



ICSD无机晶体结构数据库使用指南

北京科技大学图书馆

1 基本检索

五种检索方式

The screenshot displays the ICSD web interface with the following sections:

- Header:** FIZ Karlsruhe ICSD logo, navigation links (Home | Contact), and a welcome message: "Welcome to ICSD Web. IP authenticated (222.199.204.226). Univ Science and Technology Beijing".
- Left Navigation Panel:**
 - Login:** Fields for LoginId and Password, with a "Login Personalized" button and links for "Lost password?" and "Personalize account".
 - Navigation:** A list of search methods: "Basic search & retrieve", "Advanced search & retrieve", "Bibliography", "Cell", "Chemistry", "Symmetry", "Crystal Chemistry", "Structure Type", "Experimental Information", "DB Info", "Query Management", "Manage Queries", "List Combined Queries", and "Create Combined Query".
- Main Search Area (Basic Search & Retrieve):**
 - Bibliography:** Fields for Authors, Year of Publication, Title of Journal, and Title of Article.
 - Chemistry:** Fields for Composition and Number of Elements.
 - Cell:** Fields for Cell Parameters, Cell Volume, and Tolerance (+/- %).
 - Symmetry:** Fields for Space Group Symbol, Space Group Number, Crystal System, and Centering.
 - Exp. Info. & Ref. Data:** Fields for PDF Number, Temperature (K), ICSD Collection Code, and Pressure (MPa).
- Right Panel (Search Action):**
 - Buttons for "Run Query" and "Clear Query".
 - Search Summary:** Shows "Basic Search: -".
 - Query History:** Shows "Number of queries: 0" and a "Clear Query History" button.
- Bottom:** "Clear Basic Search" and "Count Basic Search" buttons.

参考文献

化学组成

晶胞参数

对称性

实验和代
码信息

Basic Search & Retrieve

Bibliography

Authors: Year of Publication:

Title of Journal:

Title of Article:

Chemistry

Composition: Number of Elements:

Cell

Cell Parameters:

Cell Volume: Tolerance +/-: %

Symmetry

Space Group Symbol: Space Group Number:

Crystal System: Centering:

Exp. Info. & Ref. Data

New Data Only

PDF Number: Temperature: K

ICSD Collection Code: Pressure: MPa

Search Chemistry Visual Search mode

H																	He					
Li	Be															B	C	N	O	F	Ne	
Na	Mg														Al	Si	P	S	Cl	Ar		
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr					
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe					
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn					
Fr	Ra		Rf	Db																		

→ Metals → Transition Metals → Non-Metals

Click on element or select period and/or group.

Number of Elements: Units of Coefficients:

El.Symb.	Co.(min)	Co.(max)	Ox.(min)	Ox.(max)	
AND ▼ O	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	X
AND ▼ Ti	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	X
AND ▼ Ca	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	X

Restrict total number of elements to selected number of elements

若需精确查询，则设置元素的比例系数，如 CaTiO_3 ，则O、Ti、Ca分别输入3、1、1

查看具体数据

Search Action

Search Summary

Basic Search: 81

Query History

Number of queries: 0

开始搜寻

主要是通过化学组成来搜寻晶体结构数据

2 高级检索（很少用）

Bibliography Search ⓘ

Authors
e.g. Jansen

Title of Journal
e.g. Angewandte Chemie

Title of Article
e.g. Super conducting crystals

Year of Publication
e.g. >2008 or 2000-2006 or 2001

Volume
e.g. 10

Page first
e.g. 10

Abstract
e.g. hybrid cage clusters

输入文献
信息检索

输入晶胞参
数信息检索

Cell Search ⓘ

Cell Length a

Cell Length b

Cell Length c

Cell Volume

Calc. Density g/cm³

Global Tolerance +/- %

Reduce Cell Parameters

Centering

Cell Angle α

Cell Angle β

Cell Angle γ

Units of Length Å

Search Cell Data Experimental Cell

Chemistry Search

Composition e.g. Na Cl Number of Elements

Structural Formula e.g. Pb (W O4)

