FIZ Karlsruhe

Leibniz Institute for Information Infrastructure

ADVANCING SCIENCE

SCIENTIFIC MANUAL 2021

ICSD DATABASE

ICSD is the world's largest database for fully determined inorganic structures. We want to support the community by offering an indispensable tool for materials science.

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GENERAL INFORMATION – INTRODUCTION

Find all important inorganic crystal structures
selected and curated from
more than 1.500 scientific journals worldwide

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 all 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.

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.

Around 12,000 new structures (inorganic, organometallic and theoretical) are added every year. Through our continuous quality assurance, existing content is modified and supplemented, and duplicates are removed. As a result, and by filling gaps from previous years, even the older content is not static. A summary of the current release is available at https://icsd.products.fiz-karlsruhe.de/en/about/about-icsd#facts+%26+figures+.

HIGHLIGHTS

- 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 9,000 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 physical and chemical properties are provided.
- Abstracts for a quick grasp of the article content are available.
- Simulation of Powder Diffraction Data

ACCESS OPTIONS

The following ICSD versions are available:

ICSD Web
ICSD Desktop
ICSD Intranet
ICSD API

All four versions use the same technology: The interface runs on a web server (Tomcat), which runs either at FIZ Karlsruhe (ICSD Web) or at the user's site (ICSD Desktop and ICSD Intranet). In any case, the interface is accessed with a browser. The user-friendly interface is easy to navigate with up-to-date features:

- intuitive search interface
- extensive classification in structure types, which are searchable based on descriptors defining each structure type
- structure standardization for easier comparison with other structures
- extended crystal structure visualization and analysis tools
- powder pattern simulation with the possibility of enhanced manipulation
- simple but powerful query management
- direct links to the original literature via OpenURL server

The data are encrypted and can only be accessed via the interface or ICSD API.

ICSD WEB

ICSD Web is a service enabling web access to ICSD. Its servers run at FIZ Karlsruhe and can be accessed with a common browser and an appropriate license. Authentication for single users and multiple users is handled by logins/passwords. Campus/Site users are authenticated based on their IP address; in addition, users can create personalized accounts while being IP authenticated to store searches and preferences. The advantage of the web installation is that you have access to the database regardless of where you are working.

ICSD DESKTOP

ICSD Desktop is a Windows-based solution for individual users as well as small research groups that would like to install ICSD locally on their computer/laptop. The advantage of a local installation is that you are independent of any network connection.

ICSD Desktop installs stripped-down servers to run the required services on the local machine. Access from other machines is prohibited. The software as well as the database has to be installed on each computer. Access via a network is not possible.

ICSD INTRANET

ICSD Intranet is an in-house solution based on the ICSD Web technology. It allows users to offer their own web-based access to ICSD within their university or company. Authentication is performed via a separate LDAP module, but can also be integrated into an existing LDAP solution.

API LICENSE

For applications with a large demand for structures (e.g. data mining projects) the regular ICSD licenses to ICSD Web/Desktop/Intranet may not be optimal, as there are limitations regarding the CIF export depending on the license. For example, a Campus license allows the export of a maximum of 20,000 CIF files per year. If more structures are needed for a project, the ICSD API allows the user to use unlimited CIF files for the project. With the API, searches can be performed using an advanced search language.

The API license is personalized and project-bound. To use the API license you need a regular ICSD license. For the use of the API license an additional agreement between the customer and FIZ Karlsruhe has to be concluded. The basis for this agreement is information regarding the users and the project for which the data is used.

UPDATE

The ICSD is updated twice a year. The updates take place in the second and fourth quarters. Relevant crystal structures are included as quickly as possible. However, due to the complex evaluation process and the amount of relevant crystal structure data, time delays occur and journals are prioritized. Crystal structure data that has already been recorded is only visible to the customer after the update has been carried out.

TERMS OF USE FOR THE PRODUCTS

FIZ Karlsruhe's general terms and conditions for licensing the ICSD are available at https://icsd.products.fiz-karlsruhe.de/en/support/support#terms+%26+conditions .

The general terms and conditions for the API license area available at: https://icsd.products.fiz-karlsruhe.de/sites/default/files/ICSD/documents/terms/ICSD_API_License_2019.pdf.

DEPOT CCDC /FIZ KARLSRUHE; DEPOSITING CIF FILES

"Access Structures" is a free service provided by CCDC and FIZ Karlsruhe. With this service, customers can deposit, display and access crystal structures. Access Structures is available at: https://www.ccdc.cam.ac.uk/structures/.

The structures deposited in the depot as cif files are not automatically transferred into the ICSD.

The following link explains how the structures can be deposited: https://www.ccdc.cam.ac.uk/deposit.

WHAT KIND OF STRUCTURES ARE INCLUDED AND SINCE WHEN?

ICSD contains the following types of crystal structures:

Experimentally determined inorganic structures
Experimentally determined organometallic structures
Theoretically calculated inorganic structures

When crystal structure data from relevant journals are recorded in ICSD, the main focus is on inorganic crystal structures. The inorganic crystal structure data are selected by reviewing more than 30 peer-reviewed journals and additionally by evaluating a search in specialized databases. Inorganic structures also include metals and intermetallic compounds, which were increasingly recorded from 2003 onwards. Data were also recorded retroactively. From 2003 onwards, structures containing C-H bonds or C-C bonds were also included, e.g. compounds with tetramethylammonium were included as well as oxalates. Recording these structures is a first step leading to the inclusion of organometallic structures.

