



STN is operated in North America
by Chemical Abstracts Service.

STN Database Summary Sheet

ICSD (Inorganic Crystal Structure Database) is the world's largest comprehensive database on the complete structural information for crystalline inorganic compounds. The data are carefully evaluated from relevant scientific literature. Besides the bibliographic information each dataset contains compound name, molecular formula, as well as space group, unit cell parameters, atomic coordinates and temperature factors.

ICSD also contains the following data generation package, which can be started with the Messenger RUN command:

Subject Coverage

- Crystal Structure of Inorganic Compounds
- Crystallography
- Inorganic Chemistry
- Materials Science
- Phase Transitions
- Physical Chemistry
- Physical Properties
- Physics
- Property Data
- Thermal Properties

Sources

- Journals
- Books

File Data

- 1913 to present
- More than 100,000 records (11/07)
- Reloaded and updated twice a year
- Automatic current-awareness searches (SDIs) are not available
- User Aids
- ICSD Database Description
- Online Helps (HELP DIRECTORY lists all help messages available)

Database Producer

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Copyright holder: FIZ/NIST

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ICSD

Search and Display Field Codes

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

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (1) (contains single words from CN, LSF, TI, ST)	None (or /BI)	S POWDER DIFFRACTION	CN, LSF, TI, ST
Accession Number (1,2) Atom Count (2) Author (1) Crystal Class (1) Correction Date (1,2) Crystal Lattice Parameters: Number of Formula Units (2) Cell Volume (1,2)	/AN /ATC /AU /CCLS /CDAT /CLP.NFU /CLP.VOL	S 60419/AN S 3-4/ATC S SMITH?/AU S C2H/CCLS S 880118/CDAT S 3/CLP.NFU S 20-80/CLP.VOL S 20<=CLP.VOL<=80	AN MF AU CCLS CDAT CLP CLP
Chemical Name and Mineral Name (1) Chemical Name Segment (1)	/CN /CNS	S AMARANTITE/CN S ALUMINIUM/CNS S CHLORO/CNS	CN CN
Crystallographic Space Group (1) Crystal Symmetry (1) Crystal System (1) Database Entry Date (1,2) Experimental Density (2) Element Count (2) Count for Specific Element (2)	/CSG /CSYM /CSYS /DED /DEN /ELC /Elem. Symbol	S A1A1/CSG S CEN/CSYM S CUB/CSYS S 880715/DED S 1.2-1.5/DEN S 3/ELC S 3/AL S 2.4/AL	CSG CSYM CSYS DED DEN MF MF
Element Symbol (1) Field Availability Formula Type (1)	/ELS /FA /FTYP	S BA/ELS S CSYS/FA S ABX2/FTYP S AB2X4/FTYP	MF FA FTYP
Journal Title Laue Class (1) Linearized Structural Formula (1) Molecular Formula (1) Minimum Interatomic Distance [⊗] (2)	/JT /LAU /LSF /MF /MID	S ACTA METALLURGICA/JT S M3M/LAU S AL2 O3/LSF S AG NA3 O2/MF S 1<MID<1.1 S 1-1.1/MID	SO LAU LSF MF MID
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
Oxidation State (2) Periodic Group Pearson Symbol (1) Publication Year (2) R-Value (2) Source (contains CODEN, journal title, publication year) Supplementary Terms (1) Test Flag (1) Title (1) Update (2)	/OXS /PG /PRS /PY /RVAL /SO /ST /TFLG /TI /UP	S 2/OXS S A1/PG S AP17/PRS S 1960-1970/PY S 0.3-0.4/RVAL S LESS COMMON METALS/SO S DEN/ST S 74/TFLG S ALUMINATES/TI S 890911/UP S UP>900101	OXS Not displayed PRS SO RVAL SO ST TFLG TI UP

(1) Hit-term highlighting is available.

(2) Numeric search field.

DISPLAY and PRINT Formats

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

Hit-term highlighting is available in AN, AU, CCLS, CDAT, CN, CSG, CSYM, CSYS, DED, FTYP, LAU, LSF, MF, MID, OXS, PRS, RVAL, TFLG, and TI. Highlighting must be ON during SEARCH in order to use the HIT, KWIC, and OCC formats.

Format	Content	Examples
AN (1) ATP AU (1) CCLS CDAT CIF CLP CN (1) CSG CSYM CSYS DED (1,2) DEN FA (1,2) FTYP LAU LSF MF MID (1,2) OXS (1,2) PRS RVAL (1) SO ST (1) TF TFLG (1) TI (1) UP (1,2)	Accession Number Atomic Parameters Author Crystal Class Correction Date Crystallographic Information File Crystal Lattice Parameters Chemical Name and Mineral Name Crystallographic Space Group Crystal Symmetry Crystal System Database Entry Date Experimental Density Field Availability Formula Type Laue Class Linearized Structural Formula Molecular Formula Minimum Interatomic Distance Oxidation State Pearson Symbol R-Value Source Supplementary Terms 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 CIF 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 D L9 1-6 TI D UP
ALL BIB CELL DDES IDE PARM QRD TRIAL (TRI) (1)	AN, CN, LSF, MF, TI, AU, SO, CLP, DEN, CSG, RVAL, ST, LAU, PRS, CCLS, CSYS, CSYM, FTYP, ATP, TF, TFLG AN, TI, AU, SO AN, CLP, DEN, CSG, RVAL, ST AN, LAU, PRS, CCLS, CSYS, CSYM, FTYP AN, CN, LSF, MF (IDE is the default) AN, ATP, TF, TFLG Query Related Data (default) AN, CN, TI, AU	D ALL L11 D 8 BIB D 10 CELL D 1-3 DDES D L1 1-5 IDE D L4 5 PARM D QRD D TRI TOTAL
HIT KWIC OCC (1)	Fields containing hit terms Hit terms with 20 words on either side (KeyWord-In-Context) Number of occurrences of hit terms and fields in which they occur	D HIT D KWIC NOH D OCC

(1) No online display fee for this format.

(2) Custom display only.

ICSD**SELECT, ANALYZE, and SORT Fields**

The SELECT command is used to create E-numbers or an L-number 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	Y
Chemical Name and Mineral Name	CN	Y	Y
Chemical Name Segment	CNS	Y	Y
Chemical Name Segment and Molecular Formula	CHEM	Y	Y
CODEN	CODEN	N	Y
Correction Date	CDAT	Y	Y
Crystal Class	CCLS	Y	Y
Crystal Symmetry	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	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)	Y
Source	SO	Y (2,3)	N
Supplementary Terms	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 AU.

(2) SELECT HIT and ANALYZE HIT are not valid for this field.

(3) Selects or analyzes the CODEN with /SO appended to the terms created by SELECT.

Sample Records

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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)

ICSD

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
 FTYPE 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.