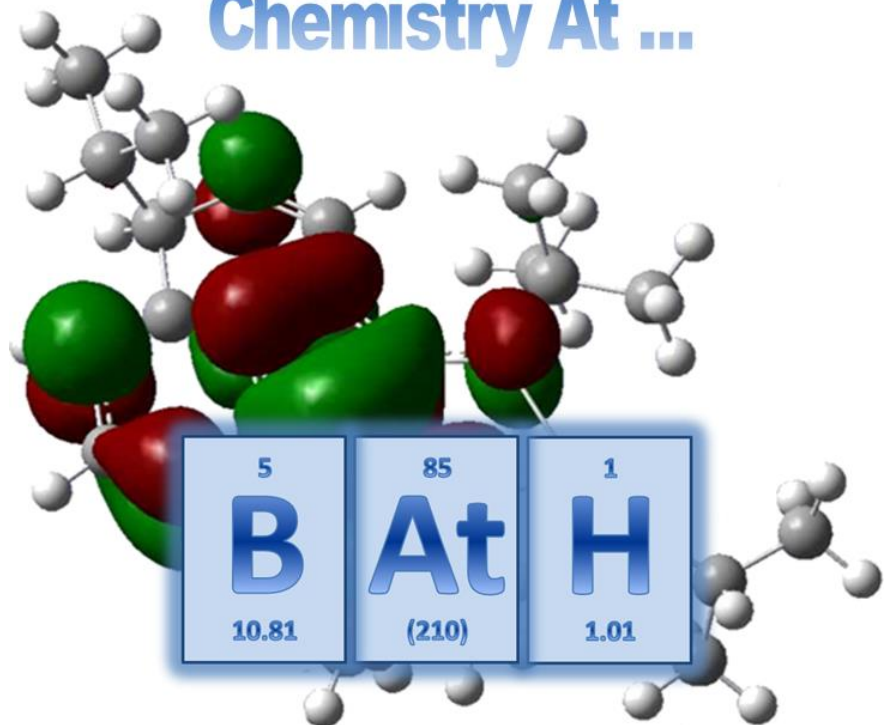


Chemistry At ...



POSTGRADUATE RESEARCH STUDENT HANDBOOK 2016/17

Department of Chemistry

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This handbook is available in electronic format via your Moodle (virtual learning environment) pages. The online version includes live links to information sources. If you require a copy in large font or other format please contact the Programme Administrator.

Every effort is made to ensure that the information contained within this handbook is accurate and up-to-date.

1. Welcome to the Faculty of Science



Welcome to the Faculty of Science at the University of Bath. I am delighted that you have chosen to pursue your postgraduate training with us. In some cases that means continuing from your previous studies at Bath, and you will be familiar with the campus and the staff. But for those of you electing to move to Bath from elsewhere, this will be an exciting new challenge. All of you will be embarking on a new phase in your lives and a move to a new style of thinking and learning inherent in postgraduate training; the Faculty of Science Graduate School is here to facilitate this transition. Above all, we want you all to succeed in your chosen course or research project, and that it should be an enriching and enjoyable experience. So do attend the induction events to meet the Graduate School team and to network with your peers. I look forward to meeting you all in the coming weeks.

Prof Sue Wonnacott, Associate Dean for Graduate Studies

1.1 The Faculty of Science Graduate School

There are 6 departments within the Faculty of Science – Biology and Biochemistry, Chemistry, Computer Science, Mathematical Science, Pharmacy and Pharmacology, and Physics. The Graduate School is the home for all postgraduate students engaged in research or taking taught Masters courses within the life sciences, physical sciences and mathematics. The Faculty has several interdisciplinary Research Centres, including the Centre for Extremophile Research (CER); the Centre for Mathematical Biology (CMB), the Centre for Regenerative Medicine (CRM) and Bath Institute for Complex Systems (BICS). These Centres foster cross-discipline interactions, both within and beyond the Faculty of Science, and support interdisciplinary postgraduate training programmes.

Role of the Graduate School

The Graduate School is responsible for supporting postgraduate students throughout their lifecycle at the University, from admission, through progression stages to submission and completion. It also provides a forum for formal and informal interdisciplinary exchanges, offering both academic and social activities. Generic skills training courses are provided by the Graduate Centre via the Graduate School.

Staff in the Graduate School

Location: Wessex House 3.33

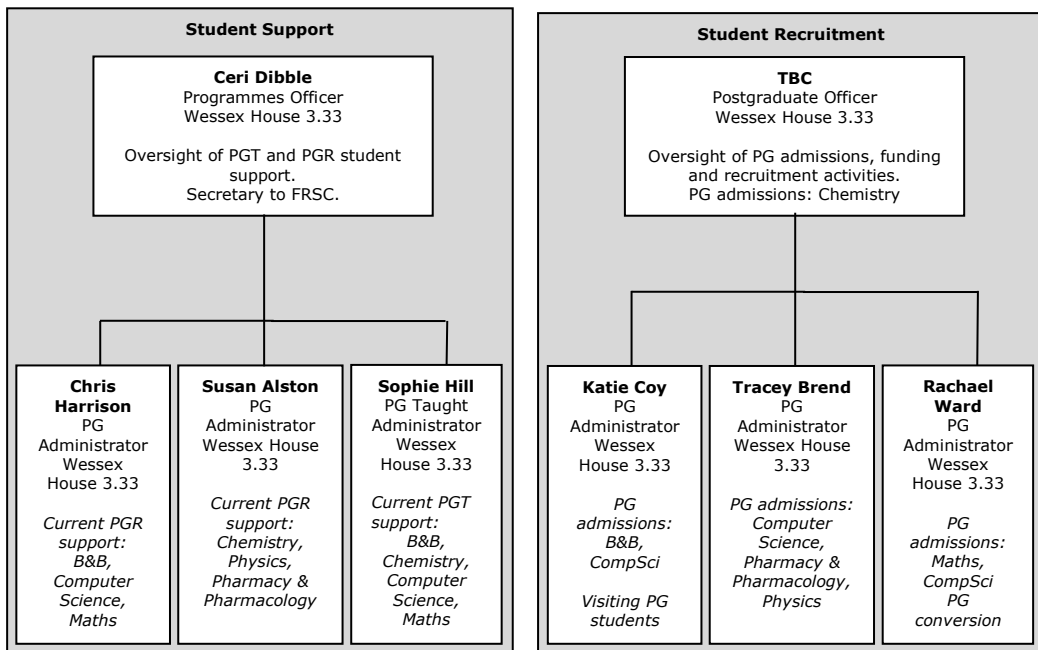
Website: <http://www.bath.ac.uk/science/gradschool/people/>