EXPERIMENTAL INORGANIC STRUCTURES

As a rule, only completely determined inorganic structures, i.e., structures for which the atomic coordinates and all other required crystallographic information are given, are recorded. In addition, there are two special cases when the cell and the associated structure type have been determined in the experiment, but the individual atomic coordinates have not. Provided that the atoms of the associated structure type are consistently located on special positions with exact positions (e.g., 0, 0, 0 or ½, ½, ½), these structures are also recorded as completely determined. However, it can also happen that the positions of the atoms in a structure type have degrees of freedom (e.g., 0, y, ½). In this case, the structure is not completely determined, because the y-coordinate was not determined experimentally. Such structures can still be included in ICSD if the number of degrees of freedom is not too large. The structure is then defined by the experimental lattice parameters and the corresponding structure type that provides the missing crystallographic data, and is included in ICSD. The missing atomic coordinates derived from the type of another structure, whereby the atomic coordinates are entered without standard deviation and only with three digits after the decimal point.

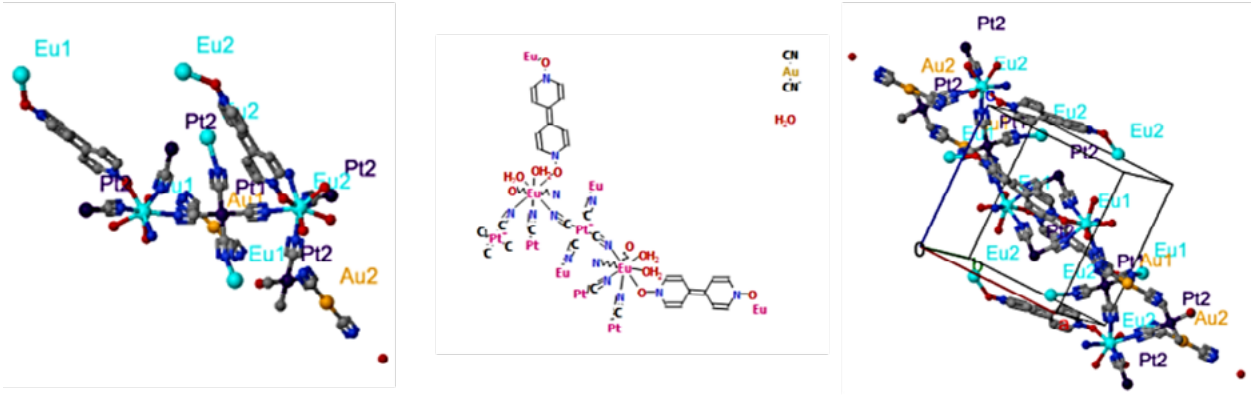
ORGANOMETALLIC STRUCTURES

Due to the increasing overlap of inorganic chemistry with organic chemistry, the regulations for recording crystal structures were extended. This was favored by the collaboration with the Cambridge Crystallographic Data Centre (CCDC). Thus, organometallic crystal structures have also been included since 2018. The relevance decision regarding the organometallic structures is made exclusively by reviewing a few particularly relevant ICSD journals. Since a large number of organometallic structures are published annually, some limiting rules have been set for the relevance decision regarding these structures.

The goal is to evaluate organometallic structures with a large inorganic part for the database. Pure organic structures will not be included. Pure organic structures include structures that contain all of the following elements: carbon, hydrogen, oxygen and nitrogen. Sulfur, phosphorus, chlorine, fluorine, or boron may also be contained.

The organometallic structures to be covered should contain at least 3 metals/semi-metals. Organometallic structures containing 2 metals can also be detected if the inorganic portion is relatively larger than the organic portion due to oxygen, sulfur or nitrogen. This is a borderline case.

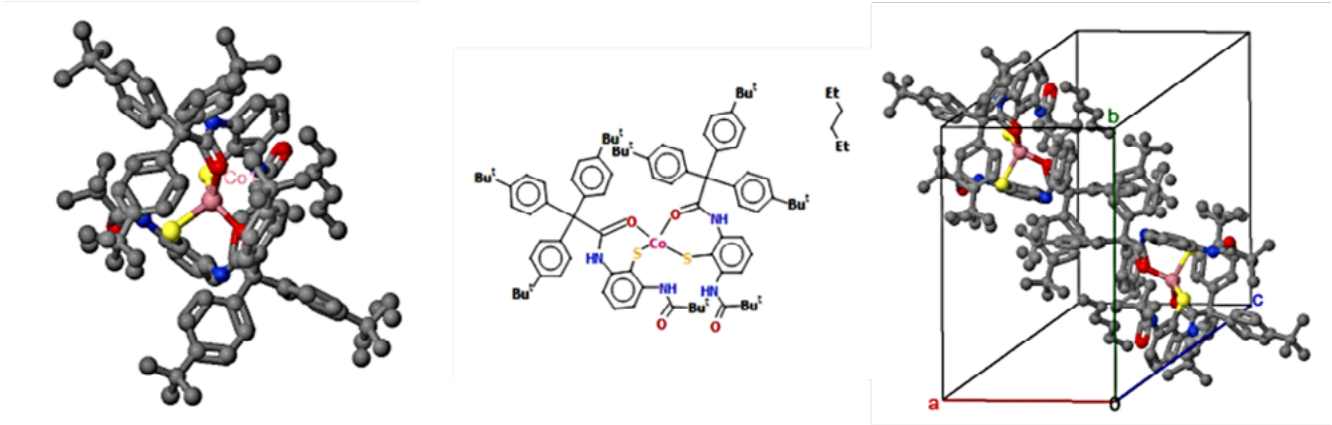
CCDC: 1921618 **Trimetallic Cyanido-Bridged Coordination Frameworks** **relevant**



