# Annual Performance Review of International Affiliations 2017

# Introduction

Dear Grants to International Affiliations Canadian National Committee Members;

Each year the National Research Council of Canada (NRC) undertakes a review of the Scientific Unions and Committees that are funded through the Government of Canada's Grants to International Affiliations Program.

CNCs are required to complete an Annual Performance Review of their activities and those of their associated international organizations. These annual assessments are conducted to help inform NRC as to whether they are meeting their outcomes, i.e., to help determine whether these memberships remain relevant and that Canada is benefiting from them.

As possible, we recommend using materials you already have such as website descriptions of your Scientific Association or CNC, and annual reports on progress you may distribute to members, trip reports from attending General Assemblies, etc.

This year we are continuing the approach initiated last year to deliver the APR questionnaire online through this form. The APR submission is due on **February 1, 2018**.

If you have any questions regarding this process, if you are no longer a contact for your committee, or if you believe you have received this email in error, please do not hesitate to contact me: Pierre-Olivier.Bedard@nrc-cnrc.gc.ca (cc Holly.Boudreau@nrc-cnrc.gc.ca).

# Section 1: Primary Review Preparer Information

**Last name (required):**
Fodje

**First name (required):**
Michel

**Primary Organization (required):**
Canadian Light Source, Inc.

**CNC Role (if held):**
Secretary

**Email (required):**
michel.fodje@lightsource.ca

**Telephone (required):**
306-657-3758

# Section 2: Scientific Union / Association

## This section pertains to the international organization itself (not the CNC)

**What is assessed in Section 2?**

The Importance of the International Affiliation in general, and in particular, within the Canadian context.

The following are provided as examples of the way in which the importance may be demonstrated. They are provided as a guide only, and your organization is not required to demonstrate that your international affiliation meets all of these objectives. As well, we understand you may have other types of examples that demonstrate the importance of the international affiliation.

1. Example ways in which the international affiliation may demonstrate importance in general are by such activities, objectives and accomplishments which:
    i. identify and address issues of importance to science and society;
    ii. facilitate interaction among scientists across all disciplines and from all countries;
    iii. promote the participation of all scientists – regardless of race, citizenship, language, political stance, or gender – in the international scientific endeavour;
    iv. provide independent, authoritative advice to stimulate constructive dialogue between the scientific community and governments, civil society and the private sector; and
    v. provide access to and participation in international industrial research and commercialization.
2. Examples of ways in which the international affiliation may demonstrate importance within a Canadian context are by such activities, objectives and accomplishments which:

    i. facilitate international scientific activity around global challenges for the benefit (health, safety, prosperity, etc.) of Canadians and the global community;
    ii. enhance Canada's position and reputation in matters of science, engineering and industrial innovation;
    iii. enable Canadian science, technology and industry to remain world-class and internationally competitive;
    iv. provide enhanced Canadian contribution, participation, and influence in international S&T and industrial efforts, action plans, policy development and decision-making;
    v. develop and sustain networks, collaborations, and partnerships;
    vi. showcase Canadian achievements, technology, and capacity;
    vii. facilitate the exchange of experience, expertise, knowledge, and technology between Canadian and international scientific and industrial communities; and
    viii. enhance opportunities for Canadian small and medium-sized enterprises (SMEs) to commercialize technologies and bring them to market.

## I. Overview of the Union

### About the union/association and what it does:

The International Union of Crystallography (IUCr) is an International Scientific Union which is a member of the International Council for Science (ICSU). It aims to (1) promote international cooperation in crystallography, (2) contribute to the advancement of crystallography in all its aspects, including related topics concerning the non-crystalline states, (3) facilitate international standardization of methods, of units, of nomenclature and of symbols used in crystallography, and (4) form a focus for the relationship of crystallography to other sciences.

The scientific activities of the Union are carried out through its 21 Commissions, which focus on individual fields such as crystal growth, inorganic and mineral structures, structural chemistry, powder diffraction, synchrotron radiation, neutron scattering, biological macromolecules, mathematical and theoretical crystallography, aperiodic structures, nomenclature, teaching, and crystallography in art and cultural heritage. Several commissions are responsible for experimental practice (e.g. Synchrotron and XFEL Radiation, Powder Diffraction, Neutron Scattering, Biological Macromolecules, Small-Angle Scattering, NMR Crystallography, Electron Crystallography, and X-ray Absorption Spectroscopy) and therefore link to large national and research infrastructures, including synchrotron facilities, neutron sources, supercomputing centers, structural genomics laboratories and curated structural databases.

The IUCr publishes its own primary research journals – Acta Crystallographica Sections A–F, IUCrJ, Journal of Applied Crystallography and Journal of Synchrotron Radiation, which communicate the highest quality peer-reviewed research findings across the many scientific areas to which crystallography is relevant. The journals require deposition of supporting data sets for published crystal structures, which are thoroughly assessed as part of the publication process. The IUCr produces International Tables for Crystallography, a multi-volume encyclopedic reference work that sets the standards for nomenclature, scientific descriptions of crystallographic symmetry, the essentials of fundamental theory, and experimental best practice.

