

## GI-MS46-O2

### The Role of CCP4 in Macromolecular crystallography

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I will discuss the role of CCP4 (UK Collaborative Computing Project 4) in the rapid expansion of structural biology laboratories in Britain and Europe during the 1980s. CCP4 helped provide state of the art software free of charge to the academic community. Developers agreed to follow a common style of organisation, and to use common formats and libraries. In exchange the project organisers provided support with maintenance and distribution. CCP4 also stimulated education in the new techniques by an annual meeting, and by organising workshops..

References:

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[1] Winn M. D. et al. (2011). *Acta Cryst. D*, 67, 235-242. doi: 10.1107/S0907444910045749

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**Keywords:** Software development, international collaborations, education

## GI-MS46-O3

### Notes on the development of crystallography in Germany with special respect to the use of neutrons

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The crystallography in Germany is based on two major roots: Out of the field of Mineralogy, research activities at German universities started already in the 18<sup>th</sup> century which lead i.e. 1877 to the foundation of the “Zeitschrift für Kristallographie und Mineralogie” by P. Groth. This journal played a major role for the publication of important crystallographic results from international authors and still exists since 2010 under the title “Zeitschrift für Kristallographie – Crystalline Materials”. Out of the field of Physics came essential contributions to the development of X-ray crystallography by German scientists: From the discovery of X-rays by W. C. Röntgen (Noble Price in Physics 1901) and the discovery of the diffraction of X-rays by crystals by M. v. Laue (Noble Price in Physics 1914) to the dynamical theory of X-ray diffraction by P. P. Ewald (Habilitation 1917).

A milestone for the practice of crystal structure determination was the publication of the first series of International Tables with the title “Internationale Tabellen zur Bestimmung von Kristallstrukturen” which were edited 1935 by C. Hermann (former Assistant of P. P. Ewald) together with W. H. Bragg (Noble Price in Physics 1915) and M. v. Laue. The IUCr (founded 1948) started a second series of “International Tables for X-ray Crystallography” 1952 and a third enlarged series of “International Tables for Crystallography” from 1983 on. In the 1960<sup>th</sup> many new crystallographic chairs were created at German Universities and research groups were established in the fields of mineralogy, physics, chemistry, biology and materials science. Crystallographic scientists were always interested to improve their experimental methods and, hence, made considerable contributions to the development of large facilities for the research using synchrotron and neutron radiation. Large facilities in Germany and with German participation (access for international users):

- Synchrotron radiation with instruments for crystallographic research: PETRA III at DESY, Hamburg; BESSY II at HZB, Berlin; ESRF, Grenoble.
- Neutron radiation with instruments for crystallographic research: FRM II at the Research Neutron Source Heinz Maier-Leibnitz, Garching; BER II at HZB, Berlin; ILL, Grenoble.

At the RWTH Aachen University a laboratory of crystallography (Institut für Kristallographie) was established 1963 with the appointment of Prof. Theo Hahn. His enthusiasm for the symmetry concept of crystallography made him an ideal editor of the third series of the “International Tables for Crystallography” (Vol. A) – 1972-2009. Research topics of the Institut für Kristallographie:

- Crystal structure analysis and crystal chemistry
- Crystal physics (structure – properties relation) and crystal growth
- Methodical development of neutron instrumentation.

Actually, the Institut für Kristallographie is operating two single crystal neutron diffractometers at the hot source of the FRM II:

- HEiDi, crystal structure analysis with short wave lengths
- POLI, investigation of complex magnetic structures using polarized neutrons.

In the last years, many crystallographic laboratories and chairs disappeared at German universities. As a result a reduction of the level of crystallographic knowledge and competence on the side of theory as well as on the application of methods is becoming clearly visible.

**Keywords:** Crystallography, Germany, Neutrons, History

## GI-MS46-O4

### Crystallography in Turkey

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The first research laboratory in Turkey was established in the 1950s by the Swedish physicist Prof. Dr. Harald PERLITZ as 'X-ray Crystallography Laboratory at Ankara University. In the mid 1960's started the X-ray crystallography studies, which used photographic single crystal data collection techniques. In 1970 a new laboratory for structural research was established at Hacettepe University in Ankara. The purchase of a CAD-4 diffractometer in 1992 attracted young scientists to do graduate work in X-ray crystallography. In 1999 a rotating anode X-ray generator was put in operation in the same department. After the purchase of Rigaku XRPD, in 2009 SWAXS system was established and nanostructure studies using HECUS SWAXS system have began.

Hacettepe University Crystallography Laboratory has become the leading centre of X-ray crystallography in the country.

Today from east (Dicle University in Diyarbakır) to west (Dokuz Eylül University DEU in İzmir) of Turkey many universities were equipped to several X-ray systems. In these laboratories Computational chemistry, particularly topological analyses of electron density-QTAIM studies, molecular spectroscopy etc.; Data mining studies on Cambridge Structural Database (CSD); Protein Purification and Structural Characterization studies ; Energetic materials; Semicrystalline Hydrogels; Structure solution studies on powder crystals; production, research and development studies of the nanostructured materials which can show interesting biophysical, physicochemical and physical ( magnetic, electric and mechanic ) properties were performed.

After these developments, in February 2001 TCA (Turkish Crystallographic Association) was founded and in August 2001, The European Crystallographic Association welcomed the Turkish Crystallographic Association as a new member . After that TCA has been accepted 53rd member by the IUCr in 2014 Canada Meeting.

The 25th European Crystallographic Meeting was organized in İstanbul in 2009. 880 delegates and 70 exhibitors were attended to the Meeting.

In the frame of IYCr2014 International Crystallography Year Activities, The Open Labs. organized in collaboration with UNESCO and IUCr and TCA were held in DEU, İzmir (2014) and Bilkent U., Ankara (2015). TCA organized a Course on Powder Diffraction for MS and PhD students. The course was held at the Hacettepe University. Furthermore crystallographic activities for schoolchildren performed to celebrate IYCr2014; Crystallography Day İstanbul Turkey (23rd May 2014) and İstanbul Crystal Growth Competition (March 10-April 18) .

**Keywords:** Crystallography, Turkey