Proposal for a new special interest group «Magnetic Crystallography" within the European Crystallographic Association

Promoters

Françoise Damay, Université Paris-Saclay, Laboratoire Léon Brillouin, CEA-CNRS, CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France

Margarida Henriques, Institute of Physics of the Czech Academy of Sciences, 18200 Prague, Czechia

Oksana Zaharko, Paul Scherrer Institute PSI, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland

Javier Campo, Aragón Nanoscience and Materials Institute, CSIC, Pedro Cerbuna 12, Zaragoza, 50009, Spain

Juan Manuel Perez-Mato, Facultad de Ciencia y Tecnología, Universidad del País Vasco, UPV-EHU, Bilbao, Spain

1. *What is magnetic crystallography?*

Magnetic ordering is the breaking of time-reversal symmetry. Similarly to the space groups of conventional crystallography, symmetry groups of three-dimensional commensurate magnetic structures, or magnetic space groups (also called Shubnikov groups, in reference to the pioneer of the antisymmetry concept), have been compiled as early as 1957 by the Soviet mathematician Zamorzaev. Despite this early work, magnetic symmetry has been used only timidly in magnetism research until recently, mostly because of the lack of standardization, and the absence of appropriate software. To determine magnetic structures, the community has been largely using instead computational tools relying on the so-called representation method, established by Bertaut around 1970, and then further developed by Izyumov in 1979.

The situation has changed drastically in the early 2000's, with the development of a substantial number of free computational tools for the analysis of magnetic structures, based on magnetic symmetry. With improvements in the standardization, computer readable listings of magnetic space groups were made available. This lead in turn to the evolution of Rietveld refinement programs, which were implemented to use magnetic space groups in the commensurate cases, and magnetic superspace groups in the incommensurate ones. These new features were supported in parallel by various programs allowing the symmetry analysis of possible magnetic orderings, given a parent structure and a propagation vector, in a magnetic phase transition. These developments have opened a new era, and magnetic symmetry is employed much more routinely today to determine a magnetic order amongst several possible alternatives. In addition, thanks to the IUCr patronage, the CIF dictionary has been extended to magnetic structures (magCIF format), allowing one to describe any magnetic structure, either commensurate or incommensurate, in an unambiguous and unified way. MagCIF is now a standard in most refinements, visualization or analysis software.

2. *Why is a Special Interest Group in Magnetic Crystallography relevant?*

Magnetic crystallography has reached a stage, nowadays, where it is supported by enough free online software to have become an, easy, efficient and powerful tool, available to the whole research community. The aim of the SIG is therefore, not only to raise awareness of its existence among researchers, but also to promote the use of good practices, in particular with respect to the new standards that are being implemented for the description of a magnetic structure, in the same fashion as crystallographic standards exist to report a crystal structure.

The funding members have at heart that all the effort which has been dedicated to the development of magnetic crystallography tools, standards, and databases for the past ten years should not benefit a small group of specialists only; rather, it should also profit the larger community of researchers working with magnetic materials, and who are already familiar with crystallography in their daily work. This positioning also comes at a time where it has been noticed by the IUCr Commission on Magnetic Structures that magnetic materials topics are often not well represented in European size crystallography events. With this new SIG, our aim is to maintain activity and dynamism in the field of magnetic crystallography.

This proposal is supported by four ECA National Members, the Association Française de Cristallographie, the British Crystallographic Association, the Danish National Committee for Crystallography, and the Swiss Society for Crystallography, and by F. Lahoz, from the Spanish Association of Crystallography, as the ECA councillor for Spain. Their support letters can be found at the end of the document. Letters of support from The Comité Español de Cristalografia, and the SFN - French Neutron Society, are also included.

3. *Topics covered by the new SIG*

The SIG on Magnetic Crystallography will be concerned with the general use of magnetic symmetry in :

- magnetic compounds in general, such as magnetic perovskites, magnetic functional materials, molecular magnets
- magnetic ordering, magnetic phase transitions, complex magnetic structures (incommensurate and quasiperiodic)
- quantum materials in which symmetry is a key element to the understanding of emergent electronic properties
- co-representations, spin space groups and their applications, including altermagnetism
- ad-hoc techniques, such as non-polarized and polarized neutron diffraction, X-ray resonant diffraction, methods for the determination of magnetic structures, magnetic crystallography computing tools

It is thus positioned over a large area of scientific interests, which will enable joint microsymposia with other ECA SIGs to be organized easily.