The IUCr also publishes a quarterly IUCr Newsletter and maintains the online World Directory of Crystallographers. Outstanding achievements within the community are recognized through the award of the Ewald Prize during the Congress and General Assembly organized triennially and also through other prizes awarded annually at meetings of regional affiliates.

## Annual Membership Due:
CHF 6000

## Category of membership adherence:
Category III

## Highlights of Activities and Accomplishments for this Year

### Annual General Assembly Meeting:

### Title (if specific):
24th Congress and General Assembly of the International Union of Crystallography

### Date:
21-28 August 2017

### Location:
Hyderabad, India

**Major Topics/Objectives:**

The IUCr General Assembly is held every three years. The Twenty-Fourth General Assembly and International Congress of the IUCr were held in Hyderabad, India from 21-28 August 2017. The General Assembly and Congress were attended by 1748 participants from 73 countries. At the Congress Opening Ceremony, the eleventh Ewald Prize was awarded to Sir Tom Blundell, recognizing his very broad contributions to the field of crystallography, and the Gjønnes Medal was awarded to Richard Henderson and Nigel Unwin. The scientific program included 1350 abstracts, of which 666 were oral presentations and the rest were poster presentations. Nine special activity micro-symposia covered topics that are of particular interest to the Union itself, such as standardization, data definitions, and education. There were also sessions for students from the emerging world to showcase the level of research capability in their countries.

Albania and Kosovo, Tunisia, Singapore, Bangladesh were accepted for Category I membership representing a significant membership growth of the Union. Upon paying their past dues, the membership of Chili was reinstated with a change in the name of their adhering body approved. Regional Committees of Crystallographers from Latvia, Tunisia, and Ukraine gave notice of withdrawal from membership of the Union prior to the General Assembly 2017. Tunisia, Bangladesh, and Singapore having secured independent membership were removed from previous regional adhering bodies. There were no changes to categories of adherence, and no changes to Statutes and By-Laws not affecting adherence to the Union.

Statement on Gender Balance: The statement was crafted in order to recognize the importance of gender diversity in addition to diversity in the geographical area, backgrounds, and scientific expertise. The IUCr will adopt procedures to promote gender balance, and several examples were included in the statement. A motion to publish gender statistics was approved.

The General Secretary and Treasurer of the IUCr presented a report on the financial state of the IUCr. Working with multiple (three) currencies has been complicated, and so the next report will only be reported in USD. The total assets decreased from CHF 4,596,542 to CHF 3,046,504, or 33%, over the triennium, due primarily to fluctuations in exchange rates, increased staff in the Chester office since IYCr2014, and a decrease in the number of submissions to Acta Cryst E (i.e. less Open Access fees collected). Cost savings and new revenue initiatives were proposed and approved after the Finance Committee meeting in March 2017.

Creation of WH & WL Bragg Prize: The new award is envisioned to be a smaller prize and will be presented for the first time at the IUCr 25th Congress to be held in Prague, Aug 22-39, 2020. It will be awarded to a promising crystallographer at an early stage of their career. It will be financed entirely from private sources and the executive committee already has indications of potential donors to fund this award. A committee will be established to oversee the parameters of the award.

The IUCr Associates Program was created to establish a professional brand of crystallographers and to serve better their needs. The voluntary program offers a series of benefits and tools to help Associates

network, share ideas and discover more about crystallography. In addition, those who join will be supporting the IUCr in its many charitable activities, such as sponsoring international meetings and schools and its OpenLabs initiative.

Publishing Commissions (Journals, International Tables): The journals are leading the field in innovative practices such as publication of data along with the articles. Eight volumes of the International tables designated A (and A1) through G are currently in print, a ninth (H, on powder diffraction) is expected to appear during 2017, and a tenth (I, on X-ray absorption spectroscopy and related techniques) is being written. Volume D needs a new editor (as the current editor is retiring.) Printed volumes can be purchased individually; online access is by subscription to the entire series. A new, considerably revised edition of the low-cost, printed Brief Teaching Edition of Volume A (Space-Group Symmetry) will appear by early 2018. Sales of subscriptions to International Tables Online have increased.

Standardization & Data Deposition: Committee for the Maintenance of the CIF Standard (COMCIFS) provided a detailed report of activities. The Diffraction Data Deposition Working Group (DDDWG) will transform into a wide-ranging Committee on Data for the IUCr from the time of the Hyderabad Congress; known as CommDat. It will aim to increase opportunities for digital archiving and sharing raw diffraction data.

Non-publishing Commissions: Before the General Assembly, the Executive Committee met with the members of all 17 Non-Publishing Committees. The reports of the commissions were received and the Chairs or a representative of the chair were present. The General Assembly also considered proposals for new commissions and reviewed the existing commissions and the number of elected members on each commission. All of the proposed changes to numbers of members on the commissions were approved by the General Assembly.

