

The idea of a closed book IT examination: a novel approach to assessing chemistry specific information technology.

PAPER

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As part of the advanced chemistry practical module in the final-year of the BSc chemistry degree at Cardiff University, students are required to take a course in chemistry-specific information technology. The problem of assessing such a module at this level is always difficult. One possible means of overcoming this problem is by setting a closed book information technology examination in chemistry. Each student is given a three-hour examination, consisting of three questions, each assessing different aspects of the IT course taken. The nature and structure of the examination paper in question is described. This paper describes some of the problems (technical and otherwise) encountered in devising such an examination. A similar structured examination could be incorporated into any BSc chemistry course to overcome this problem of assessing the IT skills required by a chemistry graduate.

Introduction

Computing skills were identified in a report of the Royal Society of Chemistry as one of the general skills which should be an integral part of a chemistry degree course¹. More recently, the Dearing Report² identified “the use of information technology” as one of the four key skills which should be developed during a university course (recommendation 21). It seems that the importance of IT skills is recognised in most chemistry courses. For example, Mason³ reports that chemistry departments have introduced special teaching in order to “fill perceived gaps in IT skills”. Furthermore, a survey carried out by the Chemical Industries Association indicates that the employers in the chemical industries are largely satisfied with the IT skills of their recently graduate employees⁴. However, a recent survey of pharmaceutical companies highlights this as a critical gap in the expertise of chemistry graduates⁵.

It is possible that the pharmaceutical industry is a special case and has particularly high expectations of IT skills. Nevertheless, it is clearly important to ensure that IT skills included in chemistry courses should be relevant to future employment, and that the time spent in developing these skills should be effectively used. At the Department of Chemistry in Cardiff we set out to design a course structure which would fulfil both these requirements.

The main objective was that, by the end of the degree course, the graduates would be able to make appropriate use of IT to prepare written and oral presentations to the professional standards expected by research journals and international conferences. This involves:

- preparation of hard copy of text;
- creation of tables, graphs, histograms, etc. from spreadsheets and databases;
- producing chemical structures in an appropriate format;
- making use of PowerPoint (or equivalent) in oral presentations.

In designing the course, we recognised the importance of assessment. Race⁶ aptly states that

- “assessment is often a major driving force which gets students down to serious studying”.
- He also reminds us that assessment has other purposes:
- “students themselves need feedback to help them to find out how their learning is going.”
- “we need feedback on how well students’ learning is going so that we can adjust and develop our teaching.”

These points are explored more deeply in a number of references⁷⁻¹⁰.

Our initial survey of available assessment procedures indicated that none met all three of the functions identified by Race as well as we wanted. We were fortunate to be given access to course modules from different universities and concluded that they were assessing skills at a lower level than was required by our third-year course. We also studied the CATS programme (Computer-Aided Assessment of Transferable Skills)¹¹ but found that it only assesses intermediate level word-processing and text editing, and not chemistry-specific programs concerned with (for example) two-dimensional drawing, modelling chemical structures or molecular graphics.

We therefore devised our own assessment procedures. This paper is based on our experiences of the two cohorts of students graduating in 1995 and 1996. It summarises the course we have designed to teach the aspects of IT we judge to be important, describes the assessment procedure (which includes a closed-book examination) which we devised to fulfil the functions given above, and evaluates the effectiveness of the examination.

The teaching of IT at Cardiff

Students studying chemistry at Cardiff University are taught aspects of IT skills throughout the three years of their course. The topics covered during the first two years are shown in Table 1. This work is assessed by selected assignments. In the third year IT course, knowledge of this material is assumed and it is included in the examination.

The third year IT course takes up two weeks of the eight week practical module. In Cardiff, students take 12 modules in a year; the practical module is a double module and therefore corresponds to 1/6th of a year's work. Material covered in the IT course is shown in Table 2.

