

Inorganic crystal structure database

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ICSD (Inorganic Crystal Structure Database) is the world's largest database for fully determined inorganic crystal structures. It is made available to the scientific community and industry by FIZ Karlsruhe. ICSD contains the crystallographic data of published crystalline inorganic structures, including atom coordinates, dating back to 1913. Organometallic and theoretical structures have been added within the past years. The ICSD data are of excellent quality. Only data that have passed thorough quality checks are included.

The ICSD database now contains more than 280,000 crystal structures. Around 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.

Highlights of ICSD:

- All important crystal structure data are available, including unit cell, space group, complete atomic parameters, site occupation factors, Wyckoff sequence, molecular formula and weight, ANX formula, mineral group, etc.
- 80 % of the structures are allocated to about 10,000 structure types. This allows for searches for substance classes.
- Continuous selection and evaluation of theoretical structures. They can serve as a basis for developing new materials through data mining processes.
- Keywords to describe to physical and chemical properties are provided.
- Abstracts for a quick grasp of the article content are available.
- Simulation of Powder Diffraction Data

Last year the revision of the mineral names took place, which included a standardization of the mineral names. The standardization of the mineral names was done following the International Mineralogical Association (IMA) and this enabled us to link mineral entries to the two mineral databases "webmineral.com" and "mindat.org", so that further information about the minerals can be retrieved.

For a large part of the minerals, we have also included the hierarchical classification. This makes it easier to find minerals in the same hierarchical level (or below) and thus can also be used in teaching for improved understanding.

Since the last update of ICSD, topological information is included in the database for about half of the inorganic structures in ICSD. As a first step, this information can be used to search for the coordination of a central atom. This coordination can then also be represented visually. The topological data provide much more information which will be made available in future updates.