

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:

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

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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 18th 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 1960th 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.