

Alliance Reshapes Crystallography Data Access

Structural chemistry's trusted crystallographic database providers join forces to provide single point access to all of the world's small molecule crystal data.

Cambridge, United Kingdom, and Karlsruhe, Germany, April, 2017.

The Cambridge Crystallographic Data Centre (The CCDC) and FIZ Karlsruhe – Leibniz Institute for Information Infrastructure (FIZ Karlsruhe) today announce the start of a joint development project that will deliver for the first time shared deposition and access services for crystallographic data across all domains of chemistry – including organic, inorganic and metal-organic structures. The resulting capability - to search over one million crystallographic structures and to deposit data for the CCDC's Cambridge Structural Database (CSD) and FIZ Karlsruhe's Inorganic Crystal Structure Database (ICSD) and their underlying CIF depots at a single source - will benefit researchers and educators across the chemistry disciplines. Two of the chemistry domain's longest-established and most trusted data organisations are combining to deliver standardised and comprehensive access to every structure ever published, with all entries discoverable through links in publications and third party information sources. This development will be of particular interest to scientists whose research spans the boundaries between organic, inorganic and metal-organic chemistry, who will no longer need to be concerned about which database to address, clearing confusion about where the database borders lie.

The CCDC and FIZ Karlsruhe have operated under an informal agreement for the decades in which they have been in existence. The CSD is the world's depository/repository of organic and metal-organic crystallographic data, containing all published structures in over 875,000 entries. The ICSD performs the same function for the inorganic chemistry community, featuring more than 185,000 structures. Each non-profit organisation respects the domain expertise of the other, and there is minimal overlap in the content of their databases. Recent advances in several areas of chemistry, such as research to design new batteries, gas storage systems, zeolites, catalysts, magnets, and fuel additives, have highlighted the challenges of researchers operating across these domains, who have had to operate across two independent data sources. The CCDC and FIZ Karlsruhe have now initiated a development project which will allow chemists to explore structures of interest simultaneously across both data sources, and for all crystallographers to deposit their data through a single, shared portal.

All of the existing expert data curation and publishing processes will remain in place, ensuring that users will still have access to the high quality data and advanced analysis capabilities on which they can depend. The new joint deposition and access portals will be built in Cambridge and based on the CCDC's recently-developed infrastructure for data deposition, processing, searching and sharing, all extended to meet the needs of the inorganic chemistry community.

“As a researcher and educator at the boundary of these domains, I am particularly excited about the promise of this partnership, both for research and for education in several areas of chemistry, where I am sure it will lead to many insights which otherwise would have been missed,” said Professor Paul Raithby, Head of Inorganic Chemistry at Bath University and Chairman of the Board of Trustees of the CCDC. “The CCDC’s considerable investment in new infrastructure to support data deposition and access has reduced the technology barriers to this project enormously, enabling a partnership which the structural chemistry community has long requested and which it sorely needs. We are very proud to be working with FIZ Karlsruhe to achieve this.”

“The community will greatly benefit from the partnership agreed between FIZ Karlsruhe and the CCDC,” emphasizes Sabine Brünger-Weilandt, President & CEO of FIZ Karlsruhe – Leibniz Institute for Information Infrastructure. “All organic and inorganic crystal structure data can be stored and made available through one central portal that is jointly operated by both partners. Thus, scientists can now more easily access the valuable information they need for their research.”

The news of this collaboration will be greeted enthusiastically by those who deposit and access structural chemistry data:

“The International Union of Crystallography welcomes this new development project and the simplification that it promises for deposition procedures for crystallographic structures.

We encourage synergistic interactions between crystallographic databases and are particularly pleased to see this collaboration between the CSD and ICSD that should lead to increased data deposition and discoverability,” said Peter Strickland, Executive Managing Editor, IUCr Journals.

“As a user of both the ICSD and CSD databases, I believe that a cooperation between FIZ Karlsruhe and CCDC will be an important step forward. The distinction between inorganic and organic structures has become artificial and realizing one central point for depositing and accessing crystallographic data will be of great help to the community,” said Professor Rene de Gelder, Radboud University Nijmegen, NL.

Planning and development work on the collaboration has already begun. The first outputs will be released through the course of 2017 and will be accessible via www.ccdc.cam.ac.uk and www.fiz-karlsruhe.de. The CSD and ICSD will continue to develop and to be available independently from the CCDC and FIZ Karlsruhe, respectively.

For more information about any aspect of this announcement, please contact:

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About the CCDC

The Cambridge Crystallographic Data Centre is dedicated to the advancement of chemistry and crystallography for the public benefit. The CCDC supports structural chemistry worldwide through collaborative research studies and by developing the Cambridge Structural Database (CSD), the world's only comprehensive, up-to-date, and fully-curated knowledge base of organic and metal-organic small molecule crystal structures.

The CSD was established over 50 years ago as the world's first numerical database and now comprises over 875,000 entries. The CCDC enhances its value to research scientists by providing state-of-the-art structural analysis software and expert research services for receptor modelling, ligand design, docking, lead optimization, formulation studies and materials research. The CSD and associated software services are delivered to around 1,400 research sites worldwide, including academic institutions in 80 countries and all of the world's top pharmaceutical and chemical companies.

Originating in the Department of Chemistry at the University of Cambridge, the CCDC is now a UK Research Council Independent Research Organisation and a University of Cambridge Partner Institute, constituted as a registered charity. With over 50 years of scientific expertise, the CCDC has demonstrated its strong track record in basic research through more than 750 peer-reviewed publications.

About FIZ Karlsruhe – Leibniz Institute for Information Infrastructure

FIZ Karlsruhe – Leibniz Institute for Information Infrastructure is a not-for-profit limited liability company. As one of the largest non-academic information infrastructure institutions in Germany, we have the public mission to provide researchers and scientists with scientific information and to develop the appropriate products and services. To this end, we edit and index large data volumes from manifold sources, develop and operate innovative information services and e-research solutions, and carry out research projects of our own. FIZ Karlsruhe is a member of the Leibniz Association which comprises 91 institutions involved in research activities and/or the development of scientific infrastructure.

The Inorganic Crystal Structure Database (ICSD) is the world's largest database for fully identified inorganic crystal structures. It contains the crystallographic data of published crystalline, inorganic compounds, including their atomic coordinates, dating back to 1913. It is produced by FIZ Karlsruhe and currently contains about 185,000 crystal structures. Updates are made twice a year (in Spring and in Fall) with data taken from scientific journals and other sources.

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