## Appendices

### Appendix A: threshold questions

- A1** (a) A mixture of  $\text{Al}_2\text{O}_{3(s)}$  and  $\text{CuO}_{(s)}$  weighing 18.371 mg was heated under  $\text{H}_2$  in a thermogravimetric analysis experiment. Under these conditions  $\text{CuO}$  is reduced to  $\text{Cu}$  but  $\text{Al}_2\text{O}_3$  does not react. When all of the  $\text{CuO}$  had been reduced the final mass was 17.462 mg. Calculate the mass percentage of  $\text{CuO}$  in the original mixture.
- (b) An atomic absorption experiment was carried out using mixed solutions containing  $\text{Fe}^{2+}$  and  $\text{Mn}^{2+}$  ions. A standard mixture containing  $2.00 \text{ mg dm}^{-3}$   $\text{Mn}$  and  $2.00 \text{ mg dm}^{-3}$   $\text{Fe}$  was analysed and gave an intensity ratio of 1.10:1 for the lines arising from  $\text{Mn}$  and  $\text{Fe}$  respectively. A mixture of  $5.00 \text{ cm}^3$  of a solution containing an unknown concentration of  $\text{Fe}$  and  $5.00 \text{ cm}^3$  of a  $2.00 \text{ mg dm}^{-3}$  standard solution of  $\text{Mn}$  was made up. This gave an absorbance of 0.128 arising from  $\text{Mn}$  and of 0.185 arising from  $\text{Fe}$ . Calculate the concentration of  $\text{Fe}$  in the unknown solution.
- A2** (a) The complex  $\text{K}_4[\text{Fe}(\text{CN})_6]$  is diamagnetic whereas  $[\text{Fe}(\text{H}_2\text{O})_6]\text{Cl}_2$  is paramagnetic.
- (i) Give the oxidation state and the number of metal  $d$  electrons in **EACH** of the complexes.
- (ii) For **EACH** complex: draw the crystal field splitting diagram inserting the metal  $d$  electrons and clearly indicate whether **EACH** complex is low spin or high spin.
- (b) When conc.  $\text{HCl}$  is added to a pink solution of  $[\text{Co}(\text{H}_2\text{O})_6]^{2+}$  the deep blue species  $[\text{CoCl}_4]^{2-}$  is formed.
- (i) Sketch the crystal field splitting diagram for the  $[\text{CoCl}_4]^{2-}$  complex and calculate the crystal field splitting energy in terms of the appropriate splitting parameter.
- (ii) Explain why the complex  $[\text{CoCl}_4]^{2-}$  is formed rather than  $[\text{CoCl}_6]^{4-}$ .
- A3** (a) Comment on the values for the following bond enthalpies which relate to the hydrogen-bonds, between, and covalent bonds within, the molecules  $\text{H}_2\text{O}$  and  $\text{H}_2\text{S}$ :

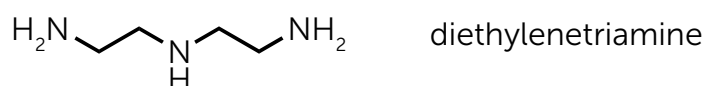
| Molecule             | Hydrogen Bond ( $\text{EH}\cdots\text{E}$ ; $\text{E} = \text{O}$ or $\text{S}$ )<br>Bond Enthalpy / $\text{kJ mol}^{-1}$ | Covalent Bond ( $\text{E}-\text{H}$ ; $\text{E} = \text{O}$ or $\text{S}$ )<br>Bond Enthalpy / $\text{kJ mol}^{-1}$ |
|----------------------|---------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------|
| $\text{H}_2\text{O}$ | 20                                                                                                                        | 463                                                                                                                 |
| $\text{H}_2\text{S}$ | 5                                                                                                                         | 338                                                                                                                 |

- (b) Explain how these bond enthalpies affect:
- (i) the melting and boiling points;
- (ii) the standard enthalpies of formation of  $\text{H}_2\text{O}$  and  $\text{H}_2\text{S}$ .
- (c) Explain what is meant by the term  *$\beta$ -hydrogen elimination reaction* as illustrated by an ethyl ( $\text{CH}_3\text{CH}_2-$ ) group coordinated to a metal centre. Sketch a plausible mechanism for such a reaction and state what the products would be.
- (d) Briefly describe an experiment that would support the mechanism that you propose in (c) above.
- (e) Explain why the following alkyl groups when coordinated to a metal centre would be relatively inert to  $\beta$ -hydrogen elimination:
- (i) Phenyl ( $\text{C}_6\text{H}_5-$ );
- (ii) Benzyl ( $\text{C}_6\text{H}_4\text{CH}_2-$ );
- (iii) Neo - pentyl ( $(\text{CH}_3)_3\text{CCH}_2-$ ).

**A4** (a) The table below shows some data for a series of octahedral chromium(III) complexes:

| Complex                                  | Colour | $\Delta_o/\text{cm}^{-1}$ | $\mu_{\text{eff}}/\text{BM}$ |
|------------------------------------------|--------|---------------------------|------------------------------|
| $[\text{Cr}(\text{H}_2\text{O})_6]^{3+}$ | Violet | 17,400                    | 3.84                         |
| $[\text{Cr}(\text{NH}_3)_6]^{3+}$        | Yellow | 21,550                    | 3.77                         |
| $[\text{Cr}(\text{CN})_6]^{3-}$          | Yellow | 26,700                    | 3.87                         |

- (i) Explain why the value of  $\Delta_o$  increases down the series for the complex ions and how this relates to the colours of the complexes.
- (ii) Determine the total number of *d* electrons in the complex ions and use the magnetic moment to confirm that these electrons are all unpaired.
- (iii) Calculate the value of the crystal field stabilisation energy (CFSE) for the  $[\text{Cr}(\text{CN})_6]^{3-}$  complex ion.
- (b) (i) Explain what is meant by the 18 electron rule as applied to transition metal complexes and describe which types of complexes tend to obey the rule. In your answer state which bonding molecular orbitals are involved in a typical transition metal complex which obeys the 18 electron rule.
- (ii) Which of the following complexes obey the 18 electron rule? Show your workings.
- $[\text{Cr}(\text{CO})_6]$  (cp =  $\text{C}_5\text{H}_5^-$ )
- $[\text{V}(\text{CO})_6]^-$
- $[\text{Pd}(\text{Me})_2(\text{PMe}_3)_2]$
- $[\text{Fe}(\text{cp})_2]$
- (iii) Explain the change in Cr-C bond length observed on replacing three carbonyl (CO) ligands in  $\text{Cr}(\text{CO})_6$  with a diethylenetriamine ligand ( $\text{HN}(\text{CH}_2\text{CH}_2\text{NH}_2)_2$ )

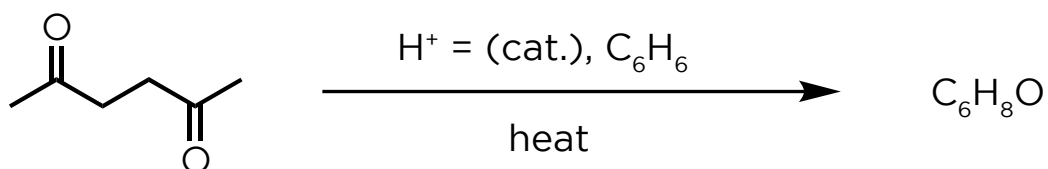


- (iv) It has been observed that the hydrolysis of  $[\text{Cr}(\text{NH}_3)_6]^{3+}$  proceeds faster when the solution is exposed to UV light. Explain, with reference to the molecular orbital diagram for the complex, why UV light accelerates this reaction.

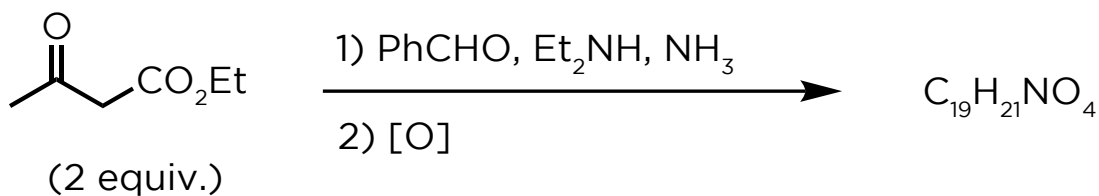
**A5** Answer **TWO** questions:

(a) Giving full mechanistic details predict the major product from **FOUR** of the following reaction sequences.

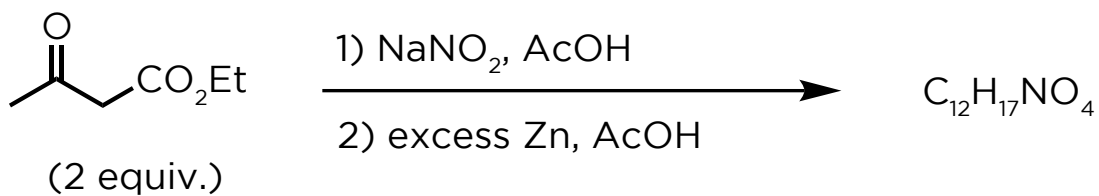
(i)



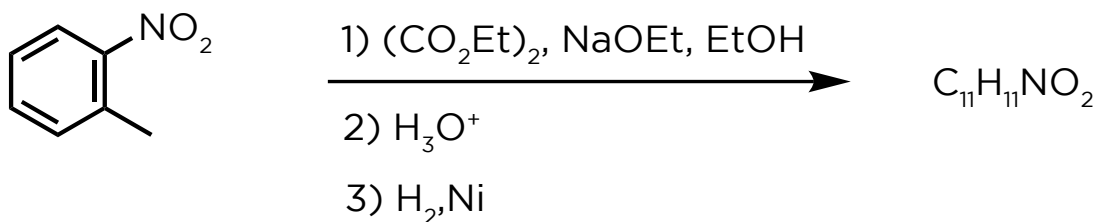
(ii)



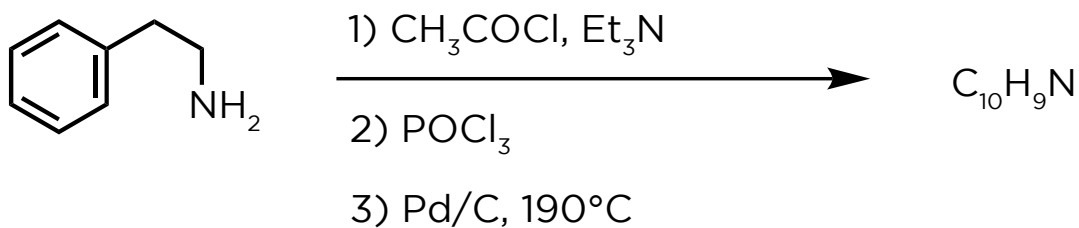
(iii)



(iv)



(v)



**A6** (a) Describe the requirements of analytical techniques that can be used with:

- (i) stopped flow;
- (ii) continuous flow;
- (iii) quenching experiments.