Email: fac-sci-gs-admin@bath.ac.uk

Tel: +44 (0)1225 38 3410 (internal ext 3410)

Professor Sue Wonnacott
Associate Dean for Graduate Studies
4 South 0.44

Simon Gane
Graduate School Manager
Wessex House 3.35



2. Welcome to the Department

2.1 Department of Chemistry

First of all, congratulations on your success in gaining a postgraduate research position and welcome to the Department of Chemistry at Bath. You are about to start on a very exciting phase of your life. If this your first time at the University Bath you'll find that it's very special place. If you're returning to Bath you will already know how special Bath is.



Postgraduate Studies is often much less structured than undergraduate studies. However, that doesn't mean you won't have lots to do: lots of work and lots of fun to be had!

There's also a lot to find out in the first few weeks - about the Department, the University and the City of Bath. We'll do our best to make sure that you settle in quickly so that you become familiar with the way that everything works at Bath, and in the Department of Chemistry. However, if you're not sure about something - please just ask.

The Department of Chemistry at Bath is a highly successful and growing department which carries out internationally recognised research in many areas of chemical sciences. Bath is the first choice for many people looking to pursue graduate studies in in Chemistry in the UK, and we have a large postgraduate community. Currently there are 42 full-time members of staff. We are a young department - the average age of academic staff is just 42. There are over 100 postgraduate students and this number is set to greatly expand in the coming years, so lots of people to meet.

Finally, I'm sure that you will have an enjoyable and rewarding time at Bath and if you do have any concerns either before you arrive or during your studies please do not hesitate to contact me by email: a.i.johnson@bath.ac.uk. Of course, once at Bath you can always pop by my office which is 1S 1.03b.

Dr. Andrew Johnson

Director of Postgraduate Studies

3. Department Structure

3.1. Who's Who in the Department

See <http://www.bath.ac.uk/chemistry/contacts/> for a full list of Department staff. Some contacts most relevant to PG students are:

Head of Department

Professor Chris Frost

Deputy Head of Department













Professor Jonathan Williams

Director of Studies (PG Research)







Dr Andrew Johnson





Departmental Coordinators

Shula Dennard / Kate Remington

 <p>Dr Antoine Buchard</p> <p><i>Whorrod Research Fellow</i></p> <p>(5W 2.28)</p> <p>a.buchard@bath.ac.uk</p>	 <p>Prof. Steven Bull</p> <p><i>Professor of Organic Chemistry; Head of Organic Chemistry</i></p> <p>s.d.bull@bath.ac.uk</p>	 <p>Prof. Andrew Burrows</p> <p><i>Professor of Inorganic Chemistry</i></p> <p>a.d.burrows@bath.ac.uk</p>	 <p>Dr Stephen Bromfield</p> <p><i>Synthetic Chemistry Teaching Fellow</i></p> <p>(WH 1.11)</p> <p>s.m.bromfields@bath.ac.uk</p>	 <p>Dr Petra Cameron</p> <p><i>Senior Lecturer in Physical Chemistry</i></p> <p>p.j.cameron@bath.ac.uk</p>	 <p>Dr Dave Carbery</p> <p><i>Senior Lecturer in Organic Chemistry</i></p> <p>d.carbery@bath.ac.uk</p>
 <p>Dr Jonathan Cox</p> <p><i>Senior Lecturer in Organic Chemistry</i></p> <p>j.p.l.cox@bath.ac.uk</p>	 <p>Prof. Matthew Davidson</p> <p><i>Whorrod Professor of Sustainable Chemical Technologies</i></p> <p>m.g.davidson@bath.ac.uk</p>	 <p>Dr Fiona Dickinson</p> <p><i>Physical Chemistry Teaching Fellow</i></p> <p>(WH 1.18)</p> <p>f.dickinson@bath.ac.uk</p>	 <p>Prof. Karen Edler</p> <p><i>Professor of Physical Chemistry; Head of Physical Chemistry</i></p> <p>k.edler@bath.ac.uk</p>	 <p>Dr Stephen Flower</p> <p><i>Lecturer in Drug Discovery; DoS Postgrad Taught</i></p> <p>(WH 1.20)</p> <p>s.e.flower@bath.ac.uk</p>	 <p>Prof. Christopher Frost</p> <p>Head of Department; Professor of Organic Chemistry</p> <p>c.g.frost@bath.ac.uk</p>