Jakub J. Zakrzewski, Barbara Sieklucka, Szymon Chorazy,
Europium(III) Photoluminescence Governed by d^8–d^{10} Heterometallophilic Interactions in Trimetallic Cyanido-Bridged Coordination Frameworks
Inorganic Chemistry, 2020, 59, 1393, DOI: 10.1021/acs.inorgchem.9b03114

If publications contain several structures, only the structures containing at least 3 metals/semimetals or 2 metals with a larger inorganic part are recorded. The other structures are not recorded.

CCDC: 1951665 **Bis(arenethiolato)cobalt(II) Complex** **not to include**



Taka-aki Okamura, Yusuke Tomita, Kiyotaka Onitsuka,
Crystal-to-Crystal Isomerization via Drastic Intramolecular Ligand Exchange: Vapochromism of a Bis(arenethiolato)cobalt(II) Complex Containing Bulky Acylamino Groups
Inorganic Chemistry, 2019, 59, 1164, DOI: 10.1021/acs.inorgchem.9b02791

THEORETICAL STRUCTURES

The experimental approach is no longer the only way to discover new compounds and structures. There are numerous computational methods for simulating and predicting structures of inorganic solids, which have produced a large amount of theoretical crystal structure data. Based on these developments, theoretically calculated inorganic crystal structure data have also been included in the ICSD since 2016. The theoretically calculated structures are evaluated and included by Dr. Dejan Zagorac , Head of the Laboratory for Theoretical Investigations of Materials at the Institute of Nuclear Sciences, Vinča, University of Belgrade, and his team.

HOW ARE RELEVANT ARTICLES REVIEWED?

Finding the long-tail of articles with crystallographic structure data makes the difference. In ICSD you can find structures from more than 1.600 journals

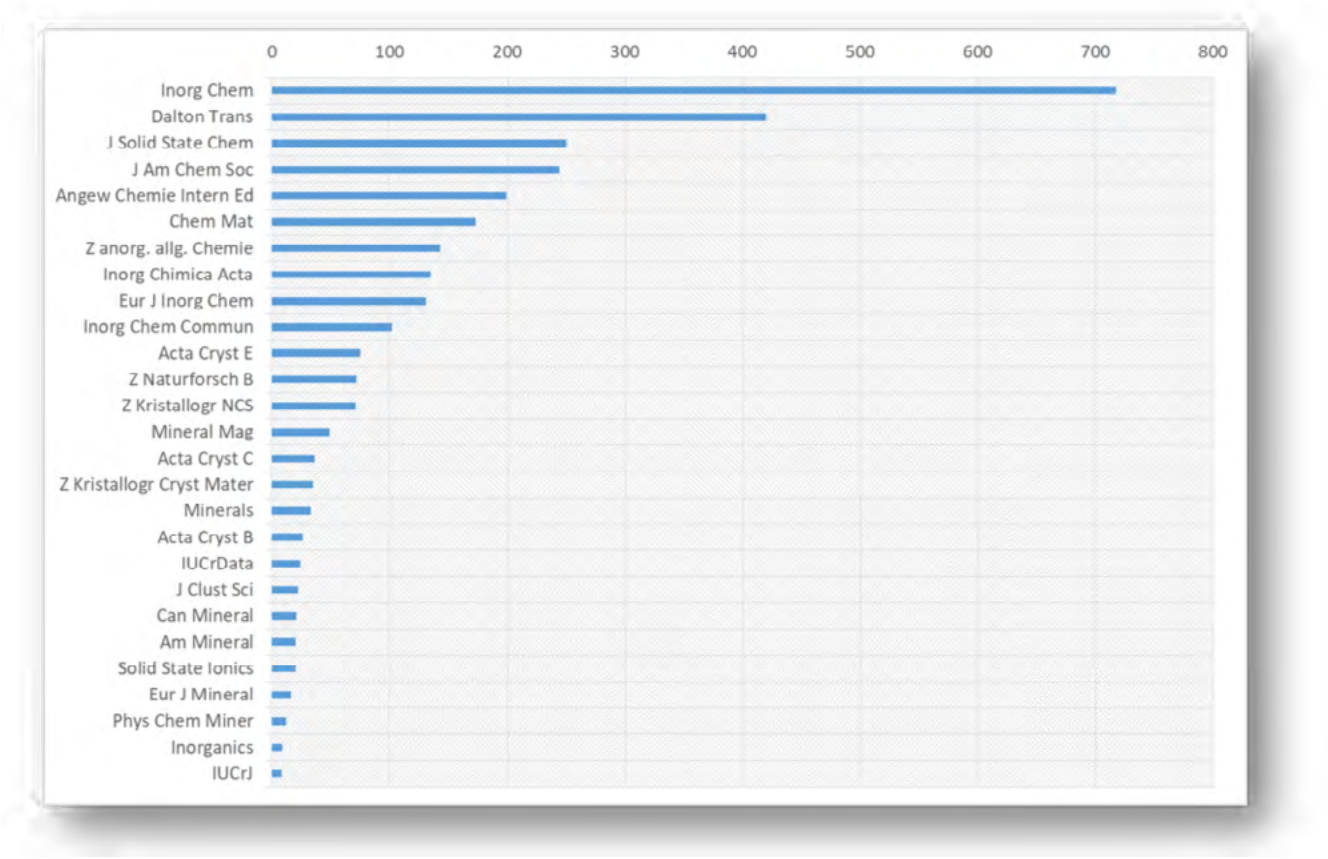
To identify relevant articles from literature, articles from relevant journals are reviewed and additional searches are carried out in databases for scientific literature. The latter mainly serves to find crystal structures published in journals that do not cover the core area of ICSD. New publications from major publishers worldwide are also regularly monitored and evaluated. The relevance decision is supported by directly inspecting possibly relevant structures in the crystal structure data repository "Access Structures". This is especially helpful in order to decide which organometallic structures are relevant. At present, more than 30 journals are checked for relevance this way; all other journals are covered by regular searches in Chemical Abstracts.