Give **ONE** example of an analytical technique that could be used in **EACH** of the above cases.

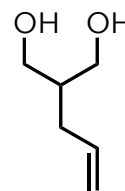
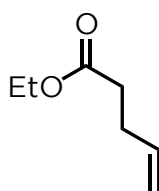
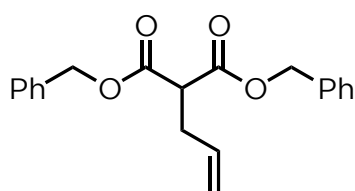
(b) An aqueous solution of the enzyme lysozyme spontaneously and irreversibly assembles into microscopic fibres in aqueous solution, when mixed with dithiothreitol (DTT). These fibres continue to grow so long as the concentration of lysozyme is above 10 mM. The shape and size of the fibres changes with time, and is to be determined using transmission electron microscopy (TEM). Sample preparation for TEM takes several hours and the sample cannot be recovered after analysis.

- (i) Describe an experiment based on the most appropriate technique in part (a) that you would use to investigate the kinetics of fibril growth, which should show how the shape and size of the fibres changes in solution during the first hour after addition of DTT.
- (ii) Discuss whether or not the experiment as you have described it would also be suitable to investigate changes occurring during the first 0.1-1 s. If not, explain why not, and suggest suitable modifications to your experiment.

Use diagrams where appropriate to help explain your answers.

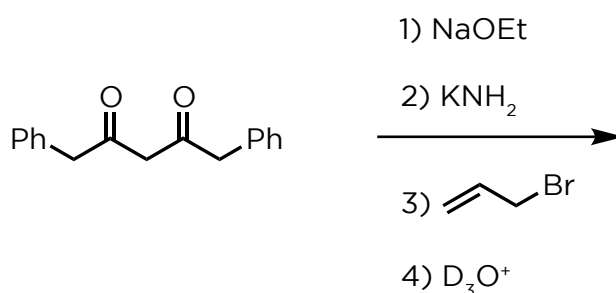
**A7** Answer three of parts (a) to (d).

(a) Starting from dibenzyl malonate suggest a synthesis for two of the compounds below. Include reagents and mechanisms in the answer.



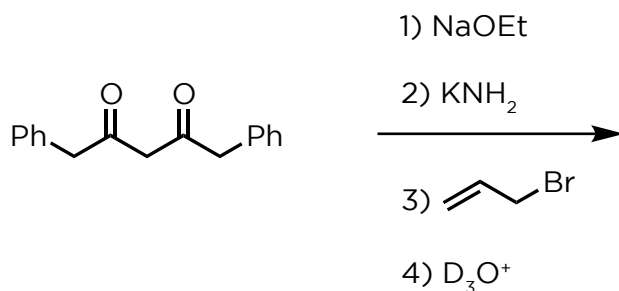
(b) Answer all parts.

- (i) Predict the product from the reaction below.



(b) Answer all parts.

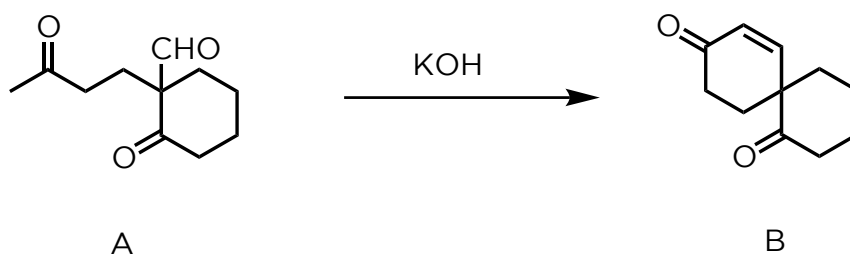
(i) Predict the product from the reaction below.



(ii) Suggest what product would be formed if the sequence of reagents were changed to: 1. NaOEt, 2. Allyl bromide, 3.  $\text{KNH}_2$ , 4.  $\text{D}_3\text{O}^+$ .

(iii) Give another example where adding reagents in the correct sequence is vital to a successful reaction.

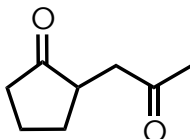
(c) Answer all parts. The reaction of tricarbonyl compound **A** with base leads to only one product **B** despite several conceivable outcomes.



- (i) Draw mechanisms to explain how **B** is formed.
- (ii) Draw two other conceivable products from the reaction.
- (iii) Explain why neither of these two products are formed.

(d) Answer all parts.

- (i) Suggest two different retrosyntheses for the diketone below. The two methods should feature the formation of carbon-carbon bonds. Each starting material should not contain more than five carbon atoms (although more carbon atoms may be introduced with reagents). Hint: cyclopentane is an inexpensive and readily available starting material.



- (ii) Draw out the synthesis based on one of your retrosynthetic analyses. Highlight and explain any modifications you make from that analysis. Mechanisms are not required.
- (iii) Highlight an element of control (chemo- or regio-selection) achieved in your synthesis.

**A8** Answer all parts.

(a) The kinetic theory of gases predicts that the diffusion coefficient is given by:

$$D = \frac{1}{3} \lambda \bar{c} \quad \text{with} \quad \lambda = k_B T / (\sqrt{2} \sigma p)$$

- (i) Identify all symbols in the two equations above and derive the S.I. units for  $\lambda$ .
- (ii) Calculate  $D$  when  $\bar{c} = 500 \text{ m s}^{-1}$ ,  $T = 300 \text{ K}$ ,  $p = 1 \text{ bar}$ , and  $\sigma = 0.4 \text{ nm}^2$ .
- (iii) Give an equation for the matter flux  $J$  arising from a concentration gradient. Calculate  $J$  (expressed in  $\text{mol m}^{-2} \text{ s}^{-1}$ ) when a pressure gradient of  $0.1 \text{ bar m}^{-1}$  is imposed for a gas with  $D = 10^{-5} \text{ m}^2 \text{ s}^{-1}$  and  $T = 300 \text{ K}$ .
- (iv) Describe briefly how gases and liquid differ.
- (b) The Gibbs free energy change on formation of a liquid droplet from a supersaturated vapour is given by:

$$\Delta G = 4\pi r^2 \gamma + \frac{4\pi r^3}{3V_l} \Delta\mu \quad (1)$$

- (i) Identify all symbols in Eq. 1. What are the physical origins of the two terms on the right-hand side of this equation?
- (ii) Starting from Eq. 1, show that the critical radius for nucleation is given by:

$$r_c = -2\gamma V_l / \Delta\mu$$

Derive an expression for the Gibbs free energy of the critical nucleus.

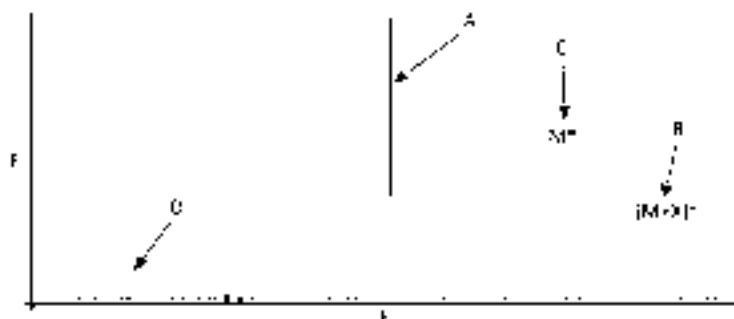
- (iii) Estimate the critical radius for nucleation of a water droplet from the bulk vapour when  $\Delta\mu = -1500 \text{ J mol}^{-1}$ , given that  $\gamma = 72.8 \text{ mN m}^{-1}$ .
- (iv) The same liquid forms a droplet against a solid surface. Assume that the interfacial energies between vapour and solid and between liquid and solid are the same, and that the droplet is hemispherical. Suggest why this implies the same critical radius as in part (ii). What is the Gibbs free energy of the critical nucleus in this case? Discuss whether nucleation will occur faster in the bulk vapour or against the solid surface.

- (c) Consider a polymer chain with  $N$  monomers of size  $a$  squeezed in a tube of size  $D$  filled with a good solvent.
- What is a good solvent?
  - The structure of the polymer chain in the tube may be considered as freely-linked, densely-packed “blobs”, with  $g$  monomers in each blob. How does  $g$  depend on  $D$ ?
  - What would be the size of the polymer chain along the tube?

**A9** Answer three of parts (a) to (d).

(a) Answer all parts.

- (i) The figure below shows a mass spectrum with typical features labelled **A** to **D** and where **E** and **F** are axis labels. Identify each feature.



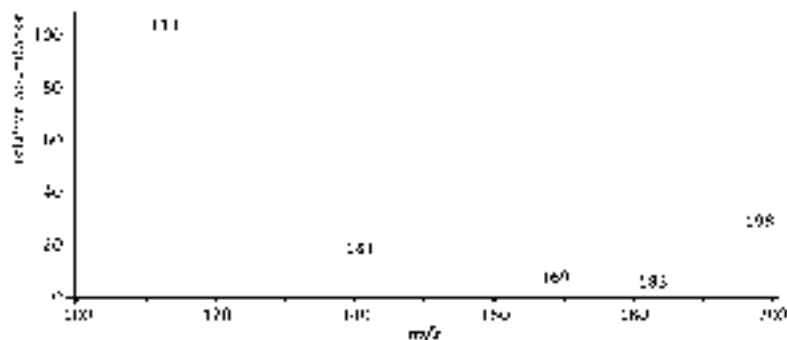
- Define the terms *nominal mass*, *isotopic mass* and *accurate mass*.
- The accurate mass of an analyte with the formula  $C_{10}H_7ClO_2$  was measured at  $m/z$  194.0142. Using the isotopic masses in the table, calculate the mass measurement error in parts per million (ppm).

| Isotope          | Exact Mass |
|------------------|------------|
| $^1\text{H}$     | 1.0078     |
| $^{12}\text{C}$  | 12.0000    |
| $^{16}\text{O}$  | 15.9949    |
| $^{35}\text{Cl}$ | 34.9689    |

- (b) An ion of mass  $m$  and charge  $z$  is extracted into a time-of-flight (TOF) mass analyser of length  $d$  by potential  $V_a$ . Given that the resulting potential energy of the ion is given by  $E_p = zeV_a$  and assuming that the potential energy is all converted to kinetic energy, derive an expression for the time-of-flight,  $t$ , in terms of the *mass to charge ratio* ( $m/z$ ) of the ion. ( $e$  is the charge on the electron.)

(c) Answer both parts.

- (i) The figure below is a simplified electron ionisation (EI) mass spectrum of a branched alkane. Determine the structure of the alkane and explain your reasoning.



- (ii) Explain why  $m/z$  113 is the most abundant ion and  $m/z$  183 is the least abundant.

(d) Answer all parts.

