Free, unified deposition and access of crystal structure data

Cambridge (UK), Karlsruhe (Germany), July 2018 – The Cambridge Crystallographic Data Centre (CCDC) and FIZ Karlsruhe – Leibniz Institute for Information Infrastructure (FIZ Karlsruhe) today announced the launch of their joint deposition and access services for crystallographic data across all chemistry. These services will enable researchers to share data through a single deposition portal and explore all chemical structures for free worldwide.

"With this joint depot, FIZ Karlsruhe supports the community's need for a reliable infrastructure for research data from crystallography." says Sabine Brünger-Weilandt, CEO from FIZ Karlsruhe. "Providing freely available research data for all chemistry is in line with our claim to Advancing Science. The announcement of the cooperation between CCDC and FIZ Karlsruhe was already enthusiastically received by the community. We are convinced that we can meet the high expectations with the new joint depot."

The Chair of Trustees for the CCDC is equally excited about the impact of this launch to researchers worldwide: "All information users, whether they admit it or not, wish that all of the information that they require was in a single location. Failing that, they are searching for a "magic bullet" that will hit exactly what they want; they want to be able to use a simple interface and locate all of their information needs. By unifying the deposition and access of organic, metal-organic, and inorganic crystal structures we get a little closer to that magic bullet, at least in the area of crystallography, and make researchers' lives that much easier." says Judith Currano, Chair of Trustees for the CCDC and Head of the Chemistry Library at the University of Pennsylvania.

Recent advances in chemistry have meant that the distinctions between inorganic and organic structures have become blurred, for instance through research to design new batteries, gas storage systems, zeolites, catalysts, magnets, and fuel additives. This, coupled with the desire from researchers for more integrated databases, has been the driving force behind the development of these joint services.

As a result, researchers and educators worldwide, working across all fields of chemistry, are able to explore over one million crystallographic structures through a joint Access Structures service enabling them to view and retrieve deposited datasets associated with structures in the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD).

Crystallographers can deposit organic, inorganic and metal-organic structures through a unified deposition service. This features a streamlined online portal for easy submission and integrates a variety of checks to alert researchers about the validity, integrity and originality of their data. Additional features include the rapid assignment of deposition numbers and the ability for depositors to choose to share their data immediately through an appropriate database. Alternatively, data destined for inclusion in a scientific article is automatically shared at the point of publication through workflows with most major publishers. Anyone looking for structures previously stored in the FIZ Karlsruhe depot can still find them using the published depot number.

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 highly curated CSD and ICSD databases and their associated advanced software will continue to develop and to be available independently from the CCDC and FIZ Karlsruhe, respectively.

For more information about these joint services, please go to the CCDC or FIZ Karlsruhe websites:

www.ccdc.cam.ac.uk
www.fiz-karlsruhe.de

And for more information about this announcement please contact:

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The Cambridge Crystallographic Data Centre

FIZ Karlsruhe
Leibniz Institute for Information Infrastructure

The **Cambridge Crystallographic Data Centre** is dedicated to the advancement of chemistry and crystallography for the public benefit. The CCDC supports structural chemistry research through the Cambridge Structural Database (CSD), the world's comprehensive, current and curated knowledge base of small molecule crystal structures.

The **Cambridge Structural Database (CSD)** was established in over fifty years ago and now comprises over 950,000 entries which are available to anyone to view and retrieve. The CCDC enhances the CSD's value to research scientists worldwide through state-of-the-art software for advanced searching and analysis, receptor modeling, ligand design, docking, lead optimization and formulation studies. The CSD products are delivered to research organizations worldwide, including over 1,400 academic institutions and the world's top pharmaceutical and chemical companies.

The CCDC itself is a not-for-profit organization as well as being a UK Research Council Independent Research Organisation and a University of Cambridge Partner Institute. With over 50 years of scientific expertise, the CCDC has demonstrated its strong track record in research through more than 750 peer-reviewed publications.

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 more than 90 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 199,000 crystal structures. Updates are made twice a year (in spring and in fall) with data taken from scientific journals and other sources.