LIST OF JOURNALS ON THE HOMEPAGE

- List of the 80 most important journals: https://icsd.products.fiz-karlsruhe.de/en/about/list-80-most-important-journals-covered-icsd
- Journal list for theoretical structures: https://icsd.products.fiz-karlsruhe.de/en/about/theoretical-structures-journal-list

FEEDBACK ON RELEVANT CRYSTAL STRUCTURE DATA

Information on publications with relevant crystal structures can be sent directly to icsd@fiz-karlsruhe.de. This can speed up the recording of the data in ICSD a bit.



NUMBER OF RELEVANT ARTICLES IN 2020 FOR THE REGULARLY EVALUATED JOURNALS

DATA CURATION

In the process of adding a structure to the database, a series of tests are run to verify data integrity and correctness. Furthermore, the data is enriched with additional or missing information.

WHAT CHECKS ARE CARRIED OUT ONCE THE CRYSTAL STRUCTURE DATA HAVE BEEN ENTERED INTO MYICSD?

Published crystal structures are recorded in the ICSD database “as given in article”. This is in line with the long-standing objective of the ICSD to “map” the literature. There are no conversions of “unusual” space group setups in particular, since authors often choose an unusual space group to emphasize an important statement in the article.

Users can also view and search for the standardized structure. Both structures (published and standardized) are available as cif files for download.

The following data are often missing in publications and are generated in addition:

- Wyckoff Sequence
- Pearson Symbol
- ANX Formula
- AN Formula
- Sum formula
- Structure types
- Standardized data
- Density
- Atom distance

We include the measured densities (if the information is available) and compare the measured with the calculated values (TestCode23).

The program also checks the following data:

- Sum formula
- Oxidation numbers
- Charges
- Space group
- R values
- Isotropic and anisotropic temperature functions

AUTOMATIC PLAUSIBILITY CHECKS

The plausibility of the space group is checked (TestCode 55). If there are discrepancies, a corresponding note is inserted automatically in the database.

If R value (TC 51), isotropic and anisotropic temperature factors (TC 53) are not available, then a corresponding comment is generated, which is then also visible in the database. Likewise, a comment is generated if the values are not within plausible limits (TC52).

The list below summarizes the automatically generated comments:

21	Deviation of the nominal from refined formula tolerable.
22	Deviation of the charge sum from zero tolerable.
23	Deviation of calculated from measured density tolerable.
51	No R value given in paper.
52	At least one temperature is implausible or meaningless
53	At least one temperature factor missing in the paper.
54	A site occupation is implausible or meaningless
55	Deviation of lattice parameters from crystal system tolerable
74	Coordinates in the paper are obviously wrong

STRUCTURE FORMULAE

For the inorganic crystal structure data, the structural formulas are structured and the charge sums are checked for agreement. The program defines a standard oxidation number for the different elements, but this can be individually adjusted at any time. In isolated cases, the hydrogens or water of crystallization in the structure under investigation are not determined or are determined incompletely. This has the consequence that the nominal sum formula (given by the author) and the calculated ("refined") sum formula differ from each other, and as a consequence also the charge sums are not balanced. In this case, "dummy atoms" are inserted to equalize the stoichiometries between nominal and refined formula.

With organometallic crystal structure data, the molecular formulae are not structured, due to the complexity of the chemical composition. Also, the oxidation numbers of the individual elements are set to 0, whereby a formal balance of the charge sums is always achieved.

ANISOTROPE DISPLACEMENT PARAMETERS

Anisotropic displacement parameters are given in one of the following three different forms:

1. ß(max 8 characters)
   $\exp(-(h^2ß_{11} + k^2 ß_{22} + l^2 ß_{33} + 2hk ß_{12} + 2hl ß_{13} + 2kl ß_{23}))$
   with standard deviations if given.