- (i) Explain why tandem mass spectrometry (MS/MS) produces greater structural information than when using electrospray ionisation (ESI) MS alone.
- (ii) Draw two possible mechanisms for the loss of water from an alcohol in ESI-MS/MS.
- (iii) McLafferty rearrangements are commonly observed in ESI-MS/MS. Draw two general McLafferty rearrangements occurring for two different functional groups.



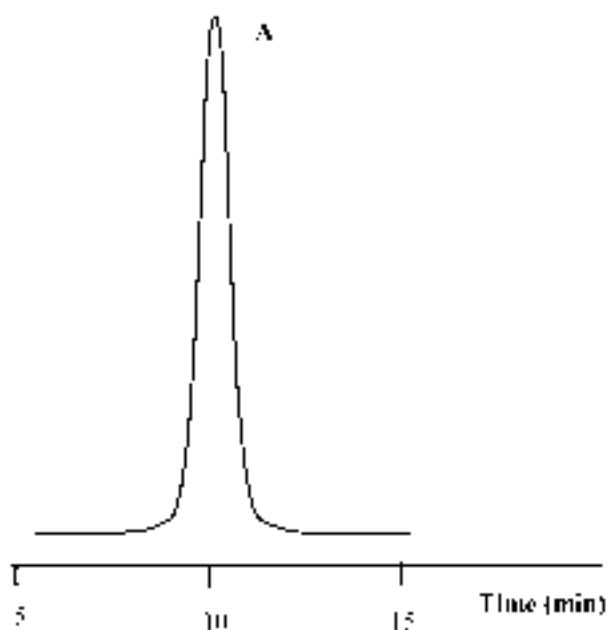
**A10** Answer all parts of this question.

- (a) Under a given set of conditions, the efficiency of a chromatography column can be expressed in terms of the number of theoretical plates, **N**, using either of the following equations:

$$N = 16(R_t/W_b)^2$$

$$N = 5.54(R_t/W_{h/2})^2$$

Define the major terms in the above equations and, from peak **A** in the chromatogram below, estimate values for **N** using both equations above. Compare the values obtained for **N** and indicate, with reasons, which of them is likely to be the more accurate.



- (b) The van Deemter equation is given below:

$$H = A + B/u + Cu$$

Provide concise definitions of the terms **H**, **A**, **B**, **C** and **u** and explain how **H** is related to **N** above.

- (c) Sketch a typical van Deemter plot as defined by the equation in part (b) and explain what useful chromatographic information can be obtained from analysis of such a van Deemter plot.
- (d) Describe the construction and operation of two types of detectors commonly used in gas chromatography. Your answer should mention the advantages and disadvantages of the GC detectors selected.
- (e) The GC analysis of a standard solution containing compounds X (22.5 mg), Y (26.5 mg) and an internal standard Z (25.5 mg) gave a chromatogram with relative peak areas of 495, 570 and 495 respectively. Following the addition of the internal standard Z (23.5 mg) to a 25 cm<sup>3</sup> sample of a solution containing unknown quantities of compounds X and Y, the gas chromatogram of the resulting solution contained peaks corresponding to X, Y and Z with relative areas 265, 375 and 310 respectively. What are the concentrations of compounds X and Y expressed in mg cm<sup>-3</sup>.

- A11** (a) Determine the concentration of fluoride in a mouthwash considering that:
- (i) measurement of 20 ml of mouthwash diluted with 20 ml of TISAB (Total Ionic Strength Adjustment Buffer) with a calomel/fluoride ISE gave a reading of -0.069V.
  - (ii) after adding 5 ml of 0.0500 M sodium fluoride and 5 ml of TISAB the reading was -0.0771. (assume T = 298.15 K)
- (b) Briefly describe the function of the membrane in a membrane electrode and one potential source of error.
- (c) Describe the experimental difference between DC Polarography, Normal Pulse Polarography and Differential Pulse Polarography.
- (d)  $\alpha$ -Benzoinoxime (cupron) is a precipitating agent for copper. In a solution consisting of 0.1 M  $\text{NH}_4\text{Cl}$  and 0.05M  $\text{NH}_3$  (pH=9), copper is reduced stepwise, giving polarographic waves at -0.2 and -0.5 V versus SCE and cupron gives a wave with  $E_{1/2} = -1.6$  V. Sketch the curves relative to the amperometric titration of copper by cupron at applied potentials of -1.0 V and -1.7 V versus SCE.

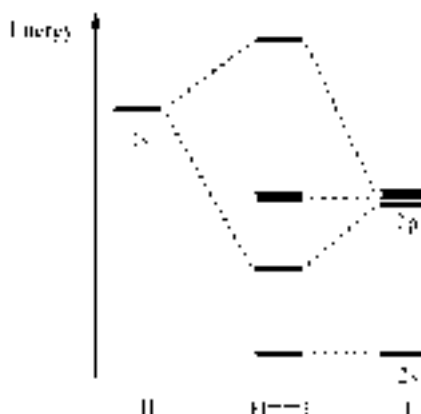
$$E = E^\circ + \frac{0.0592}{n} \log \frac{a_A^a}{a_B^b}$$

$$E_{\text{cell}} = K - \frac{0.0592}{n} \log [\text{A}^-]$$

**A12** (a) What is meant in symmetry by the term *Principal Axis*?

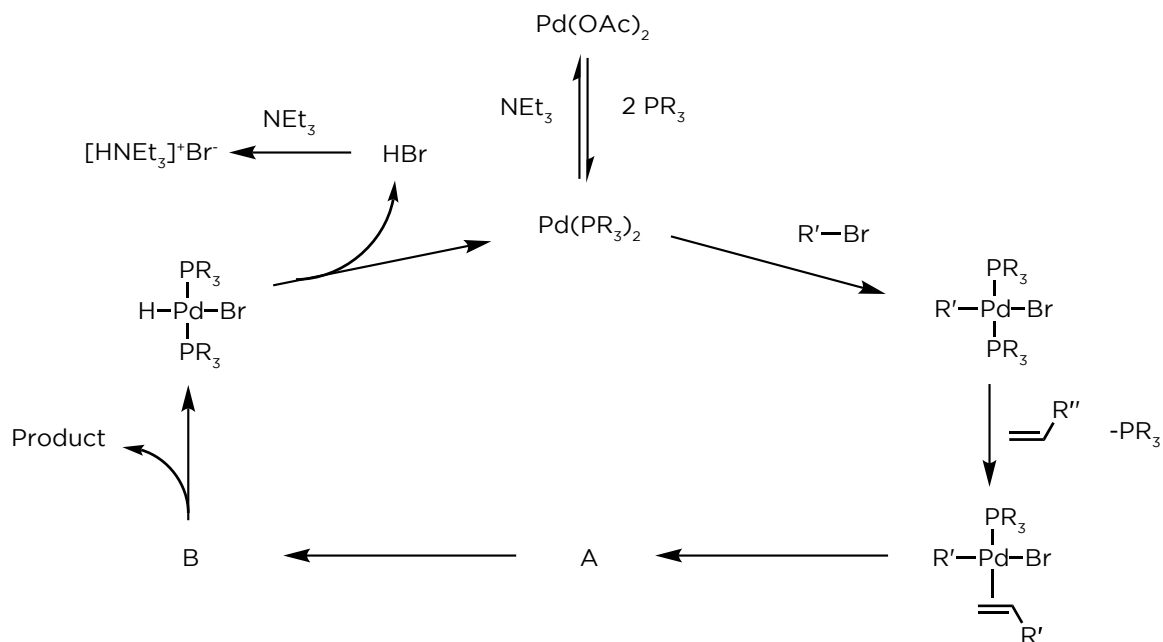
Draw structures and identify the Principal Axes of each of the following:

- (i)  $\text{SF}_6$
  - (ii)  $\text{SeF}_5^-$
- (b) Describe the procedure for the assignment of a chemical species to a particular symmetry point group.
- (c) Assign each of the following species to a point group, in each case explaining your reasoning.
- (i)  $\text{AsF}_4^-$
  - (ii) cyclohexane (chair conformation)
  - (iii)  $\text{OCN}^-$
- (d) Give the definition of a 'node', as used in molecular orbital theory. State how  $\sigma$ -,  $\pi$ - and  $\delta$ -molecular orbitals are distinguished in terms of the number and position of the nodes present in these species.
- By taking linear combinations of the appropriate **d-orbitals** draw an example of (i) a  $\sigma_u^*$ , (ii) a  $\pi_u$ , and (iii) a  $\delta_u^*$  molecular orbital. In each case show clearly the presence of any nodes.
- (Remember, by convention the internuclear axis lies along the z-direction)
- (e) Below is an incomplete energy level diagram for the heterodiatomic molecule H-F. Copy this diagram into your answer booklet.

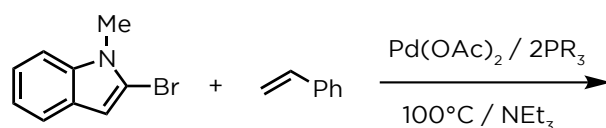


- (i) Complete the energy level diagram by adding the appropriate number of electrons. Would you expect H-F to be paramagnetic?
- (ii) Draw shorthand representations of the *occupied* molecular orbitals of H-F and assign each a symmetry label.
- (iii) Explain how the distribution of electron density in the occupied molecular orbitals of H-F is consistent with the idea of polar covalent bonding in this molecule.

**A13** (a) A partial mechanism for the Heck reaction is shown below:



(i) Give the organic product formed in the following Heck reaction:



- (ii) What type of phosphine is used in the Heck reaction? Give a reason for this choice.
- (iii) Draw the structures of Intermediates **A** and **B** and give the fundamental organometallic reaction steps involved in their formation. Show how the structures of **A** and **B** determine the selectivity of the overall reaction.
- (iv) The following substrates are not suitable for the Heck reaction.
- (a) Ph-Cl      (b) Et-Br      (c) MeHC=CMe<sub>2</sub>

By considering the individual steps involved in this process, suggest a reason why the Heck reaction is less efficient in each of these cases.

- (b) Calculate the magnitude (in Tesla) of the applied magnetic field for an NMR spectrometer operating at 1000 MHz for  $^1\text{H}$ .

$$\frac{\Delta E}{h} = \frac{g\beta_N B_z}{h}$$

(where  $g = 5.585$ ,  $\beta_N = 5.05 \times 10^{-27} \text{ J T}^{-1}$  and  $h = 6.63 \times 10^{-34} \text{ J Hz}^{-1}$ )

- (c) (i) Tin has a number of naturally occurring isotopes. Data for three of them are tabulated below. Giving one reason, identify which is the most favourable nucleus for NMR spectroscopy.

| Isotope           | Natural Abundance (%) | Spin          | Receptivity  |
|-------------------|-----------------------|---------------|--------------|
| $^{115}\text{Sn}$ | 0.36                  | $\frac{1}{2}$ | <b>0.693</b> |
| $^{117}\text{Sn}$ | 7.68                  | $\frac{1}{2}$ | <b>19.54</b> |
| $^{119}\text{Sn}$ | 8.58                  | $\frac{1}{2}$ | <b>25.2</b>  |

- (ii) A fourth naturally occurring isotope,  $^{120}\text{Sn}$ , has a high natural abundance (32.59%) but cannot be used in NMR spectroscopy. Suggest a likely reason for this.

