3. Computer Keyboard Skills

Summary

Outline of the exercise

In this exercise students participate in the production of material for a new World Wide Web-based undergraduate 'book'. They are required to include text and a variety of chemistry graphics in a specific format. A number of different scenarios are outlined in the tutor's guide including one in which the preparation of structures and brief text on four natural products, and an outline for the mechanism of the Wittig reaction, are required. The aim of the exercise is to develop the ability to use chemical drawing packages and prepare text and graphics in an effective manner and it therefore provides a useful introduction to some of the most important computer keyboard skills required by chemists. The notes assume that students have access to appropriate computing facilities.

Key aims

- to practise using standard computer drawing and word-processing packages for the production of effective visual aids

Time requirements

- 1 hour introduction (tutor contact time)
- 9 hours private study
- 10 hours total student time

Timetable

The following timetable is suggested:

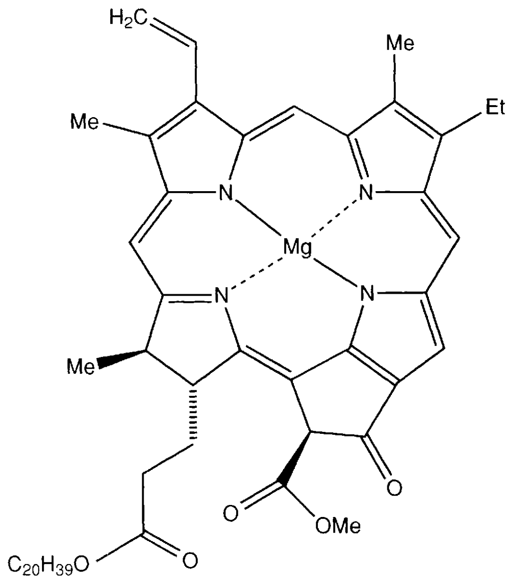
1 hour	Introduction	(possibly in small groups, in a computer room)
9 hours	Preparation	(private study)

S3 Computer keyboard skills

A publisher is putting together a new undergraduate chemistry course on the World Wide Web, and is collecting samples of possible material before commissioning the whole course. You are an undergraduate chemist – you know the types of format and style which catch your attention, and make chemistry clear to you, so you are in an ideal position to win the deal for us! In this exercise you must construct two sample pages for the new course.

1. Natural Products

Prepare one page showing four natural products. Display their structures and describe some of their chemistry and properties. An example of chlorophyll a is shown below, to illustrate the layout required:



Chlorophyll a

- A green pigment found in most plants
- One of several natural products containing a porphyrin ring (four pyrroles connected by CH groups)
- A catalyst for photosynthesis
- First total synthesis by Woodward

Prepare the following four structures:

- Cholesterol (using a 3D representation to show ring conformations)
- Strychnine
- Quinine
- Another interesting natural product, of similar complexity, of your choice.

The sample must fit on one side of A4, and must use text with added graphics (so that hyperlinks can be added for the final publication). A 'table' format can be used to achieve this.

2. Wittig Reaction

Prepare a one-page summary of the Wittig reaction of a stabilised ylid with an aldehyde, clearly explaining the stereochemistry. The sample must fit on one side of A4, and can be constructed entirely in a chemical drawing package. The summary should contain:

i) A detailed mechanism for the reaction of $Ph_3P{=}CHCO_2Et$ with Ph–CHO, showing the intermediates and stereochemistry leading to ***E***- and ***Z***-products.

ii) A verbal description of the main features of the reaction mechanism and comments on the stereoselectivity – this can be in the form of annotations of the mechanism.

iii) A diagram of the reaction profile (reaction co-ordinate versus energy), including the key intermediates in the reaction sequence, namely the betaine and the oxaphosphetane, expected for this particular Wittig reaction.

Specific formats are required for both pages. Times 12 point font should be used for most of the text, although headings can be larger. The following settings must be used within the chemical drawing package:

Drawing settings

- Chain angle 120°
- Bond spacing 12 %
- Fixed length 0.773 cm
- Bold width 0.902 cm
- Line width 0.026 cm
- Margin width 0.053 cm
- Hash spacing 0.071 cm

Text settings

Caption Text Settings
Helvetica 8 pt Normal

Label Text Settings
Helvetica 10 pt Bold
Fractional character width x

Preferences

Units cm

Tolerance 5 pixels

Remember – computers, disks and printers often go wrong at the last minute. Prepare your submissions in good time, prepare back-up copies of your work every 5 minutes, and make sure it is printed well before the deadline.