2. *B* (max 8 characters each)
   $\exp(-1/4(h^2B_{11}a^{*2} + k^2B_{22}b^{*2} + l^2B_{33}c^{*2} + hkB_{12}a^*b^* + klB_{23}b^*c^* + hlB_{13}a^*c^*))$
   with standard deviations if given.

3. U (max 8 characters each)
   $\exp(-2\varpi^2(h^2U_{11}a^{*2} + k^2U_{22}b^{*2} + l^2U_{33}c^{*2} + 2hkU_{12}a^*b^* + 2klU_{23}b^*c^* + 2hlU_{13}a^*c^*))$
   with standard deviations if given.

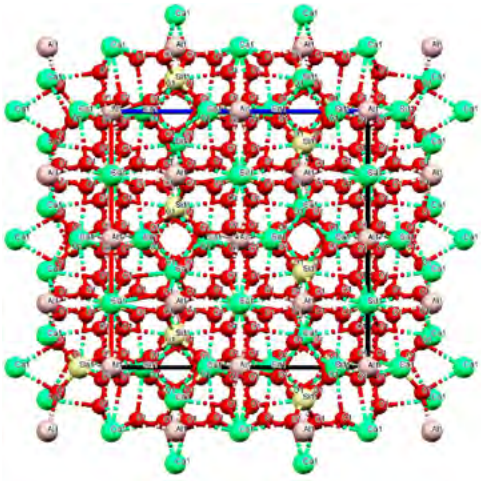
Published Crystal Structure Data

Cell parameter	11.917(4) 11.917(4) 11.917(4) 90. 90. 90.	Space group	I a -3 d (230)
Cell volume	1692.39 Å³	Z	8
Crystal system	cubic	Crystal class	m-3m
Laue class	m-3m		
Structure type	Garnet#Ca3Al2Ca3Al2(SiO4)3		
Pearson symbol	cl160		a/b b/c c/a
Wyckoff sequence	h d c a	Axis ratios	1.0000 1.0000 1.0000
Calc. density	3.54 [g/cm³]		

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	B
Ca	1	+2.00	24 c	0	0.25	0.125	1	
Al	1	+3.00	16 a	0	0	0	1	0.94
Si	1	+4.00	24 d	0	0.25	0.375	1	
O	1	-2.00	96 h	0.0381(5)	0.0450(5)	0.6515(4)	1	

EL	Lbl	Beta(1,1)	Beta(2,2)	Beta(3,3)	Beta(1,2)	Beta(1,3)	Beta(2,3)
Ca	1	0.00089(35)	0.00264(43)	0.00264(43)	0	0	0.00001(30)
Si	1	0.00209(57)	0.00209(57)	0.00110(51)	0	0	0
O	1	0.00233(35)	0.00208(34)	0.00148(31)	-.00008(33)	0.00002(30)	0.00021(30)

CRYSTAL STRUCTURE DATA OF A GARNET STRUCTURE CALLED GROSSULAR WITH THE COLLECTION CODE (CC) 24946 COPIED FROM ICSD.



CRYSTAL STRUCTURE OF GROSSULAR (CC24946)

GROSSULAR, PHOTO: ROB LAVINSKY, IROCKS.COM

https://de.wikipedia.org/wiki/Grossular#/media/Datei:Grossular-137781.jpg

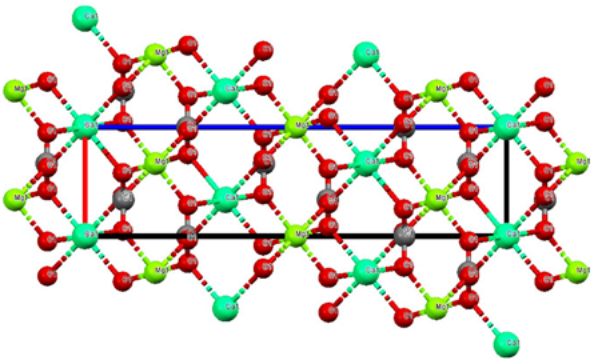
▾ Published Crystal Structure Data

Cell parameter	4.8033(9) 4.8033(9) 15.984(4) 90. 90. 120.	Space group	R -3 H (148)
Cell volume	319.37 Å³	Z	3
Crystal system	trigonal	Crystal class	-3
Laue class	-3		
Structure type	Dolomite#CaMg(CO3)2		
Pearson symbol	hR10		
Wyckoff sequence	f c b a	Axis ratios	a/b 1.0000 | b/c 0.3005 | c/a 3.3277
Calc. density	2.88 [g/cm³]	Meas. density	2.9 [g/cm³]

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	TF
Ca	1	+2.00	3 a	0	0	0	1	
Mg	1	+2.00	3 b	0	0	0.5	1	
C	1	+4.00	6 c	0	0	-.2423(2)	1	
O	1	-2.00	18 f	0.2829(3)	0.0350(4)	-.24397(9)	1	