The Date and Place of the 25th Congress and General Assembly was confirmed as Prague, Czech Republic, August 22-30, 2020. There were two groups applying for consideration to hold the 26th Congress and General Assembly. The Australian Academy of Science on behalf of the Society of Crystallographers in Australia and New Zealand (SCANZ) to hold the Congress in Melbourne, Australia and the US National Committee for Crystallography proposed to hold the Congress in San Diego, United States. After a secret ballot, 26th General Assembly and Congress were provisionally scheduled for Melbourne, Australia in 2023, with 72.7% of the vote. This will be confirmed at the General Assembly in Prague in 2020. The Budget estimates for the period to the 25th General Assembly was considered and the recommendation that the Unit Contribution remain at its current level was approved. This Contribution level was set at the Beijing meeting in 1993, 24 years ago.

Elections: The recommendation of the Executive Committee for appointments and re-appointments were approved by the General Assembly. The Executive Committee presented five candidates for the position of President, two for Vice President and one for General Secretary and Treasurer of the Union and a slate of 10 candidates to serve as ordinary members. A vote was taken for President and Sven

Lidin (Sweden) was elected for a three-year term (with 51.72% of the vote after all rounds). For Vice President, Hanna Dabkowska (Canada) was elected for a three-year term (with 95.45 % of the vote, after only one round). The General Assembly had no problem with the recommendation of Luc Van Meervelt (Belgium) for the General Secretary and Treasurer. Three members for 6-year appointments were required – 1 from Asia/Oceana (India/Australia/Other); 1 from Americas, and 1 from any geographic region. The election results were: Asia/Oceania - Jenny Martin (Australia) (60.23 %; after first round), Americas - G. Diaz de Delgado (Venezuela) (80.68 %; only one round), Member-at-Large – M. Takata (Japan) (63.64 %; after all rounds).

## Other Major Meetings or Events (e.g., meetings, research programs, work-program, commission, panels)?

| Name of Event | Location | Date | Major Topics / Objectives |
|---|---|---|---|
| The 67th Annual Meeting of the American Crystallographic Association | New Orleans, Louisiana | May 26th-30th 2017 | Crystallographic research with sessions on sources, methods, and results. |
| São Paulo School on Scattering: Diffraction and Imaging using Light, Neutrons and X-rays | São Paulo, Brazil | July 17-21st, 2017 | advanced school on scattering, diffraction, and imaging using X-rays, neutrons and light |
| IUCr-UNESCO OpenLab Costa Rica | San Jose, Costa Rica | Dec 4-9th, 2017 | Single-crystal X-ray diffraction, X-ray powder diffraction |
| IUCr-UNESCO OpenLab Senegal | Ziguinchor, Senegal | Nov 20th-Dec 2nd, 2017 | Laboratory and synchrotron X-ray crystallography and applications to emerging countries |
| The 31st Biennial Conf. of the Society of Crystallographers in Australia and New Zealand | Pullman Bunker Bay, Western Australia | 3 – 7 December 2017 | Topics range from macromolecular structure through chemical crystallography and materials research to new methodologies in X-ray, neutron or electron diffraction and imaging |

## Report on accomplishments and key activities for this review year

Richard Henderson, IUCrJ Editorial Board member and winner of the 2017 Gjønnes Medal in Electron Crystallography with Nigel Unwin has been awarded the 2017 Nobel Prize in Chemistry with Jacques Dubochet and Joachim Frank “for developing cryo-electron microscopy (cryoEM) for the high-resolution structure determination of biomolecules in solution”. In August 2017 Richard delivered his Gjønnes Medal lecture at the 24th Congress and General Assembly of the IUCr in Hyderabad, India

Both the IUCr and IUPAP celebrated the start of their joint project LAAMP (Light sources for Africa, the Americas and Middle East Project), funded by the 2016–2019 ICSU Grants Programme, by hosting a kick-off event during the 24th Congress and General Assembly of the IUCr and the 29th IUPAP General Assembly (São Paulo, Brazil, October 11–13, 2017), respectively. LAAMP promotes utilization of light

source and crystallographic sciences to facilitate the enhancement of knowledge and improve the economic and social conditions in targeted regions of the world.

The symmetry database at http://it.iucr.org/resources/symmetrydatabase/ has been updated and expanded to include a wealth of new data. Information is now available for the Euclidean, chirality-preserving and affine normalizers of the space groups; these aid many crystallographic calculations including the comparison of different but equivalent coordinate descriptions of a crystal structure (and the accompanying changes in structure factors) and the derivation of phase restrictions for use indirect methods, as described in Chapter 3.5 of the new edition of International Tables Volume A.

IUCr Journals are doing well despite the fact that the publishing environment is very challenging. The journals are the main source of financing for all IUCr activities. In January 2016, the IUCr launched a new open-access data publication, IUCrData, which enables authors to rapidly publish brief, peer-reviewed Data Reports on individual crystal structures.

The Executive Committee created the IUCr Outreach and Education Fund which supports activities such as the Africa initiative and IUCr-UNESCO OpenLabs. The IUCr successfully applied to the International Centre for Theoretical Physics and the International Union of Pure and Applied Physics (IUPAP) for funding of a joint workshop in Senegal in 2017.