4. *Scope of the magnetic Crystallography SIG*

- Contribution to the recognition of magnetic crystallography in the research community
- Collaboration and joint actions with other SIGs to enlarge its impact in the European community

- Promotion of the common magCIF standard
- Promotion of a magnetic structure database built on the sharing of magCIF files
- Support for microsymposia and symposia on magnetic crystallography related topic in workshops and conferences
- Sponsorship of schools or satellite meetings
- Elaboration of teaching materials, such as tutorials, for students and scientists in need
- Promotion of pertinent publications in IUCr journals

5. Supporters

Dr. José Antonio Alonso Alonso
Instituto de Ciencia de Materiales de Madrid, Spain

Dr. Angel Arevalo-Lopez
UCCS, Université de Lille, France

Dr. Stanislaw Baran
Jagiellonian University, Poland

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Paul Scherrer Institute, Switzerland

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Institut de Chimie de la Matiere Condensée de Bordeaux, France

Dr. Alexander Tsirlin
University of Leipzig, Germany

Dr. Joost van Duijn
University of Cordoba, Spain

Dr. Andrew Wills
University College London, UK

6. Proponents

The SIG founding Chair, Vice chair and Secretary are proposed to be Françoise Damay, Margarida Henriques, and Oksana Zaharko, respectively.

This document was prepared by
Françoise Damay, Margarida Henriques, Oksana Zaharko, Javier Campo, J. Manuel Perez-Mato
November 14th, 2024

Association Française de Cristallographie

https://www.afc.asso.fr/

Strasbourg, July 5, 2024

Dr Claude Sauter
President of the French Crystallographic Association
CNRS Research Director
Institut de Biologie Moléculaire et Cellulaire
2, allée Conrad Roentgen, 67084 Strasbourg, France
c.sauter@ibmc-cnrs.unistra.fr

Dear colleagues,

With the support of the IUCr Commission on Magnetic Structures, our colleague Françoise Damay, along with Margarida Henriques, Javier Campo and Manuel Perez-Mato, is working on a new SIG project “Magnetic Crystallography” for the European Crystallographic Association.

Nowadays, magnetic symmetry can be employed almost routinely when describing a magnetic order, thanks to the development of free computational tools, in parallel with an improved standardization of magnetic space groups. This new SIG is a great way to strengthen bonds between the ECA and the magnetism community. Moreover, it will be a key tool in promoting the use and power of existing online tools amongst crystallographers, or in advertising new features and abilities. This new SIG will also drive more efficiently the development of a magnetic structure database, akin to those already existing in classical crystallography, and the learning of good practice with respect to the descriptions of magnetic structures using standards.

The board of the AFC gives therefore its full support to this new project, which will greatly benefit the community.

Yours sincerely,

Dr Claude Sauter

British Crystallographic Association

School of Chemistry
University of St Andrews
North Haugh, St Andrews
KY16 9ST, UK
Email:
president@crystallography.org.uk

16 July 2024

To whom it may concern,

I am writing in support of the application by the IUCr Commission on Magnetic Structures to establish a **new Special Interest Group (SIG) attached to the European Crystallographic Association entitled "*Magnetic Crystallography*"**.

The analysis of magnetic systems through crystallographic means has developed dramatically in the last 20 years, and the pace of change continues to increase. New tools with firm foundations in symmetry considerations have increasingly broad usage within the scientific community interested in magnetism. Within our membership it is clear that these developments are improving the accessibility and understanding of magnetic structure analysis. The MagCIF format, as developed and promoted by the IUCr Commission on Magnetic Structures provides a unique way to store and transmit magnetic structure information in a format analogous to that of the traditional CIF, and database creation and international meetings focusing on magnetic crystallography are developing correspondingly.

The proposed SIG will provide significant benefit to the UK and European community by e.g. activities developing of the European magnetic crystallography community, encouraging and supporting the use of the MagCIF format and magnetic crystallography database, increasing the availability of training and conference opportunities related to magnetic crystallography and providing a nexus for a Europe-wide network of crystallographers with interest and specialisation in magnetism.

The British Crystallographic Association (BCA) was established in 1982 to represent and connect scientists across UK industry and academia who use diffraction and complementary techniques to study materials ranging from metals and minerals to proteins and medicines. As such, the BCA is able to engage a significant proportion of the UK crystallographic community when the SIG is formed and we look forward to the significant benefits to our members, and other scientists in the UK, that the SIG would provide.

The individual Members of the IUCr Commission on Magnetic Structures have outstanding international reputations, as does the work they have done collectively on behalf of the Commission through projects such as the MagCIF. This combined with the significant benefits that a SIG on Magnetic Crystallography would bring to the community that we represent leads to the British Crystallographic Association being in strong support of their initiative to form a new 'Magnetic Crystallography' SIG.