For the 8 week practical module, the cohort of about 80 students is split into four (approximately) equal groups. Each group spends two weeks on each of the four courses which make up the module: inorganic chemistry, organic chemistry, physical chemistry and information technology. The information technology course is based in the department's computer laboratory which (at the time) contained 23 networked Pentium 75 MHz PC's running Windows 3.1. During the two week period the students are required to attend the laboratory for two 6 hour periods per week (10.00 – 17.00hrs). During these sessions two postgraduate demonstrators and one member of the academic staff were available to offer help and advice. In addition, the students

Table 1: Information on the modular course content and nominal time allowances spent on chemistry specific IT in years one and two

<i>Year 1:</i>	<i>HRS</i>
• Introduction to the student network, e-mail, WWW and computer-aided learning (CAL) chemistry tutorials Introduction to Windows and MS-DOS	1
• Introduction to Microsoft Word - letter-writing, CV's, chemical abstracts, formatting, subscripts, superscripts, symbols	1
• Molecular graphics	3
<i>Nominal IT time in the microcomputer laboratory:</i> <i>(Note this does not include the time for completion of assignments)</i>	5
<i>Year 2:</i>	<i>HRS</i>
• Advanced word-processing - Tabs, tables, use of the equation editor in chemistry	3
• Two-dimensional chemical structure drawing - Chem-Window	6
• Introduction to Microsoft Excel - chemical spreadsheets (use of the function wizard, formulae) and graphs in chemistry (line graphs and scatter plots)	6
<i>Nominal IT time in the microcomputer laboratory:</i> <i>(Note this does not include the time for completion of assignments)</i>	15

are expected to complete assignments based on the work in each session; the full assignment must be completed within two weeks after the last formal session in the computer laboratory. Since the notional time available for the IT course is about 50h (one quarter of a double module), adequate time has been allowed for this work.

This summary of the course structure shows that it introduces the individual techniques required to achieve the stated objective. By the end of the third year module, the students are expected to be able to integrate their skills and to apply them to a specific context.

Assessment

Assessment may be based on work completed during a particular course or module, or after the whole course has been delivered. An advantage of assessing coursework is that it can be to some extent formative: it is not too late for staff or students to take action before the end of the course to overcome any deficiencies. Assessing coursework has disadvantages as well as advantages. For example, it is not possible to give an assignment which requires students to integrate all their knowledge of the course until all the ground

Table 2: Final-year BSc advanced chemistry practical module - IT section - time allowances, assessment and sample assignments

<i>Year 3:</i>	<i>HRS</i>
• Databases using Access	6
• Presentations in chemistry using PowerPoint	6
• Molecular modelling using DTMM for Windows	9
• Information technology examination	3
<i>Nominal IT time in the microcomputer laboratory:</i> <i>(Note this does not include the time for completion of assignments)</i>	24
<i>Assessment:</i> <i>(Selected examples of the types of assignment shown)</i>	%
• Assignment 1 (databases) Example: Using the Opac search facility and Microsoft Access compile and print a suitable comprehensive database for all the textbooks, printed since 1985 on coordination chemistry in the library. Save the file on disk. The database should include all relevant information, such as name of author, name of textbook, publishing company, edition, year, no. of copies, location in library etc.	10
• Assignment 2 (research presentation) Example: Present the chemistry of boron, using PowerPoint. Save the short presentation on disk as Bor.ppt and print copies of the presentation, with summary Spider diagrams for your audience.	10
• Assignment 3 (molecular modelling) Example: You are asked to model the structure, Dopamine. Explain your design process and give the minimised energy in kJ mol ⁻¹ respectively. Save the minimised structure on disk as Dopa.mol. Print the structure in DTMM.	15
• End-of-module IT examination. (Example given in appendix)	65

has been covered. Furthermore, in-course assessment is normally based on assignments carried out under circumstances in which students can plagiarise¹²⁻¹⁴.