EL	Lbl	Beta(1,1)	Beta(2,2)	Beta(3,3)	Beta(1,2)	Beta(1,3)	Beta(2,3)
Ca	1	0.0055(5)	0.0055(5)	0.00038(7)	0.00275(25)	0	0
Mg	1	0.0041(9)	0.0041(9)	0.0004(1)	0.00205(45)	0	0
C	1	0.0050(15)	0.0050(15)	0.0001(1)	0.00250(75)	0	0
O	1	0.0041(19)	0.0100(15)	0.0008(1)	0.0041(15)	-.0003(1)	-.0009(1)

CRYSTAL STRUCTURE DATA OF A CARBONATE STRUCTURE CALLED DOLOMITE WITH THE COLLECTION CODE (CC) 10404 COPIED FROM ICSD



CRYSTAL STRUCTURE OF DOLOMITE (CC10404)

DOLOMITE (WHITE) AND MAGNESITE, PHOTO: DIDIER DESCOUENS

https://de.wikipedia.org/wiki/Dolomit_(Mineral)#/media/Datei:Dolomite-Magn%C3%A9site-_Navarre.jpg

OXIDATION STATES

From the atomic coordinates the program calculates a sum formula, which should agree with the entered sum formula. With inorganic entries, the sum formula is structured intellectually. If these two sum formulas do not match, a comment is automatically generated (see list of automated test codes below) and inserted.

The oxidation numbers of the elements are assigned automatically. If the positive and negative charge sums do not match, then the oxidation numbers of the individual elements are changed manually.

It is also possible to specify an average oxidation number for a given element (average charge calculation is triggered), in which case a corresponding comment is generated. In some cases, the hydrogen from the present water is not specified in the refinement, but in the structural formula. Here the missing hydrogens can be added. If the positive and negative charges do not match, a corresponding comment will be visible in the database at the respective entry.

R VALUES

Of course, the R value can only be specified if it is quoted in the present publication. The definition of the R value is then entered in the Comment field. The message "R value is missing" is automatically inserted when the entry is set to productive.

EXAMPLE

R = R(wp)

ATOMIC COORDINATES, ISOTROPIC DISPLACEMENT PARAMETERS, SITE OCCUPATION, BONDED H-ATOMS

The atomic coordinates x, y, z are given with a maximum of 7 characters each. The isotropic displacement (temperature) factor is given as "B" if defined by

$$\exp(-B (\sin^2 \theta)/\lambda^2)$$

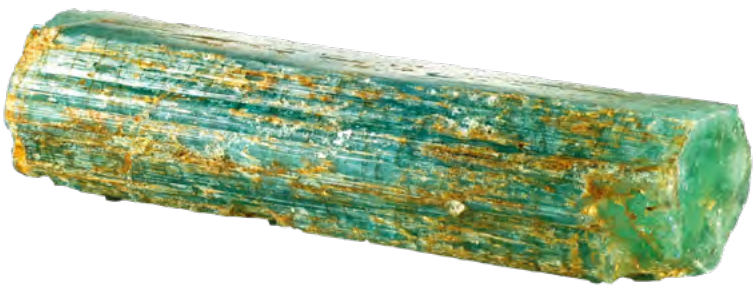
or "U" if defined by

$$\exp(-8\pi^2 U (\sin^2 \theta)/\lambda^2) .$$

Since 2003 isotropic and anisotropic temperature factors are given if both are available. Older records contain either isotropic or anisotropic temperature factors (if anisotropic temperature-factors are available). Displacement factors may have a maximum of 6 characters. The site occupation (max 5 characters) describes the statistical occupation of the site, i. e. the quotient of the actual amount of atoms and the maximum number of positions of the site. A special remark is generated for defect structures with SOF < 1. They need a special treatment when the Pearson symbol or the ANX formula is generated (see chapter 4). The number of undetermined H atoms bonded to another atom (e. g. H bonded to O in H_2O, or N in NH^{4+}) is noted.

FEEDBACK ON RECORDED CRYSTAL STRUCTURE DATA

Discrepancies may occur in the recorded crystal structure data despite multiple checks. Discrepancies include, for example: errors in writing the article by authors or in recording the structures by FIZ Karlsruhe. They can be reported to icsd@fiz-karlsruhe.de. Until the next update, the discrepancies will be corrected.



REMARKS

There are standard remarks, free text remarks, and test remarks that are messages from the test program. The standard remarks consist of three characters. They are searchable and listed below. Please note that the remarks TEM (temperature in K) and PRE (pressure in MPa) contain numerical values and will be made numerically searchable in future updates. All remarks will be displayed in a full sentence.

Standard remarks and the related full text that may be completed by additional information if available:

ABC	Absolute configuration given
AHT	Anharmonic temperature factors given
COA	Published data has been corrected through correspondence with the author
COR	This publication corrects errors in an earlier one
DIS	Disordered structure that cannot adequately be described by numerical parameters
EDP	Electron diffraction (powder)
EDS	Electron diffraction (single crystal)
EMP	Electron microscopy of a single powder particle
ESC	Electronic structure calculations
MAG	Magnetic structure also determined
MIN	Compound with mineral name
MOD	Modulated structure or misfit-layer structure
NDP	Neutron diffraction (powder)
NDS	Neutron diffraction (single crystal)
NMR	NMR spectroscopy data given
ODS	Order-disorder structure
PDF	The structure has been assigned a PDF number
POL	Polytype structure
PRE	Pressure in MPa
RVP	Rietveld profile refinement applied
SFP	Structure determined from projections
SNP	Synchrotron radiation (powder)
SNS	Synchrotron radiation (single crystal)
TEM	Temperature in Kelvin
THE	Structure calculated theoretically
TWI	Structure determined on a twinned crystal
XDP	X-ray diffraction (powder)

In addition to the standard remarks there is a free text field for additional comments (e. g. cells of isomorphic compounds if given in the paper).

