



SHORT INFORMATION

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Commission on Aperiodic Crystals

Terms of Reference

In the following, by "crystal" is meant any solid having an essentially discrete diffraction diagram, and by "aperiodic crystal" is meant any crystal in which three dimensional lattice periodicity can be considered to be absent. As an extension, the latter term will also include those crystals in which three dimensional periodicity is too weak to describe significant correlations in the atomic configuration, but which can be properly described by crystallographic methods developed for actual aperiodic crystals.

- To promote the development of common methods and nomenclature for the crystallographic investigation of aperiodic crystals, including modulated structures, polytypes, incommensurate misfit or composite crystals, and quasicrystals.
- To promote and coordinate scientific interchange among groups working in the field of incommensurate structures, quasicrystals, polytypes and aperiodic crystals in general. In particular, to promote the dissemination of the existing methods for structural analysis, and support the development of new ones.
- To promote the exchange of adequate samples and / or experimental data sets of these crystals, so that they can be made available to a larger number of groups.
- To cooperate with the Commission on Crystallographic Nomenclature and other interested groups in the development of a standard nomenclature for dealing with higher dimensional descriptions of aperiodic crystals.
- To promote cooperation between crystallographers working on aperiodic crystals and mathematicians working in the field of high-dimensional symmetry groups and/or aperiodic systems, and to stimulate the development of mathematical crystallography.
- To promote knowledge among crystallographers of superspace or high- dimensional space methods as tools which can also be used to advantage investigation of certain periodic crystal structures.
- To cooperate with other Commissions of the IUCr in establishing adequate guidelines and standards for articles to be published in IUCr journals reporting structural investigations of aperiodic crystals and theoretical investigations of aperiodic patterns.
- To promote and coordinate scientific meetings dealing with aperiodic crystals; in particular to continue the triennial series of meetings begun by the preceding Commission.
- To advise the IUCr on organizing or sponsoring sessions on aperiodic crystals and/or high-dimensional crystallography at Congresses.

Commission on Crystallographic Computing

Terms of Reference

After the close of the Fourth General Assembly, the Executive Committee appointed an ad-hoc Committee to consider what action the Union could take with respect to a number of questions raised at that Assembly concerning crystallographic computing. The final report of this ad-hoc Committee was sent to the National Committees in June as an appendix to the Agenda, and it is added to these Minutes as Annex I, Appendix C (b) (see p. 19).

Following the recommendation of the ad-hoc Committee, the Executive Committee proposed that a Commission on Crystallographic Computing be set up, with the following terms of reference:

- (a) The Commission shall promote the collection and dissemination on an international scale of information relating to crystallographic computing, with special reference to general-purpose digital computers;
- (b) The Commission may undertake any activity related to crystallographic computation;
- (c) The Commission shall have power to appoint: (i) Consultants to assist and advise in all matters relating to specific machines, and (ii) Regional Correspondents to assist in the collection and distribution of information on a geographical basis.

After a short discussion, during which the General Secretary explained that the Executive Committee had already presented nominations for the new Commission subject to the approval of its establishment by the General Assembly, the Assembly approved the formation of a Commission on Crystallographic Computing with the above terms of reference, and decided that its elected membership should be five.

Commission on Biological Macromolecules

Terms of Reference

The Commission on Biological Macromolecules was established at the Ottawa General Assembly in 1981, with the following terms of reference:

- To advise the IUCr in organizing or sponsoring sessions on macromolecular crystallography at Congresses and conferences
- To promote and coordinate scientific exchange between countries in the field of macromolecular crystallography
- To cooperate with other Commissions of the Union on matters dealing with macromolecular crystallography
- To cooperate with other international bodies interested in macromolecular crystallography and allied subjects

Commission on Powder Diffraction

Terms of Reference

The Commission on Powder Diffraction was established at the Perth Congress in 1987, with the following terms of reference:

- To advise the IUCr in organizing or sponsoring meetings, schools and Congress sessions on powder diffraction and related subjects.
- To promote and coordinate scientific exchange between countries in the field of powder diffraction.
- To cooperate with other IUCr Commissions on matters concerning powder diffraction.
- To cooperate with other international bodies interested in powder diffraction and allied subjects.
- To promote useful interactions of the IUCr with the large world-wide body of X-ray and neutron powder diffractionists.
- To promote the scientific growth and development of the field of powder diffraction.