T3 Computer keyboard skills

Many students will have already received training in word-processing, and guidance on the use of a range of other computing facilities, for example email, the World Wide Web (WWW), databases and spreadsheets. The simple format of this short exercise requires them to develop several skills that will be particularly useful in other aspects of communicating chemistry including:

- confidence with a basic chemical drawing package;
- a feel for the range of chemical drawing graphics available;
- mixing text and graphics; and
- following a precise format.

A one hour session can be used to introduce students to word-processing and chemical drawing packages, although the content of the session will depend on students' previous experience and the specific hardware and software available. It is effective to carry out this session in a computer room. This exercise provides a useful introduction to some of the most important keyboard skills required by chemists.

The Exercises

Examples of two exercises concerning Natural Products and the Wittig Reaction are given in the student's guide. Model answers for these exercises are given below. These exercises are specific to organic chemistry, however similar exercises in inorganic or physical chemistry can be put together easily. For example:

a Draw the structures of four important inorganic molecules and describe some of their chemistry and properties. For example:
- Cp-Fe(CO)(PPh_3)(COMe) – what is it used for? See *Chem. Br.*, 1989, **25(3)**, 268.
- 3-(η–Cp)-3,1,2,-*closo*-$CoC_2B_9H_{11}$ – discuss its isomerisation. See *J. Am. Chem. Soc.*, 1972, **94**, 6679.
- XeF_6 – what is its shape, and why was this unexpected?
- *cis*-$PtCl_2(NH_3)_2$ – what is its medicinal use, and how does it work?

b Discuss the mechanism by which $Mn(CO)_5Me$ isomerises to $Mn(CO)_4(COMe)$. Clearly show the mechanism for the reaction, explain the key experiments that aided the elucidation of the mechanism and draw a reaction co-ordinate/energy profile diagram; also indicate why the elucidation of this mechanism was important for other organometallic processes.

c Explain four important physical chemistry terms; each explanation should include an equation and a graphic (eg 'Boltzmann distribution', 'first order kinetics', 'the Arrhenius equation', 'diatomic dissociation energy').

d Explain how a specific piece of equipment can be used to determine a key physical constant (*eg* bond length from infrared spectroscopy, second order rate constant measurements using conductivity apparatus, heat of evaporation of a compound from vapour pressure measurements).

The explanation should include a schematic drawing of the equipment, a description of the experiment, a graphical representation of the results, and how these would be interpreted.

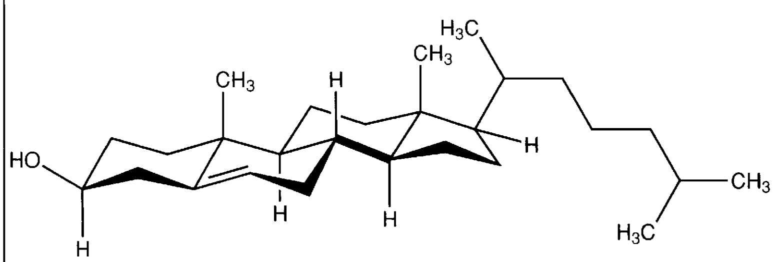
Adapting the exercise

It is easy to adapt this exercise to specific course requirements. One variant is to have a pool of about twenty natural products, and about six reactions, from which the students are randomly allocated their task. This reduces the risk of copying and adds a little more interest and individuality to the exercise.

Assessment

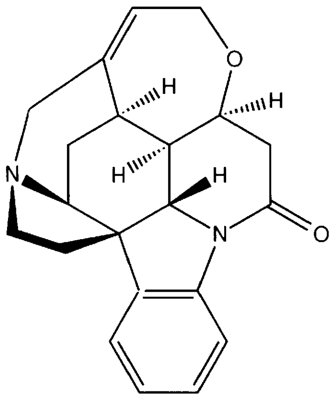
It is simple to mark the submissions with a grade (A: excellent, B: good; C: average; D: poor; E: very poor; X: unsatisfactory), and peer-assessment could easily be used.