REFERENCES

References in ICSD only quote the initial publication. References in ICSD contain the following information:

- Title of the publication
  The Title of the publication is given in English, French or German.
- Citation
  The citation includes the year, the CODEN (with check-letter) for journals, volume, first page and last page.
- Authors
  The surname is given followed by the initials of the first name. Some authors may be written differently depending on the language of the publication, e. g., Gladyshevskii (in Russian) or Hladyshevsky (in Ukrainian). In a few cases in Chinese author names first or last name may be interchanged. Please inform us about any wrong writings.
- DOI
  The Digital Object Identifier for the article is retrieved through CrossRef or supplied by the publisher and inserted in the reference of ICSD as a link to assure direct access to the full text
- Article ID
  Several online-only journals publish articles that have article numbers. In those cases an article ID number will usually replace the familiar pagination because this numbering system simplifies the publication process. In cases where we can define a page number, we will include it in addition to the Article ID.

MINERALS

The names of minerals are included according to the publication. The names acknowledged by the IMA are listed in an additional field if they are available.

We distinguish between natural and synthetic minerals. In the case of natural minerals, the place of discovery is also mentioned.

EXAMPLES

CC10404
Mineral name: Dolomite
Mineral origin: Binnenthal, Switzerland

CC16916
Mineral name: Anglesite
Mineral origin: Monte Poni, Sardinia, Italy

CC24946
Mineral name: Grossular
Mineral origin: Asbesto, Quebec, Canada

CHEMICAL NAMES

This field contains the chemical name in English with oxidation state where necessary and corresponding to the first formula. This formula is calculated from all atoms with defined atomic coordinates. If undetermined atoms are included a remark is displayed in the atomic coordinates list. Oxidation state is given in Roman numbers.

Phase information may be given after the hyphen. If two structures seem to be identical and have slight differences only due to special conditions details are given after a hyphen (e. g. doped material).

EXAMPLES

CC10404 Calcium magnesium dicarbonate
CC16916 Lead sulfate(VI)
CC24946 Tricalcium dialuminium silicate

The chemical name for organometallic compounds is very complex. In the case of organometallic compounds, only parts are also used as the chemical name.
In most cases, the chemical name is taken from the corresponding publication. The chemical name does not always correspond to the IUPAC standards.

HERMANN–MAUGUIN SPACE GROUP SYMBOL

This symbol is used according to the International Tables for X-Ray Crystallography. If different origin choices are available, those space groups with origin at center are characterized by an additional “z”, while an additional “s” is being used for special origins. Rhombohedral space groups with hexagonal cells are marked with an additional “h” (“hr” for reverse setting). Full symbols are used for monoclinic space groups to show the choice of the unique axis.
For all other space groups a list of coordinate triplets of a general position is given. Space groups that are not included in the International Tables need a critical evaluation. In a numerical database, a space group “F1$\bar{3}$2/m” may cause some trouble in statistical searches. It should be replaced by R$\bar{3}$mH (with 3/4 volume).

EXAMPLE

CC10404	R$\bar{3}$H
CC16916	Pnma
CC24916	Ia$\bar{3}$d

ANX FORMULA

The ANX formula is generated according to the following rules:

- H+ is not taken into account, even if coordinates are available.
- The coordinates for all sites of all other atoms must be determined.
- Different atom types on the same position (e. g. for solid solutions) are being treated as

one single atom type. The relevant atom type is the one with the highest site occupation factor. If the SOFs are equal the first atom type is the relevant atom type.

- Exception to this rule: if anions and cations occupy the same site they will not be treated as one atom type.
- All sites occupied by the same atom type are combined unless the oxidation state is different.
  $Fe^{2+}(Fe^{3+})_2O_4$ → AB2X4
  $(Fe^{2.6667+})_3O_4$ → A3X4
- For each atom type the multiplicities are multiplied by the SOFs and the products are added. The sums are rounded and divided by the greatest common divisor.
- If the rounded sum is equal to zero all sums are multiplied by a common factor so that the smallest sum is equal to 1.0, so no element will be omitted.
- Cations are assigned the symbols A–M, neutral atoms N–R and anions are assigned X, Y, Z, S–W.
- The symbols are sorted alphabetically and the characters are assigned according to ascending indices: AB2X4, not A2BX4.

All ANX formulae with more than 4 cation symbols, 3 neutral symbols or 3 anion symbols are deleted. This measure limits the number of different ANX formulae.