According to Thomson Reuters, over half of the IUCr journals saw impact factor increases in 2016, with the new Open-Access Journal IUCrJ receiving an impact factor of 5.3. According to Scimago Journal Ranks (SJR), Acta Crystallographica D has an h-index of 123 and is among the top-ten highest ranked Journals in Structural Biology. In addition, all nine IUCr Journals met the recently announced open-access publication requirements of the Wellcome Trust. Three of the Nobel Prize winners in 2016, Yoshinori Ohsumi of the Tokyo Institute of Technology, Tokyo, Japan; Sir J. Fraser Stoddart of Northwestern U., Evanston, USA; and Bernard L. Feringa of Groningen U., The Netherlands, have published in IUCr Journals.

## Report on the importance of the international affiliation to Canada

Crystallography and associated diffraction, spectroscopy and microscopy methods are used in basic research and industrial applications in each of the Federal Government's four priority areas – 1) environmental science and technologies 2) natural resources and energy, 3) information and communications technologies and 4) health and life sciences technologies. These methods include a wide variety of fundamental methodologies that are used to identify the structures, chemistries, and properties of natural and synthetic materials of all types. Diffraction is used in the development of stronger and lighter construction materials, energy-efficient refrigeration devices, display devices, catalysts, pharmaceuticals, and drug delivery media. It is also used in failure analyses, quality control, and characterization of mechanical devices, medical implants, pharmaceuticals, and electronics. Diffraction is also used in the workplace and environmental safety and in forensics. Structural analysis, as uniquely provided by crystallographic techniques, is central to almost all areas of applied and fundamental chemistry and materials science. Crystallography is used in earth sciences, and geology to

understand the structures and chemistries of natural materials including minerals, meteorites, glasses, sediments and soils, to address basic questions about the formation and history of the Earth. Similar methods are used industrially in the development and monitoring of mining processes. These applications bridge the environmental sciences and the natural resources priority areas. The petroleum industry is a major player in the Canadian natural resources arena, where powder diffraction methods are used to monitor the progress of drilling and extraction operations and to provide information regarding the surface chemistries of the materials from which the petroleum products are extracted. Monitoring the sulfur content of coals and heavy oils are readily accomplished using diffraction methods.

Crystallographic techniques are employed in the development of more sustainable green energy technologies and associated sources and storage devices, including fuel cells, batteries, and solar cells. The development of new semiconductor, superconductor and nano-materials and devices is greatly facilitated by the structural and chemical information readily provided by crystallography. These materials are critical to the development of the communications equipment and integrated circuits that power the information age. Macromolecular and small molecule crystallography contribute heavily to uncovering and understanding the molecular basis of disease. Determination of the structures of biological macromolecules which control essential biological processes greatly accelerates the design of novel pharmaceuticals, drug delivery media, and the engineering of new proteins with novel activities.

The Canadian science and technology network in crystallography and associated methods are dispersed among biochemistry, geology, chemistry, physics, biology, and engineering departments of most universities, government, and industrial labs throughout Canada. The Canadian faculty, post-doctoral researchers, and students involved in crystallographic and diffraction applications number in the thousands. In the past decade, the Canadian government has invested over $300 million to build the Canadian Light Source and its 14 operational beamlines in Saskatoon in support of Canadian research and technology development requiring crystallography associated techniques. Beamline applications range from macromolecular structure determination to medical imaging and nano-device fabrication. There are currently more than 60 labs specialized in biological crystallography, towards understanding the molecular basis of diseases and drug design. In addition, there are over 30 research groups using small molecule crystallography, and many more, using powder diffraction techniques, carrying out research in organic, inorganic, organometallic, and solid-state supramolecular chemistry. The Electron-Micro Beam and X-ray Diffraction facility at UBC serves about 100 companies involved in the mining and energy industries. The Canadian Center for Electron Microscopy at McMaster University provides an international resource for high-quality electron diffraction. The academic research activities of the various labs using crystallographic approaches are supported by a variety of sources including CIHR, NSERC, and private foundations. These labs are providing a new generation of highly trained researchers.

The IUCr International affiliation is therefore highly relevant to the Canadian context.

## Section 3: Canadian National Committee

# This section pertains to the Canadian National Committee (not the international organization)

### What is assessed in Section 3?

The Effectiveness of the supporting NRC Partner Organization and CNC.

The following are provided as examples of the way in which the effectiveness of the supporting NRC partner organization (PO) and CNC may be demonstrated. They are provided as a guide, and your organization is not required to demonstrate that the PO and-or CNC meet all of these objectives. As well, we understand you may have other types of examples which you wish to include to demonstrate the effectiveness of the PO and-or CNC.