 <p>Prof. Mike Hill</p> <p><i>Professor of Inorganic Chemistry</i> Director of Research</p> <p>m.s.hill@bath.ac.uk</p>	 <p>Dr Ulrich Hintermair</p> <p><i>Whorrod Research Fellow</i> (5W 3.36b)</p> <p>u.hintermair@bath.ac.uk</p>	 <p>Prof. Saiful Islam</p> <p><i>Professor of Computational Materials Chemistry</i></p> <p>m.s.islam@bath.ac.uk</p>	 <p>Prof. Tony James</p> <p><i>Professor of Organic Chemistry</i></p> <p>t.d.james@bath.ac.uk</p>	 <p>Prof. Toby Jenkins</p> <p><i>Professor of Bio-Physical Chemistry;</i> Admissions Tutor (Postgraduate)</p> <p>a.t.a.jenkins@bath.ac.uk</p>	 <p>Dr Andrew Johnson</p> <p><i>Lecturer in Inorganic and Materials Chemistry;</i> Postgraduate Director of Studies</p> <p>a.l.johnson@bath.ac.uk</p>
 <p>Dr Matthew Jones</p> <p><i>Reader in Inorganic Chemistry.</i></p> <p>m.jones2@bath.ac.uk</p>	 <p>Dr Barbara Kasprzyk-Hordern</p> <p><i>Reader in Environmental Chemistry</i></p> <p>b.kasprzyk-hordern@bath.ac.uk</p>	 <p>Dr Randolph Köhn</p> <p><i>Senior Lecturer in Inorganic Chemistry;</i></p> <p>r.d.kohn@bath.ac.uk</p>	 <p>Dr Simon Lewis</p> <p><i>Senior Lecturer in Organic Chemistry;</i></p> <p>s.e.lewis@bath.ac.uk</p>	 <p>Dr Mary Mahon</p> <p><i>Senior Lecturer in Inorganic Chemistry;</i></p> <p>m.f.mahon@bath.ac.uk</p>	 <p>Prof. Frank Marken</p> <p><i>Professor of Physical Chemistry</i></p> <p>f.marken@bath.ac.uk</p>
 <p>Dr Benjamin Morgan</p>	 <p>Dr Claire McMullin</p>	 <p>Dr Dan Pantos</p>	 <p>Prof. Steve Parker</p>	 <p>Dr Sofia Pascu</p>	 <p>Prof. Gareth Price</p>

<p><i>Royal Society Research Fellow</i></p> <p>b.j.morgan@bath.ac.uk</p>	<p><i>Computational Chemistry Teaching Fellow (WH 1.24)</i></p> <p>c.mcmullin@bath.ac.uk</p>	<p><i>Senior Lecturer in Organic Chemistry</i></p> <p>g.d.pantos@bath.ac.uk</p>	<p><i>Professor of Physical Chemistry</i></p> <p>s.c.parker@bath.ac.uk</p>	<p><i>Reader in Inorganic Chemistry</i></p> <p>s.pascu@bath.ac.uk</p>	<p><i>Professor of Physical Chemistry</i></p> <p>g.j.price@bath.ac.uk</p>
 <p>Prof. Paul Raithby <i>Professor of Inorganic Chemistry</i></p> <p>p.r.raithby@bath.ac.uk</p>	 <p>Dr Asel Sartbaeva <i>Royal Society Research Fellow</i></p> <p>a.sartbaeva@bath.ac.uk</p>	 <p>Dr Janet Scott <i>Reader in Physical and Sustainable Chemistry</i> (5W 3.36a) j.l.scott@bath.ac.uk</p>	 <p>Dr Gan Shermer <i>Teaching Fellow</i></p> <p>g.shermer@bath.ac.uk</p>	 <p>Dr Ruth Webster <i>University of Bath Prize Research fellow</i></p> <p>r.l.webster@bath.ac.uk</p>	 <p>Prof. Mark T. Weller <i>Professor of Energy Materials</i></p> <p>m.t.weller@bath.ac.uk</p>

 <p>Prof. Michael Whittlesey <i>Head of Inorganic Chemistry; Professor of Inorganic Chemistry</i></p> <p>m.k.whittlesey@bath.ac.uk</p>	 <p>Prof. Ian Williams <i>Professor of Theoretical Organic Chemistry; Third and Final year Director of Studies</i></p> <p>i.h.williams@bath.ac.uk</p>	 <p>Prof. Jonathan Williams <i>Professor of Organic Chemistry; Deputy Head of Department</i></p> <p>j.m.j.williams@bath.ac.uk</p>	 <p>Prof. Chick Wilson <i>Professor of Physical Chemistry</i></p> <p>c.c.wilson@bath.ac.uk</p>
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All staff are in 1 South unless indicated otherwise. The telephone numbers listed can be dialled from any internal University telephone. From outside the University, add (01225) 38 to the number (e.g. x 6504 becomes 01225 386504).

The directory of staff names and room numbers is located in the Foyer of the Chemistry Building, 1 South. If necessary, please contact Computing Services (using the "help" button [at http://www.bath.ac.uk/bucs/help/contact/index.html](http://www.bath.ac.uk/bucs/help/contact/index.html)) with your details if you need to be added to the appropriate list and email list.

3.2 Research Areas in the Department

Research in the department is divided into Physical, Inorganic, Organic and Computational Chemistry, with much of the research spanning two or more of these disciplines, facilitating multidisciplinary programmes of research. The Centre for Sustainable Chemical Technologies and the associated Centre for Doctoral Training link research between Chemistry and Chemical Engineering in many areas of green chemistry and renewable energy research, and also facilitates collaboration with other departments across the university.

Physical Chemistry

Solar cell research, electrochemistry, laser optical and microwave methods, LB films, biomimetic functional thin films, nanoscale & hierarchically structured materials and self-assembly, polymer-surfactant interactions, DNA electrochemistry, new polymer synthesis and sonochemistry, studies of protein-protein and enzyme binding, heterogeneous catalysis, materials for biofuel production.

Inorganic Chemistry

Catalysis, novel organometallic synthesis, hydrogen bond interactions, supramolecular coordination chemistry, bio-inorganic chemistry, X-ray crystallography and powder diffraction, synthesis of ALD and MOVCD precursors, transition metal chemistry, organometallic polymers, clusters and nanomaterials.

Organic Chemistry

Asymmetric synthesis, development of transition metals and enzymes as catalysts, asymmetric catalysis, biomimetic catalysis, bioorganic chemistry, antibody engineering, molecular evolution, enantioselective synthesis of aminoacids, supramolecular chemistry, molecular sensor design, natural product synthesis.

Computational Chemistry

Computer simulation of crystal growth, zeolite structures and minerals, studies of transition states of reactions, simulations of oxide materials for fuel cells and ceramic membranes and intercalation materials for lithium batteries.