- (d) What is meant by the following terms:

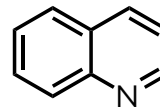
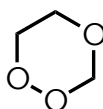
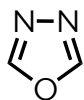
- (i) Relaxation Delay;
- (ii) Free Induction Decay;
- (iii) Exchange Spectroscopy.

- (e) (i) The following figure shows the  $^{27}\text{Al}$  NMR spectrum of  $\text{NaAlH}_4$ . Interpret this spectrum, explaining the origins of the observed splittings and their relative intensities.

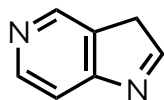


- (ii) Isotope  $^{27}\text{Al}$  has  $I=5/2$ . Describe an effect that this value of  $I$  may have on the appearance of the  $^{27}\text{Al}$  spectrum.

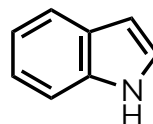
A14 (a) Name the following heterocycles:



(b) Explain why **5-azaindole** is a weak base and easily protonated in water, whereas **indole** is not.

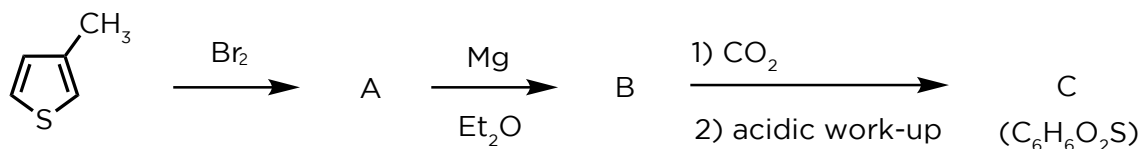


5-azaindole

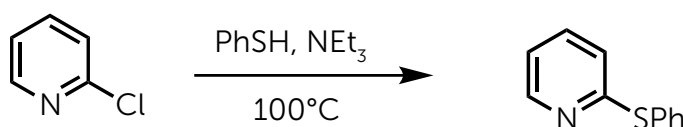
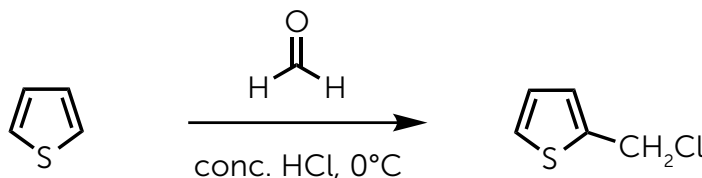


indole

- (c) Why is it much more difficult for pyridine to undergo electrophilic aromatic substitution than benzene?
- (d) The Friedel-Crafts acylation of pyrrole with trichloroacetyl chloride ( $\text{Cl}_3\text{CCOCl}$ ) proceeds at room temperature and yields a single isomer.
- Identify the product of this reaction. Using resonance structures of the intermediates involved, justify why only one isomer is formed.
  - The subsequent nitration of the product from i. with  $\text{HNO}_3$  gives  $\text{C}_6\text{H}_3\text{Cl}_3\text{N}_2\text{O}_3$ , again as a single isomer. Suggest the structure of this product.
- (e) Identify the products **A** – **C** in the reaction scheme below.



- (f) Propose a structure for the heterocyclic product,  $\text{C}_{18}\text{H}_{21}\text{NO}_4$ , from the reaction of ammonia, phenylacetaldehyde ( $\text{PhCH}_2\text{CH}=\text{O}$ ) and two mole equivalents of methyl acetoacetate. Suggest suitable reagents to convert it into a pyridine.
- (g) Suggest plausible curly arrow mechanisms for the following transformations.



## Appendices

### Appendix B: depth questions

**B1** Answer ALL parts (a), (b) and (c).

- (a) (i) Describe the origin of the X-ray radiation described as Cu K $\alpha$  in terms of the electronic transitions involved.
- (ii) A substance known to have a cubic unit cell gives reflections with Cu K $\alpha$  radiation (1.54 Å) at glancing angles 20.06°, 24.61°, 43.17° and 50.31°. The reflection at 43.17° is known to be due to the (221) planes. Index the other reflections and determine the unit cell parameter,  $a$ .
- (b) (i) What are the essential conditions for laser action?
- (ii) Draw and label the energy level diagram for a ruby laser.
- (iii) How many energy levels are essential for laser action in this laser, and how are the conditions necessary for laser action achieved with this system?
- (iv) Why is it not possible to populate the  ${}^2\text{E}$  level in the ruby laser directly from the ground state?
- (v) Why is the ruby laser almost always used as a pulsed laser and not a continuous laser?
- (c) State in words what is meant, in statistical thermodynamics, by a *partition function*. Write down an expression showing how a typical molecular partition function is commonly factorized into four terms, each involving a different kind of energy. State what molecular properties determine the values of each term. (For example, one factor is  $q_{\text{trans}}$ , a term which relates to translational motion, whose value is determined by the molecular mass).

**B2** Answer BOTH parts (a) and (b).

(a) The Debye equation is:

$$-\left(\frac{\epsilon_r - 1}{\epsilon_r + 2}\right) = \frac{M}{\rho} \frac{N_A}{3\epsilon_0} + \left(\frac{\mu^2}{3kT}\right)$$

The left hand side is called the molar polarisation,  $P_m$ .

- (i) Describe the physical significance of the two separate terms on the right hand side of the Debye equation.
- (ii) Suggest molecular examples in which you would expect either the first or the second of the two terms to dominate.
- (iii) State the effect of increasing temperature on  $P_m$ , and suggest a physical reason for it.
- (iv) Suggest a means of determining the static relative permittivity,  $\epsilon_r$ .
- (b) The static optical and dielectric characteristics of a pure molecular liquid were measured at 295 K. The refractive index,  $n$ , was determined as 1.45 and the static relative permittivity,  $\epsilon_r$ , as 18. Given the formula weight of the molecules as  $M = 128 \text{ g mol}^{-1}$  and the liquid density,  $\rho = 0.9 \text{ g cm}^{-3}$ , calculate the polarisability of the molecule and its dipole moment.

$$\epsilon_0 = 8.85 \times 10^{-12} \text{ J}^{-1} \text{ C}^2 \text{ m}^{-1}$$

$$N_A = 6.02 \times 10^{23} \text{ mol}^{-1},$$

$$k = 1.38 \times 10^{-23} \text{ J K}^{-1} \text{ mol}^{-1}$$

**B3** Answer BOTH questions.

- (a) (i) In transition-metal complexes, ligand-to-metal charge-transfer (LMCT) and metal-to-ligand charge-transfer (MLCT) transitions have different requirements for the ligand orbitals.

- Distinguish between these requirements
- The four ligands below are important in bioinorganic chemistry. Identify the type of CT transition expected for each of them:

CO

CN<sup>−</sup>

Cysteinate = [RCH<sub>2</sub>S]<sup>−</sup>

tyrosinate = [RCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>O]<sup>−</sup>

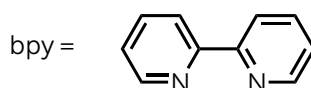
- (ii) By considering the electron configurations of the metal and the ligands, show that the purple colour of MnO<sub>4</sub><sup>−</sup> must be associated with an LMCT transition.
- (iii) In addition to their LMCT bands, FeO<sub>4</sub><sup>2−</sup> and MnO<sub>4</sub><sup>2−</sup> show absorption bands with low molar absorption coefficients (ca. 10 m<sup>2</sup> mol<sup>−1</sup>), as listed below. In contrast, CrO<sub>4</sub><sup>2−</sup> shows no such bands.

FeO<sub>4</sub><sup>2−</sup> λ<sub>max</sub> = 790, 550, 340 nm

MnO<sub>4</sub><sup>2−</sup> λ<sub>max</sub> = 830 nm

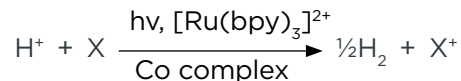
For each of these **three** tetrahedral doubly charged ions, draw a labelled *d*-orbital splitting diagram and show the corresponding ground state electron configuration.

- Using your diagram, account for the 830 nm absorption band of MnO<sub>4</sub><sup>2−</sup> and calculate Δ<sub>t</sub> in units of cm<sup>−1</sup>.
  - An explanation of the three absorption bands of FeO<sub>4</sub><sup>2−</sup> requires consideration of the ground and excited electronic states (terms). Explain how electronic states differ from electron configurations with the aid of this example, and explain qualitatively why the spectrum contains more than one spin-allowed *d-d* band.
- (b) (i) [Ru(bpy)<sub>3</sub>]<sup>2+</sup> has an MLCT absorption band at 450 nm and an emission maximum at 600 nm. Describe the difference in recording methods between an emission spectrum and an excitation spectrum. Explain how an excitation spectrum of [Ru(bpy)<sub>3</sub>]<sup>2+</sup> would be recorded and predict what would be observed.



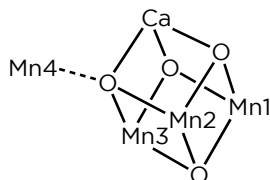


- (ii) Irradiation of an aqueous solution of  $[\text{Ru}(\text{bpy})_3]^{2+}$  in the presence of a  $\text{Co}(\text{II})$  complex and a reducing agent  $\text{X}$  generates  $\text{H}_2$  according to the equation below. The hydrogen derives from water and the reaction is catalytic with respect to  $\text{Ru}$  and  $\text{Co}$  complexes.



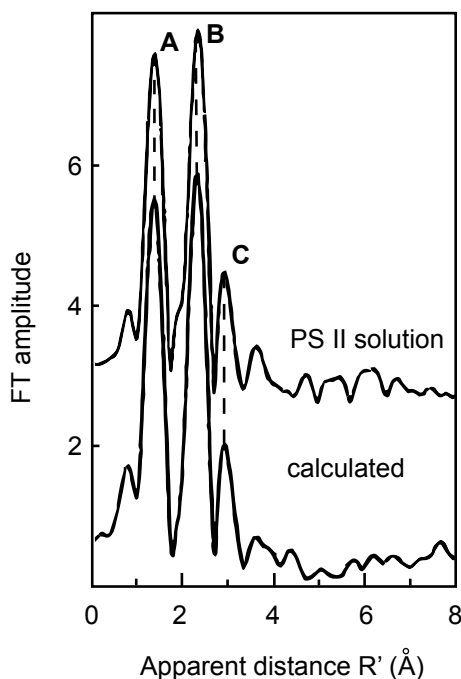
With the aid of this example and the data in part b(i), explain the role of the ruthenium complex as a photocatalyst and comment on the significance of the reaction.