Commission on Synchrotron and XFEL Radiation

Terms of Reference

The Commission on Synchrotron Radiation was formally established at the Bordeaux General Assembly in 1990, with the following terms of reference.

- Crystallography of small molecules and large molecules in the areas of very high resolution, large unit cells, microcrystals, reduced radiation damage, kinetic crystallography and multi-wavelength anomalous-dispersion phasing.
- Fibre diffraction and small-angle scattering including time-resolved studies.
- X-ray topography
- EXAFS (extended X-ray absorption fine structure).
- Diffuse scattering
- X-ray optics and detectors of particular relevance to the utilization of the unique properties of synchrotron radiation.
- Magnetic scattering.
- High pressure diffraction
- To assist in the organization of relevant sessions at IUCr Congresses and other meetings that will catalyze developments and innovations in the subject.
- To catalogue information on the available synchrotron-radiation sources and the instrumentation relevant to the above topics. This information will be made freely available and so improve the future planning, use and effectiveness of the global resources available for the community of crystallographers and diffractionists represented by the IUCr.
- To provide a forum for comparing and contrasting the policies of the various centralized synchrotron facilities.
- To facilitate scientific and technical studies aimed at improving standards of sources, equipment and procedures.
- To try to provide a mechanism whereby potential users of synchrotron radiation from anywhere in the world can be directed to the appropriate facility and helped with gaining access there.

The Commission will serve several functions as follows.

Commission on Neutron Scattering

Terms of Reference

The Commission on Neutron Diffraction was established at the Moscow General Assembly in 1966. The proposal at that time is given below.

The Commission on Neutron Diffraction shall be concerned with those aspects of crystallography which can be studied almost uniquely by using neutron beams. Broadly these fall into three classes:

- Satisfactory detection of light atoms (particularly hydrogen)
- The detection and description of magnetic architecture
- The study of crystal dynamics from inelastic scattering data

It is considered that there are several ways in which these aims can be directly advanced and that there is a substantial need for action at the present time in these various directions.

- Tabulation and critical evaluation of data on the neutron scattering amplitudes of elements and isotopes, including complex scattering amplitudes, and of magnetic form factors. There are wide variations of accuracy among the accepted values and the accuracies of many of them are not known.
- Collection of information and recommendations on technical procedures, e.g. choice of initial colli-

mation, the uses of Soller slits, choice and availability of monochromators, corrections for secondary extinction, multiple scattering and series termination.

- Cataloguing of information on reactor types, neutron flux, background, instrumentation, methods of data collection and handling, design of cryostats and magnet assemblies.
- Encouragement of monographs, e.g. on Shubnikov groups, and their application to the determination of magnetic structures, inelastic scattering techniques. Cooperation in the production of Structure Reports for the description of magnetic structures.
- Support for symposia, in particular to ensure that the various aspects of neutron diffraction techniques, such as those mentioned above, get adequate coverage in meetings of the International Union of Crystallography. This need is quite distinct from providing coverage of the results of neutron-diffraction investigations.

The name was changed to Commission on Neutron Scattering by the General Assembly at the Beijing meeting in 1993. The Commission requested the change in name because it wished to represent and serve all neutron scatterers who consider that they use crystallographic techniques.

Commission on NMR and Related Methods

Terms of Reference

The Commission on NMR Crystallography and Related Methods was established at the Montreal General Assembly in August 2014. The Commission will serve several useful roles for the community that studies the crystalline state using magnetic resonance, as well as for the larger crystallographic community. The terms of reference are as follows:

Establish, implement and maintain standards

The NMR community already operates under some guidelines put forward by IUPAC. These mostly concern chemical shift referencing – a not unimportant issue for the proper collection, analysis and reporting of spectral data. The proposed Commission will first identify areas in need of common spectral standards, and then serve as a clearinghouse for these issues. Members will be chosen who have familiarity with the technical complexities that arise in this area. The Commission may work toward the development of a common format for sharing magnetic resonance crystal information – modeled on the Crystallographic Information File format – that would keep track of raw NMR data and extracted information. At present, there is no such common standard in the NMR community, though some national crystallographic societies are already active in proposing such extensions. Additionally, integration of

NMR data into structure search formats is already under development or may be soon, in packages such as FOX and Jana2006. Such integration could also be linked to topological crystallography software packages, such as TOPOS.

