ICSD (Inorganic Crystal Structure Database)

Subject Coverage

- Crystal structures of inorganic compounds
- Crystallography
- Inorganic chemistry
- Materials science
- Phase transitions
- Physical chemistry
- Physical properties
- Physics
- Property data
- Thermal properties

File Type

Numeric

Features

Alerts (SDIs)	Not available		
CAS Registry Number® Identifiers	☐	Page Images	☐
Keep & Share	☑	SLART	☐
Learning Database	☐	Structures	☐

Record Content

- Bibliographic information, each dataset contains compound name, molecular formula, as well as space group, unit cell parameters, atomic coordinates and displacement factors.

File Size

- 188,631 records (06/2017)

Coverage

1913-present

Updates

Reloaded and updated twice a year with about 5.000 new or updated records

Language

English

Database Producer / Supplier

FIZ Karlsruhe
STN Europe
P.O. Box 2465
76012 Karlsruhe
Germany
Phone: +49-7247-808-555
Fax: +49-7247-808-259
Email: helpdesk@fiz-karlsruhe.de

In cooperation with

National Institute of Standards
and Technology (NIST)
Gaithersburg, MD 20899
U.S.A

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User Aids	• Online Helps (HELP DIRECTORY lists all help messages available) • STNGUIDE
Cluster	• AUTHORS • NUMERIC STN Database Cluster information: http://www.stn-international.com/en/customersupport/customer-support#cluster+%7C+subjects+%7C+features

Search and Display Field Codes

There are no fields that allow left truncation in this file.

General Search Fields

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single words from Chemical Name (CN), Linearized Structural Formula (LSF), Title (TI), and Supplementary Term (ST) fields)	None or /BI	S POWDER DIFFRACTION	CN, LSF, TI, ST
Accession Number **(1,2)**	/AN	S 60419/AN	AN
Atom Count **(2)**	/ATC	S 3-4/ATC	from MF
Author **(1)**	/AU	S SMITH?/AU	AU
Cell Volume **(2)**	/CLP.VOL	S 20-80/CLP.VOL S 20<=CLP.VOL<=80	CLP
Chemical Name and Mineral Name **(1)**	/CN	S HALITE/CN	CN
Chemical Name Segment **(1)**	/CNS	S ALUMINIUM/CNS S CHLORO/CNS	CN
Correction Date **(1,2)**	/CDAT	S 880118/CDAT	CDAT
Count for Specific Element **(2)**	/Elem. Symbol	S 3/AL S 2.4/AL	from MF
Crystal Class **(1)**	/CCLS	S C2H/CCLS	CCLS
Crystal Lattice Parameters: Number of Formula Units **(2)**	/CLP.NFU	S 3/CLP.NFU	CLP
Crystal Symmetry (Centering, Polarity) **(1)**	/CSYM	S NCEN/CSYM	CSYM
Crystal System **(1)**	/CSYS	S CUB/CSYS	CSYS
Crystallographic Space Group **(1)**	/CSG	S A1A1/CSG	CN
Database Entry Date **(2)**	/DED	S 19880715/DED	DED
Element Count **(2)**	/ELC	S 3/ELC	from MF
Element Pair	/MID.ELP	S AG-AG/MID.ELP S AL-AG/MID.ELP AND 2-3/MID S AG-AG/MID.ELP AND 0.5-0.6/MID	MID
Element Symbol **(1)**	/ELS	S BA/ELS	from MF
Experimental Density **(2)**	/DEN	S 1.2-1.5/DEN	DEN
Field Availability	/FA	S CSYS/FA	FA
Formula Type (ANX-Form) **(1)**	/FTYP	S ABX2/FTYP S AB2X4/FTYP	FTYP
Journal Title	/JT	S ACTA METALLURGICA/JT	SO
Laue Class **(1)**	/LAU	S MMM/LAU	LAU
Linearized Structural Formula	/LSF	S AL2 O3/LSF	LSF
Minimum Interatomic Distance **(2)**	/MID	S 1<MID<1.1 S 1-1.1/MID	MID
Molecular Formula **(1)**	/MF	S AG3 AL22 O34/MF	MF
Oxidation State **(2)**	/OXS	S 2/OXS	OXS
Pearson Symbol **(1)**	/PRS	S AP17/PRS	PRS
Periodic Group	/PG	S A1/PG	not displayed
Publication Year **(2)**	/PY	S 1960-1970/PY	SO
R-Value **(2)**	/RVAL	S 0.3-0.4/RVAL	RVAL
Source (contains CODEN and journal title)	/SO	S LESS COMMON METALS/SO	SO
Supplementary Term **(1)**	/ST	S STRUCTURE CALCULATED?/ST	ST
Test Flag **(1)**	/TFLG	S UNUSUAL/TFLG	TFLG
Title **(1)**	/TI	S ALUMINATES/TI	TI
Update Date **(2)**	/UP	S UP>JAN 2000	UP

(1) Hit term highlighting is available.
(2) Numeric search field that may be searched with numeric operators or ranges.