- B4** (a) In photosynthesis, the oxidation of water to dioxygen is catalysed by a tetranuclear manganese centre of PSII, for which the structure is shown in **Figure 1**.



**Figure 1**

- (i) Give a balanced half-equation for the light-induced oxidation of water to dioxygen. Identify **two** reasons why this oxidation is particularly challenging, indicating how they are overcome in nature.
- (ii) Suggest three reasons why manganese as opposed to copper is present in the reaction centre of PSII.
- (iii) Using the structure in Figure 1 and giving your reasons, assign the three peaks labelled **A**, **B** and **C** in the manganese EXAFS spectrum of PSII in solution shown in Figure 2.



- (b) The O-O stretch vibration band positions of  $\text{O}_2$ ,  $\text{O}_2^-$  and  $\text{H}_2\text{O}_2$  are listed in Table 1 and may be used to interpret vibrational data from dioxygen-binding proteins.

**Table 1**

| Compound               | $\nu_{\text{O-O}} / \text{cm}^{-1}$ |
|------------------------|-------------------------------------|
| $\text{O}_2$           | 1555                                |
| $\text{O}_2^-$         | 1107                                |
| $\text{H}_2\text{O}_2$ | 878                                 |

- (i) The O-O stretch vibration band of a hypothetical dioxygen-binding protein is observed at  $1102 \text{ cm}^{-1}$ . By comparison with the values given in **Table 1**, assign a bond order to the bound dioxygen in the hypothetical protein and sketch a simplified MO diagram for the frontier orbitals.
- (ii) Excluding EXAFS and vibrational techniques, give **one** experimental method that could be used to obtain information about the metal centre in the hypothetical protein, explaining what information would be obtained.
- (iii) Identify the dioxygen transport proteins that contain each of the metal-dioxygen units given in Table 2, and sketch the active site of the oxygenated form of **each** protein.

**Table 2**

| Metal dioxygen unit       | $\nu_{\text{O-O}} / \text{cm}^{-1}$ |
|---------------------------|-------------------------------------|
| $\text{Fe}_2(\text{O}_2)$ | 848                                 |
| $\text{Cu}_2(\text{O}_2)$ | 730                                 |
| $\text{Fe}(\text{O}_2)$   | 1100                                |

- (iv) Explain why the  $\nu_{\text{O-O}}$  band at  $730 \text{ cm}^{-1}$  observed for the  $\text{Cu}_2(\text{O}_2)$  unit is the lowest of the series given in Table 2.

**B5** (a) Marine sediments accumulated on the ocean floor can provide information about past climates and the age of the sea floor. They are complex mixtures, containing thousands of organic compounds, and are an analytical challenge for oceanographers.

- (i) Identify **two** types of mass analysers that can be used to separate sediment compounds with the same *nominal* molecular weight but different molecular formulae.
- (ii) For **one** of the analysers given in your answer to part (a)(i), describe the method of ion introduction and separation.

- (iii) Three compounds, **A**, **B** and **C**, found in a Pacific Ocean sediment sample, were studied using a high resolution mass spectrometer with positive ionisation. Using the measured masses and the proposed protonated ion molecular formulae given in **Table 1**, calculate the average mass accuracy in ppm of this mass analyser.

Atomic masses:

C = 12.00000 Da

O = 15.99492 Da

H = 1.00783 Da

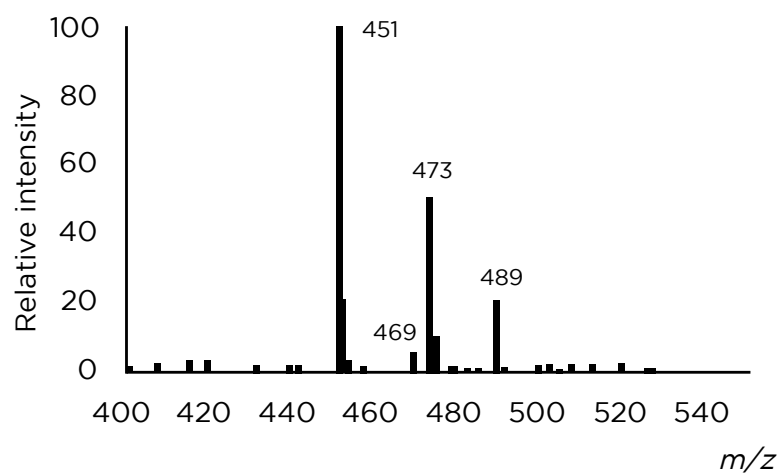
N = 14.00307 Da

S = 31.97207 Da

**Table 1**

| Compound | Measured Mass / Da | Proposed Protonated Ion Formula |
|----------|--------------------|---------------------------------|
| <b>A</b> | 451.05222          | $C_{19}H_{15}O_{13}$            |
| <b>B</b> | 451.20913          | $C_{22}H_{31}O_8N_2$            |
| <b>C</b> | 451.23900          | $C_{21}H_{39}O_8S$              |

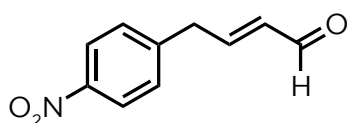
- (iv) Electrospray ionisation coupled to ion trap mass spectrometry was used to investigate the structure of compound **A**, and the positive ionisation mass spectrum obtained is shown in **Figure 2**. Considering the four peaks labelled in **Figure 2**, determine which peak is the protonated molecular ion and identify the **three** adducts present.



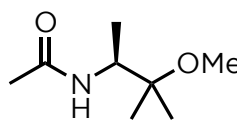
- (v) The  $[M+H]^+$  ion of compound **A** was fragmented using collision induced dissociation, and  $[M-18]^+$  and  $[M-42]^+$  ions were observed.
- Suggest possible structures for each of these neutral losses.
  - Is the  $[M-42]^+$  fragment ion of compound **A** an even electron or odd electron species?
- (b) A scientist working at a Regulatory Agency is given a river water sample that has been contaminated with an unknown pesticide.
- Giving your reasons, suggest a suitable mass spectrometric method to identify and quantify the pesticide in the water sample. Include in your answer a suitable ion source, mass analyser and separation technique (if appropriate).
  - The pesticide has also been released into the atmosphere and it has reacted to form a range of volatile organic compounds. An air sample has been collected and returned to the laboratory. Explain how you would modify the method you suggested in part (b)(i) to analyse this air sample.
  - Suggest a mass spectrometric method that could be used to analyse the volatile organic compounds in the atmosphere at the location of the contamination at high time resolution, and outline any limitations of your chosen method.

**B6** Answer **ALL** parts (a), (b) and (c).

- (a) Predict the  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for compounds **7** and **8**, giving multiplicities and estimates of the coupling constants (for  $^1\text{H}$ ), chemical shifts and intensities. Also, for each compound predict the major bands in the infrared spectra in the region of  $4000 - 1500\text{ cm}^{-1}$ .

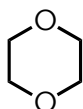


**7**



**8**

- (b) Suggest a method to both distinguish between, and confirm the identity of, compounds **9** and **10**, based on the molecular ions generated by mass spectrometry.