Facilities and equipment

The department has a new research building with state-of-the-art laboratories and first class research facilities including:

- Atomic force and scanning tunnelling microscopes
- Surface plasmon resonance and surface plasmon enhanced fluorescence
- Mass spectroscopy suite
- Five NMR instruments (250, 300, 400 and 2 × 500 MHz)
- Extensive single crystal and powder diffraction facilities
- Small angle X-ray scattering instrumentation
- High power molecular modelling facilities
- Modern electrochemical instrumentation
- State-of-the-art laser optics
- Peptide synthesiser
- Fully equipped hazards-high pressure lab
- Raman, UV - Vis, FTIR, CD and fluorescence spectrometers

International and Industrial links

The Department has international links with countries including Germany, Sweden, the Netherlands, Switzerland, USA, Japan, China, Sri Lanka, France, Spain, Ireland, Malta, Singapore, Brazil, South Africa, Australia and New Zealand.

There are industrial links with companies including Glysure Ltd, National Physical Laboratory, Molecular Sensing plc, EpiChem, Unilever, Pilkington, Johnson Matthey, GlaxoSmithKline, Takeda, and Astra Zeneca.

4. Working in the Department

4.1 Department Website

Please regularly refer to the Department webpages as these contain the most recent and continually updated sources of information
<http://www.bath.ac.uk/chemistry/>

4.2 Keys and security registration

You must complete a security registration form as soon as you arrive to work in the Department. This will be arranged as part of your Induction to the Department. You will be issued with a swipe access card for access to the Department out of normal working hours and any keys which are required to access your research laboratories. You will need to sign for these and a small deposit may be required.

We will also arrange for your photograph to be taken and added to the board in the foyer.

4.3 Stationery

If you require any stationery items, please speak to the Department Coordinators in room 1S 0.16.

4.4 Mail Pigeonholes

Post is delivered/collected twice per day, between 9.00 and 9.30 am and between 3.45 and 4.00 pm.

Incoming post: Any post received for you by the Department will be put in the postgraduate/postdoctoral pigeon holes located in the connecting corridor at the rear of the Chemistry Building, 1 South. Please check your pigeon hole **daily** and discard any unwanted junk mail immediately.

Outgoing post: Please place in either the internal or external post tray in the Post Room (1S 0.16).

Academic and support staff pigeonholes are located in the by the drinks machine (1South ground floor "pool" area).

General information is placed on the noticeboard adjacent to the postgraduate/postdoctoral pigeon holes. There is another noticeboard located outside the Department Coordinators' room (0.16) for more general wide-ranging University notices.

4.5 Printing

Printers/photocopiers have been provided for use by the postgraduate and postdoctoral staff in Building 1 South. Your library card can be swiped against the card reader to allow photocopying and the cost will be charged directly to your research grant. Printing can be done to any printer in the department by sending the document to the printer labelled Postscript on myprint.campus.bath.ac.uk. To retrieve your printout, swipe your card on the card reader on a printer. Follow the instructions on the screen and your printout will be printed to that machine. Printing via this method will also be charged directly to your research grant, so discuss use of colour printing or printing in large amounts with your supervisor before doing it. In theory, the printout can be collected from any printer on campus using this method.

4.6 Finances

Financial matters are dealt with by the Faculty Science Finance Office located in Wessex House 3.50A.

All queries regarding salaries and pensions should be addressed to either the Payroll Office within the University's Finance Office (4 Manvers Street) or the Human Resources (Personnel) Department (Wessex House, Level 3).

Training Support Fund

Your supervisor may have access to a Training Support Fund (TSF) to support your research. With their approval, this can be used to purchase books, equipment, computing, travel to conferences, plus other expenditure that your supervisor believes will benefit your work. The amount available in this fund varies considerably depending on the source of your funding, and the programme of study you are on. Please check with your supervisor regarding arrangements for this. You will be given a unique code by your supervisor to use for all items of expenditure connected with your research project.

Purchasing Travel

Although you are able to purchase travel tickets yourself and claim the costs back with a receipt, the University can buy these tickets upfront on your behalf. This is charged directly to the University. The University's travel agent, Ian Allan Travel, is available to postgraduate students to book their own journeys and accommodation online (see uob.ianallantravel.com to register). You will need to know your project code, so if you don't know this, please ask your supervisor.

Conference fees and associated costs can be arranged through the Faculty Finance Office (fac-sci-finance-admin@bath.ac.uk). Please check with your supervisor before making any purchases for travel.

Expense Claims

The process for claiming back research expenses you have paid yourself is the same for postgraduate students as for staff. This is done with the Agresso system online at <https://agresso.bath.ac.uk>. If you do not have access to Agresso, or require some help completing your claim, please speak to the BUCS helpdesk in the Library. Agresso web expenses enables you to enter the costs online and print out a summary to which you attach your receipts and hand in to the Faculty of Science Finance Office in Wessex House 3.50. Please check with your supervisor before claiming any expenses.

Student Maintenance Payment (Stipend)

If your study is funded from a Studentship (i.e. URS, ORS, DTG) you will most likely be receiving a quarterly payment for living costs during your degree. This is not applicable for self-funded students. Maintenance is paid directly to your bank account in October, January, April and July. Please be aware though, that this payment will stop for periods of suspense, and status changes from full or part time study (i.e. Writing-Up, Thesis Submitted etc.) Any questions about maintenance can be directed to the Student Finance Office (stufin-stipends@rt.bath.ac.uk).

Purchasing and stores

To make a purchase, you need to obtain either a [BLUE Order Request form](#) (for external supplier orders) or a [GREEN Order Request form](#) (for internal stores orders, i.e. items kept in stock) which you can obtain from your research write-up room. If you wish to order chemicals/consumables that will be used in medical research (VAT exempt), please see the Stores technician(s); they will provide the necessary [PINK form](#).

Fill in all the details – suppliers should normally be an SUPC approved supplier. Ask your supervisor to authorise the purchase by stamping the form with their numbered stamp and place the form in the tray just outside 1South 0.58, from where they will be processed.

Goods will be delivered directly to your laboratory or office by the technical staff, so it is very important to specify the exact room for the delivery on the order form. Any goods which need to be returned (e.g. damaged) must be handled back through the 3S stores – with all paperwork attached.

