Tools for teaching molecular spectroscopy

M. Dalibart

LPCM, UMR 5803, Université BORDEAUX I, France

Abstract

From our experience in teaching molecular spectroscopy it appeared that specific teaching tools could be useful. We describe here self-training packages, instrument simulators and tools for classroom demonstration developed for this purpose and report on their usefulness for teaching various target groups: university students, chemical school engineers, and technicians during part time courses.

Keywords: self-training, self-assessment, e-learning, FTIR, UV, Raman, luminescence, optical spectroscopy, spectrometer simulator, classroom demonstration.

1 Introduction

Teaching spectroscopy means teaching several disciplines at the same time: chemistry, optics, classical mechanics, quantum mechanic, electronics and data processing. Many students have gathered some basic knowledge in these fields during their studies; it is nevertheless always difficult and time consuming to refresh memories. From our experience in teaching molecular spectroscopy to audiences such as university students at various levels, technicians, and engineers, it appeared that specific teaching tools might be useful for this purpose. They would be particularly useful for the in-house crash or part time courses nowadays often in demand. For this purpose, we have been working on self-training programs, spectrometer simulators and classroom demonstration software. Descriptions of these tools and reports on their introduction through teaching practices are presented in this paper.
2 Description

2.1 Self-training software

The first self-training software was already written in the eighties, at the very beginning of FTIR spectroscopy. This was partly motivated by the fact that at that time FTIR spectrometers were too expensive for our teaching laboratory. However, we had received a donation of small personal computers (4 K memory, two 80 K floppies), the French "Goupil 3". Using BASIC and machine language, chaining programs and using one floppy as common memory, we were able to illustrate the concepts on which FTIR is based, i.e. Fourier transformation, resolution, sampling, aliasing, etc. This software was subsequently distributed by Bomem and Mattson, two FTIR manufacturers. A few years later, a special issue was made available under the European Program "COMETT II" Dalibart [1].

Today, we make available more elaborate software Dalibart [2] which allows self-teaching in Fourier transform infrared spectroscopy (ISIR), photoluminescence spectroscopies (ISPL) and Raman scattering (ISR). Modules covering ultraviolet absorption are presently under development. In the near future, all molecular spectroscopy techniques will thus be covered. Besides molecular spectroscopy, a special package (IC) devoted to colour and colorimetry was also written. The packages are distributed by WinLab [3]. A demonstration package can be downloaded [4].

Figure 1: A screen capture from ISIR.

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Each package includes modules for theory, instrumentation, and practice. Theory obviously includes some amount of revisited classical and quantum theory. The instrumentation part introduces interference, gratings, monochromators, the Michelson interferometer and also spectral sources, detectors and optical fibers. A large section is devoted to data treatment, introducing sampling, subtraction and specific spectral corrections. Numerous sampling methods for liquids, solids and gases are described. For example, in ISIR, we start from a simple KBr pellet, moving to more advanced methods like attenuated total reflectance, specular reflectance and diffuse reflectance. Reflectance theory, accessories and specific data treatments are included (see figure 1), chromatography and microscopy coupling are not forgotten.

More practical aspects such as spectral interpretation, spectral searching, and modern quantitative analysis are also covered extensively. Various databases dealing e.g. with instrument manufacturers, accessories dealers, optical properties of materials, and solvents are also supplied. Numerous web links are available through a mouse click.

![Figure 2: Self-assessment in action.](image)

Each chapter contains lessons and a tutorial for experiments. A self-assessment is proposed to check the advancement of learning and the correct answers can be consulted (see figure 2). Being an e-book, the software makes use of navigation tools such as search functions, glossary and bookmarks. Thus, using these interfaces the user can access the desired topic instantly. Help is available through an email interface. In order to allow an easier understanding of this encyclopaedic content, numerous figures, applets and movies are used.
showing e.g. black body curves, vibrational modes of molecules and instruments in action. Two levels (a basic level and an advanced one) are available and the user can readily choose his own curriculum.