Examples of ways in which the NRC Partner Organization and-or CNC may demonstrate effectiveness are by such activities, objectives and accomplishments which:

i. facilitate international scientific activity around global challenges for the benefit of Canadians and the global community;
ii. enhance Canada's position and reputation in matters of science, engineering and industrial innovation;
iii. identify, represent and promote the capabilities and distinctive competence of this Canadian scientific community internationally;
iv. enhance the depth and breadth of the participation of this Canadian scientific community in the activities and events of the international organization, and related organizations;
v. facilitate the collecting, reconciling and representing of the views of their stakeholder community on relevant issues;
vi. ensure the promotion of Canadian contributions to international decision-making;
vii. encourage and support their stakeholder community to take advantage of emerging international networking opportunities;
viii. encourage and support their stakeholder community to take advantage of opportunities to showcase Canadian achievements, technologies, and capacity;
ix. encourage their stakeholder community to take active roles in international conferences, symposia, and workshops; and disseminating relevant information obtained about developments in the wider international community to Canadian stakeholders;
x. ensure membership of the CNC is representative of researchers, and disciplines within its community;
xi. establish the mechanisms for communicating to the Canadian scientific community the views and information about the activities of the CNC and the international organization;
xii. attract and stage international events of value to the Canadian scientific community; and
xiii. facilitate the nomination of the Canadian Delegate(s) to the international organization's general assemblies, general meetings or council meetings.

## I. Overview of the Canadian National Committee (CNC)

### About the Canadian National Committee and what are its primary role and activities

The Canadian National Committee for Crystallography (CNCC), which is similar to the equivalent Committees on Crystallography of other nations, represents Canada internationally within the International Union of Crystallography (IUCr). It exists to promote the advancement of the science of crystallography in Canada and throughout the world, and to effect appropriate Canadian participation in the International Union of Crystallography (IUCr). The CNCC is currently a Category III Adhering-Body to the IUCr, thus has three delegates and three votes at IUCr General Assembly business meetings.

The CNCC's primary functions are: (1) to advise, and receive advice and directives from the National Research Council of Canada (NRC) on matters pertaining to Canadian participation in the International Union of Crystallography (IUCr); (2) to inform crystallographers in Canada concerning the activities of the IUCr; (3) to nominate persons to represent the crystallographers in Canada as delegates to the General Assemblies of the IUCr; (4) to provide information and guidance for such delegates; (5) to plan and sponsor scientific meetings in Canada as is consistent with the objectives of the IUCr; (6) to perform such other duties as are required of national committees of adhering countries under the statutes of the IUCr; and (7) to take any other action directed toward the benefit and advancement of the science of crystallography in Canada and throughout the world.

To achieve these objectives, the CNCC organizes workshops and meetings within Canada, maintains the Larry Calvert Fund, revenues from which are used to offer travel awards to deserving students and post-doctoral trainees, and non-faculty members at Canadian academic institutions, to enable their attendance at courses, scientific meetings, and the triennial IUCr Congresses. The main capital for the Larry Calvert Fund came from surplus revenues from IUCr Congresses and General Assembly Meetings organized by the CNCC and held in Canada in 1981 and 2014.

The CNCC also maintains a website (http://xtallography.ca) with information about the CNCC, minutes and the reports from the Canadian delegates of the IUCr General Assembly, links to conferences and workshops, training resources in crystallography, Canadian research facilities and research facilities worldwide, winners of the Canadian Poster Prize at the ACA annual meeting, and special interest groups of the ACA. The CNCC site provides links to information on the Larry Calvert Travel Fund and other Canadian student funding resources, links to the IUCr site, the CLS and to the Canadian Institute for Neutron Scattering (CINS) – the two major research facilities in Canada. The CNCC maintains a Twitter (https://twitter.com/CNC_Crystals) and Facebook (https://www.facebook.com/CNCCrystallography/) social media account for additional outreach to the members of the community.

In support of Canada's affiliation with an International Organization (IO), the National Research Council of Canada (NRC) enters into a Canadian Partner agreement with a Canadian Partner Organization.

**Partner Organization name:**

Canadian Light Source, Inc.

The Canadian Partner is responsible for creating and maintaining a Canadian National Committee (CNC) for this international affiliation, composed of leading Canadian researchers, to support Canada's affiliation with organizations.

**Canadian National Committee name (if a specific one exists):**

Canadian National Committee for Crystallography (CNCC)

## Composition of the CNC

**Please provide an up to date list of CNC secretariat members, and some information as follows about the members:**

| Title | Name | CNC Position | Affiliated Institution | E-mail address | CNC Term (if applicable) |
|---|---|---|---|---|---|
| Dr | Patrick Mercier | Chair | NRC | Patrick.Mercier@nrc-cnrc.gc.ca | 2015-2018 |
| Professor | Tomislav Friščić | Vice-Chair | McGill University | tomislav.friscic@mcgill.ca | 2015-2018 |
| Dr | Michel Fodje | Secretary | Canadian Light Source, Inc. | Michel.fodje@lightsource.ca | 2015-2018 |
| Dr | Brian Patrick | Treasurer | University of British Columbia | bpatrick@chem.ubc.ca | 2015-2018 |
| Professor | Andreas Decken | | University of New Brunswick | adecken@unb.ca | |
| Dr | Jim Britten | | McMaster University | britten@mcmaster.ca | |
| Dr | Joe Schrag | | BRI-NRC | joe.schrag@cnrc-nrc.gc.ca | |
| Professor | Louise Dawe | Outreach Coordinator | Wilfrid Laurier University | ldawe@wlu.ca | |
| Professor | Lynne Howell | | Hospital for Sick Children | howell@sickkids.ca | |
| Professor | Marie Fraser | | University of Calgary | frasm@ucalgary.ca | |
| | | | | | |