DISPLAY and PRINT Formats

Any combination of formats may be used to display or print answers. Multiple codes must be separated by spaces or commas, e.g., D L1 1-5 TI AU. The fields are displayed or printed in the order requested.

Hit-term highlighting is available for some fields (see page 3). Highlighting must be ON during SEARCH to use the HIT, KWIC, and OCC formats.

Format	Content	Examples
AN	Accession Number	D AN 1-6
ATP	Atomic Parameter	D L5 ATP
AU	Author	D L8 AU 10-20
CCLS	Crystal Class	D CCLS 5-10
CDAT	Correction Date	D CDAT L3 1-5
CLP	Crystal Lattice Parameters	D CLP
CN	Chemical Name and Mineral Name	D 1-4 CN
CSG	Crystallographic Space Group	D CSG
CSYM	Crystal Symmetry (Centering, Polarity)	D CSYM 10
CSYS	Crystal System	D CSYS
DED	Database Entry Date	D DED
DEN	Experimental Density	D DEN
FA	Field Availability	D FA
FTYP	Formula Type (ANX-Form)	D FTYP 1-3
LAU	Laue Class	D LAU 1-5
LSF	Linearized Structural Formula	D L6 10-15 LSF
MF	Molecular Formula	D MF
MID **(1)**	Minimum Interatomic Distance	D MID
OXS **(1)**	Oxidation State	D OXS
PRS	Pearson Symbol	D PRS
RVAL	R-Value	D RVAL 1-10
SO	Source	D SO
ST	Supplementary Term	D L10 1-5 ST
TF	Temperature Factor	D TF
TFLG	Test Flag	D TFLG 2
TI	Title	L9 1-6 TI
UP **(1)**	Update Date	D UP
ALL	IDE, BIB, CELL, DDES, PARM	D ALL L11
BIB	AN, TI, AU, SO	D 8 BIB
CELL	AN, CLP, DEN, CSG, RVAL, ST	D 10 CELL
CIF	ALL, with special formatting (see HELP DNLDFORMATS)	D CIF
DDES	AN, LAU, PRS, CCLS, CSYS, CSYM, FTYP	D 1-3 DDES
IDE	AN, CN, LSF, MF	D L1 1-5 IDE
PARM	AN, ATP, TF, TFLG	D L4 5 PARM
QRD	Query Related Data (default)	D QRD
TRIAL	AN, CN, TI, AU	D TRI
HIT	Hit term(s) and field(s)	D HIT
KWIC	Up to 50 words before and after hit term(s) (KeyWord-In-Context)	D KWIC
OCC	Number of occurrences of hit term(s) and field(s) in which they occur	D OCC

(1) Custom display only.

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Accession Number	AN	Y	N
Author	AU	Y	N
Chemical Name	CHEM	Y	N
Chemical Name and Mineral Name	CN	Y	Y
Chemical Name Segment	CNS	Y	N
CODEN	CODEN	N	Y
Correction Date	CDAT	Y	N
Crystal Class	CCLS	Y	Y
Crystal Symmetry (Centering, Polarity)	CSYM	Y	Y
Crystal System	CSYS	Y	Y
Crystallographic Space Group	CSG	Y	N
Database Entry Date	DED	Y	Y
Field Availability	FA	Y **(2)**	N
Formula Type (ANX-Form)	FTYP	Y	Y
Journal Title	JT	Y **(2)**	Y
Laue Class	LAU	Y	Y
Linearized Structural Formula	LSF	Y	Y
Molecular Formula	MF	Y (default)	Y
Occurrence Count of Hit Terms	OCC	N	Y
Pearson Symbol	PRS	Y	Y
Publication Year	PY	Y **(2)**	N
Source	SO	Y **(2,3)**	N
Supplementary Term	ST	Y	N
Test Flag	TFLG	Y	N
Title	TI	Y	Y

(1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set, e.g., SEL HIT TI.
(2) SELECT or ANALYZE HIT are not valid with this field.
(3) Selects or analyzes the CODEN with /SO appended to the terms created by SELECT.

