

Report of the NATIONAL WORKSHOP ON CRYSTAL STRUCTURE DETERMINATION USING POWDER XRD organized by the KHWARZIMIC SCIENCE SOCIETY, 15 – 17 August, 2007

KHWARZIMIC SCIENCE SOCIETY, PUNJAB UNIVERSITY REPORTING

<http://www.khwarzimid.org>

The Khwarzimid Science Society (KSS), Lahore (Pakistan) organized a three-day National Workshop on Crystal Structure Determination using Powder X-ray Diffraction (XRD). This workshop dealt with various aspects of determining crystal structures and touched upon symmetry, crystal lattices and structures, Fourier description of diffraction, peak indexing, determining unit cell shapes and sizes and atomic positions, crystal structure refinement and peak profile analysis.

The workshop was inaugurated at the Institute of Biochemistry and Biotechnology, Punjab University. The opening lecture was given by Dr. N. M. Butt, Chairman Pakistan Science Foundation on “diffraction studies of nanostructures”. The President of the Khwarzimid Science Society and Chair of the Advisory and Organizing Committees, Dr. Saadat Anwar Siddiqi then presented an overview of the KSS, coinciding with the tenth anniversary of the Society. He recounted the hundred and fifty events organized by the Society and recapped the Society’s major strengths. He also remarked that with very meager resources, the Society has been able to maintain an unmatched track record of scientific events of very high quality and caliber. More than 95 percent of the events are open and free for all, focusing on students and specialists alike. Events feature workshops, seminars, symposiums, scientific publication, public meetings, exhibitions and patronage of student science projects.

The Chief Guest for the opening session, Dr. Jamil Anwar, Dean of Sciences, the Punjab University praised the efforts of the KSS and its team in organizing the Workshop and maintaining an illustrious record of uplifting the popular science culture in the Punjab University in particular, and the educational institutions of Lahore, in general.

The Workshop was hosted with the collaboration of the Centre for Solid State Physics, Punjab University and the financial support of Bana International and Bruker-AXS, Germany. The latter also invited Dr. Menges Goetz, one of our leading speakers, who traveled all the way from Germany for the workshop.

The first day of the workshop covered the basics of crystallography including symmetry, point and space groups, crystal lattices and the seven crystal systems. Special emphasis was laid on crystallographic notation and the seasoned speakers, especially Dr. Saadat Anwar Siddiqi (Professor Centre for Solid State Physics, Punjab University, Lahore), carefully addressed the myriad problems students routinely faced while trying to understand crystal systems. He was very clear in marking the difference between lattices and structures, and explained Miller indices, planes, directions and fractional coordinates. An exercise worksheet was also handed out to the students.

The second day dealt with diffraction and crystal structure determination. It featured marathon lectures by Dr. Falak Sher (Pakistan Institute of Engineering and Allied Sciences) who very methodically covered peak indexing, space group determination using systematic absences and the phase problem. His lectures were remarkably clear, excellently organized and presented and he never lost attention from the students. Dr. Sabieh Anwar (School of Science and Engineering, LUMS, Lahore) carefully covered the physical basis of diffraction focusing on the duality between the real and reciprocal spaces, the Fourier and the convolution connections to crystal structure determination.

On the third and final day of the workshop, Dr. Falak Sher wrapped up his discussion with the Rietveld method of refining trial crystal structures. He then took, as a case example of computer-based refinement methods, the freely available programme, GSAS. He went through the working of the application with real examples. Finally the students were allowed to practice on the computers under the careful instruction of the Dr. Sher. On the same day, Dr. Menges Goetz from Bruker-AXS, Germany very succinctly described the instrumental, sample and background contributions to peak profiles. He then went on to elaborate the “fundamental parameters” approach to analyzing peak profiles and its role in refining crystal structures.

The event was made even more versatile and colourful by the introduction of topics of allied interest, interspersed over the three days of the workshop. Dr. Arshad Bhatti (COMSATS Institute of Information Technology, Islamabad) was invited to lecture on “microscopic characterization of nanostructures” and Dr. Umair Manzoor from the same University was invited to speak on “Electron microscopy and electron diffraction”. Various references were also given to neutron diffraction and synchrotron radiation throughout the lectures, adding all the more to the utility of the workshops.

The concluding session was presided by Dr. Ijaz M. Ghauri, General Secretary of the KSS and the Director of the CASP (Centre for Advanced Studies in Physics), Government College University, Lahore. Dr. Jamil Khan (Gomal University, D.I. Khan) and Rizwan Adeel (PCSIR, Lahore) also offered their valuable thoughts on the organization of the workshop and lauded the efforts of the KSS – especially its role of filling in a very deep-trenched vacuum in the dissemination of scientific knowledge, and that too with selfless dedication and without monetary benefits.

The National workshop has been rated as an overall success, especially looking at the feedback forms retrieved from the participants towards the end of the workshop. More than a hundred individuals applied from around Pakistan and about fifty were selected. These were either users of XRD equipment, crystallographers or science students who were interested in learning about crystal structures. There were also a few HEC Ph.D. scholars who were proceeding abroad to undertake research in the same subject. The attendees represented three provinces of the country and came from, for example:

Sindh University (Jamshoro), Karachi University, U.E.T. Lahore, the Punjab University (School of Biological Sciences, Physics and Chemistry Departments, Centre of Excellence in Molecular Biology, Centre for Solid State Physics), Bahauddin Zakarriya University (Multan), PIEAS, Quaid-e-Azam University, Islamia University Bahawalpur, Government College of Technology (Bahawalpur), Dyal Singh College Lahore, PCSIR Labs Lahore, Pakistan Atomic Energy Commission, University of Peshawar, University of Agriculture (Faisalabad), NIBGE (Faisalabad), COMSATS(Islamabad), Vienna University (Austria).

The participants came from a carefully selected mix of backgrounds: physics, chemistry, biology, soil and environmental sciences, materials science, agriculture, engineering and geology – another proof to the KSS's strongly inter-disciplinary appeal. More details of the events, lecture notes and photographs can be accessed from <http://www.khwarzimidc.org>.



Group photo of the participants.



Dr. Menges Goetz (Bruker), Dr. Nazma Ikram (CSSP, PU), Dr. Ijaz M. Ghauri (CASP, GCU), Dr. Saadat A. Siddiqi (CSSP, PU), Dr. Falak Sher (PIEAS) and Dr. Jamil Khan (Gomal University, D.I. Khan).



Dr. N.M. Butt (Chairman Pakistan Science Foundation) in his inaugural address.



Dr. Falak Sher, lead speaker, describing the diffraction from body-centred iron.



A section from the participants during a lecture.