Taking these advantages and disadvantages into account we decided to divide the mark for the third year IT module into two components:

- 35% for assignments based on each IT practical session;
- 65% for a closed book examination at the end of the module and covering all the IT skills included in the course (including first and second year work).

For the assignments we considered various options for detecting plagiarism¹²⁻¹⁴, and concluded that it was preferable to try to prevent it from occurring. The strategy we adopted was to set an assignment on each session in the computer laboratory. The forms of assignment are shown in Table 2. The requirement that part of the assignment be submitted in printed format at the end of the session was introduced in order to ensure that it was the student's own work.

The closed book examination is taken during the final 3 hours of the last session in the computer laboratory. It consists of three questions which between them assesses the IT skills which students are expected to develop over the 3 year period. The students were not allowed to bring in any IT manuals or other material into the examination, but they were encouraged to make full use of the Help facility within the software. Each student had to print their final document on completion of the examination.

Question 1 aims to assess the ability of a student to reproduce an academic paper to professional research journal publication standard. This involves using some or all of the skills covered in the 3 years of the IT course (Word, Excel, Chem-Window, etc.).

Question 2 assesses some of the more specific features of the programmes including:

- generation of scatter plots using the function wizard;
- formulae and graphical features of Excel;
- use of the equation editor using Microsoft Word (to produce mathematical equations such as those found in physical chemistry);
- more difficult features of two-dimensional structure drawing using Chem-Window, such as perspective drawings, Newman, Fischer and saw-horse projections, inorganic complexes and clusters, aspects of chemical structure modelling, etc.

Question 3 is the most challenging; a knowledge of basic chemistry is required in order to answer it. The intention is to concentrate on aspects of chemistry where understanding is particularly helped by the use of molecular graphics or molecular modelling¹⁵. Examples are VSEPR theory, point group symmetry, conformational analysis, and space group symmetry.

A specimen examination paper is included in the Appendix. Additional examples and marking schemes are available from the authors on request. After the examination, marked scripts with appropriate detailed comments were returned to the students in order to provide feedback. The comments identify not only weaknesses, but also sections of the scripts which were of particularly high standard.

Table 3: Student marks, 1995 and 1996

	1995	1996
Number of students	60	59
Examination Mark/%		
Highest	100	86
Mean	67	55
Lowest	30	15
IT course (Examination and Assignment)		
Highest	98	98
Mean	67	61
Lowest	33	28

Results

At the time of writing, the third year IT course and its associated examination had been taken by two cohorts of Cardiff students (in 1995 and 1996), a total of 119 students.

A summary of the marks obtained for these students is shown in Table 3. The mark obtained by each student was added to the marks obtained for the inorganic, organic and physical chemistry laboratory courses. The marks for all of the four courses were comparable; the mean varied between 56% to 62%, with the IT mark at 61%.

In 1995 there is some evidence that the mark for the assignments slightly helped the students who were the weakest in the examination. In 1996, the overall performance in the assignments was better than that in the examination.

No specific pass mark was set for the IT course.

Discussion

Avoiding technical problems

When about 20 students are taking a closed book examination based on computers, it is clearly important to avoid technical problems due to failure of computers, or the network, or of the printers.

We have always limited the number of students taking the examination at any one time so that there have always been 3 or 4 surplus PCs. To date, this has been sufficient to avoid any problems with the individual computers.

Networking has not, so far, caused problems. If there is a network failure, it would be necessary to reschedule the examination.

Our classroom PCs do not all have their own printer, but are connected to 2 central laser printers. Examinees can print directly to these without having to move. Naturally, the examinee must check the printout; this is particularly important because there can sometimes be loss of complex characters (e.g. when using an equation editor) when using parallel printing set up. For this reason, we located all the students as close as possible to the printer; the computers furthest away were the ones we chose to keep vacant. Printing has not been a problem; but we take the precaution of ensuring the students have a disk so that, if necessary, documents can be printed later.