**Additional Space for listing CNC members or for other Comments on CNC membership**

The CNCC membership represents various regions of Canada, with members from British Columbia, Alberta, Saskatchewan, Ontario, Québec and New Brunswick

**What Canadian research, scientific, innovation or other communities and/or particular organizations does the CNC act as representative for to the scientific union or association?**

| Community or organization | Comments (if any) on how they are engaged | Additional comments (if any) |
|---|---|---|
| Mineralogy and Materials Science Diffraction community | Patrick Mercier represents this community on the CNCC | |
| Solid State Crystallography community | Represented by Tomislav Friščić on the CNCC | |
| Synchrotron Crystallography community | Represented by Michel Fodje on the CNCC | |
| Chemical Crystallography and Powder Diffraction community | Represented by Brian Patrick, Jim Britten, Andreas Decken, Patrick Mercier and Louise Dawe | |
| Macromolecular Crystallography community | Represented by Marie Fraser, Lynne Howell, Joe Schrag | |
| American Crystallographic Association (ACA) | Tomislav Friščić is the Canadian representative to the ACA Council. And writes a column in the ACA Newsletter which is distributed to all members of the ACA. | |

**Comments**

In general, the CNCC represents service crystallographers, crystallography faculty members at Canadian universities, crystallography researchers at government institutions (e.g. Department of Agriculture, National Research Council of Canada) and Canadian crystallographers in industry. The committee engages with the community through our website, social media, and meetings of the Canadian Division at the American Crystallographic Association. The committee also engages with the community through newsletters published by the American Crystallographic Association and the IUCr.

## II. Highlights of activities and accomplishments for this year

### Does the CNC host an annual meeting?

Yes

### What form does the meeting take?

Teleconference

## Report on the CNC's accomplishments and key activities for this review year

* If available, please feel free to copy any annual (or biannual, etc.) communications to your membership, and-or stakeholders that might provide such highlights.

The committee held seven teleconferences in 2017, on Feb 16th, Mar 23rd, May 3rd, June 26th, July 18th, Oct 17th and Dec 11$^{th}$ with numerous follow-up discussions via email throughout the year on key topics. Topics discussed included: (1) planning of Crystallography Workshops to be held in Canada; (2) community outreach activities; (3) nominations of Canadians to represent Canada on IUCr

Commissions and the Executive Committee; (4) decisions related to the management of the Larry Calvert Fund; and (5) planning Canadian participation in IUCr 2017 Congress.

The committee organized a competition for the Larry Calvert Travel awards to students wishing to attend the 2017 IUCr Congress in India. Four applicants were approved, three of whom ultimately received the awards. The winners of the 2017 Larry Calvert Travel awards were Jenna Marie Skieneh (University of Western Ontario), Ghada Ayoub (McGill University), Naheda Sahtout (University of Saskatchewan), and Thirumalai Ulaganathan (University of Saskatchewan).

The committee made key decisions about the future of the Larry Calvert Fund, such as investment options to preserve and/or grow it. After consultation with the community, the committee approved a resolution to amend the terms of the Larry Calvert Travel awards, effectively expanding the scope to support students, post-docs and non-academic staff at Canadian academic institutions. The scope was also expanded to include support for travel to other national and international workshops, courses and scientific meetings, in addition to the IUCr congress held every three years.

Several successful workshops and meetings were organized and/or sponsored by the CNCC and other members of the community in Canada during 2017: Jim Britten organized the 8th Canadian Chemical Crystallography Workshop which was held May 22nd-26th 2017, in Hamilton, ON as a satellite to the 100th Canadian Chemical Society Conference. The students participating were given hands-on training on methods of crystal structure solution and refinement from experts in the field. Dmitriy Soldatov and Kathryn Preuss from the University of Guelph organized a symposium on Crystalline and Semi-crystalline Molecule-based Materials, May 30-31, 2017. The 7th Annual CLS MX Data Collection School was held at the Canadian Light Source, in Saskatoon from June 5th to 9th 2017. The 20 students and postdocs who participated were given hands-on training on synchrotron data collection, refinement and structure solution in crystallography. The special topic for 2017 was structure solution using PHENIX, taught by Dr. Jeffrey Lee from the University of Toronto. The 5th Annual Meeting on Protein Structure, Function, and Malfunction (PSFaM) was held on June 14th-16th, 2017 in Saskatoon, Saskatchewan. Louise Dawe and Kenneth Maly organized the 4th Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec (CEMWOQ-4) at Wilfrid Laurier University, in Waterloo, ON, from May 26-28, 2017. Patrick Mercier organized the 10th Canadian Powder Diffraction Workshop, which was held June 2nd-4th, in Edmonton, Alberta as a satellite to the 54th Annual Clay Minerals Society Conference. The 26th Annual Buffalo/Hamilton/Toronto Crystallography Meeting was held on November 3rd at McMaster University. The Plenary Speaker was Dr. Bernhard Rupp, Medical University Innsbruck, Austria.