4.7 Technical Information

Waste disposal

'Tradebe' handle the waste from Sigma and they have given instructions on how they would like the waste to be segregated. Please recycle all your empty SIGMA bottles in the bins outside 1 South. Please put a line through all the labels (glass & plastic) and remove the lids from the glass bottles. All lids can go in the plastic bin along with any plastic Sigma tubs. Any size of bottle can be taken but they should be washed out first.

Halogenated and Non Halogenated waste bottles: Please ensure that these bottles are not overfilled and the black lids not overtightened. Only use "venting" lids for solvent waste bottles (identified by a special label), not normal lids. All full bottles must be placed in crates and not on the floor.

Each laboratory should regularly remove its hazardous chemical waste and take it down to the 1S waste holding area. Each bottle must be properly labelled (Aqueous or Non-Aqueous) and then stored according to chemical compatibility. Halogenated and Non-Halogenated solvents must be segregated. Waste labels can be obtained from the stores technicians. Vented caps **MUST** be used on all chemical waste bottles. Do **NOT** dispose of any chemical waste down the laboratory sinks or drains. Separate procedures exist for the disposal of unusual or highly hazardous waste – email bbcwaste@bath.ac.uk for further advice or with any queries.

NMR Spectroscopy

The NMR facility in the Department of Chemistry at Bath currently consists of five instruments; one Agilent and four Bruker spectrometers. 1S 0.57 houses a Bruker AV300 and a Bruker AV400 spectrometer, located next door to our Bruker AV500 in 1S 0.03. The Bruker AV250 and the Agilent ProPulse 500 are in 1S 0.42. Basic training and safety guidance is provided to all researchers by Dr John Lowe or Dr Catherine Lyall before use of NMR instruments running in automation. Training will be arranged as part of your induction week.

The main purpose of the AV250 is to provide high throughput, rapid turnaround ¹H spectra. It is fitted with a 60 position sample changer to allow continuous data acquisition throughout the day and night – ¹H only during the day and ¹H/¹³C during the night. Local users can keep track of samples submitted on the AV250, and print out spectra once complete, using a link from the 250MHz

NMR webpage. A PDF of the processed spectrum is also emailed to the user immediately after acquisition.

The AV300 is also fitted with an automatic sample changer with capacity for 60 samples, allowing high-throughput data acquisition round the clock. Any researcher can use this machine, including final year undergraduate students during their research projects. It is normally used for the acquisition of standard 1D and 2D data. Like the 400 and 500, a fully autotunable probe allows data from a large range of NMR-active nuclei to be acquired. Local users can also keep track of samples and print out spectra online as for the 250, in addition to the emailed PDFs of spectra.

The AV400 is normally reserved for more specialised 'hands-on' applications, and a small group of students, postdocs and staff are trained to operate it. It is fitted with an autotune probe and, along with the 500, can acquire data from a wide range of nuclei (including ^1H , ^{13}C , ^{11}B , ^{15}N , ^{19}F , ^{29}Si , and ^{31}P). In addition a separate probe allows the acquisition of ^{19}F - ^1H correlations. Currently, it is often used for NMR studies of diffusion. A wide selection of modern gradient-based experiments is available, and spectra can be acquired at temperatures from -150 to $+150$ °C. Most research groups will have at least one person trained; anyone wanting training on the AV400 or the AV500 should contact Dr John Lowe in the first instance.

As with the AV400, the Bruker AV500 is used in manual mode by researchers who have opted to be trained in its operation. Complete with two autotune probes, it is capable of examining a broad range of nuclei (including ^1H , ^{13}C , ^{11}B , ^{15}N , ^{19}F , ^{29}Si , ^{31}P and ^{103}Rh). A full selection of modern gradient-based 1D and 2D experiments are available, and spectra can be acquired at temperatures from -150 to $+150$ °C.

In 2014, we have had our most recent spectrometer installed. The Agilent ProPulse 500 has a 96 position sample changer, for continuous data acquisition at a higher field strength. The autotune probe is capable of examining ^{19}F spectra in automation, in addition to all other nuclei available on the AV300. When used in manual mode, samples can be acquired at temperatures between -80 and $+100$ °C.

An external NMR service is offered to customers from outside the University. Prices start at £30 per sample, please contact Dr John Lowe, j.lowe@bath.ac.uk, for further information.

Mass Spectrometry Service

The Department of Chemistry Mass Spectrometry facilities have recently been upgraded and consist of a new electrospray Time-of-Flight mass spectrometer (ESI-TOF), and a new electrospray quadrupole Time-of-Flight mass spectrometer (ESI-QTOF). These are used for a wide range of applications, including:

- Organic and inorganic synthesis product confirmation
- Impurity profiling and identification of unknowns
- Reaction monitoring

The **micrOTOF** (ESI-TOF) is used for routine accurate mass analysis, with high resolution acquisition. It is controlled by open access software, with a choice of generic methods for different mass ranges and polarities. Generally it is run using an autosampler to inject the sample into a solvent stream supplied by the LC pump, without any chromatographic separation. There is also the capability for liquid chromatography to precede the mass spectrometric analysis (LC-MS).

The **micrOTOF-Q** (ESI-QTOF) instrument is operated as a research instrument where users will have full interaction with the operating methods. As for the micrOTOF, this instrument is capable of acquiring high mass accuracy data, of publication quality. In addition, the inclusion of a 'Q' (quadrupole) allows for fragmentation experiments to be carried out, allowing for some structural elucidation to be done. In combination with the excellent NMR and X-ray facilities in the department, full structural identification and characterisation should be possible. A glove box is located next to the spectrometer making it possible to prepare samples in an inert environment and then to infuse them directly into the mass spectrometer via a break in the glove box, allowing for 'inert' mass spectrometric analysis to be conducted.

In order to use the facilities, it is important that you first receive some training. You can be trained to use the OpenAccess micrOTOF, or the research micrOTOFQ, or both. Contact Dr Anneke Lubben (a.t.lubben@bath.ac.uk) or visit the Mass Spectrometry Service web pages for more details or to sign up for training. Once you have been trained, you will be allocated a user name which will give you access to the service. Outside the normal working hours of 8.00am to 6.30pm weekdays, access is restricted using a card reader on the door to the foyer. In addition there is a keypad on the lab door to allow for access to the instruments themselves. This requires a 4 digit key-code, which is only given to you once you have undergone training.