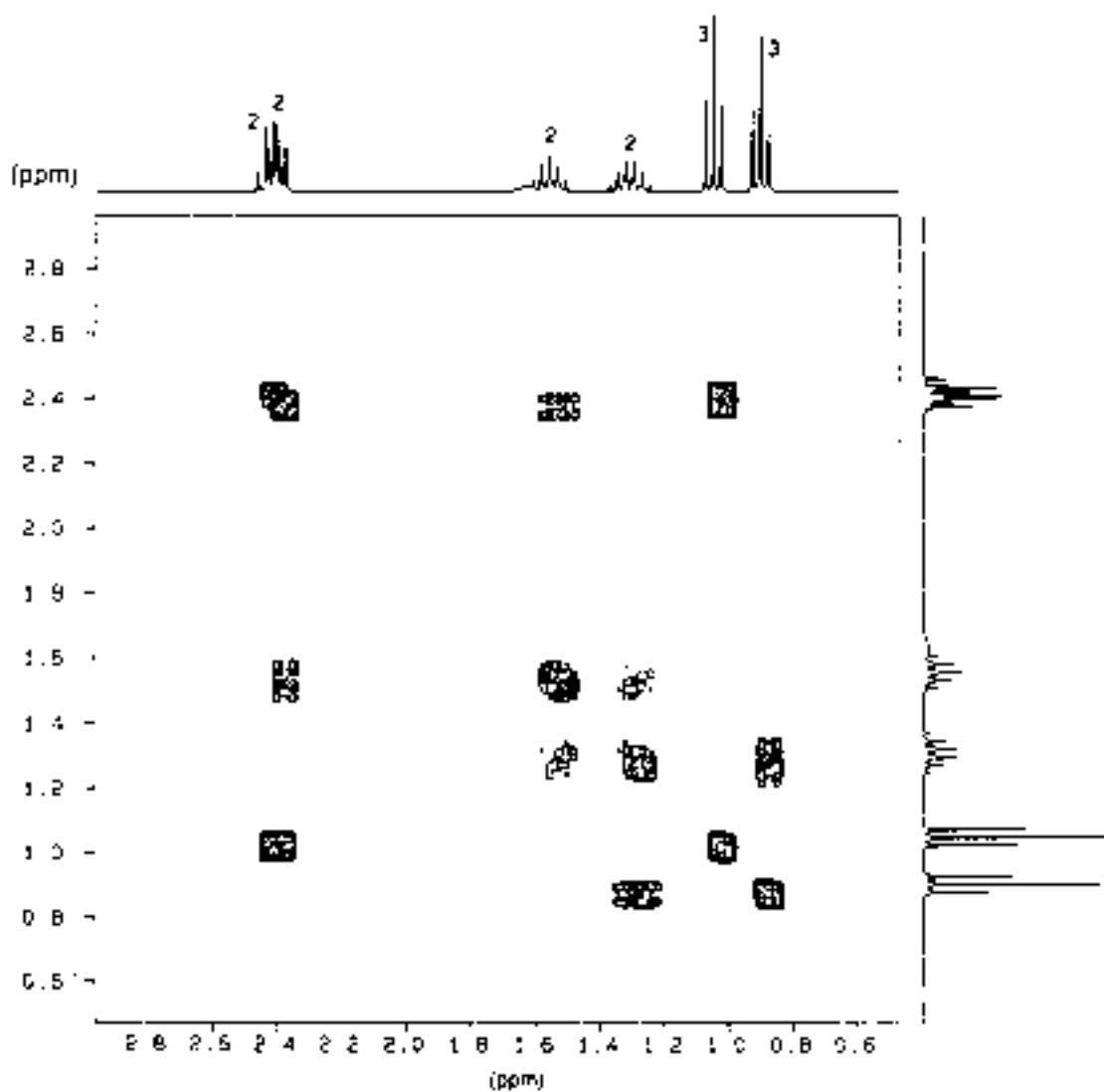
**9**



**10**

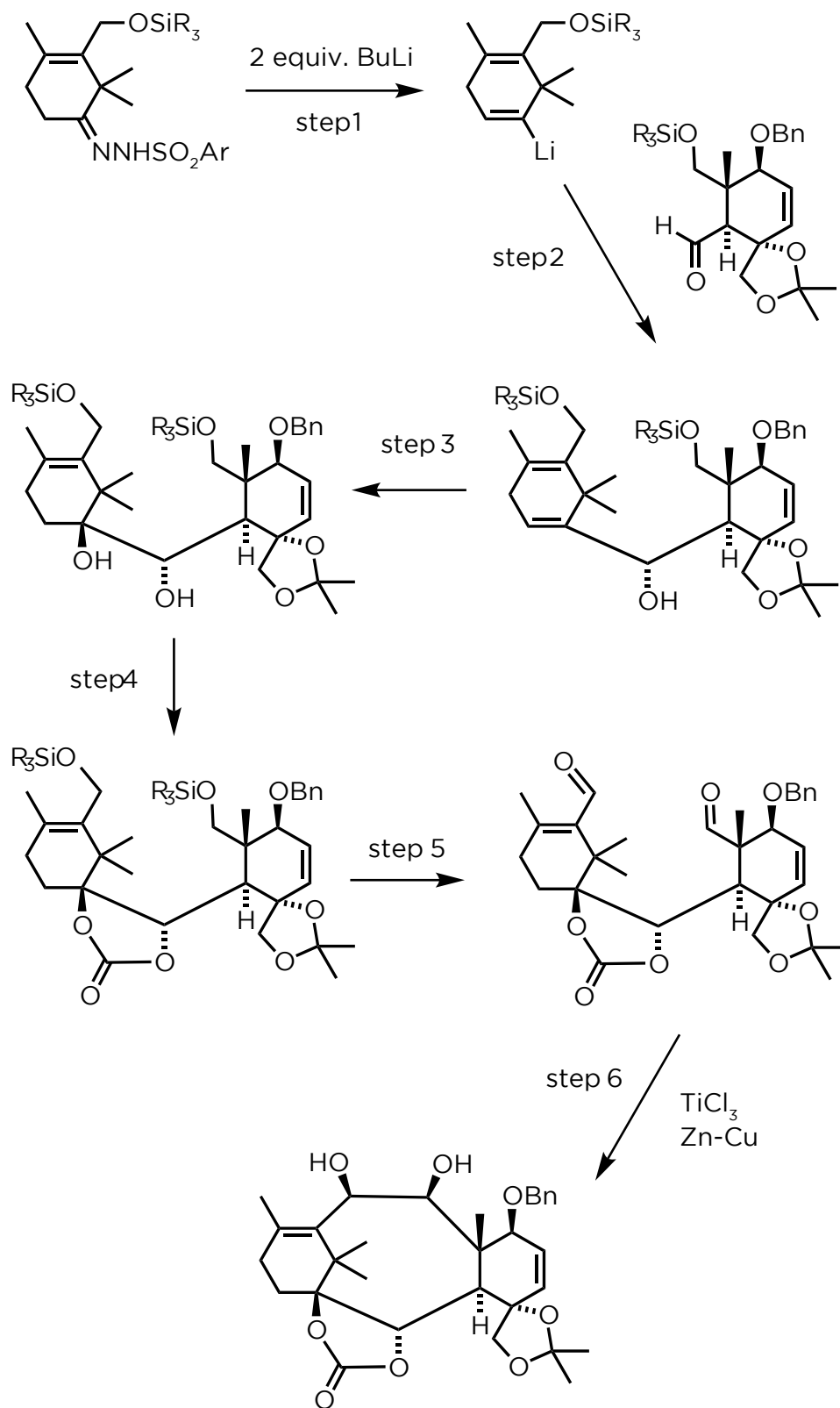
- (c) Identify the compound  $C_7H_{14}O$  from the following COSY spectrum. Illustrate all of the connectivities and show how these support the identity of the structure given. In the COSY spectrum, the diagonal runs from upper left to lower right.

The spectrum was recorded in  $CDCl_3$  at 300 MHz. The integers indicate the number of hydrogen atoms associated with each multiplet.



**B7** Answer **ALL** parts (a), (b), (c), (d) and (e).

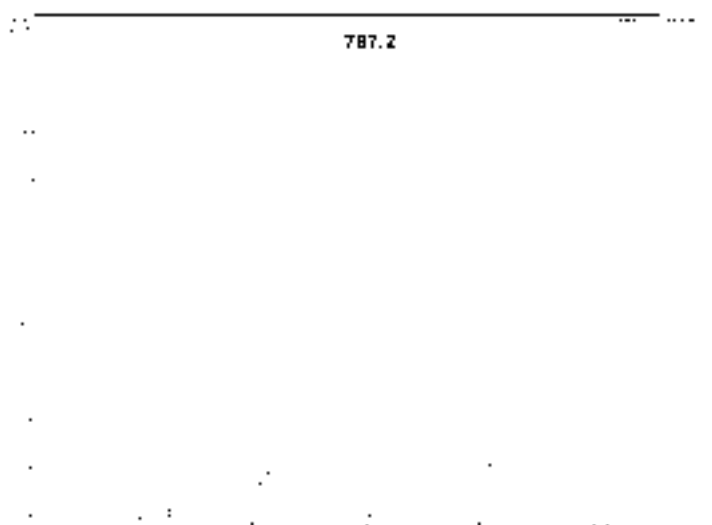
The following scheme is taken from the synthesis of taxol by Nicolaou.



- (a) Step **1** involves a Shapiro reaction in the generation of the vinyl lithium species. Provide a mechanism for the reaction.
- (b) Step **3** involves a sequence of reactions. Suggest possible reactions and reagents to achieve the transformation shown.
- (c) Step **4** generates a cyclic carbonate. The molecule also contains a cyclic acetal. What was the reason for incorporating the two different types of diol protection in this molecule? Indicate the reaction conditions that could be used to hydrolyse each type.
- (d) Suggest possible reactions and reagents to achieve the transformation shown in step **5**.
- (e) Step **6** involves a McMurry coupling of a dialdehyde species to give a diol. Suggest a mechanism for the reaction.

**B8** Answer ALL questions

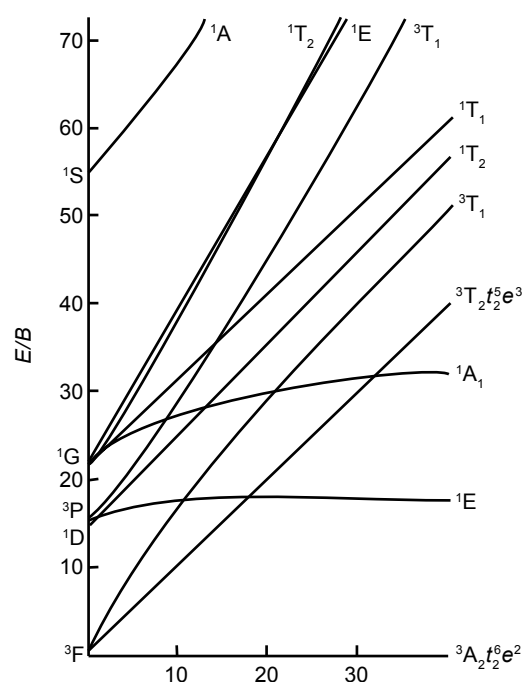
- (a) Name two ionisation techniques suitable for analysis of high molecular weight biomolecules.
- (b) A sample of sucrose in 20 mM potassium dihydrogenphosphate buffer was analysed by electrospray ionisation mass spectrometry using direct injection (*i.e.* without chromatographic separation) . A repeating series of ions 175 Da apart was observed in the spectrum, and no ions from the analyte were seen. What has gone wrong with this experiment? Suggest how you could improve the results.
- (c) What are the main advantages of ambient ionisation techniques?
- (d) Name two hybrid mass analysers suitable for MS-MS experiments.
- (e) Calculate the resolution of the ion shown below using the full width at half maximum (FWHM) method.



- (f) How many orientations does a deuterium nucleus adopt in an applied magnetic field? Deuterium has a spin quantum number,  $I$ , of 1.

- (g) Calculate the resonance frequency for a  $^{31}\text{P}$  nucleus when viewed on an NMR spectrometer operating with an applied magnetic field,  $B_0$ , of strength 9.4T ( $\gamma_{^{31}\text{P}} = 10.84 \times 10^7 \text{ rad sec}^{-1} \text{ T}^{-1}$ ).
- (h) Explain how the line intensities in multiplets arise. Illustrate consideration of an  $\text{AX}_2$  spin system.
- (i) Explain the purpose of the following steps in an NMR experiment:
- Locking
  - Shimming
  - Tuning
- (j) Why is it essential to use deuterated solvents in NMR experiments?

- B9** (a) Identify the ground-state term symbols of the free ions  $\text{Rh}^{3+}$ ,  $\text{Ti}^{3+}$  and  $\text{Fe}^{3+}$ .
- (b) Use Diagram 1 to estimate  $\Delta_{\text{oct}}$  and  $B$  for  $[\text{Ni}(\text{NH}_3)_6]^{2+}$  which shows absorptions in its UV/Visible spectrum at 10 750, 17 500 and 28 200  $\text{cm}^{-1}$ .



**Diagram 1:** Tanabe-Sugano Diagram for a d8 Transition Metal Complex

- (c) Sketch the ESR spectra expected for a solution of  $\text{Cu}^{2+}$  in water, and of the same solution after it has been frozen. Assume that only coupling to  $^{63}\text{Cu}$  ( $I = 3/2$ ) is observed.



**B10** Answer all parts.

- (a) (i) Write down the formula relating the electron density  $\rho(\vec{r})$  to the wavefunction:

$$\Psi(\vec{r}_1 s_1, \vec{r}_2 s_2, \dots, \vec{r}_n s_n).$$

- (ii) Consider the following two-electron density for helium in its ground electronic state:

$$\rho_2(\vec{r}_1, \vec{r}_2) = 2\Phi^2(\vec{r}_1)\Phi^2(\vec{r}_2).$$

where  $\Phi(\vec{r}) = \sqrt{\frac{8}{\pi}} e^{-2r}$  is a normalized atomic orbital. Show that the electron density is:

$$\rho(\vec{r}) = \frac{16}{\pi} e^{-4r}$$

[Hint: For a two-electron system, the two-electron density is:

$$\rho_2(\vec{r}_1, \vec{r}_2) = 2 \int ds_1 \int ds_2 |\Psi(\vec{r}_1 s_1, \vec{r}_2 s_2)|^2]$$

- (iii) For the exact Hohnberg-Kohn energy functional,  $E_{HK}[\rho]$ , state whether the energy obtained using  $\rho(\vec{r}) = \frac{16}{\pi} e^{-4r}$  would be greater than, less than or equal to the exact ground state energy of helium, explaining your reasoning.
- (b) (i) The Kohn-Sham energy functional is:
- $$E[\rho] = T_s + V_{nuc}[\rho] + J[\rho] + E_{xc}[\rho].$$
- List the four energetic components that are contained in  $E_{xc}[\rho]$ .
- (ii) Give two examples where Kohn-Sham DFT using the B3LYP functional fails to give qualitatively correct predictions. Explain the reasons for the failures and describe how these problems can be overcome.

