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# THE INORGANIC CRYSTAL STRUCTURE DATABASE (ICSD) – PRESENT AND FUTURE

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The Inorganic Crystal Structure Database (ICSD) is a comprehensive collection of crystal structure entries for inorganic materials. ICSD is produced by Fachinformationszentrum Karlsruhe, Germany, and the National Institute of Standards and Technology, US. The WWW interface is developed in cooperation with the Institut Laue-Langevin, Grenoble. The ICSD is disseminated in computerized formats with scientific software tools to exploit the content of the database. ICSD includes records of all inorganic crystal structures with atomic coordinates published since 1913. The data base contains 70 102 records as of July 2003. All data are recorded by experts and are checked several times. Apart from updating, data integrity and completeness are important objectives. Incorporation of missing structures, evaluation and correction of data, with the help of authors, users and experts are ongoing activities. This review article gives an overview of the product portfolio and the current activities.

*Keywords:* Inorganic Crystal Structure Database (ICSD); Crystal structure; Database; Inorganic compounds

**Contents**



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## 1. INTRODUCTION

As the number of crystal structures determined increases, full exploitation of this higher throughput requires coherent access to the full range of structures. We describe here the primary implementation of this concept for inorganic structures.

The idea of the Inorganic Crystal Structure Database (ICSD) goes back to an initiative of Professor Günter Bergerhoff in 1978 at the Institute for Inorganic Chemistry of the University of Bonn, Germany (Bergerhoff and Brown, 1987). Between 1985 and 1989 ICSD was maintained with the collaboration of the University of Bonn and Fachinformationszentrum (FIZ) Karlsruhe, and from 1989 up to 1998 in a joint venture between the Gmelin Institute, Germany and FIZ Karlsruhe. Since 1997 ICSD is produced cooperatively by FIZ Karlsruhe, Germany, and the National Institute of Standards and Technology (NIST), US. ICSD is continually updated by FIZ Karlsruhe, a non-profit scientific organisation dedicated to collecting, editing and distributing crystal structure data. The production, quality control and general software development is done at FIZ Karlsruhe, the PC-Windows based graphical interface (FindIt) is generated under the responsibility of NIST. The WWW interface is developed in cooperation with the Institut Laue-Langevin, Grenoble. ICSD is a comprehensive collection of crystal structure information for non-organic compounds including inorganics, ceramics and minerals. Metals and intermetallic compounds will be incorporated in future. As of July 2003 (update 2003/1) the database comprises 70 102 records. The annual increase is about 4000 new entries delivered to users in two updates.

At about the same time as the database was initiated the mechanism of Crystal Structure Deposition (CSD) at FIZ Karlsruhe began. It started as an archive of crystal structure records, as important crystal structure information was found to be lacking in many relevant publications. Since then, many publishers provide footnote references to the crystal structure deposit of FIZ Karlsruhe, where additional structure information can be obtained on request using a CSD number. Since February 1999, there has been an agreement between the Cambridge Crystallographic Data Centre (CCDC) and FIZ Karlsruhe that all organic and organometallic compounds should be deposited at CCDC and all inorganic and intermetallic compounds at FIZ Karlsruhe. The deposited data are also required as input for the respective databases.

## 2. INFORMATION CONTENT

The ICSD contains information on compounds of all inorganic crystal structures including pure elements and minerals. Selection criteria for compounds are

– no C–C and C–H bonds in any of their residues
– contain at least one of the non-metallic elements H(D, T), He, B, C, N, O, F, Ne, Si, P, S, Cl, Ar, As, Se, Br, Kr, Te, I, Xe, At, Rn
– fully characterised structure
– atomic coordinates determined (though coordinates of hydrogen and vagabonding ions like sodium in zeolites may be missing)
– composition fully specified
– author, title and literature citation (or flag ‘private communication’)

Added by experts or generated by computer programs are

– Wyckoff sequence
– Pearson symbol
– molecular formula
– molecular weight
– calculated density
– element charge
– ANX formula
– minimum interatomic distances
– reduced cell information
– mineral group name

The entries in the database are characterised and can be retrieved by chemical identification data (name, formulae, mineral name and group), by bibliographic data (author, title, citation) and by crystallographic parameters (unit cell dimensions, space group, atomic parameters, thermal parameters and the reliability index R).

## 3. INPUT DATA FLOW

The data acquisition for the input into the database is done by scanning the original papers from relevant crystallographic journals (printed or electronic form), performing additional searches in the online databases, using information from CSD deposition and via direct contributions from authors and crystallographic experts. Even taking all these sources of information into account no one can be sure that everything has been found.

Original publications are excerpted from about 1200 journals. Each structure determination reported in the literature yields a separate record in the database. The following list reflects that most of the entries (41 862) come from 12 journals (data according to update 2003/1, July 2003 with 70 102 records):

| Journal Title | Entries |
|---|---|
| Acta Crystallographica | 8881 |
| Journal of Solid State Chemistry | 6842 |
| Zeitschrift f. Anorg. u. Allg. Chemie | 5691 |
| Zeitschrift für Kristallographie | 4120 |
| American Mineralogist | 2666 |
| Journal of Alloys and Compounds | 2524 |
| Inorganic Chemistry | 2071 |
| Zeitschrift für Naturforschung | 2017 |
| Kristallografiya | 1977 |
| Journal of the Less-Common Metals | 1792 |
| Materials Research Bulletin | 1704 |
| Physica C | 1577 |

After the data acquisition the data are excerpted by scientists, checked by computer programs and experts, further data not given in the original publication are added and the information is finally stored in a relational database format.