4.8 You and your Supervisors

You should maintain close contact with your lead supervisor throughout your career as a research student. He/she will establish the directions of your research and will ensure that you receive the correct training in the different specialised techniques that are required and in the material that forms the background to your research. He/she will also arrange for the facilities necessary for your research to be available. You will also be assigned a second supervisor.

Research is increasingly a strongly collaborative activity and you should make sure that you work closely not only with your supervisor but also with other members of the research group. They, and other students and staff in the Department, can often provide you with specialised knowledge or advice that can prove invaluable. Make sure, too, that you share *your* experience with others: this means learning to communicate your ideas well.

These are a few suggestions for students to consider:

- Full-time students are advised to meet their lead supervisor on a *formal* basis for supervision at least once a fortnight (it is expected that there will also be more frequent informal contact).
- Part-time students are advised to meet their supervisor on a formal basis for supervision about three times a semester.
- It is the responsibility of students to arrange meetings with their supervisors.
- The expertise of other staff is also available to all students, but again the student is responsible for making contact with the appropriate member of staff.
- Students must be prepared to go out and seek help and advice. They should not rely on other people approaching them.
- Any problems that arise that cannot be solved by direct student – supervisor discussion should be brought initially to the Director of Postgraduate Studies, who may refer the matter to the Head of Department.

4.9 Some differences between First and Higher Degrees

The nature of study for higher degrees by research is very different from that for first degrees. In undergraduate courses, students' activities are very well defined, with comprehensively timetabled formal commitments.

Postgraduate studies are far less structured and consequently students have a much greater responsibility for organisation of their work and for time management.

4.10 How to get things done

As your research progresses, especially if your area of work is experimental, you will need to make the best use of the University's technical resources.

Your supervisor will advise you about the ways in which equipment and other items can be ordered and who to see when you need items manufactured. The University has its own mechanical workshop in the basement of 4E for the making of equipment and there is also a glass-blowing workshop. The personnel are highly skilled and produce excellent items of apparatus: however, there is a high demand for their services which are not cheap or available on instant demand. Remember also that there will be a waiting time of around 3-4 weeks (and sometimes longer) so think well ahead so that your research is not delayed. Simple pieces of apparatus and electronics can sometimes be made in the Department's own workshops, perhaps with the help of our own technical staff. Again, discuss your needs with your supervisor before committing technical staff to major tasks. If you wish to make small items yourself, you can obtain the necessary training and clearance from the Department's technical staff. When using communal research areas such as the workshop or clean room, please keep everything as tidy as possible!

5. Health and Safety

5.1 Safety policy

All safety matters are treated with the utmost importance within the Department of Chemistry, and a separate safety manual will be issued to all new researchers. To emphasise the importance of safety, some of the key points are repeated here.

The University has a Health and Safety Policy which is displayed throughout the campus. There is also a Safety, Health and Environment Unit (WH3.26) with staff who are able to advise on health and safety issues and who monitor the health and safety management of the University.

For further information, the Safety, Health and Environment website is:

<http://www.bath.ac.uk/hr/stayingsafewell/hs-policy/index.html>

or email r.bott@bath.ac.uk.

The University has a public liability insurance policy to cover any claims brought by students or members of the public against the University where the University has been negligent. This policy does not, however, cover students who come to harm because of their own fault, or cause damage of their own volition.

Risk Assessment and Operating Procedures

The Management of Health & Safety at Work Regulations, 1992, and other Regulations as well, require us to "suitably and sufficiently assess the risks to the health and safety of employees to which they are exposed whilst they are at work". This means that we must make "risk assessments" for every work activity carried out by, in particular, students and other researchers. This page indicates how the procedure may be put into effect in the Department of Chemistry.

Hazards and Risks

"Hazard" and "risk" are words which are synonymous in common use but in the technical jargon of Safety Management have different meanings: **the hazard** presented by a substance or activity is its potential to do harm (rock-climbing is a hazardous activity) and **risk** from a substance or activity is the likelihood that it will cause harm in the circumstances of actual use or that the hazard will be realised (rock-climbing may be of low risk if the proper equipment is used and the rules are followed).

The aim of making a "risk assessment" is to identify the hazards associated with an activity, to assess the seriousness of these hazards and to formulate systems of work, training or other methods (controls) to reduce the associated risks to a minimum or at least to an acceptable level.

This procedure has to be carried out by someone who is experienced and fully familiar with the activity *i.e.* a "competent person".

The Risk Assessment Procedure

We are required to

- identify hazards associated with activities or situations.

- somehow or other quantify the associated risk. (How likely is it that any hazard will be realised? How severe will the consequences be? How often does exposure to the hazard occur?)
- identify who is at risk.
- identify the control measures to be used to reduce the risk to a "reasonable" level.
- quantify the residual risk, and then
- record the assessment and implement the control measures.

Application to Chemistry

Straightforward as this procedure is, its translation to the variety of activities carried out in the Department of Chemistry is clearly not trivial, thus the following practice should be adopted.

How to Do it?

- **Identify** Which activity is to be assessed? Has it been done before or can it be broken down into tasks that have already been assessed (see the [chemistry department safety wiki](#)). If there is no existing Assessment, you will have to do it yourself.
- **Carry out the procedures 1), 2) and 3) above, i.e. identify the hazards, quantify the risks and identify who is at risk.** This is where you have to put in the work, reading around the subject and so on. The conclusions here may be subjective but you must be clear about the person or persons you are considering and their likely level of ability or competence. There is a possibility of using sliding scales of likelihood for the hazard being realised (unlikely, likely, very likely, certain) and for the severity of any injury (slight (Elastoplast), moderate (stitches), severe (hospitalisation), death), and frequency of exposure.
- **Formulate control measures.** These will include:
 - physical or engineering controls (e.g. sturdy, custom-built trolleys for moving gas cylinders, the provision of fixed racks for cylinders when they are in use) and this will allow you to spot any possible deficiencies in the physical provisions of laboratories;
 - protective equipment to be worn (e.g. safety glasses, lab. coats);
 - procedures to be followed (e.g. solvent bottles to be transported in proper carriers) and
 - any training that is required.

