

CRYSTALLOGRAPHY NEWS

British Crystallographic Association

No.84 March 2003

BCA Spring Meeting - York 2003
Software patents and Crystallography
CCP4 Meeting and BSG School



Charging for Crystallography Services
Synchrotron Radiation School
Book Reviews

QUARTERLY



HTC technology for the rapid identification of novel drug candidates, reported the successful collection and subsequent analysis and interpretation of 53 data sets in 3.5 days in a home laboratory using ACTOR and other instrumentation from Rigaku/MSC. Dr. Andrew J. Sharff of Astex said, "Based on a standard working day/week, this represents an increase in throughput of over 3 fold, compared to manual data collection."

Since its inception in Japan in 1923, Rigaku Corporation has been at the forefront of analytical and industrial instrumentation technology. With hundreds of major innovations to its credit, Rigaku and its subsidiary companies are world leaders in the fields of x-ray spectrometry, diffraction, x-ray optics, as well as small molecule and protein crystallography. Rigaku employs over 800 people in the manufacture and support of its analytical equipment. Its products are in use in more than 70 countries - supporting research, development, and quality assurance activities. Through its U.S. subsidiary, Rigaku/MSC, it continuously promotes partnerships, dialog, and innovation within the global scientific and industrial community.

Paul Swepstun

Workshop on Magnetic Rietveld Refinement

So what were the hottest tickets in town over the Christmas 2002 holiday period? Ronan Keating live at Wembley? Frank Bruno's triumphant return with Sooty in "Goldilocks and the Three Bears" at the Southend Pavilion? Jerry Springer the Opera? No, despite stiff competition, the award has to go to the "Magnetic Rietveld Refinement Workshop" organised by Paolo Radaelli and co-sponsored by RAL/IOP/PCG, whose 25 places were snapped up within 24 hours of the course being announced.

The lucky delegates gathered at Cosener's house on the 12th of December for what was advertised as an intensive 2 day course on the theory and practice of magnetic structure determination. Day one was taken up with a mixture of lectures on the Shubnikov groups for describing magnetic symmetry by Paolo Radaelli (RAL) and the theory of magnetic structures, their description and determination by Juan Rodriguez-Carvajal (LLB). These lectures were then backed up by an evening practical session determining the possible magnetic symmetries allowed for simple perovskite structures. On day two, these approaches were generalised by Andrew Wills (UCL) who gave a series of lectures on the application of group theory to understanding magnetic structures. This more general approach both reinforced and complemented the first day's work on Shubnikov groups. The rest of day two was taken up with

a series of demonstrations and practical classes involving some of the main software packages required for magnetic structure determination: GSAS, SARAH (AW) and Fullprof (JRC). Hearing about the second two packages directly from their authors was particularly informative.

Following an excellent Christmas dinner the true meaning of the "intensive" nature of the course was brought home to everybody, with post-dinner "games" including "Flip the Spin", "Prime the Symmetry Operator" and "Reduce the Representation". It was clear from the number of participants (and tutors) still working away at magnetic refinements at midnight, that people were enjoying the course greatly.

The final morning was taken up with computer-based exercises giving people the opportunity to tackle both test examples and real data they had brought along. This was a rare and valuable opportunity to learn directly from the experts about an area of condensed matter science that is topical, important, and perhaps poorly understood by many. The fight for places on the course and the wide variety of nationalities represented (attendees came from, *inter alia*, the UK, Spain, Finland, Sweden, Japan, Greece, France, Germany) clearly showed the huge demand for a forum such as this. We can only hope that Paolo, Andrew and Juan can be persuaded to make this the first in a regular series of workshops.

John Evans