Model Answers



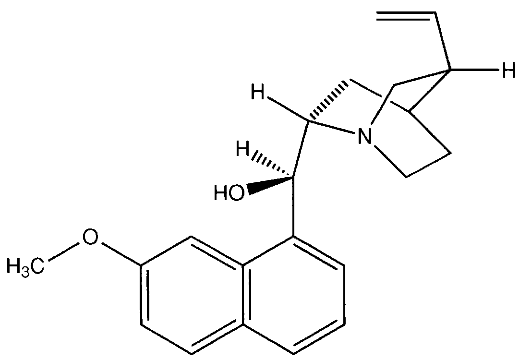
Cholesterol

- Polycyclic, hydrophobic hydrocarbon with a single hydrophilic OH group
- Constituent of cell walls
- Biosynthesised from C_5 building blocks
- Can be deposited on the walls of arteries, leading to heart disease



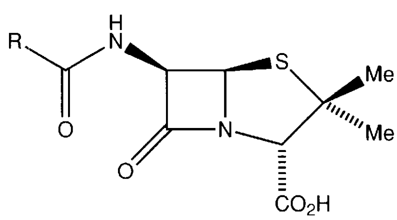
Strychnine

- Alkaloid (naturally occurring base)
- Extremely toxic
- First synthesis by Woodward, but Overman has recently completed the first enantiospecific synthesis



Quinine

- Alkaloid isolated from Cinchona tree
- Structure determined in 1908
- Used to treat malaria
- First synthesis by Woodward in 1944

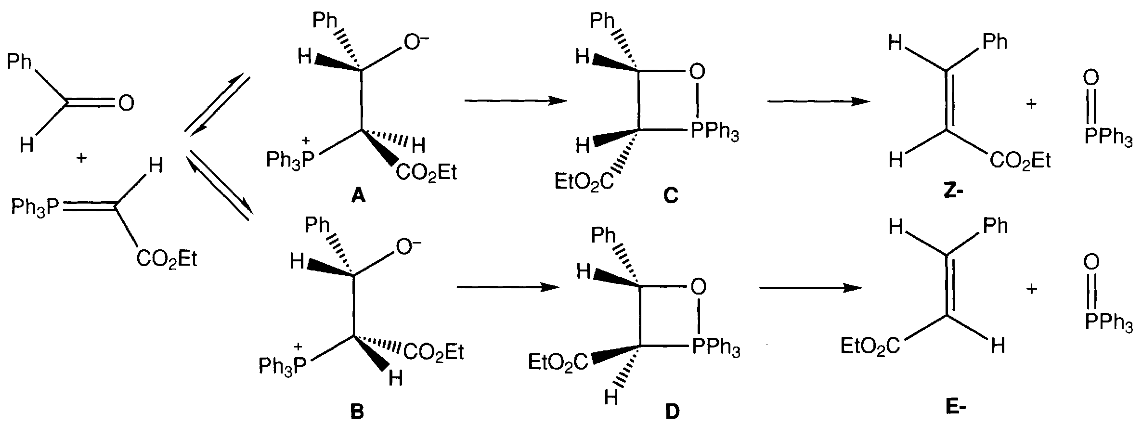


Pencillin G: R = CH_2Ph

Penicillin G

- The penicillins are fungal antibiotics
- They all contain the strained 4-membered β-lactam ring, and an additional 5-membered N/S ring
- They work by inhibiting a key enzyme involved in the construction of bacterial cell walls
- Penicillins with various R groups are used medicinally, of which penicillin G (R = CH_2Ph) has been used extensively.

The Wittig reaction between benzaldehyde and the phosphorus ylid of ethyl bromoethanoate



1. Initial attack of the ylid on the C=O is as shown, forming **A** (Ph_3P and O *anti*, and Ph and CO_2Et *anti*.).

2. But the first step is reversible, so the betaines **A** and **B** can both be formed.

3. The betaines are converted into the oxaphosphetanes **C** and **D**. **D** forms much faster.

4. Intermediate **D** rapidly collapses to *E*-alkene, and the initial equilibria allow almost all of the reaction to proceed *via* **B** and **D**.

The following diagram illustrates the energy versus reaction co-ordinate profiles for the two reaction pathways.