

ICSD – Inorganic Crystal Structure Database

Evaluated crystal structure data of high quality

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, material testing laboratories and researchers at universities and research institutions are dependent on evaluated crystal structure data.

The ICSD data, comprising about 140,000 peer-reviewed entries including atomic coordinates dating back to 1913, are of excellent quality. Only data which have

passed through quality checks are included. About 7,000 new structures are recorded annually for ICSD, and the existing structures are regularly revised, corrected and updated.

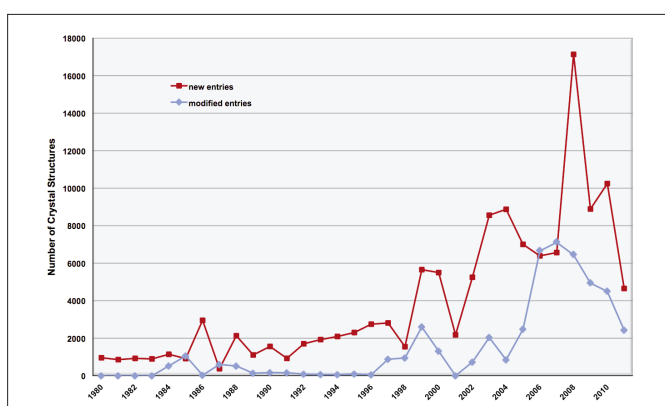
The number of modified structures has been raised extensively during the past. This included also the deletion of many duplicates, which had been incorporated into ICSD in the 1980s as a result of distributed update procedures among the partners.

About 90% of the entries in ICSD are represented by compounds with 2 - 5 elements.

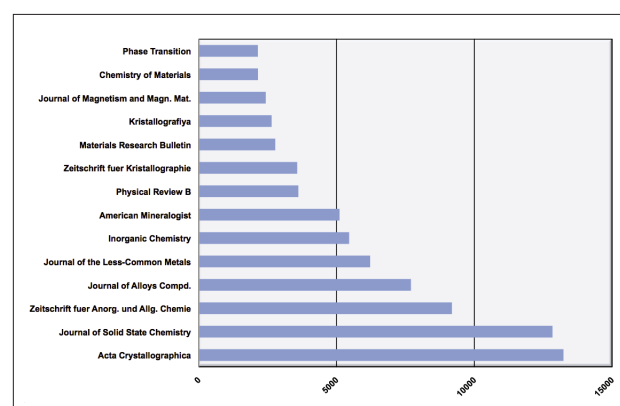
The atomic coordinates of all structures contained in ICSD have been fully determined or were derived from the corresponding structure types.

Structures in ICSD

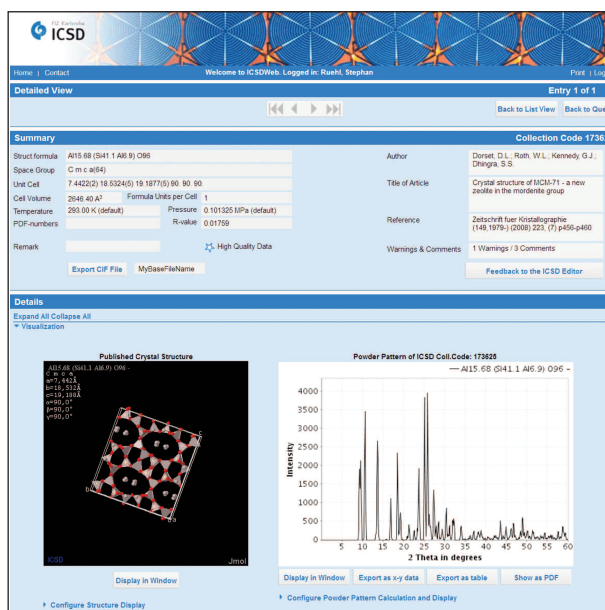
- do not have C–C and C–H bonds and
- do not include organic/heteroorganic cyclic systems



Input development in ICSD over the years 1981-2011.



The most relevant journals for ICSD.



Many options are available for display and analysis of results.

ICSD Web is available at <http://icsd.fiz-karlsruhe.de>

FIZ Karlsruhe's Crystal Structure Depot

The Crystal Structure Depot enables authors to store their extensive crystal structure data and to refer to the stored record(s) in their publications.

FIZ Karlsruhe started its depot more than 25 years ago for organic and inorganic compounds in printed form; today, only electronic data for inorganic compounds are stored in the depot.

Many publishers inform their authors that in parallel to a publication in a scientific journal, crystal structure data should also be stored in the Crystal Structure Depot at FIZ Karlsruhe. A CSD number will be assigned to the data for later reference in the publication. The data can then be ordered from the Crystal Structure Depot at FIZ Karlsruhe.

Access to the Crystal Structure Depot is free on request for scientists.

More information on FIZ Karlsruhe's Crystal Structure Depot is available at www.fiz-karlsruhe.de/crystal_structure_dep.html

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