The Commission may undertake the compilation of basic NMR crystallographic knowledge into usable International Tables for NMR crystallography. Such a compendium may contain a list of irreducible crystallographic symmetries – akin to listings used in infrared, Raman and UV spectroscopy – as well as symmetries related to NMR pulse sequences used for selective extraction of spin interactions. Another specific contribution would be a section for correspondences between the quantum description of NMR observables and the associated structural parameters. Most of these notions, familiar to spectroscopists manipulating phase coherence, are not commonplace for methods without such phase coherence. The Commission may also endeavour to simplify and systematize the taxonomy (and terminology) to bridge NMR and diffraction based fields. Additionally, cross-Commission efforts should be made to integrate recent developments in other areas. One such example is the incorporation of topological crystallography, which is under the purview of the Commission on Mathematical and Theoretical Crystallography, into NMR crystallography.



Assist journals and editors

As the number of manuscripts submitted to peer-reviewed journals that employ magnetic resonance in the study of the crystalline state rises, editors and referees unfamiliar with NMR may need some guidelines for how to assess the quality of data reported, as well as the level of experimental detail that is commonplace in NMR forums. The proposed Commission could put forward a set of recommendations for journals in the larger crystallographic community. As such, there should be some representation within the Commission from the community of current or former journal editors. This could also provide a fruitful intersection with the existing Commission on Journals. Several leading journals have had recent themed issues on NMR crystallography. The Commission may promote the use of IUCr journals as a stable forum for NMR crystallographic articles, which are currently scattered in many different broad-audience journals.

Help organize conferences and workshops

Conferences in NMR crystallography have already been organized in recent times. The SMARTER series of conferences is the most obvious example with an approximate audience of about 100 participants. This conference has been supported since its birth in 2005 by the IUCr Commission on Inorganic and Mineral Structures. Other conferences, such as the Gordon Research Conference (GRC) on Computational Aspects – Biomolecular NMR and the Experimental NMR Conference (ENC), have held themed sessions on NMR crystallography. Judging by the recent publication and conference activity, it is clear that the magnetic resonance and crystallographic communities are cross-fertilizing. For graduate students in one area, accessibility to working knowledge in the other field will be critical in their training. There is great potential for targeted workshops to help such students. For example, a hands-on workshop for a graduate student in crystal engineering in solid-state NMR would be of great value. A series of re-

gional workshops, which would reduce travel costs and showcase local NMR capabilities, might cover theory basics and simple data collection. A short course – in the spirit of the Gordon Research Seminars – that precedes a major meeting could also be of useful service to the NMR crystallographic community. Such a mechanism would provide an efficient way to leverage against existing travel plans, and it could serve as an international networking opportunity for young researchers.

Serve as a liaison to commercial vendors

Both diffraction and NMR rely on expensive equipment, which is sold by a handful of vendors that market diffraction and magnetic resonance instruments. The IUCr likely does not want to get involved in the commercial side of crystallography, yet the truth is that researchers in both NMR and diffraction have a symbiotic relationship with the vendors that manufacture and sell the instruments. Researchers rely on healthy Research & Development that stems from friendly competition between the vendors to spur innovation, which, in turn, leads to the next generation of capabilities. The Commission could serve in some capacity as the representative for the research community, giving feedback and gentle encouragement to the vendors as warranted. A working relationship between the Commission and leading vendors can also be tapped to support conferences, workshops and student travel, as the need arises. In NMR, the main vendors are Bruker, Agilent and Jeol, with many small companies providing consoles, magnets, probes, software packages and services. The three main companies in NMR also have a significant presence in the diffraction community.

Other activities

The Commission will tailor its efforts in conjunction with regional and international bodies, such as the International Society for MAGnetic Resonance (ISMAR) or the American Crystallographic Association (ACA), to advance its agenda.

Commission on Crystallographic Teaching

Terms of Reference

The Commission on Crystallographic Teaching was established at the Paris Congress in 1954, with the following terms of reference:

- To exchange information on teaching on an international scale.
- To promote publication of articles on teaching.
- To arrange for discussions on teaching under the auspices of the Union.