Chemical Name

Mineral Name e.g. Adamite

Mineral Group e.g. Pyroxene

ANX Formula

AB Formula

输入化学
信息检索

Symmetry Search

Note: Restrictions apply to Experimental Cell

Space Group Symbol e.g. Fm-3m

Include All Settings

Space Group Number e.g. 1 or 3-120

Crystal System ▼ Centering ▼

Crystal Class Crystal Class Notation HM- or Schoenflies-Notation ▼

Laue Class ▼

Wyckoff Sequence

Pearson Symbol

输入对称性
信息检索

Crystal Chemistry Search

Interatomic Distances

	Atom A	Ox. A		Atom B	Ox. B	d_{\min}^{AB}	d_{\max}^{AB}
	<input type="text"/>	<input type="text"/>	-	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
AND	<input type="text"/>	<input type="text"/>	-	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
AND	<input type="text"/>	<input type="text"/>	-	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
AND	<input type="text"/>	<input type="text"/>	-	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Crystal Structure is

Polytype Structure
 Order/Disorder Structure
 Structure Type
 Defect Structure
 Misfit Layer Structure
 Disordered Structure
 Mineral

输入晶体化学信息检索

输入结构类型信息检索

Structure Type Search

Pre Defined Structure Types

Structure Type

e.g. Mg₂SiO₄

Search in predefined structure types

Structure Type Descriptors

<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/> SpaceGrp	<input type="checkbox"/> Wyck	<input type="checkbox"/> Pearson	<input type="checkbox"/> ANX
-	-	-	-

Experimental Information Search

Temperature K

Pressure MPa

Comments e.g. stable above

R-Value

Radiation Type

- X-Ray
- Electrons
- Neutrons
- Synchrotron

Sample Type

- Powder
- Single Crystal

输入实验
信息检索

Additional Properties

- Twinned Crystal Data
- Rietveld Refinement employed
- Anharmonic Temperature Factors given
- Absolute Configuration determined
- Theoretically calculated structures
- NMR Data available
- Magnetic Structure
- Correction of earlier data

输入数据库
信息检索

DB Info Search

ICSD Collection Code e.g. 9061 or 90000-95000

PDF Number e.g. 47-1360

Release Tag e.g. 2007.1 or 2005.1-2007.1

Recording Date yyyy-mm-dd, e.g. 1998-06-26

Modification Date yyyy-mm-dd, e.g. 2006-04-01

New Data Only

3 检索结果

查看细节

Navigation

Search & Retrieve

Display

- List View
- Detailed View**
- Synoptic View
- Export Data

Quality Filter

- All Data
- High Quality Data only
- Standard Data only

对结果按要求过滤

以CaTiO3为例

Results: List View # of Hits: 75

Select All Deselect All Show Detailed View Show Synoptic View Export Selected Data Back to Query

Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Reference	☆	📄
<input checked="" type="checkbox"/> 37263	P c m n	Ca (Ti O3)	Perovskite-GdFeO3	Powdwer neutron diffraction study of the perovskites Ca Ti O3 and Ca Zr O3	Koopmanns, H.J.A.; van de Velde, G.M.H.; Gellings, P.J.	Acta Crystallographica, Section C: Crystal Structure Communications (1983) 39, p1323-p1325	☆	📄
<input type="checkbox"/> 62149	P b n m	Ca (Ti O3)	Perovskite-GdFeO3	Orthorhombic perovskite Ca Ti O3 and Cd Ti O3: structure and space group	Sasaki, S.; Prewitt, C.T.; Bass, J.D.	Acta Crystallographica, Section C: Crystal Structure Communications (1987) 43, p1668-p1674	☆	📄
<input type="checkbox"/> 71915	P b n m	Ca (Ti O3)	Perovskite-GdFeO3	Electron difference density and structural parameters in Ca Ti O3	Buttner, R.H.; Maslen, E.N.	Acta Crystallographica, Section B: Structural Science (1992) 48, p644-p649	☆	📄
<input type="checkbox"/> 71916	P b n m	Ca (Ti O3)	Perovskite-GdFeO3	Electron difference density and structural parameters in Ca Ti O3	Buttner, R.H.; Maslen, E.N.	Acta Crystallographica, Section B: Structural Science (1992) 48, p644-p649	☆	📄
<input type="checkbox"/> 74212	P b n m	Ca (Ti O3)	Perovskite-GdFeO3	X-ray powder diffraction study of Ca Ti O3 perovskite at high temperatures	Liu, X.; Liebermann, R.C.	Physics and Chemistry of Minerals (1993) 20, p171-p175	☆	📄
<input type="checkbox"/> 74213	P b n m	Ca (Ti O3)	Perovskite-GdFeO3	X-ray powder diffraction study of Ca Ti O3 perovskite at high temperatures	Liu, X.; Liebermann, R.C.	Physics and Chemistry of Minerals (1993) 20, p171-p175	☆	📄
<input type="checkbox"/> 74214	P b n m	Ca (Ti O3)	Perovskite-GdFeO3	X-ray powder diffraction study of Ca Ti O3 perovskite at high temperatures	Liu, X.; Liebermann, R.C.	Physics and Chemistry of Minerals (1993) 20, p171-p175	☆	📄
<input type="checkbox"/> 74215	P b n m	Ca (Ti O3)	Perovskite-GdFeO3	X-ray powder diffraction study of Ca Ti O3 perovskite at high temperatures	Liu, X.; Liebermann, R.C.	Physics and Chemistry of Minerals (1993) 20, p171-p175	☆	📄
<input type="checkbox"/> 74216	P b n m	Ca (Ti O3)	Perovskite-GdFeO3	X-ray powder diffraction study of Ca Ti O3 perovskite at high temperatures	Liu, X.; Liebermann, R.C.	Physics and Chemistry of Minerals (1993) 20, p171-p175	☆	📄
<input type="checkbox"/> 82487	P b n m	Ca (Ti O3)	Perovskite-GdFeO3	A single-crystal infrared spectroscopic and X-ray diffraction study of untwinned San Benito perovskite containing O H groups	Beran, A.; Libowitzky, E.; Armbruster, T.	Physics and Chemistry of Minerals (1993) 20, p171-p175	☆	📄

[1-10] [11-20] [21-30] [31-40] [41-50] [51-60] [61-70] [71-75] [LastPage]

高质量数据

保存成cif文件用其它软件实现结构可视化

查看细节信息

Summary				Collection Code 37263	
Struct.formula	Ca (Ti O3)		Author	Koopmanns, H.J.A.; van de Velde, G.M.H.; Gellings, P.J.	
Space Group	P c m n(62)		Title of Article	Powdwer neutron diffraction study of the perovskites Ca Ti O3 and Ca Zr O3	
Unit Cell	5.3829(3) 7.6453(4) 5.4458(3) 90. 90. 90.		Reference	Acta Crystallographica, Section C: Crystal Structure Communications (1983) 39, ▲ ▼	
Cell Volume	224.12 Å ³	Formula Units per Cell	4	Warnings & Comments	0 Warnings / 1 Comments
Temperature	room temperature	Pressure	atmospheric		
PDF-numbers	01-076-2400 22-153	R-value	0.0452		
Remark			☆ High Quality Data		
Export CIF File		<input type="text" value="MyBaseFileName"/>	Show Synoptic View	Feedback to the ICSD Editor	

Details
Expand All Collapse All
▶ Visualization
▶ Chemistry
▶ Published Crystal Structure Data
▶ Standardized Crystal Structure Data
▶ Distances & Angles
▶ Bibliography
▶ Experimental Information
▶ Warnings & Comments
▶ Compare Published & Standardized Structure

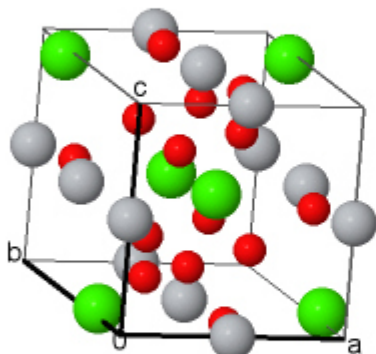
- 结构可视化
- 化学信息
- 出版的晶体结构数据
- 标准化的晶体结构数据
- 键长和键角