Feedback from students

Feedback from students was obtained via representatives reporting to the staff student meeting. Four representatives (one for each of the four IT groups) was appointed; their role was to collate the views of all their respective group members (about 20) on the IT course, and to pass the collective views on to the nominated student representatives at the staff-student meeting. Informal discussion with the representatives indicated that they had taken their role very seriously.

The staff-student meetings are held regularly, and are attended by the Head of Department and by members of staff of the Teaching Committee. The meetings allow ample time for discussion and detailed comments are passed on to the relevant member(s) of staff for action. It is evident from the level of discussion at these meetings that the representatives do their best to reflect fairly the view of the whole class.

There was some feeling that the weight of the examination should be reduced by awarding the assignments more than 35% of the total marks. The counter arguments to this are that the examination provides a valuable test of the students' ability to work independently at the keyboard for a 3 hour period, and also that it covers all of the material included during the 3 years of the course. Furthermore, the closed book examination avoids all problems with plagiarism.

Some students felt that they should be allowed to use manuals in the examination. The arguments for and against this have been well rehearsed and can be summarised as the conflict between allowing students to spend valuable time consulting manuals and the realism of providing access to information which would be available in the real world. In this case we felt that the students had ready access to the on-line Help facility built into all Windows programs, and that this should be sufficient for the style of question we set. Denying access to additional manuals focuses the students' attention on the need to be completely familiar with basic concepts and with the Help facility – both aspects which are stressed throughout the course.

Many students were critical of question 3 in the examination on the grounds that it required knowledge of chemistry as well as of IT skills. Interestingly, at the end of the final year, it turned out that many students recognised that this question had highlighted for them areas of general chemistry in which they were weak. The discovery of this weakness at the end of the IT module gave them time to address it.

With these three reservations, which led to valuable exchange of views between staff and students, the students commented very favourably on both the content of the IT course and on the assessment procedures.

Students were particularly appreciative of the feedback they received on the examination paper. Students scoring below 45% (approximately 13% of the class) were given additional advice before starting to write their project report. These two methods for providing feedback allowed all students to identify weaknesses and improve their skills before they needed to apply them in the preparation of project reports at the end of the year.

The class representatives also reported that those scoring marks over 75% (approximately 16% of the class) were particularly motivated and identified IT skills as one of their significant strengths.

Feedback to the course tutor

Four members of staff were involved in the planning, teaching and examining of this course. They were able to form an impression of the students' progress by observation during the session in the computer classroom. These impressions were reinforced and enhanced by careful analysis of the strengths and weaknesses of the examination scripts. The identification of specific weaknesses (failure to use the spellchecker, problems with modelling, etc.) allowed the course tutors to improve the delivery of the course.

The teaching of IT throughout the 3 year course is reviewed at regular meetings of the four members of staff. On the basis of the evidence presented here, we are convinced that the closed book examination we have designed is a fair procedure for assessing the students' competence at the skills we wish them to learn. Furthermore, it meets the three criteria specified earlier.

The students respond positively to the examination; they see the virtue of being able to apply all appropriate aspects of IT to a particular problem and, through question 3, they are encouraged to see IT as an integral part of chemistry.

By holding the examination at the end of the third year of the course, the students receive useful feedback in time to improve their skills before they use them in preparing their final year project reports.

The tutors are able to make use of the examination scripts to identify aspects of the course which need improvement.

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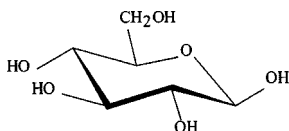
Appendix:

Sample chemistry IT examination paper

Instructions to Candidates: Candidates are required to answer all three questions. No IT manuals are allowed in the examination. Each document must be printed by the end of the examination. Each file must be saved to disk, which is collected at the end of the examination. Time: 2.00-5.00 PM

