

ICSD (Inorganic Crystal Structure Database)



Subject Coverage	<ul style="list-style-type: none">• Crystal structures of inorganic compounds• Crystallography• Inorganic chemistry• Materials science• Phase transitions	<ul style="list-style-type: none">• Physical chemistry• Physical properties• Physics• Property data• Thermal properties	
File Type	Numeric		
Features	Alerts (SDIs) Not available		
	CAS Registry Numbers® <input type="checkbox"/>	Page Images <input type="checkbox"/>	STN AnaVist <input type="checkbox"/>
	Keep & Share <input checked="" type="checkbox"/>	SLART <input type="checkbox"/>	STN Easy <input type="checkbox"/>
	Learning Database <input type="checkbox"/>	Structures <input type="checkbox"/>	STN Viewer <input type="checkbox"/>
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	135,468 records (04/11)		
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 E-mail: helpdesk@fiz-karlsruhe.de In cooperation with National Institute of Standards and Technology (NIST) Gaithersburg, MD 20899 U.S.A Copyright Holders		

Sources

- Journals
 - Books
-

User Aids

- Online Helps (HELP DIRECTORY lists all help messages available)
 - STNGUIDE
-

Clusters

- AUTHORS
 - NUMERIC
- [STN Database Clusters](#) information (PDF).
-

Pricing

See the [STN Price List](#) or enter HELP COST at an arrow prompt.

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) Atom Count (2) Author (1) Cell Volume (2)	/AN /ATC /AU /CLP.VOL	S 60419/AN S 3-4/ATC S SMITH?/AU S 20-80/CLP.VOL S 20<=CLP.VOL<=80 S HALITE/CN	AN from MF AU CLP
Chemical Name and Mineral Name (1) Chemical Name Segment (1)	/CN /CNS	S ALUMINIUM/CNS S CHLORO/CNS	CN CN
Correction Date (1,2) Count for Specific Element (2)	/CDAT /Elem. Symbol	S 880118/CDAT S 3/AL S 2.4/AL	CDAT from MF
Crystal Class (1) Crystal Lattice Parameters: Number of Formula Units (2)	/CCLS /CLP.NFU	S C2H/CCLS S 3/CLP.NFU	CCLS CLP
Crystal Symmetry (Centering, Polarity) (1) Crystal System (1) Crystallographic Space Group (1)	/CSYM /CSYS /CSG	S NCEN/CSYM S CUB/CSYS S A1A1/CSG	CSYM CSYS CN
Database Entry Date (2) Element Count (2) Element Pair	/DED /ELC /MID.ELP	S 19880715/DED S 3/ELC 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	DED from MF MID
Element Symbol (1) Experimental Density (2) Field Availability Formula Type (ANX-Form) (1)	/ELS /DEN /FA /FTYP	S BA/ELS S 1.2-1.5/DEN S CSYS/FA S ABX2/FTYP S AB2X4/FTYP	from MF DEN FA FTYP
Journal Title Laue Class (1) Linearized Structural Formula Minimum Interatomic Distance (2)	/JT /LAU /LSF /MID	S ACTA METALLURGICA/JT S MMM/LAU S AL2 O3/LSF S 1<MID<1.1 S 1-1.1/MID	SO LAU LSF MID
Molecular Formula (1) Oxidation State (2) Pearson Symbol (1) Periodic Group Publication Year (2) R-Value (2) Source (contains CODEN and journal title) Supplementary Term (1) Test Flag (1) Title (1) Update Date (2)	/MF /OXS /PRS /PG /PY /RVAL /SO /ST /TFLG /TI /UP	S AG3 AL22 O34/MF S 2/OXS S AP17/PRS S A1/PG S 1960-1970/PY S 0.3-0.4/RVAL S LESS COMMON METALS/SO S STRUCTURE CALCULATED?/ST S UNUSUAL/TFLG S ALUMINATES/TI S UP>JAN 2000	MF OXS PRS not displayed SO RVAL SO ST TFLG TI 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 ATP AU CCLS CDAT CLP CN CSG CSYM CSYS DED DEN FA FTYP LAU LSF MF MID (1) OXS (1) PRS RVAL SO ST TF TFLG TI UP (1)	Accession Number Atomic Parameter Author Crystal Class Correction Date Crystal Lattice Parameters Chemical Name and Mineral Name Crystallographic Space Group Crystal Symmetry (Centering, Polarity) Crystal System Database Entry Date Experimental Density Field Availability Formula Type (ANX-Form) Laue Class Linearized Structural Formula Molecular Formula Minimum Interatomic Distance Oxidation State Pearson Symbol R-Value Source Supplementary Term Temperature Factor Test Flag Title Update Date	D AN 1-6 D L5 ATP D L8 AU 10-20 D CCLS 5-10 D CDAT L3 1-5 D CLP D 1-4 CN D CSG D CSYM 10 D CSYS D DED D DEN D FA D FTYP 1-3 D LAU 1-5 D L6 10-15 LSF D MF D MID D OXS D PRS D RVAL 1-10 D SO D L10 1-5 ST D TF D TFLG 2 L9 1-6 TI D UP
ALL BIB CELL CIF DDES IDE PARM QRD TRIAL	IDE, BIB, CELL, DDES, PARM AN, TI, AU, SO AN, CLP, DEN, CSG, RVAL, ST ALL, with special formatting (see HELP DNLDIFORMATS) AN, LAU, PRS, CCLS, CSYS, CSYM, FTYP AN, CN, LSF, MF AN, ATP, TF, TFLG Query Related Data (default) AN, CN, TI, AU	D ALL L11 D 8 BIB D 10 CELL D CIF D 1-3 DDES D L1 1-5 IDE D L4 5 PARM D QRD D TRI
HIT KWIC OCC	Hit term(s) and field(s) Up to 50 words before and after hit term(s) (KeyWord-In-Context) Number of occurrences of hit term(s) and field(s) in which they occur	D HIT D KWIC 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
```

6
ICSD

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.

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