- 参考文献
- 实验信息
- 警告和评论
- 出版和标准化的结构比较

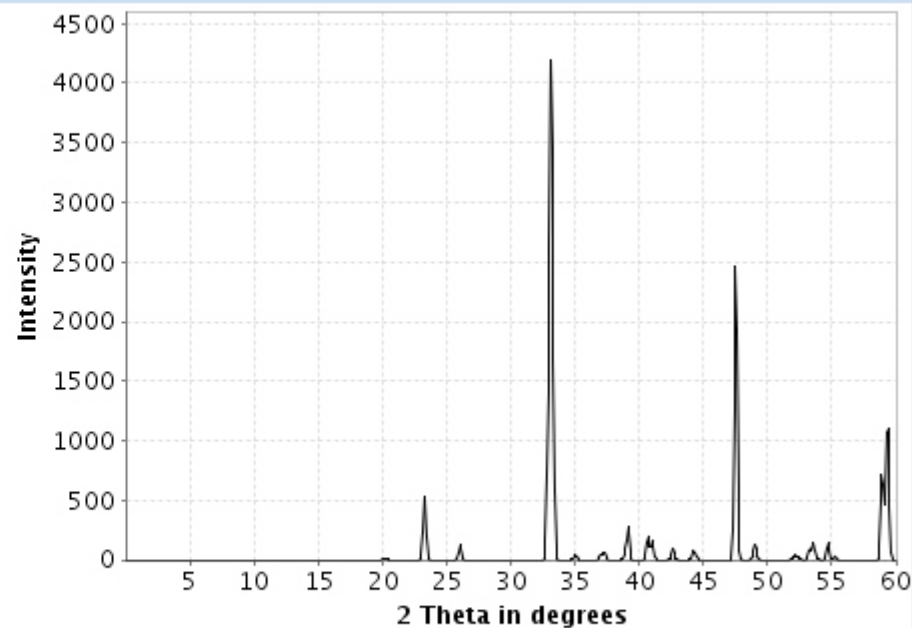
可视化

Published Crystal Structure

HM: P c m n
 a=5.383Å
 b=7.645Å
 c=5.446Å
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=90.000^\circ$


[Interactive Visualization](#)
[结构三维可视化](#)

Powder Pattern


[Display in Window](#)
[Export as x-y data](#)
[Export as table](#)
[Show as PDF](#)
[Configure Powder Pattern Calculation and Display](#)

Chemistry

Sum Form Ca1 O3 Ti1

Struct.Form. Ca (Ti O3)

Chemical Name Calcium titanate

Mineral Name Perovskite

Mineral Group Perovskite

Number of Formula Units 4

ANX Formula
Cryst.Comp. ABX3AB Formula
Chem.Comp. ABC3

化学信息

▼ **Published Crystal Structure Data**

Cell Parameters	5.3829(3) 7.6453(4) 5.4458(3) 90. 90. 90.								
Volume	224.12	Formula Units per Cell	4	Calc. Dens.	4.03				
Space Group	P c m n(62)	Pearson Symbol	oP20	Meas. Dens.	4.03				
Crystal System	orthorhombic	Crystal Class	mmm	Laue Class	mmm				
Wyckoff Sequence	d c 2 b	Structure Type	Perovskite-GdFeO3						
Axis Ratios	a/b 0.7041	b/c 1.4039	c/a 1.0117						
Remark									
EL	Lbl	Ox State	Wyck Symb	X	Y	Z	B	SOF	H
Ca	1	+2.00	4c	0.0083(7)	0.25	0.0360(5)	1.01(7)		
O	1	-2.00	4c	0.5726(5)	0.25	-0.173(4)	0.94(6)		
O	2	-2.00	8d	0.2901(3)	0.0369(2)	0.2877(3)	0.94(6)		
Ti	1	+4.00	4b	0.5	0	0	0.59(12)		

▼ **Standardized Crystal Structure Data**

Cell Parameters	5.4458 7.6453 5.3829 90.000 90.000 90.000								
Volume	224.12	Formula Units per Cell	4	Calc. Dens.	4.03				
Space Group	P n m a(62)	Pearson Symbol	oP20						
Crystal System	orthorhombic	Crystal Class	mmm	Laue Class	mmm				
Wyckoff Sequence	d c 2 a								
Axis Ratios	a/b 0.7123	b/c 1.4203	c/a 0.9884						
Transformation Method	Tidy								
Transformation Info	Multiple transformations possible, first one selected REMARK Transformed from setting P c m n. TRANS c,-b,a origin 0 0 1/2								
Remark									
EL	Lbl	Ox State	Wyck Symb	X	Y	Z	B	SOF	
Ca	1	+2.00	4c	0.4640	0.2500	0.0083	1.0100		
O	1	-2.00	4c	0.5173	0.2500	0.5726	0.9400		
O	2	-2.00	8d	0.2123	0.0369	0.2901	0.9400		
Ti	1	+4.00	4a	0.0000	0.0000	0.0000	0.5900		