This process of categorisation is not simple. It calls on our own expertise and experience, our knowledge of the abilities of our students and our knowledge of how far any reasonable control measures to be used are going to be effective and it decides who gets to do what.

Write all this down: This is a legal requirement but, more than that, performing a Risk Assessment is not simply an end in itself. Rather it is a tool to help us to protect the health and well-being of our students and workers. As such, what is written down in the Risk Assessment document should be included as part of the training. The document should be fully available to, in fact required reading for, researchers to enable them to realise the hazards associated with the tasks they are to perform and to see what must be done or what they must do to protect themselves. The Risk Assessment document should be as full as possible and include within it a description of recommended operating procedures, if relevant, action to be taken in an emergency and any suitable references. So in fact this recording becomes part of the next stage.

Implement the control measures. *e.g.* provide the trolleys and racks and carry out the training, including reading the full text of the Risk Assessment.

Finally, if you think that the Assessment you have just made will be of use to others, make it available and have it included in the Department of Chemistry [library of Risk Assessments on the Safety Wiki](#).

5.2 Safety Induction and Registration

As part of your induction week you **must** attend a Safety induction **BEFORE** starting any work in a COSHH regulated area. You will then be given a copy of the latest Departmental Safety Manual which you are required to read. You must complete **Form A** (page 15) and return it to the Health & Safety coordinator. A register of all attendees will be kept in the department.

Your induction will cover Fire and Chemical Safety. This will involve a presentation (including watching some videos) by the Departmental Health and Safety Officer.

You **MUST** also attend a session in the practical use of Fire Extinguishers, and will be expected to attend the next available training session arranged for research staff. Your certificate of attendance will be held on file and will cover a 3-year period (after which you will be required to attend for a refresher). To sign up for this session, send an e-mail to Mrs Sarah Elkins (s.l.elkins@bath.ac.uk).

If you will use gas cylinders in your work, you **MUST** also attend a session on Gas Cylinder Manual Handling. To sign up for this session send an email to Mr Russell Barlow (r.w.barlow@bath.ac.uk).

If your work involves use of lasers you **MUST** view the laser safety video (online) and complete the Laser Safety form. Contact Prof. Toby Jenkins (a.t.a.jenkins@bath.ac.uk) to obtain the form and directions for watching the video.

You should familiarise yourself with all the Safety noticeboards and where the Fire Extinguishers and First Aid kits are in your main work areas. You should know who is your postgraduate [safety committee](#) representative and your Laboratory Custodian.

If you are required to attend the University Medical Centre for Occupational Health Surveillance, please make sure you keep to your appointments. This can be normal for new research workers.

5.3 Safety Contacts

The Faculty of Science Health & Safety co-ordinator is Robyn Bott, who can be contacted at r.bott@bath.ac.uk. Alternatively, any queries about safety can be directed to your supervisor.

5.4 COSHH

COSHH Assessments must be completed **JOINTLY** by the Research Worker and the Research Supervisor BEFORE the procedure is carried out. The purpose of the assessment is to give careful consideration to the risks involved in using particular chemicals in a defined procedure such as a synthesis.

COSHH forms and much other useful safety information can be downloaded from the University Safety website:

<http://www.bath.ac.uk/hr/stayingsafewell/index.html>

6. Training and Seminars

Training is recognised as a crucial element of any PhD programme. The Department of Chemistry and the Faculty of Science have developed a complementary series of training courses, details of which are given in the accompanying lists. It is both a requirement of the Research Councils and the policy of the Department that all students must attend appropriate training courses. It is generally regarded that around 10 days per year of skills training is appropriate over the three years of PhD study. A record sheet which covers

most aspects of training supplied by the Department is included here and on the web, and you should use it to keep a record of what you have done. This must be shown to your assessors during meetings before the 6, 24 and 30 month reports and a copy must be completed and handed in with your First Year Transfer Report.

The Faculty also provides courses in more generic aspects of doing a PhD. While there are a number of courses for those just starting a PhD, other topics, such as writing a thesis, are aimed at final year postgraduates. Thus, training should be viewed as an on-going process throughout the PhD degree.

Other training options are outlined on the **University website** (<http://www.bath.ac.uk/learningandteaching/rdu/courses/pgskills/>). Information on these topics will be available at the Graduate School Welcome and Lunch on Monday 3rd October 2016.

6.1 Training Sessions

Mandatory Courses

Important: All new postgraduates MUST attend the Safety Induction on Monday 26th September 2016 (14:15 in room 1S 0.01) before starting any experimental work.

Fire Safety Training: will be held soon after the start of term (date TBC) and is **compulsory** for **all** new staff and postgraduate students. Sign up for one of the two sessions on the list during the Departmental Welcome or, if you miss this session, email Mrs Sarah Elkins (S.L.Elkins@bath.ac.uk) to reserve a place.

Courses which are compulsory for certain activities

Laboratory Demonstrating: If you wish to take part in demonstrating in the undergraduate laboratories this year, you must attend this course, organised by Dr Andrew Johnson and Dr Fiona Dickinson. The date is to be confirmed – more details will be given in the Departmental Welcome. There are also equivalent courses run centrally, later in the year. These can be booked through the PGSkills website.

Solvent Purification System Training: If you will need to take dried pure solvents from this system, you must attend a training session before you use

it. Attend the course run by Dr Randolph Köhn. The date and time for this training is to be confirmed – more details will be given in the Departmental Welcome. (no need to sign up, an attendance record will be taken during the course).

Gas Cylinder Manual Handling Training: This is **mandatory** if you will use gas cylinders during your PhD work, and you will not be allowed to move cylinders unless you attend this training. You will be contacted to sign up for this session near the start of term; if you miss this session, email Mr Russell Barlow (r.j.barlow@bath.ac.uk) to sign up for this course.