Yours sincerely

Dr Alexandra Gibbs
President, British Crystallographic Association

UNIVERSITY OF COPENHAGEN
DEPARTMENT OF PHARMACY

To Whom It May Concern

In support of the SIG for magnetic crystallography

25 SEPTEMBER 2024

MANUFACTURING AND MATERIALS

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KØBENHAVN Ø

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Anders Østergaard Madsen, PhD
Associate Professor
Department of Pharmacy
University of Copenhagen

I am writing to express my strong support for the establishment of the new Special Interest Group (SIG) in Magnetic Crystallography within the European Crystallographic Association (ECA). As the Chair of the Danish National Committee for Crystallography, I recognize the significant advancements and contributions that magnetic crystallography has made to the broader field of crystallography and materials science.

Magnetic crystallography, which involves the study of magnetic ordering and the use of magnetic symmetry, has evolved remarkably over the past few decades. The development of computational tools and the standardization of magnetic space groups have transformed this once niche area into a vital and accessible tool for researchers worldwide. The introduction of the magCIF format, supported by the International Union of Crystallography (IUCr), has further unified and clarified the description of magnetic structures, facilitating their study and application.

The proposed SIG aims to promote awareness and good practices in magnetic crystallography, ensuring that the benefits of recent advancements are widely disseminated and utilized. This initiative is particularly timely, as magnetic materials are often underrepresented in major European crystallography events. By fostering collaboration and organizing joint microsymposia with other SIGs, the Magnetic Crystallography SIG will enhance the visibility and impact of this important field.

The SIG's objectives, including the promotion of the magCIF standard, the creation of a magnetic structure database, and the support for educational and outreach activities, align perfectly with the goals of the ECA. These efforts will not only benefit specialists but also the larger community of researchers working with magnetic materials, thereby advancing the field as a whole.

I wholeheartedly endorse the formation of the Magnetic Crystallography SIG and look forward to the positive impact it will have on the crystallographic community.

Sincerely yours,

Anders Østergaard Madsen

SGK
SSCr

UNIVERSITÄT
BERN

University of Bern, Faculty of Science
Department of Chemistry, Biochemistry and Pharmaceutical Sciences, Freiestrasse 3, CH-3012 Bern

European Crystallographic Association
Executive Committee

Bern, September 17th, 2024

Letter of Support for the Foundation of a SIG on Magnetic Crystallography

Dear Dr. van der Lee,

As the national representative for Switzerland in the ECA Council, it is with great enthusiasm that I express my support for the project of a new Special Interest Group “Magnetic Crystallography”.
Magnetic Crystallography focuses on the intricate relationships between symmetry of magnetic structures, magnetic properties, and crystallographic structures. Its use has developed tremendously within the last 20 years, thanks to new online tools, the development of standards (magCIF), and a dynamic teaching activity, exemplified by dedicated schools, online tutorial materials, and practical sessions in conferences such as the IUCr. The new SIG will be a great place for the European magnetism community to share results, learn about new developments, and continue to improve the accessibility and understanding of magnetic structure analysis. This European initiative would reflect similar already existing activities at the IUCr level, specifically with its Commission on Magnetic Structures.

Neutron scattering is one of the best techniques to probe magnetism. With its own national spallation neutron source, SINQ at Paul-Scherrer Institute (PSI), Switzerland is an important actor in the neutron landscape, and the community of Swiss Crystallographers using SINQ will certainly benefit from this new SIG. It will increase in turn the attractiveness of neutron techniques and scientific output of neutron facilities in general.

PD Dr. Simon Grabowsky
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3012 Bern
Switzerland

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I am therefore confident that this new SIG will have an invaluable positive impact for the crystallographers, and more generally, researchers working in magnetism, spanning solid state chemistry to fundamental physics.

Yours sincerely,

PD Dr. Simon Grabowsky
Swiss Society for Crystallography
National Councilor

Prof. Fernando J. Lahoz
Senior Researcher
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Dr **Arie VAN DER LEE**,
President of the European Crystallographic Association, ECA
Institut Européen des Membranes
CNRS, Université de Montpellier,
Montpellier, France

Zaragoza, 31 October 2024

Dear President, dear Arie

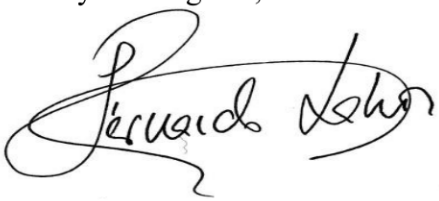
As councilor member of the ECA Council representing Spain, in accordance with the collegiate decisions of the Spanish association of crystallography (*Grupo Especializado de Cristalografia y Crecimiento Cristalino, GE3C*),- adhering body from Spain in the ECA,- and of the Spanish Committee of Crystallography,- working group nominated by Spanish Government to represent Spain at IUCr,- I should express my full support for the initiative presented by Dr. Francoise Damay and other renowned colleagues, for the creation of a new SIG, focused on Magnetic Crystallography.

