Computing in Spectroscopy: Discussion Meeting at EUCMOS XXIV in Prague—27 August 1998

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During the recent European Congress on Molecular Structure in Prague, Czech Republic, one afternoon session was devoted to spectroscopic computing. The round-table discussion meeting followed an introductory plenary lecture. The meeting took the form of a review of the current status, an assessment of the future needs and a short question and answer session with the panel of experts. The answers given to the current status of spectroscopic computing provide an interesting snapshot of life in a spectroscopic laboratory at the end of the twentieth century. Unfortunately many of the comments from the participants show that we are still a long way from satisfying the needs of the spectroscopist.

Current status

Hardware

In an attempt to discover what was the level of spectroscopic computing amongst the participants at the discussion meeting, a show of hands was used to answer basic questions about computing use.

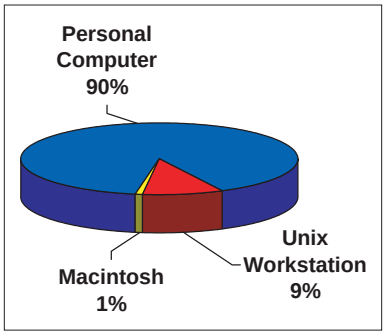

Figure 1. Distribution of computer hardware in use amongst the participants at the discussion meeting.

Figure 1 shows that dominance of the personal computer has inevitably also reached the spectroscopic computing workplace.

The figures have been normalised to give a percentage based on total usage amongst those voting. Quite often a single participant would vote for more than one answer.

Operating systems

Figure 2 shows a breakdown of the operating systems in use amongst the 150 or so participants at the discussion meeting.

This figure is more interesting showing a disproportionately large percentage of OS2 users compared to the normal population. This can clearly be attributed to the use of OS2 by a well-known spectrometer manufacturer as the main PC operating system for their spectrometer control computers. It will be interesting to see—now that this manufacturer has switched to Windows NT4—if this anomaly disappears in the near future. It is also interesting to see a surprisingly large percentage of Windows'98 users considering that the operating system has only recently been released. Unfortunately the question was not asked as to whether this was in use as an upgrade or had been pre-installed on a newly purchased computer.

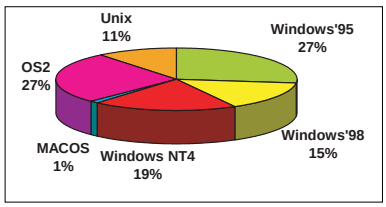

Figure 2. Distribution of operating systems in use by the participants at the discussion meeting.

Software/spectroscopic software

The third question as to the software currently employed by the participants produced an enormous and very broad based response. Figure 3 shows most of the packages mentioned.

Spectrometer control software was deliberately left off this list although later comments [saved up until after the discussion meeting had finished(!)] showed that this software is often employed off-spectrometer at the scientists' desk to continue data analysis

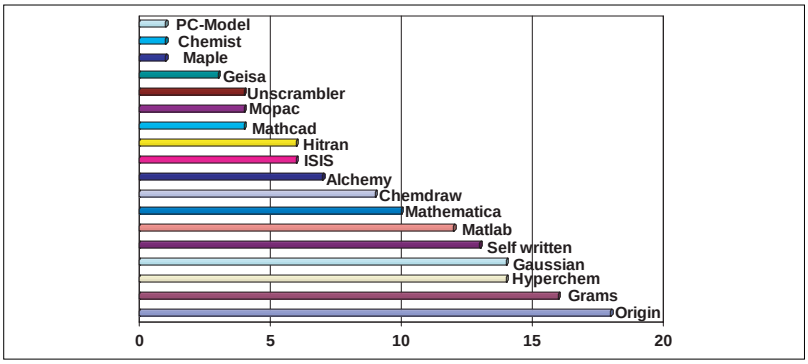

Figure 3. Various software products were in use amongst the participants. Software used primarily for spectrometer control was deliberately left off this list.

and so should really have been included when used in that role.

It is also clear to see from the list of packages that the European Congress on Molecular Spectroscopy XXIV was heavily dominated by theoretical scientists. Apart from a number of general scientific programs there are only a few examples of packages used specifically by analytical spectroscopists.

Future needs

Changes planned?

To start off the debate on future needs the question was asked as to whether or not any changes were planned to the status recorded at the start of the meeting. Although the general feeling of the meeting was that changes were due—there seemed a lack of a specific strategic direction as if changes would of course take place but somewhat out of control of the participants. Whether this was due to participants feeling as if their purchasing policy in this area was left to the whim of spectrometer and operating system manufacturers was not clear. What did come out of the discussions was a definite lack of identification with particular software products.

Advice needed?

Surprisingly—or maybe not so surprisingly—nobody felt the need to ask in public for the advice of the expert panel on any aspects of the subjects covered. Although after the meeting several requests for information were received.

What do we lack?

During the plenary lecture introducing this session much was made of the greatly improved interoperability of software systems used by spectroscopists, either in the spectroscopic laboratory or on the desktop. The lecture discussed the use of standard formats, Chemical MIME, the use of the Java programming language for internet/intranet applications and also the extended implementation amongst spectrometer manufacturers and third-party software houses of each others data formats.

Despite all this apparent progress the main complaint amongst the participants was a lack of interoperability between their software packages!

Furthermore the failure of the international spectroscopic community as a whole and the various standards bodies in particular to come up with intensity standards in various wavelength ranges was strongly criticised. This complaint will now be brought up with different bodies in the hope of starting some action in this direction.

Another area of worry has evolved out of the increased implementation of chemometric software in normal spectrometer control packages. This can be seen as an excellent development with powerful tools once reserved for the mathematician becoming available to everyone—but the drawback seems to be a lack of in-built intelligent warnings about over-modelling of data. It is quite possible to set up calibration models which give superb standard errors of prediction, way beyond what is realistic for the data involved. A.M.C. Davies has written substantially in this column about the dangers inherent in such over-modelling and I can only appeal to spectroscopists starting down the chemometrics path to heed his warnings and always validate against completely independent data that was not used in any way in the calibration step!

The point should be made that no independent software house producing spectroscopic (or chemical) software—of many invited—accepted the invitation of the organisers to participate in EUCMOS XXIV and this discussion. It is hoped that this will change in the future.

Finally, the meeting wished for better teaching software and it was observed that the Coblentz Society is heavily involved in running short courses of this nature.

Conclusion

The discussion meeting continued through the planned coffee break and threatened the ensuing poster session before it was wound up. This is unfortunately a sign that we have much to do before spectroscopists can be truly happy with their software tools.

Thanks are due to Professors Mantsch, Iwata, Nafie and Dr Heise as well as the staff of EUCMOS XXIV for providing the expert panel and technical support during the meeting.