1. (i) Attached is a recent academic paper (1995 *Tetrahedron Letters* **36** 21 3745-3748) by C J Richards, D E Hibbs and M B Hursthouse. Using 12 point Times New Roman font type, 1" margins all round, 1.5 line spacing, portrait page and full justification, reproduce: (a) The reaction scheme number 2, on P.3746 forming complex 10, from reactant 7; (b) Reference 6 on P. 3748; (c) Table 1 on P.3746. For Table 1, use a List 2 type format. Centre the table horizontally and vertically on a landscape page with the same criteria as listed above. Include the title and footnote for the table. Include a bottom centre-aligned page numbering scheme in your document, starting at i etc. Save the document as Pap.doc file in Word, and print your document on single-sided A4 paper. (25 marks)

(ii) Draw the following structure in Chem-Window, and paste it into the Pap.doc Word document using the Paste Special facility. Print the structure in Word. Print a ball and stick representation of the structure in DTMM also. (15 marks)



(iii) **Either:** Type the following passage in Word, using Times New Roman 12 point font type, 1.5 line spacing, full justification, portrait page and 1" margins all-round. Give the page number as 65 (bottom, centre-aligned). Save the file as Cryst.doc. Print the document.

Crystal data for $C_{28}H_{28}FeNOP$, $M_r = 481.33$, orthorhombic, $P2_12_12_1$, $a = 9.098(4)$, $b = 10.924(3)$, $c = 23.448(8)$ Å, $V = 2330.4(14)$ Å³, $Z = 4$, $D_c = 1.372$ g cm⁻³, $\mu(MoK\alpha) = 0.737$ mm⁻¹, $F(000) = 1008$, $T = 120$ K. Intensity data were collected on a FAST area TV detector diffractometer with $MoK\alpha$ radiation ($\lambda = 0.71069$) as previously described. 10654 reflections were measured giving 3731 unique data. The structure was solved by direct methods (SHELX-S) and refined by full-matrix least squares on F_o^2 (SHELXL-93) using all

unique data. Final wR_2 (on F_o^2) and R (on F) were 0.0719 and 0.0445 for all data
or type the Schrödinger wave equation in Word:

[Object too big for pasting as inline graphic. | In-line Graphic *]*

Save the document as Wave.doc file in Word, and print your document. (15 marks)

2. Using the formulae, function wizard and graphing facilities of Excel, find $E_{act.}$, the activation energy and A , the pre-exponential factor, of the reaction $A_{2(g)} + B_{2(g)} \rightleftharpoons 2AB$, given that $R = 8.314$ J K⁻¹ mol⁻¹ and the following data:

T/K	540	642	733	792	877
$k/(Ms^{-1})$	7.36×10^{-7}	6.32×10^{-5}	2.37×10^{-3}	7.65×10^{-2}	3.19×10^{-1}

Plot the graph in Excel (save the file as Act.xls) using the following criteria:

(a) Full size portrait page; (b) No header or footer; (c) Times New Roman, 10 point for the title of the graph and 8 point for the x and y axes numbers; (d) Times New Roman, 9 point for the x and y axes titles (include units); (e) Insert a trendline for the plot (use a fine weighted thin line); (f) Use a white background for the plot area; (g) Include the correlation coefficient on the same line as the title of the graph; (h) Use bold and italics for the title of the graph, and bold for the titles of the axes; (i) Do not include a legend on the plot; (j) Ensure that all units are given, with appropriate superscripts etc. (if applicable). (30 marks)

3. Either: Use VSEPR theory to deduce the structure of the nitrate oxyanion. Print the structure in Word (save the file as *Symm.doc*), including the determination of the shape and approximate bond angle and hybridisation. List also the elements of symmetry and the point group symmetry of the oxyanion

or model the cage compound, cubane. Minimise the energy, and comment on the stereochemical aspects of the structure in terms of the contributing terms of the force field. Save the structure on disk as *Cube.mol*. Print the minimised structure in DTMM, and draw a two-dimensional representation of the structure in Chem-Window. Import and print this structure in Word, and express the minimised value in kJ mol⁻¹. (15 marks)