Magnetic properties have extraordinary relevance in numerous applications used in our daily lives. Magnetic crystallography offers a unique entry into the interpretation and possible improvement of those properties.

The creation of a Specialized Group in this topic should channel the interaction of European scientists working in this area and stimulate the entry of new young researchers into this field.

As a member of the ECA Council, I declare my determined support for the proposal to create this new SIG on "Magnetic Crystallography"

With my best regards,



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Fernando J. Lahoz

ECA Councillor representing Spain

MINISTERIO
DE CIENCIA, INNOVACIÓN
Y UNIVERSIDADES

INSTITUTO DE QUÍMICA FÍSICA
"BLAS CABRERA"

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Prof. J.M. Garcia-Ruiz
Donostia International Physics Center
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En Madrid, a 19 de junio de 2024

Dear Prof. Marijana Dakivic,

We are writing to express our enthusiastic support for the creation of a new Special Interest Group (SIG) within the European Crystallographic Association (ECA), dedicated to Magnetic Crystallography. This initiative is timely and of paramount importance to the advancement of the crystallographic sciences and their applications in understanding magnetic materials.

Magnetic Crystallography has emerged as a crucial field within the broader scope of crystallography, focusing on the study of magnetic structures and the intricate relationships between magnetic properties and crystallographic structures. The establishment of a SIG focused on this area will provide a formal platform for scientists, researchers, and practitioners to collaborate, share knowledge, and drive forward innovative research.

As presidents of the Spanish adhering bodies to the ECA and IUCr, we have witnessed firsthand the growing interest and need for focused research on magnetic crystallography. We are confident that the creation of this SIG will not only support existing research initiatives but also inspire new projects and collaborations, ultimately leading to groundbreaking discoveries and technological advancements.

Thank you for considering this proposal. We are available for any further discussions or to provide additional support as needed.

Sincerely,

ALBERT DE LA CRUZ ARMANDO JOAQUIN - DNI 02616640E
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Firmado por GARCIA RUIZ JUAN MANUEL - DNI ***0241** el día 20/06/2024 con un certificado emitido por AC Sector Público

Armando Albert
Presidente del Grupo Especializado
de Cristalografía y Crecimento Cristalino

Juan Manuel García-Ruiz
Presidente del Comité Español
de Cristalografia

Prof. Marijana Đaković
President of the European Crystallographic Association
Faculty of Science, Department of Chemistry
University of Zagreb
Zagreb, Croatia

SIG 'Magnetic crystallography' – Letter of Support

Dear Professor Đaković,

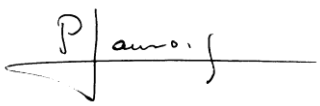
As the President of the Société Française de la Neutronique (SFN, French Neutron Association), it is my great pleasure to express our strongest support for the SIG project entitled "Magnetic Crystallography". Indeed, its spin makes the neutron a direct probe of magnetism on the atomic scale. Neutron diffraction is thus at the core of many experimental studies concerned with magnetic orders or magnetic transitions, whether in solid-state chemistry or physics.

The field of magnetic structure concerns many "hot topics" of today. To illustrate this, we'll mention just a few of them here. A very obvious one is superconductivity, where research efforts are focused on elucidating the microscopic mechanisms behind the fascinating properties of the so-called "unconventional" superconductors, i.e. superconductors with high critical temperatures. They are characterized by complex phase diagrams in which superconductivity coexists or competes with other states of matter, in particular magnetic phases. One should also mention information and new quantum technologies, which are based on magnetic phenomena such as skyrmions. The proposed SIG will provide a natural way to promote the very dynamic research in the field of magnetic structures and phase diagrams.

In recent years, there has been a tremendous amount of work by the IUCr Commission on magnetic structures to facilitate the use and standard reports of magnetic space groups for everyone working with magnetic structures. The proposed SIG should also open the currently available easy-to-use software to a wide scientific community.

We are confident that this new SIG will have an extremely positive impact on research on magnetism as well as on research that uses neutron diffraction. This in turn should lead to larger and stronger user communities at large-scale facilities, both at the French and European level.

Yours sincerely,



Pascale Launois
President of the Société Française de la Neutronique, on behalf of its board of directors