**B11** Answer all parts.

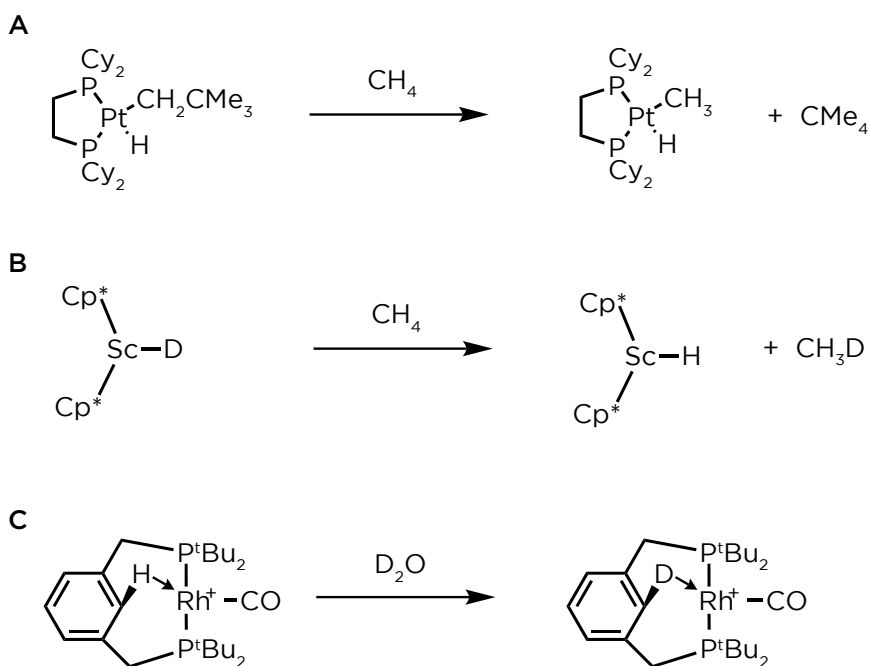
- (a) An alkali metal hydride, **A**, contains just 0.75% hydrogen by mass. When **A** is dissolved in THF solution with 1 equivalent of 18-crown-6, nmr spectroscopy using the alkali metal as the spin active nucleus shows one resonance at  $\delta = -44$  ppm. Electrolysis of **A** yields the elemental alkali metal and a gas **B**. When the elemental alkali metal is dissolved in THF solution with 1 equivalent of 18-crown-6, nmr spectroscopy using the alkali metal as the spin active nucleus shows two peaks at  $\delta = -44$  and  $-212$  ppm. In contrast, if the crown ether is added in excess then only the peak at  $\delta = -44$  ppm is seen. In a typical reaction, an excess of **A** reacts with  $\text{TiCl}_4$  to give Ti metal, a gas, **B**, and a salt **C**. Identify **A-C** and explain these observations.

What products would be expected from reaction of **A** and  $\text{PCl}_3$ ?

- (b) You are tasked to design a stable singlet carbene. Explain the design features, in particular with respect to the following:
- Bond angle at the carbene centre;
  - Substituents bonded to the carbene centre;
  - Whether the molecule would be cyclic or acyclic;
  - If the design is based on a cyclic five membered ring, would your choice contain a saturated or unsaturated backbone?

- (c) An organophosphine **A** contains 15.3% P, 71.3% C and 13.4% H, and displays a singlet in the  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum at  $\delta = 61$  ppm and a doublet in the  $^1\text{H}$  NMR spectrum at  $\delta = 1.3$  ppm ( $J_{\text{P-H}} 10$  Hz). Solutions of mixtures of **A** and  $\text{B}(\text{C}_6\text{F}_5)_3$  show  $^{31}\text{P}$  and  $^{11}\text{B}$  NMR signals representative of the parent compounds. However, under an atmosphere of  $\text{CO}_2$ , reaction occurs rapidly to give a zwitterionic compound **B** which exhibited resonances in the  $^{31}\text{P}\{^1\text{H}\}$  and  $^{11}\text{B}\{^1\text{H}\}$  NMR spectra at  $\delta = 46.1$  and  $2.7$  ppm, respectively. The  $^{13}\text{C}$  NMR spectrum of **B** showed resonances expected for the constituent phosphorus and boron fragments as well as a signal at  $\delta = 161.6$  ppm, which exhibited a PC coupling of 93 Hz; the IR spectrum of **B** showed an absorption at  $1695\text{ cm}^{-1}$ . When heated to  $70^\circ\text{C}$ , **B** loses  $\text{CO}_2$  to reform **A** and  $\text{B}(\text{C}_6\text{F}_5)_3$ . Identify **A** and **B** and explain the reactivity and spectroscopic data.

- B12** (a) (i) The three reactions shown below each involve a C-H activation step. Draw a reasonable reaction pathway in each case. State the mechanism by which any C-H bond activation steps occur and sketch the transition state involved.



- (ii) For each reaction identify the factors that promote the C-H activation process.

- (b) (i) Draw an energy level diagram showing the key orbital interactions that occur between a dihydrogen ligand and a  $d^6 C_{4v} ML_5$  metal fragment.

Use your diagram to explain why the barriers to rotation about the M-H<sub>2</sub> axis in  $L_5M(\eta^2-H_2)$  complexes are usually very low.

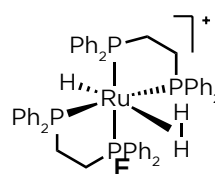
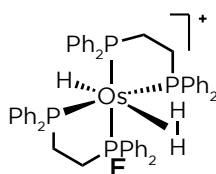
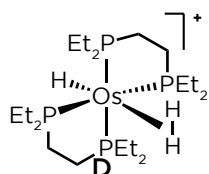
- (ii) NMR data for three  $\eta^2-H_2$  dihydrogen complexes are given below:

Data set 1:  $^1J_{HD} = 40 \text{ Hz}$ ;  $T_1^{\min} = 25.5 \text{ ms}$

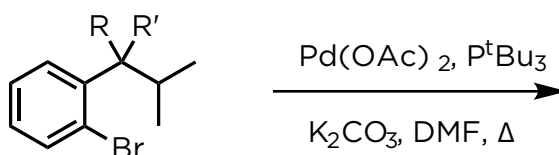
Data set 2:  $^1J_{HD} = 21 \text{ Hz}$ ;  $T_1^{\min} = 32.0 \text{ ms}$

Data set 3:  $^1J_{HD} = 11.4 \text{ Hz}$ ;  $T_1^{\min} = 80.0 \text{ ms}$

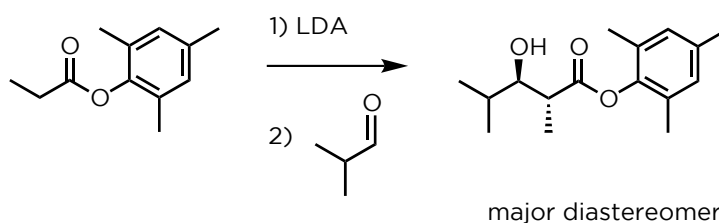
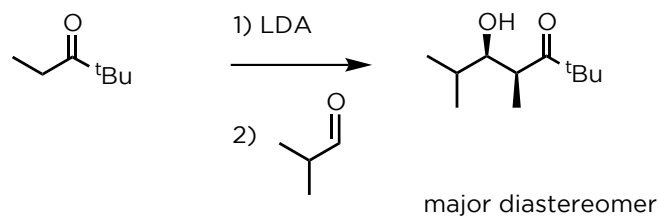
Match each of these data sets to one of the three  $\eta^2-H_2$  complexes, **D** to **F** below, and fully account for all the data. Hence place the complexes in order of increasing H-H distance and show how this is consistent with the nature of the complexes involved.



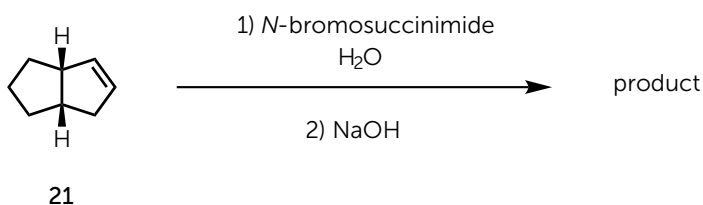
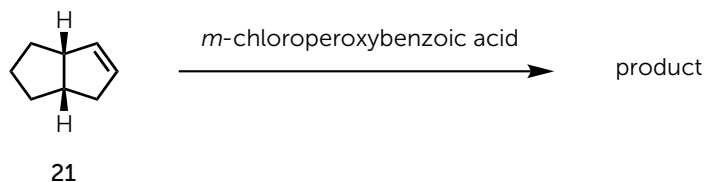
- (c) C-H activation is now being incorporated into catalytic cycles for the synthesis of organic molecules. For the following reaction draw (i) the structure of the product formed and (ii) the structure of the species involved in the C-H activation step. For the latter highlight the key features that enable C-H bond activation to occur.



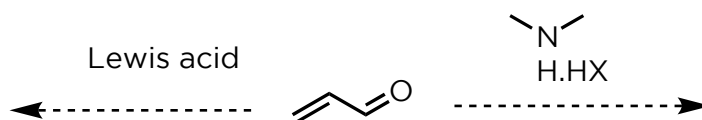
- B13 (a)** Rationalise the stereochemical outcome of the aldol reactions below. You should illustrate your answer with an appropriate transition state diagram for the key aldol step in each case, highlighting any similarities and differences.



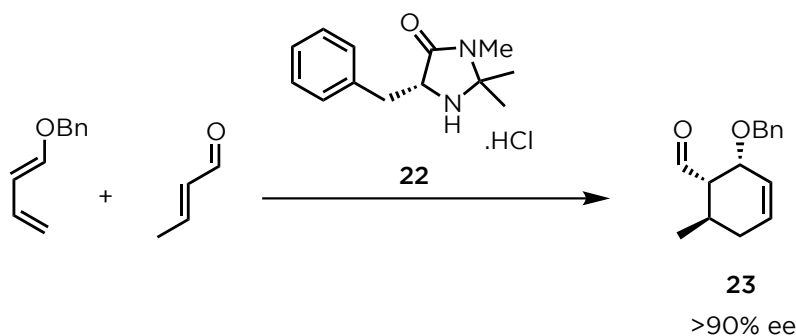
- (b) Predict the structures of the major product arising from each reaction of the alkene (**21**) below, rationalising your answer in terms of the reaction mechanisms.