### Highlights of Canadian or CNC engagement at the international organization's annual general assembly meeting (if no general assembly this year, please leave blank)

The 24th IUCr General Assembly meeting was held in Hyderabad, India from Aug 21st to 28th, 2017. Jim Britten (McMaster University) and Pawel Grochulski (Canadian Light Source, Inc) were members of the International Program Committee and Patrick Mercier (NRC) was a member of the programme committee for the 2017 IUCr Crystallographic Computing School held in Bangalore (August 2017).

Three Canadian delegates were selected to participate in the 2017 IUCr Congress. They are Louise Dawe (*chair*), Pawel Grochulski (*delegate*), Tomislav Friščić (*delegate*), and Patrick Mercier (*alternate delegate*). The chair of the delegation coordinated with all participating Canadians before and during the Congress and prepared the final report about the General Assembly deliberations. Canadians were invited to present 2 keynotes, 9 oral presentations, and 12 poster presentations. Additionally, 4 microsymposia were co-chaired by Canadians. Overall, there were 25 Canadian registered participants at the meeting.

Various Canadians were nominated and most were eventually successfully voted to fill vacancies on IUCr commissions and the Executive Committee of the IUCr. Hanna Dabkowska (McMaster University), was elected Vice-President of the Union. This will increase Canadian visibility and reputation in the international crystallographic community. Canadians were elected/renewed to serve as members on 8 commissions with two acting as Chairs. Hanna Dabkowska is the IUCr representative on the ICSU Committee on Space Research (COSPAR). Three Canadians are co-editors of the IUCr Journals: Albert Berghuis (McGill University, Acta D and IUCrData) and Alan Lough (University of Toronto, Acta E and IUCrData), Gil Privé (University of Toronto, Acta F and IUCr Data).

The Canadian delegates voted in favor of the Statement on Gender Balance and Creation of WH & WL Bragg Prize, and the recommendation that the unit contribution remain unchanged.

**Notable highlights of Canadian or CNC engagement at other major meetings or events (if any).**

The American Crystallographic Association is the North American Regional Affiliate of the International Union of Crystallography (IUCr). The Canadian Division of the ACA is a branch of the ACA which serves to represent the interests of Canadian crystallographers within the ACA. The CNCC is heavily involved in these activities. Each year, there is a face-to-face meeting of the Canadian Division held during the annual ACA meetings, where all Canadian participants are invited to attend. Topics discussed usually include communications from the CNCC, Crystallography events planned in Canada.

Dr. Tomislav Friščić (vice-Chair of the CNCC) is currently the Canadian Representative on the ACA Council and authors a column in the quarterly ACA newsletter titled “RefleXions from Canada”. The newsletter is widely distributed in print and on the web to members of the community. The columns written in 2017 highlighted the contributions of Canadian crystallographers to the field of crystallography. Examples include the contributions of Daniel Leznoff (Simon Fraser University) and Stephen Loeb (University of Windsor) to crystal engineering, and the contributions of James Wuest (Université de Montréal), to solid-state chemistry and chemical crystallography. Louise Dawe (Wilfrid Laurier University) and David Rose (University of Waterloo) were on the Nominating Committee for the ACA for 2017-2018, with Louise Dawe chairing the committee for 2017.

At the ACA Annual meeting held in New Orleans in May 2017, Michael James (University of Alberta) co-organized a symposium on “Conformational Dynamics of Ligand Binding”, Tomislav Friščić co-organized the first ever symposium on “NMR Crystallography” at the ACA. This symposium included two speakers from Canada: Mihails Arhangelskis (McGill, University) and Darren Brouwer (Redeemer University). Other sessions co-sponsored by the Canadian Division of the ACA include:

"Joint Methods for High Rate Data Processing: XFEL and Synchrotron", "NMR Crystallography", "Enzymes of Post-Translational Modifications", "Home-Built Software", "Hot Structures", and "Structural Biology of Infectious Diseases".

The 68th ACA Annual meeting in 2018 will be held 20–24 July in Toronto, Ontario, Canada. Louise Dawe and David Rose will be co-chairing the poster program. David Rose will be chairing the Nominating Committee of the ACA for 2018.

