ICSD OFFERS

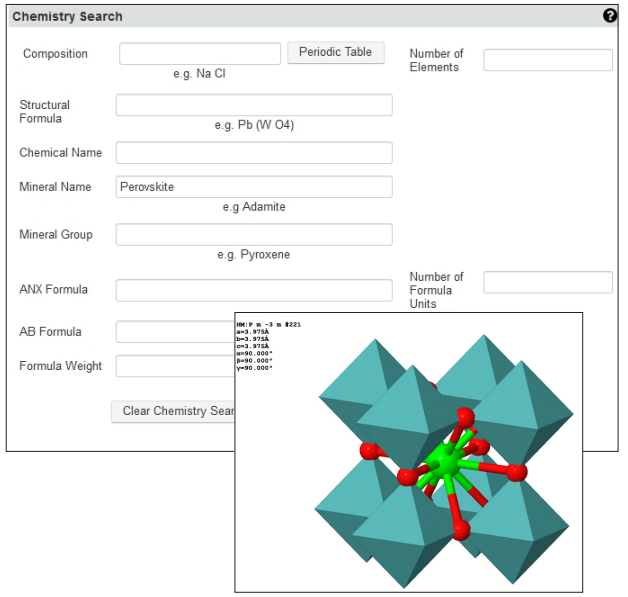
- All important crystal structure data, including unit cell, space group, complete atomic parameters, site occupation, Wyckoff symbols, ANX formula, mineral name/group, etc.
- Simulation of powder diffraction data
- Structure types as a sophisticated classification scheme
- Theoretical structures that can serve as a basis for developing new materials
- Keywords providing information about material properties, applications, and methodology
- Abstracts for a quicker grasp of the article content

ACCESS TO ICSD – OPTIONS TAILORED TO YOUR NEEDS

Customers may choose the way of accessing ICSD data which best suits their needs:

- ICSD Web: our web portal at https://icsd.fiz-karlsruhe.de
- ICSD Desktop: a Windows-based PC version.

  Typically used for local installations within smaller research groups
- ICSD Intranet: in-house solution for easy integration into corporate intranets
- ICSD API Service: allows to download large amounts of data for data mining projects



MORE INFORMATION

www.fiz-karlsruhe.de/en/icsd

ICSD
FIZ Karlsruhe

Zertifikat seit 2016
audit berufundfamilie

Leibniz Gemeinschaft

FIZ Karlsruhe – Leibniz-Institut für Informationsinfrastruktur GmbH
Hermann-von-Helmholtz-Platz 1 · 76344 Eggenstein-Leopoldshafen · Germany
Phone: +49 7247 808-555 · helpdesk@fiz-karlsruhe.de · www.fiz-karlsruhe.de
Februar 2024

ICSD
FIZ Karlsruhe

ICSD
RELIABLE CRYSTAL STRUCTURE DATA

FIZ Karlsruhe provides the scientific and the industrial community with ICSD (Inorganic Crystal Structure Database), the world's largest database for completely determined inorganic crystal structures.

Reliable crystal structure data of high quality play an important part in optimizing the development of new materials which foster innovation in various areas. Crystallographic data can serve to explain and predict material properties. Therefore, materials scientists are dependent on evaluated crystal structure data.

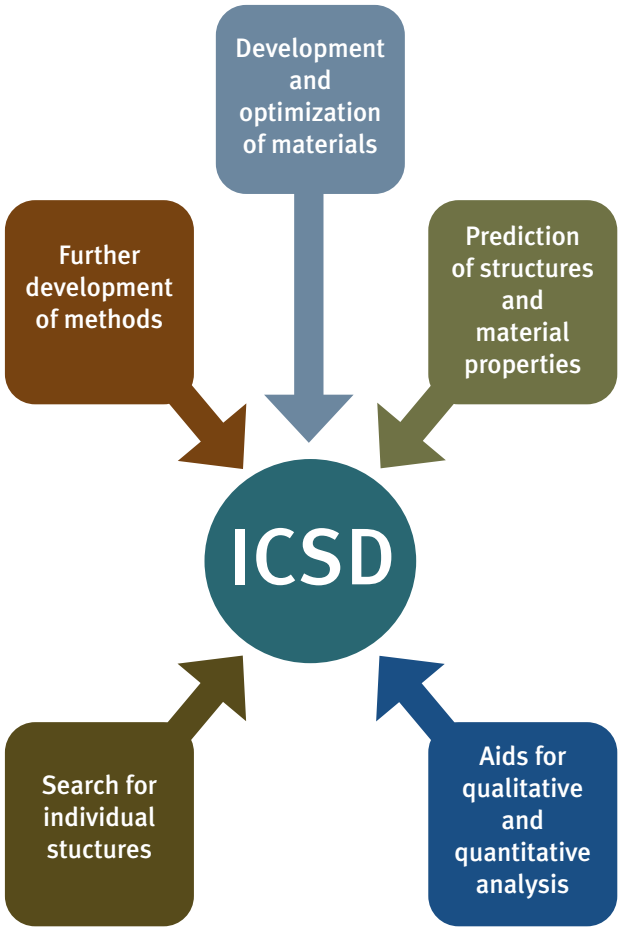
The ICSD data, comprising more than 290,000 peer-reviewed entries dating back to 1913, are of excellent quality. Only data which have passed thorough quality checks are included. About 16,000 structures are recorded annually and existing structures are regularly revised, corrected and updated.

ORGANOMETALLIC STRUCTURES

Recent advances in chemistry show that the distinction between inorganic and organic structures has become vague. This becomes more obvious in research areas on, for example, zeolites, catalysts, batteries, or gas storage systems.

This is why the scope of ICSD has been recently extended to organometallic structures. We now include pure inorganic structures plus organometallic structures where material properties are available or where inorganic applications are known. Biotechnological, medical or pharmaceutical contents are still not included.

NEW FIELDS OF APPLICATION



TRADITIONAL APPLICATION

We offer the following search functionalities:

- Group search for organometallic compounds
- Sum formula, linearized sum formula
- Compound name, name segments
- Elements, periodic groups, element count
- Text searches in abstracts
- Keywords for applications and material properties

THEORETICAL STRUCTURES

One can already observe a strong tendency to shift materials research from the traditional synthesis-oriented approach to a more theory-oriented approach. Especially crystal structure predictions become more and more reliable.

Therefore, FIZ Karlsruhe has already started to include theoretically calculated structures together with available material properties into the ICSD. This extends the typical use cases of ICSD to more data-mining based applications.

We offer some special search functionalities for theoretical structures:

- Group search for theoretical structures
- Calculation methods
- Technical details