出版的和标准化的晶体结构数据比较

键长和键角计算

Distances & Angles

Select Pairs of Elements

Atom A	Atom B	Atom C
Ca	Ca	Ca
O	O	O
Ti	Ti	Ti

Select/Unselect all Select/Unselect all Select/Unselect all

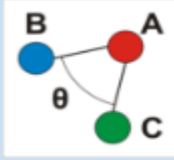
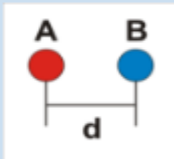
Select from Atom Positions

Configure Bonds & Angles Calculation

Distance [Å] min: 0.7 max: 3.0

Ionic radii [%] min: 80.0 max: 120.0

Save As Default Restore Default Reset to System



柱状分布图显示 → Histograms Calculate ← 计算键长键角

参考文献

Bibliography

Title of Article Powder neutron diffraction study of the perovskites Ca Ti O₃ and Ca Zr O₃

1st Reference Acta Crystallographica, Section C: Crystal Structure Communications (1983) 39, p1323-p1325

DOI: [10.1107/S0108270183008392](https://doi.org/10.1107/S0108270183008392) Get full text by: [CrossRef](#) [Google](#)

2nd Reference Golden Book of Phase Transitions, Wroclaw (2002) 1, p1-p123

Get full text by: [CrossRef](#) [Google](#)

3rd Reference

文献来源

实验信息

Experimental Information

External Conditions

Temperature Pressure

Radiation Type

X-ray Electrons Neutrons Synchrotron

Sample Type

Powder Single Crystal R-Value

Additional Information

Twinned Crystal Data Theoretically calculated structures NMR Data available

Rietveld Refinement employed Magnetic Structure Available Correction of Earlier Work

Absolute Configuration Determined Anharmonic temperature factors given

Properties of Structure

Polytype Structure Order/Disorder Structure Disordered Structure

Defect Structure Misfit Layer Structure Mineral

Structure Prototype

相关评论

Warnings & Comments

Warnings

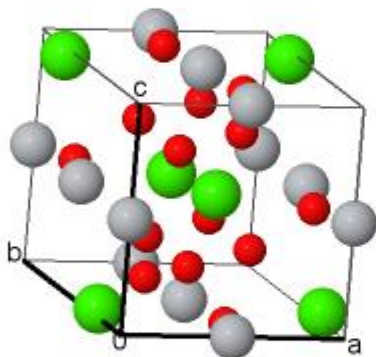
Comments

Stable up to 1330 K (2nd ref., Tomaszewski), 1330-1533 K: I4/mcm, above Pm3-m

▼ Compare Published & Standardized Structure

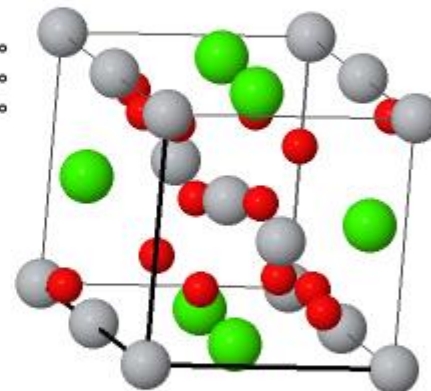
Published Structure

HM: $P\ c\ m\ n$
 $a=5.383\text{\AA}$
 $b=7.645\text{\AA}$
 $c=5.446\text{\AA}$
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=90.000^\circ$



Standardized Structure

HM: $P\ n\ m\ a$
 $a=5.446\text{\AA}$
 $b=7.645\text{\AA}$
 $c=5.383\text{\AA}$
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=90.000^\circ$



Interactive Visualization

出版的和标准化的晶体结构数据比较

Thanks for your attention

