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European Crystallographic Meeting ECM20 Kraków, Poland - Meeting Report

25th-31st August 2001

CCDC Poster Prize winners at ECM20

The CCDC poster prizewinners at ECM20 were:

L. Dobrzycki (Warsaw University, Poland).

Structure of YAG crystals substituted with Erbium and Ytterbium.

G. Paliwoda (Jagiellonian University, Krakow).

Mutual recognition between diastereoisomers, quinine and quinidine, in the solid state.

M.U. Schmidt (Clariant GmbH)
Ternary mixed crystal

$C_{22}H_{12}C_{12}N_6O_4/C_{23}H_{14}C_{12}N_6O_4/C_{24}H_{16}C_{12}N_6O_4$
Structure solved by crystal structure predictions and X-ray powder diffraction

The Prizes - an amethyst geode and \$250 to each winner - were presented by CCDC Scientific Director, Dr Frank Allen, at the Closing Ceremony on 31 August 2001.



CCDC Prize presentation to L. Dobrzycki (Warsaw University, Poland)

The CCDC Prize Committee comprised:

Gautam R. Desiraju
(Hyderabad, India)

Robert O. Gould
(Edinburgh, Scotland)

Mariusz Jaskolski
(Poznan, Poland and ECA Executive Committee)

Paul T. Beurskens
(Nijmegen, The Netherlands and ECA Executive Committee).

Computing and Teaching Microsymposia at ECM

The ancient Jagiellonian University (founded in 1364) of the splendid architectural city of Kraków, was the host of one of the contrasting final morning Microsymposia on the contemporary topic of Computing and Teaching. Six speakers delighted the audience with a wide range of topics on using the Internet for distance learning, virtual courses in crystallography and a number of different models for delivery of the curriculum. Some key issues regarding the pace of introducing the new technologies, the role of government in delivering mass education and the pressures on institutions in responding to the novel methods of education were raised during the talks.

Y. Epelboin (CNRS, Paris) [1] in the opening address asked, "What can we learn from actual experience?" and compared the US experience with the European paradigm. He projected that the world education market [2] by 2005 would be worth an

estimated 90 billion US dollars. Distance learning would open up the accessibility to virtual documents and libraries facilitating politicians to contain the budget for education. However, the case was argued that the rich diverse tapestry of language and traditions that is European culture could not so easily be swayed by an economic model. Co-operation via Brussels would ensure that the "Revolution would go marching on..." was the idiosyncratic Gallic rally.

At the heart of G. Chapuis' talk (Lausanne, Switzerland) was the "nuts and bolts" of implementing interactive web applications of Java applets to provide simulation of some key crystallographic concepts. He listed the ingredients for a virtual course in crystallography concentrating on the tools for simulation and provided a number of real time demonstrations of the Ewald sphere, Laue pattern diagrams and Fourier transforms. The didactic road is long to a complete course on the Internet although within a Java environment using a web browser simulations can be performed, directly independent of the computer platform being used. This time the baton was passed on to the IUCr to promote and establish structured learning modules for potential crystallography students. C. Sansom (Birkbeck, London) described at length the Masters level distance learning courses in Structural Biology offered by Birkbeck College since 1996. She gave an overview profile of the

average student taking the course as mature with demanding professional careers quipping "that there were no typical students". The communication links between students and teachers were maintained using a purpose built Internet chat room or MUD for short (multi-user Dimension). Much of the material is written in simple HTML which can be run on a low specification computer, course material being made available at regular intervals throughout the year. It was stressed that fees were kept low to encourage wide student participation in the Advanced certificate on the Principles of Protein Structure (PPS) [4].

The first of two talks on powder diffraction commenced with A. Le Bail (Université du Maine, France) who challenged the audience to think "Where is all the knowledge." and reminded us that distance learning was in its centenary. The dangers of online education are well-established [5] with the automation of Higher Education likened to creating "Digital diploma mills" as the pervasive new information technologies advance. The provision of a powder diffraction course was inspired by the Birkbeck model and the speaker emphasised the deliberation in choosing between a synchronous and asynchronous mode of learning. The course material with pedagogic exercises is available on Structure Determination by Powder Diffractometry (SDPD) [6] and can be viewed on the web. Caution was advised that expert systems could kill the interest of deep

learning and that an explosion of software diversity could pose a nightmare for student and teacher alike. An anachronistic talk on Crystallographic Autostereograms was given by A. Katrusiak (Poznan, Poland) using handouts for the audience to practice on. The speaker presented a clear reminder of the optics of the eye and its ability to perceive perspective by binocular vision. An interesting talk that prompted a member of the audience, R. Shirley (Surrey, England), to remark that confusion over the term stereogram could be avoided if it referred only to that normally used in stereographic projection.

Returning to the topic of powder diffraction on the Internet J. Cockcroft (Birkbeck, London) stressed again the need for life-long learning and the proud tradition that Birkbeck has maintained in teaching during its 178-year history. The compatibility of the Powder Diffraction on the Web course [7] with both Netscape and Internet Explorer 3 was mentioned as well as being Java/Java script free. As it is easy "to get lost in hyperspace" the material makes extensive use of course navigation buttons on the web pages. With such an undertaking a priori knowledge cannot be assumed, but full use of colour is made in pictures and photographs contained in the HTML documents. Awareness of copyright is also an issue. The material itself is organised into three areas; experimental methods covering basic crystallography, diffraction and symmetry, data analysis covering

both quantitative & qualitative aspects and a project on Rietveld refinement. On the topic of programming options it was revealed that the space group diagrams used in the course were written in Fortran code, a spin off being a commercially available CD-ROM. The debate over interactive versus downloadable software was touched upon again. Finally the matter of assignments was mooted and their role in good housekeeping recorded. They act as an aid to learning, are complementary to the course material and provide model answers and feedback to the students in their distance learning environment away from the more traditional face to face approach that is being challenged more and more in the 21st Century.

References

- [1] <http://www.lmcp.jussieu.fr/~epelboin>
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- [4] <http://www.cryst.bbk.ac.uk/pps/index.html>
- [5] Noble D. - <http://communication.ucsd.edu/dl>
- [6] <http://sdpd.univ-lemans.fr/course/index.html>
- [7] <http://pd.cryst.bbk.ac.uk/pd/welcome.htm>

Bursary Report

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