## 4. DATA EVALUATION

Data validation is an essential point in the whole input procedure. Various careful data checks have to be taken into consideration in this context. Data checking by computer is applied as far as possible. For this purpose, use is made of formal checking procedures, of plausibility considerations, of constraints following from mathematical and physical laws and of the fact that redundant data have to be consistent. The most important relations which are used for checks are

– Formal checking of:
  correct structure, missing field contents, plausibility, duplication, syntax

– Verification of contents:
  plausibility and validity of cell
  matching of cell and space group
  validity of oxidation state, multiplicity, site occupation, electroneutrality and molecular formula
  plausibility of isotropic temperature factors and interatomic distances

– Mineralogical nomenclature
– Authors spelling

Details of the data checking are described in an article by Behrens (1996).

## 5. ICSD AVAILABILITY

A major effort has been made during recent years to re-create the ICSD in relational database format. This format allows searches to be undertaken based on several criteria and fields that are not searchable in a flat-file format. By combining individual search conditions using Boolean operators, improved access to the stored data is possible. During this redesign additional improvements have been made to the content, for example, mineral names and associated mineral group names are now both included, space groups and symmetry record tables have been edited, the author names checked for unique spelling, and more than 9000 entries have been re-evaluated on an individual basis. We are indebted to Prof. Dr. R. Allmann who reviewed, supplemented and corrected many entries, and contributed many missing crystal structures. All versions available for our users (Windows-based PC version, internet/intranet version, database on STN International) are created from this relational database source.

### 5.1. PC Version – ICSD for Windows ('FindIt')

A recent Windows-based ICSD version on CD ROM replaced the DOS version with RETRIEVE in July 2002. This new software product is tabular in design and allows for searching in five general categories: Chemistry, Crystal Data, Reduced Cell, Symmetry and Reference Data. The software includes enhanced features for the characterisation of materials based on lattice search and chemistry search modules, and provides three-dimensional visualisation and powder pattern simulation for inorganic structures. Distances and angles can be calculated and export function allows download in CIF and a user-definable display format. Details are given

in a publication from Belsky *et al*. (2002). [A demo version of the PC-Windows version with 3380 records is available for downloading from the page: http://www.fiz-informationsdienste.de/en/DB/icsd/produkte.html.]

### 5.2. Internet/Intranet Versions

The WWW interface was developed with our partner Dr. Alan W. Hewat, Diffraction Group Leader at ILL Grenoble, who also provides a detailed online documentation. Access to the ICSD Internet Version is possible via a personal password or IP address. ICSD-for-WWW can display the VRML structures in three dimensions and also calculate, display and print X-ray and neutron powder diffraction patterns on-screen. In addition the output of a list of references in the Refer/BibIX format used by Endnote for Windows and Macintosh is possible. A demo database together with the WWW software may be freely downloaded from ILL and installed on your own WWW server, providing an ideal resource for teaching crystallography. [If you later purchase the full ICSD for WWW database from FIZ Karlsruhe (not the individual CD license), you may use this WWW software to make it available to your entire laboratory (according to your particular contract).] (To get an idea of the WWW version of the ICSD database, feel free to access the demo database at http://icsdweb.FIZ-karlsruhe.de.)

The Intranet Demo Versions (ftp://ftp.ill.fr/pub/dif/icsd/) can be installed on a local intranet server that supports PHP-MySQL and a WWW-server such as Apache. We recommend Suse Linux on a modern PC, but any other variety of Linux, Unix, Windows or Macintosh computer should also be able to run the new ICSD database server. [The PHP-MySQL WWW interface is copyright (2003) by Peter Hewat, while the three-dimensional crystal structure visualisation software, xtal-3d is copyright (1994–2003) by Marcus Hewat.] The Linux version has been made available by Dr. Alan W. Hewat (ILL) with help from Dr. Michael Wanitschek (MPI Stuttgart). These free versions are complete with powder pattern simulation and three-dimensional structure drawing, but contain only a subset of the complete ICSD database which must be licensed from FIZ Karlsruhe.

The retrieval options are equivalent to those of the PC FindIt version of ICSD. There are web pages with structure images made by M. Hewat that will give you an idea of the various possibilities of graphic display of crystal structures. Some of the applications require additional software which in many cases is available on the web for free downloading. The Internet/Intranet versions are completely redesigned at the moment and with the next update in July 2003 more on-line copies of journal articles will be available. You will then be able to generate queries to CrossRef and Litlink.

### 5.3. ICSD on STN International

Of course, ICSD can also be accessed through STN International. The data can be searched and displayed using the Messenger retrieval language, special features like the display of the structures are not supported.

## 6. FUTURE DEVELOPMENTS

The main focus in the future development of the ICSD will stay on accuracy and reliability of the data. Numeric properties currently available only in remarks will be extracted in separate search fields. In addition to the current input, the inclusion of metals and intermetallic phases will be undertaken by abstracting the original publications. With the help of expert colleagues we have also started to assign structure types to compounds in the database. The next ICSD release will show the first results of this effort. Colleagues with a special knowledge in this area are invited to offer comments and help in this task. The new Intranet/Internet version is based on MySQL and will contain hyperlinks to original publications. Bibliographic cross referencing and links to numeric properties and phase diagrams are under discussion and evaluation.

This overview may help to give an impression of the input and distribution policy of the ICSD database. We always have to find the right balance between cost-effectiveness and quality of a database as determined by completeness, accuracy and actuality. Any comments are welcomed. Please contact us under crysdata@FIZ-karlsruhe.de.

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