The ISIR and ISPL software was first used as a didactic support in classroom teaching. These packages have proven to be very efficient tools for teaching students. Tedious concepts such as Fourier transform or convolution product are easily illustrated. Movies showing vibrational modes of molecules such as acetone, nitromethane or benzene are more efficient that a descriptive text! Furthermore, this allows students to practice open lectures and to focus easily on specific problems.

Students at the Engineering School of Chemistry and Physics of Bordeaux (ENSCPB) are evaluated in spectroscopy on the basis a short oral presentation. Typical topics are e.g. ATR, diffuse reflectance, FFT, IR sampling methods, 3D fluorescence spectra, synchronous scanning etc. They can be easily researched by the student with the help of the software. It is true that on several topics a web search could yield similar results, but for a beginner it is quite time consuming to find the perfect query giving related links and only relevant links, not to mention language problems. ISIR and ISPL were also available in the spectroscopy teaching laboratory and some instructive projects have been elaborated using this software.

During in-house courses, technicians have been successfully instructed on molecular vibrations and Fourier transform. However, such people are often afraid to of the self-learning approach due to the encyclopaedic contents and want more guidance. Thus, we have undertaken to develop a new line of basic packages dedicated to applied spectroscopy for in-house use. A first version dealing with near-infrared and chemometry applied to quality control is under development. After a brief introduction to mid-infrared and near-infrared spectroscopies the specific instrumentation is presented. A third step is devoted to PLS data processing through chemometry: clustering and prediction.

The future of new learning leads to e-learning. Of course, updating and helping will be easier on-line, but at the present time, limited range web colours and access time required for such large movies are limiting this approach.

2.2 Spectrometer simulator

Nowadays a relatively cheap computer can be turned into another powerful tool: a spectrometer simulator. A tedious and time-consuming training is always necessary to acquire experimental skill. This is particularly true in the case of luminescence and Raman scattering since numerous artifacts are possible and the number of parameters to be optimized is very large. In this view, a spectrofluorimeter simulator Dalibart and Belin [5] appears to be a valuable tool to render this training easier and faster. After choosing a set of experimental parameters, the computer displays immediately the corresponding spectrum. The influence of all experimental parameters is simulated: monochromator slit width, excitation or emission wavelengths, xenon source type, photomultiplier tube high-voltage, etc. The nature of solvents with first and second orders Rayleigh and Raman scattering is taken into account. Sample geometries and
concentrations with corresponding inner filter are also simulated. Obviously, there is no risk of damaging the virtual photomultiplier tube! Figure 3 exhibits a screen capture from this simulator.

Figure 3: Using the spectrofluorimeter simulator.

2.3 Classroom demonstration

Computers are essential for modern spectroscopy. Unfortunately, experimental skills disappear concomitantly and the instrument appears as a black box. In order to demystify the instrumental layout, our last development is a software dedicated to low cost "Ocean Optics optical fiber spectrometers", allowing classroom demonstrations. Using a notebook, an usb spectrometer, a diode-laser, a linear variable filter, a halogen-deuterium source, some optical fibers, and a cell holder it is easy to build "real life" typical instruments and then to demonstrate how they work. Besides the spectrum window, the video frames coming from an usb webcam are displayed on the screen.

Figure 4 shows an ultraviolet-visible absorption spectrometer in action. Introducing a band filter and moving the collecting fiber to the 90° port leads to a spectrofluorimeter as shown in figure 5.
Figure 4: Manufacturing the UV spectrometer.

Figure 5: Demonstrating fluorescence.
Finally, a Raman spectrometer can be manufactured if a (rather expensive) green (532 nm) solid laser or an ionised argon laser (514 nm) is available (see figure 6).

### 3 Conclusion

At the University of Bordeaux and at the Engineering School of Chemistry and Physics of Bordeaux (ENSCPB) we have introduced some didactic tools for spectroscopy in our teaching practices. These packages have proven to be efficient tools for teaching students in traditional classroom teaching and open lectures. Specific tools are currently developed for in-house course. Spectrometer simulators are efficient for acquiring experimental skill and may save money.

### References

[3] WinLab Instruments, 33 Avenue Gambetta, F-93170 Bagnolet, France,