Sample Record

DISPLAY ALL

```
AN   75479  ICSD
CN   Aluminium oxide
LSF  Al2 O3
MF   Al2 O3
TI   Neutron diffraction measurements of the residual stresses in Al2 O3 - Zr
     O2 (Ce O2) ceramic composites
AU   Wang, X.-L.; Hubbard, C.R.; Alexander, K.B.; Becher, P.F.
SO   Journal of the American Ceramic Society. (1994) Vol. 77 p. 1569-1575;
     CODEN=JACTAW
```

```
CLP  A=4.7554(3) B=4.7554(3) C=12.9910(6)    unit: Angstrom
     ALPHA=90. BETA=90. GAMMA=120.    unit: Degrees
     NFU  6
     VOL  254.42  Angstrom**3
CSG  R3-CH; 167
     1 'x-y, -y, -z+1/2'
     2 '-x, -x+y, -z+1/2'
     3 'y, x, -z+1/2'
     4 'x-y, x, -z'
     5 'y, -x+y, -z'
     6 '-x, -y, -z'
     7 '-x+y, y, z+1/2'
     8 'x, x-y, z+1/2'
     9 '-y, -x, z+1/2'
     10 '-x+y, -x, z'
     11 '-y, x-y, z'
     12 'x, y, z'
     13 'x-y+2/3, -y+1/3, -z+5/6'
     14 '-x+2/3, -x+y+1/3, -z+5/6'
     15 'y+2/3, x+1/3, -z+5/6'
     16 'x-y+2/3, x+1/3, -z+1/3'
     17 'y+2/3, -x+y+1/3, -z+1/3'
     18 '-x+2/3, -y+1/3, -z+1/3'
     19 '-x+y+2/3, y+1/3, z+5/6'
     20 'x+2/3, x-y+1/3, z+5/6'
     21 '-y+2/3, -x+1/3, z+5/6'
     22 '-x+y+2/3, -x+1/3, z+1/3'
     23 '-y+2/3, x-y+1/3, z+1/3'
     24 'x+2/3, y+1/3, z+1/3'
     25 'x-y+1/3, -y+2/3, -z+1/6'
     26 '-x+1/3, -x+y+2/3, -z+1/6'
     27 'y+1/3, x+2/3, -z+1/6'
     28 'x-y+1/3, x+2/3, -z+2/3'
     29 'y+1/3, -x+y+2/3, -z+2/3'
     30 '-x+1/3, -y+2/3, -z+2/3'
     31 '-x+y+1/3, y+2/3, z+1/6'
     32 'x+1/3, x-y+2/3, z+1/6'
     33 '-y+1/3, -x+2/3, z+1/6'
     34 '-x+y+1/3, -x+2/3, z+2/3'
     35 '-y+1/3, x-y+2/3, z+2/3'
     36 'x+1/3, y+2/3, z+2/3'
RVAL 0.070000
ST   Neutron diffraction (powder)
     The structure has been assigned a PDF number (calculated powder
     diffraction data): 01-082-1399
     Rietveld profile refinement applied
     Structure type : Al2O3
LAU  3-m
PRS  HR10
CCLS 3-M; D3D
CSYS TRI
CSYM NCEN; NPOL
FTYP A2X3

ATP  Atomic Parameters
==========================================================================
At  Nr  Ox  Wy       X       Y       Z       SOF
---+---+---+----+----------+--+----------+-----
Al  1  3   12c  0           0  0.3520(3)  1
O   1  -2  18e  0.3063(4)   0  0.25       1
```

```
TF  Temperature Factors      unit: Angstrom **2
=====================================================================
At  Nr
---+----
Al  1  B= 0.17(7)
O   1  B= 0.17(5)
TFLG At least one temperature factor is implausible or meaningless but agrees
     with the value given in the paper.
```

In North America
CAS
STN North America
P.O. Box 3012
Columbus, Ohio 43210-0012 U.S.A.

CAS Customer Center:
Phone: 800-753-4227 (North America)
614-447-3700 (worldwide)
Fax: 614-447-3751
Email: help@cas.org
Internet: www.cas.org

In Europe
FIZ Karlsruhe
STN Europe
P.O. Box 2465
76012 Karlsruhe
Germany
Phone: +49-7247-808-555
Fax: +49-7247-808-259
Email: helpdesk@fiz-karlsruhe.de
Internet: www.stn-international.com

In Japan
JAICI (Japan Association for
International Chemical Information)
STN Japan
Nakai Building
6-25-4 Honkomagome, Bunkyo-ku
Tokyo 113-0021, Japan
Phone: +81-3-5978-3601 (Technical Service)
+81-3-5978-3621 (Customer Service)
Fax: +81-3-5978-3600
Email: support@jaici.or.jp (Technical Service)
customer@jaici.or.jp (Customer Service)
Internet: www.jaici.or.jp