## In-kind contributions of CNC (or partner organization)

### Time

**For each member of the CNC secretariat, please provide the following information:**

| Committee Member | Estimated In-kind hours contributed to running/participating in CNC this year | Participated in International Union/Affiliation AGM (Y/N) | Participated in CNC Annual Meeting (Y/N) | Comments (if any) on any other contributions |
|---|---|---|---|---|
| Michel Fodje | ~90 Hours | N | Y | Website System Administrator |
| Louise Dawe | ~20 Hours | Y | Y | Webmaster |
| P. Lynne Howell | ~15 Hours | N | Y | |
| Andreas Decken | ~15 Hours | N | Y | |
| Tomislav Friščić | ~15 Hours | Y | Y | |
| Brian Patrick | ~15 Hours | N | Y | Treasurer |
| Patrick Mercier | ~75 Hours | Y | Y | |
| Jim Britten | ~15 Hours | N | Y | |
| Joe Schrag | ~15 Hours | N | Y | |
| Marie Fraser | ~15 Hours | N | Y | |

### Financial

**Does the partner organization hold a separate budget for the support/running of the CNC and/or Canadian science community engagement with the international affiliation/union?**

No

**If yes, what is the value of that budget?**

N/A

**If yes, what kinds of activities does it support (Please check all that apply)?**

N/A

**Please provide details on any specific instruments or ways in which the CNC has been established? E.g., is it incorporated as a non-profit? Is there an agreement between the Canadian Partner organization and the CNC, etc.?**

In April of 2016, a Memorandum of Understanding was signed between the NRC and the Canadian Light Source, Inc (CLS) allowing the CLS to become the Canadian Partner responsible for creating and maintaining the CNCC. Under that agreement, the CLS provides hosting for the CNCC Website, nominates the Executive Secretary of the Committee, and provides teleconferencing resources to the committee.

While the committee itself is not incorporated as a non-profit, the Larry Calvert CNC/IUCr Trust Fund has been incorporated as a non-profit, with the members of the committee acting as its trustees. The Fund offers travel awards to deserving students, post-doctoral and non-faculty trainees at Canadian academic institutions, to enable their attendance at courses, scientific meetings, and the triennial IUCr Congresses, in order to further their expertise and education in crystallography and related disciplines.

## Participation

### Please provide the details of any Canadian union members sitting on the executive body of your international affiliation/union in the last year

| Name of Canadian Researcher | Executive Role | Title/ Position and Affiliated Institution | Term |
|---|---|---|---|
| Hanna Dabkowska | Vice President of IUCr | Research scientist, McMaster University | 2017-2020 |
| | | | |

### If the information is available, please provide the details of any Canadian union members participating in non-executive committees, research programs, work-program, commission, panel position or other sub-structures/groups managed through the international affiliation:

| Name | Position on the international affiliation body | Committee/Research Program/Other | Title/ Position and Primary place of work | Term on the international affiliation body |
|---|---|---|---|---|
| Patrick Mercier | Member | Commission on Crystallographic Computing | Senior Research Officer—Energy, Mining and Environment National Research Council Canada | 2012-2020 |
| Patrick Mercier | Chair | Commission on Inorganic and Mineral Structures | Senior Research Officer—Energy, Mining and Environment National Research Council Canada | 2017-2020 |
| Pawel Grochulski | Chair | Commission on Synchrotron and XFEL Radiation | Bio/Life Science Manager, Senior Scientist, Canadian Light Source | 2017-2020 |

| Name | Position on the international affiliation body | Committee/Research Program/Other | Title/ Position and Primary place of work | Term on the international affiliation body |
|---|---|---|---|---|
| Pawel Grochulski | Member | Commission on Biological Macromolecules | Bio/Life Science Manager, Senior Scientist, Canadian Light Source | 2017-2020 |
| Chérif Matta | Member | Commission on Quantum Crystallography | Professor and Chair, Department of Chemistry and Physics Mount Saint Vincent University | 2017-2020 |
| Howard Young | Member | Commission on Electron Crystallography | Associate Professor, University of Alberta | 2017-2020 |
| Roderick Wasylishen | Member | Commission on NMR Crystallography and Related Methods | Professor, University of Alberta | 2017-2020 |
| David Bryce | Member | Commission on NMR Crystallography and Related Methods | Research Chair, University of Ottawa | 2017-2020 |
| Jim Britten | Consultant | Commission on Crystallographic Teaching | Scientific Directory, Analytical X-Ray Diffraction Facility McMaster University | 2017-2020 |
| Michel Fodje | Consultant | Commission on Crystallographic Computing | Senior Scientist, Canadian Light Source | 2017-2020 |
| Louise Dawe | Member | IUCr Sub-Committee on the Union Calendar | Assistant Professor, Wilfrid Laurier University | 2017-2020 |

**If the information is available, please provide the details of any Canadian union members participating in ICSU related work including on committees, research programs, work-program, policy or position documents, commissions or other sub-structures/reporting exercises managed through the ICSU secretariat:**

| Name | Contribution | ICSU Participation | Title/ Position and Primary place of work | Term for ICSU Work |
|---|---|---|---|---|
| Hanna A. Dabkowska | IUCr representative | ICSU Committee on Space Research (COSPAR) | Research scientist, McMaster University | 2005-2020 |
| | | | | |
| | | | | |