6.2 PG Skills Training

In addition to the specialised training that you will need for your particular project, the University and Department also provide training in a number of more generic skills. There are also external training courses, operated for example by EPSRC.

At the end of your postgraduate studies you will be expert in a highly specialised field, but to be successful in your future career a number of 'generic skills' are required. Developing generic skills will help to make you a more effective researcher, produce better research, be more aware of your skills, make informed career choices and be more employable. Such skills are identified by the Researcher Developer Framework. www.bath.ac.uk/learningandteaching/rdu/tna/rdf.html

Generic skills will be developed in the normal course of your studies, and by attendance at some of the courses offered by the University's PGSkills Programme. An important first step in developing generic skills is to carry out a self-assessment of your strengths and weaknesses, and for you to develop a plan to strengthen the weaker areas. It is very useful to think about how the 'generic' skills are embedded in your everyday work, and to record these in the training log too.

You should NOT attempt to attend everything in the first few months. Instead, discuss your priorities with your supervisor, and determine the development activities that you need to do now for the next 6-12 months of your project, and also to prepare you for your future career. You should be planning and reviewing your development all the way through your research project, and discussing this regularly with your supervisor.

The University PG Skills Programme runs over 100 training sessions throughout the year that address all aspects of the Joint Statement of Skills Training. These courses are free to research students. To browse courses and book online, see: <http://www.bath.ac.uk/learningandteaching/rdu/courses/pgskills/>

The PG Skills Programme includes sessions delivered by BUCS and the Library, however you may also wish to visit their websites to look for other opportunities they may offer.

External activities

A range of courses are also run on a national level by “Vitae” to support the personal development and teamwork skills of postgraduate schools. For details, see the link at the PG Skills Homepage. Other opportunities may also be offered by specific funding bodies. You should take the initiative in finding such courses and you should discuss possible funding with your supervisor.

6.3 Seminars

A programme of research colloquia is organised within the various sections in the Department and postgraduate and postdoctoral researchers are expected to attend. Your supervisor will provide you with more information. Details of forthcoming seminars and conferences are sent by email and posted either on the postgraduate/postdoctoral noticeboard or adjacent to the pigeonholes. Students are informed of upcoming seminars directly by emails from the staff members who organise them

1. **Weekly Research Seminars** usually held on Tuesdays at 13:15 in 1South room 0.01, and given by invited scientists. ***Postgraduates from the relevant section are expected to attend and a sign-in book will be passed around to record attendance.***
2. **Weekly Departmental Research Presentations.** Three seminars are given Wednesday afternoons starting in January, between 1.15-2.15 pm in Room 0.01, in 1 South, by Postgraduate Students. It is a requirement that every student gives a presentation during their second year and in the final year of their PhD (see 4. below). ***Giving these presentations is a requirement for progression and for year 1 and 2 students, attendance at the lunchtime seminars is mandatory. A sign-in book will be passed around to record attendance.***

3. **Ad hoc Guest Seminars.** Occasional seminars may be given by visitors to the Department. These are often from eminent scientists or from active younger researchers, and offer a further opportunity for learning, discussion and possibly finding out about potential employment opportunities. In addition, other departments, especially *Biology & Biochemistry, Pharmacy and Pharmacology, Physics, Chemical Engineering* have seminar programmes that include work highly relevant to research within the Chemistry Department. *Postgraduate students are encouraged to attend.*

4. **Final Year Symposium.** All students in final year are required to give a presentation on their research during a two-day symposium in May to an audience which includes staff and students from other departments, as well as from Chemistry and which also frequently includes industrial representatives. As well as the talks, all students at the end of their first year of PhD studies are required to present a poster on their work which will be displayed outside the lecture room or nearby, and to present it during a poster session in the evening. Prizes are generally awarded for the best talks and posters in the various sections. ***Giving these presentations is a requirement of progression, and attendance at this symposium is mandatory for ALL postgraduates.***

Why do you need to go to seminars?

Research Seminars are a fundamental part of academic life. For postgraduates, they not only advance knowledge but also provide training in communication skills. Thus they constitute an important element in the PhD training programme, and are recognised as such by the Research Councils that fund most of the studentships. Postgraduate students are expected to want to attend not only those seminars related to their own research but also those covering other topics, to keep up to date with current advances in their general discipline and to get an insight into other fields. Moreover, students will often encounter solutions to their own technical problems by attending seminars outside their own research group. Finally, when you apply for jobs elsewhere, your interviewers will expect you to know about the research going on in your Department.

Chemistry Seminar Programme 2016-2017

Most seminars are in 1S 0.01. Further details about the seminar program will be sent by email during the year.

6.4 Preparing Your Presentation

Aims of the Presentation

- To give you practice in presenting a talk
- To tell the audience about your work
- To get constructive feedback

The audience will be composed of other postgraduates, post-docs and academic staff from across the Department. They will be knowledgeable but will not know your specialisation in detail. Pitch the talk at the appropriate level.

Objectives of your talk

To explain:

- **What** you are trying to do
- **Why** it is important
- **How** you are planning to do it (or did it).

The schedule for second year talks allows for three talks in an hour, which means about 15 minutes plus five minutes of questions for each speaker.

Practical points

- Use Powerpoint.
- Learn by observing current presenters about good (and bad) practice. Go to the postgraduate session on presentations and learn how to improve. Practise your talk until you feel confident.
- Arrive early and practise in the lecture room (Room 0.01 in 1 South). Make sure that you know how the computer, projector, etc, work.

6.5 2nd Year Postgraduate Talks

Semester 2, 2016-17

Postgraduate talks this year will take place in 1 hour sessions, on every Wednesday. Each talk should last for approximately 15 minutes, leaving 5 minutes for questions, and describe the research carried out during the project to date. The full timetable for these will be provided around Christmas time.

7. The PhD/EngD lifecycle

The diagram below illustrates the typical lifecycle for standard PhD or integrated PhD/EngD students and includes details of the key progression milestones and when they occur. Further details about these progression milestones can be found in the *University Handbook for Research Students*, which will be included in your welcome pack.



The PhD/EngD lifecycle