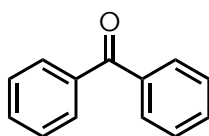
- (c) (i) What are the similarities and differences between activation of an unsaturated aldehyde with a Lewis acid and an organocatalyst (illustrated below)?



- (ii) State two possible advantages of using organocatalysis as compared to metal catalysis.
- (iii) Catalyst **22** (below) promotes Diels-Alder reaction of dienes and unsaturated aldehydes. Account for the relative and absolute stereochemistry of the product (**23**) shown. Illustrate your answer with appropriate annotated diagrams showing iminium geometry and facial selectivity.



- B14** (a) In the context of organic photochemistry, define the terms *sensitiser* and *quencher*.
- (b) When carrying out a photochemical reaction, explain why molecular oxygen is usually rigorously excluded from the reaction mixture whereas it is sometimes necessary to add small amounts of benzophenone (**24**).



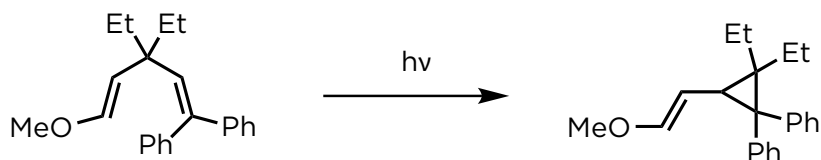
**24**

- (c) (i) Outline a mechanism for a Paterno-Buchi reaction between benzaldehyde and *cis*-but-2-ene and hence identify the likely product(s).
- (ii) Benzaldehyde, *cis*-but-2-ene and penta-1,3-diene have triplet state energies of 72, 78 and 58 kcal mol<sup>-1</sup> respectively.

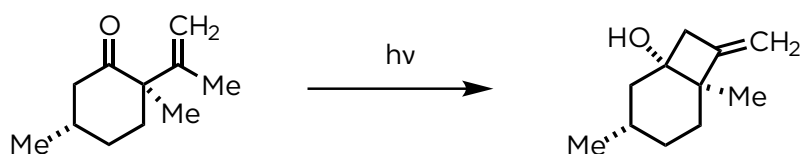
With reference to the above data, explain why benzaldehyde and but-2-ene are suitable partners in the Paterno-Buchi reaction whereas, under similar photochemical conditions, benzaldehyde and penta-1,3-diene do not undergo the Paterno-Buchi reaction.

(d) Provide a plausible mechanism for *one* of the following photochemical transformations:

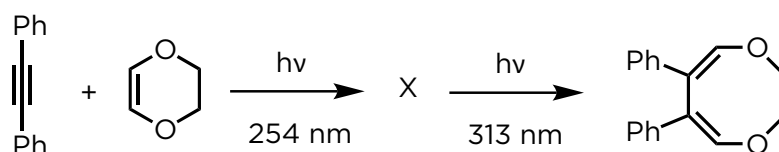
(i)



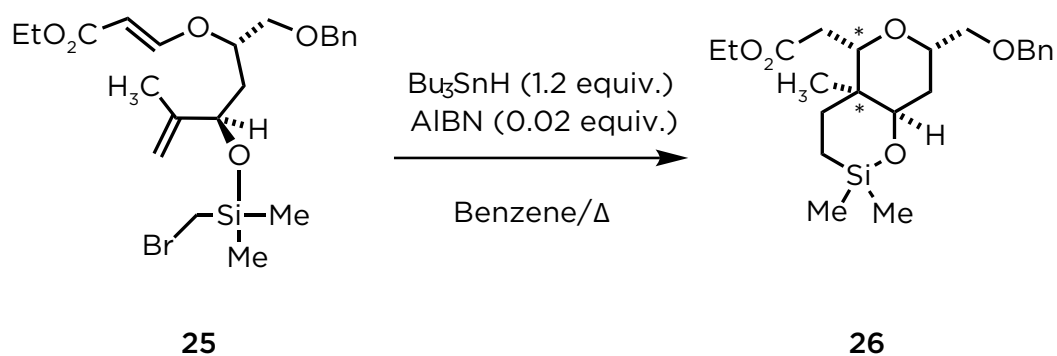
(ii)



(iii)



(e) Treatment of a dilute solution of the unsaturated bromosilyloxy ether **25** in benzene with tri-*n*-butyltin hydride and azobis(isobutyronitrile) (AIBN) at 80 °C results in the formation of the bicyclic compound **26** in ca. 80% yield.



$\text{Bn} = \text{CH}_2\text{Ph}$

Suggest a mechanism (including radical initiation and propagation steps) for the transformation of **25** into **26**, and account for any aspects of regioselectivity and the stereochemistry of the chiral centres in **26** indicated by asterisks.

## Appendices

### Appendix C: examples of transferable/professional Skills matrix

"Here at Leeds we have an Industry Advisory Board that provides advice on embedding transferable skills development in our programmes. The board is composed of an independent chair and representatives from ~10 companies from multiple sectors. With their help, we have a consolidated list of all the professional skills our students should develop during their degree. We then ask each module leader to identify which of these key transferrable skills students develop through each of the modules they run. The module leaders are required to mark which professional skills students develop on a comprehensive mapping document forming a large matrix which gives a clear overview of exactly which professional skills are covered in each of our chemistry units. This enables us to ensure that we effectively embed professional skills within the chemical curriculum, while also helping our students recognise the skills that they develop. This instils an important confidence in our students, helping them know that they have developed the skills that future employers require.

Our Industry Advisory Board also provides additional opportunities for students, eg networking opportunities and bespoke advice on c.v./job application preparation that complements opportunities/information disseminated through the School's LinkedIn group."

**Professor Steve Marsden** University of Leeds

**Figure 1.**  
Example of the  
matrix used at the  
University of Leeds

|          | Analytical skills | Commercial awareness | Communication skill | Confidence | Creative problem solving | Critical thinking | Ethical awareness | Flexibility | Independent working | Initiative | Leadership | Planning & organisation | Professionalism | Research skills | Social/cultural sensitivity | Team working | Time management | Use of knowledge |
|----------|-------------------|----------------------|---------------------|------------|--------------------------|-------------------|-------------------|-------------|---------------------|------------|------------|-------------------------|-----------------|-----------------|-----------------------------|--------------|-----------------|------------------|
| CHEMXXXX | X                 |                      | X                   |            |                          | X                 |                   |             | X                   |            |            |                         |                 |                 |                             |              |                 | X                |
| CHEMXXXX | X                 |                      | X                   |            |                          | X                 |                   |             | X                   |            |            |                         |                 |                 |                             |              |                 | X                |
| CHEMXXXX | X                 |                      | X                   |            |                          | X                 |                   |             | X                   |            |            |                         |                 |                 |                             |              |                 | X                |
| CHEMXXXX | X                 |                      |                     |            | X                        | X                 |                   |             | X                   |            |            |                         |                 |                 |                             |              |                 | X                |
| CHEMXXXX | X                 |                      | X                   |            | X                        | X                 |                   |             | X                   |            |            |                         |                 |                 |                             |              |                 |                  |
| CHEMXXXX | X                 |                      |                     |            | X                        |                   |                   |             | X                   |            |            |                         |                 |                 |                             |              | X               | X                |
| CHEMXXXX | X                 |                      |                     |            | X                        | X                 |                   |             |                     |            |            |                         |                 |                 |                             |              |                 | X                |
| CHEMXXXX | X                 |                      |                     |            | X                        | X                 |                   |             | X                   |            |            |                         |                 |                 |                             |              |                 | X                |

At the University of Reading we have a stream of modules running vertically through our courses to fully embed professional skills for chemists. Through problem based learning, our chemistry students develop professional skills that are fundamental to any career and can then use their experiences as anecdotal evidence in interviews and applications.

Our first and second year Chemical Concepts modules encourage students to think about the skills they need and how to develop them, and we use the Royal Society of Chemistry Undergraduate Skills Record for recording these skills.

In year 1, students carry out a number of group problem based learning activities. They give presentations, write reports and design a poster to explain how they have completed the task and obtained the solutions. The first activity requires students to identify and research elements suitable for a variety of industrial applications which links nicely to an introductory module in inorganic chemistry on the periodic table and solid state structures. In the following term students carry out an IT and numeracy skills based challenge, which uses team work and communication skill. Besides these group tasks there are individual activities, such as summarizing an article from Education in Chemistry.

The 2nd year module focusses on the chemical industry and career management. The challenge is based on the Titan project. Teams of students act as the management group for a company producing TiO<sub>2</sub> in the UK. The teams have to prepare a pitch to justify the continuation of production at the UK site and are required to produce videos explaining their 5 year plans. Additionally, students develop entrepreneurial skills as they have to produce reasoned and financially sound plans for TiO<sub>2</sub> production. The teams then have to defend their plans in an “Apprentice-style” board room interview held with the heads of the parent company, Titan Industries. The activity runs in parallel to sessions delivered by our Careers Advisor on cv preparation and career planning and so students can clearly see the relevance of the professional skills developed to placement applications.

The development of professional skills culminates in the final years. Students carry out research projects and draw on their experiences of independent

investigative and analytical skills, problem solving, ICT and communication as they write project reports, deliver presentations and attend vivas.

#### **Professor Elizabeth Page, the University of Reading**

“At York, we focus on developing the skills a chemist requires in the context of chemical knowledge taught in the core of our course.

All first year students participate in a team-building industrial-style day event in which they meet their peers, engage in small group activities, and solve real-world chemical problems in teams. They also give a short oral presentation, getting guidance on presentation skills, and carry out a public understanding of science exercise in which they either write a popular science article or create a YouTube video.

Students develop skills in maths, biology and physics, take workshops in scientific ethics and methodology, one whole course is taught in an independent-learning style, and a team practical on ‘the chemistry of a night out’ encourages them to develop experiment design and time-management skills. In year 2, we have a highly innovative assessed six-lecture course teaching Chemical Health and Safety. Students do a wide range of contextualised assessed activities in their option modules from industrial field trips to geology practicals, and in end of year ‘Group Exercises’, students work as mock industrial companies to solve real-world chemistry problems. They have to organise meetings, keep minutes and consider financial implications, as well as watching-back a recorded oral presentation.

Third year students develop scientific writing and literature comprehension skills in a Scientific Literacy module, while MChem Group Research Mini-Projects prepare students for their major final year research projects, introducing extended report writing, preparation of a poster and planning of open-ended research. All of these professional skills come together in the students’ final year extended research projects where they must show independence and self-reliance to effectively plan, develop and manage their own project.”

**Professor David K. Smith,**  
**Department of Chemistry, University of York**



## Notes

## Notes

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