EXAMPLE

Structural formula		ANX formula
CC10404	$CaMg(CO_3)_2$	ABC2X6
CC16916	$Pb(SO_4)$	ABX4
CC24946	$Ca_3Al_2(SiO_4)_3$	A2B3C3X12

PEARSON SYMBOLS

Three datasets are required to create a Pearson symbol:

1. Symbol for the crystal system
   - a = triclinic (anorthic)
   - m = monoclinic
   - o = orthorhombic
   - c = cubic
   - h = trigonal
   - h = hexagonal
   - t = tetragonal

- 2. Symbol for Bravais-Type
- P = primitive
- F = face centered
- I = body centered
- R = rhombohedral

In ICSD the older A, B, C notation for Pearson symbols has been substituted by "S" symbol (one side centered) for monoclinic and orthorhombic space groups (for monoclinic also I). This way the Pearson Symbol has become independent of the cell transformations.

3. The number of atoms in the unit cell

This number is calculated from the sum of all multiplicities and the respective site occupation factors for each atom type. The data are rounded. The number of atoms rhombohedral space groups depends on the trigonal or hexagonal setting of the space group. In ICSD the number of atoms in hexagonal settings of rhombohedral space groups should be divided by 3 to match the data from Pearson's Handbook and to get numbers invariant to cell transformations.

EXAMPLE

CC10404	hR10
CC16916	oP24
CC24946	cI160

WYCKOFF SEQUENCE

Sites with SOF < 1 are treated in analogy to the treatment for the ANX formula (see above). Symmetrically equivalent sites (represented by a Wyckoff letter) are counted, and the number is given along with the Wyckoff letter.

The Wyckoff letters are sorted alphabetically (descending sort) and written along with their number, each new Wyckoff letter is separated by a blank.

EXAMPLE

CC10404	f c b a
CC16916	d c4
CC24946	h d c a

This sequence is not unique, but depends in some space groups on the choice of origin. E.g., for spinels the sequence changes from "f d a" to "f c b" after an origin shift of ½ ½ ½.

STRUCTURE TYPES

Structure types were introduced into ICSD in 2007 as an approach to describe structural similarity between inorganic structures. This is still an ongoing process, i.e. quality enhancements resp. introducing new types is continuously in progress in the background. ICSD structure types may best be classified as "isoconfigurational", according to the definition by IUCr [1]. In this definition, isoconfigurational structures must conform to certain structural parameters (descriptors) like:

- Space group
- Pearson symbol
- Wyckhoff sequence
- ANX formula

Of these descriptors the Wyckhoff sequence is crucial, because it describes the atomic arrangement in the unit cell. Each structure type is defined by a set of some or all or even more than of the listed descriptors, as has been explained in detail in [2].

In the ICSDWeb interface just the most basic descriptors (the listed ones above) are available for searching in the ICSD database, whereas the assignment of type information indeed is realized in a batch procedure step for each new ICSD update. This data mining process makes use of more than the previously listed descriptors. The total list of descriptors is shown in the Excel file, see information box).

In this listing there appear further important descriptors as c/a-ratio, monclinic angles, chemical restraints (forbidden elements), and essential for correct labelling entries with type information.

EXAMPLE

CC10404	Dolomite#$CaMg(CO_3)_2$
CC16916	Barite#$BaSO_4$
CC24946	Garnet#$Ca_3Al_2Ca_3Al_2(SiO_4)_3$

LITERATURE

[1] Lima-de-Faria, F., Hellner, E., Liebau, F., Makovicky, E. & Parthé, E., Acta Cryst. (1990). A46, 1-11, "Nomenclature of inorganic structure types. Report of the International Union of Crystallography Commission on the crystallographic Nomenclature Subcommitte on the Nomenclature of Inorganic Structure Types", https://doi.org/10.1107/S0108767389008834

[2] Allmann, R. & Hinek, R., Acta Cryst. A63 (2007), 412–417, "The introduction of structure types into the Inorganic Crystal Structure Database ICSD", http://dx.doi.org/10.1107/S0108767307038081

[3] Excel list containing all structure type descriptors is available in ICSD on the Structure Type search mask

EXISTING PUBLICATIONS

Original publication to be cited in scientific work referring to the ICSD database:
Bergerhoff, G. & Brown, I.D. in "Crystallographic Databases", F.H. Allen et al. (Hrsg.) Chester, International Union of Crystallography, (1987).

Zagorac, D., Müller, H., Ruehl, S., Zagorac, J. & Rehme, S., J. Appl. Cryst. 52 (2019), 918-925, "Recent developments in the Inorganic Crystal Structure Database: theoretical crystal structure data and related features", https://doi.org/10.1107/S160057671900997X.

Behrens, H., Luksch, P., Acta Cryst. B62 (2006), 993–1001, "A bibliometric study in crystallography", https://doi.org/10.1107/S0108768106030278.

Belsky, A., Hellenbrandt, M., Karen, V. L. & Luksch, P., Acta Cryst. B58 (2002), 364–369, "New developments in the Inorganic Crystal Structure Database (ICSD): accessibility in support of materials research and design". http://dx.doi.org/10.1107/S0108768102006948.

Further publications see: https://icsd.products.fiz-karlsruhe.de/en/about/about-icsd#publications

LINKS

Link to homepage
https://icsd.products.fiz-karlsruhe.de/

Access to the database
https://icsd.fiz-karlsruhe.de/search/basic.xhtml

»The important thing in science is not so much to obtain new facts as to discover new ways of thinking about them«

Wiliam Lawrence Bragg (1890-1971)

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