

Details

Inorganic Crystal Structure Database (ICSD) (ICSD WEB)

FIZ Karlsruhe provides the scientific and the industrial community with the world's largest database for completely identified inorganic crystal structures, ICSD. The ICSD data are of excellent quality and its first records date back to 1913. Only data which have passed thorough quality checks are included. As the world's leading provider of scientific information on inorganic crystal structures, we take full responsibility for database production, maintenance and quality control, and we ensure that the ICSD database and our software solutions meet the highest possible quality standards. More than 12,000 new structures are added every year. Through our continuous quality assurance, existing content is modified, supplemented or duplicates removed. As a result, and by filling gaps from previous years, even the older content is not static.

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[To website](#)

Host Institution

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<https://www.fiz-karlsruhe.de/>

Scientific Domain

Primary Subjects:

- Chemistry
- Physics
- Geosciences (including Geography)
- Materials Science and Engineering

Secondary Subjects:

Category

Research data repositories

Scientific Services

The database (status Nov. 2020 > 232.000 entries) contains the following types of crystal structures: a) Experimental inorganic structures, which can be: - either fully characterized where the atomic coordinates are determined and the composition is fully specified - or the structure is published with a structure type so that the atomic coordinates and other parameters can be derived from existing data. b) Experimental metal-organic structures - only structures with known inorganic applications or where relevant material properties are available. c) Theoretical inorganic structures - Extracted from peer-reviewed journals - Showing a low E(tot) - Methods which lead to comparable experimental results. In particular, the database provides information on: - structural data of pure elements, minerals, metals, and intermetallic compounds - structural descriptors (Pearson symbol, ANX formula, Wyckoff sequences) - bibliographic data and abstracts - keywords on methods, properties and applications

Scientific Equipment

Keywords

- structural data

- pure elements
- minerals
- metals
- intermetallic compounds
- complete atomic parameters
- structure types
- theoretical data
- metal-organic structures
- material properties

Networks

Users per annum

Internal Users:

External Users in total: >1.000.000 Zugriffe

External Users:

External Users in the EU:

External Users outside of EU: