

ICSD-无机晶体结构数据库 使用指南

iGroup · 上海

ICSD主页 <https://icsd.fiz-karlsruhe.de/index.xhtml>



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Logout

Content Selection

- Experimental Structures only
- Theoretical Structures only
- All Structures

Navigation

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
- Create Combined Query

Basic Search & Retrieve

Bibliography

Authors Year of Publication

Title of Journal

Cell Parameters

Number of Elements

Space Group Number

Crystal System Centering

Temperature K

Pressure MPa

ICSD Collection Code

基本检索

高级检索

检索式管理

Search Action

Search Summary

Basic Search: -

Query History

Number of queries: 10

2018-07-18T04:34	58
2018-05-28T09:40	61
2017-10-25T08:11	(23)
2017-04-07T04:39	(6)
2017-04-07T04:38	(391)
2017-04-07T04:36	(41)
2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

高级检索-依据文献检索



检索相应作者提供的晶体结构

检索来源于某期刊的晶体结构

检索来源于某文章的晶体结构

限定来源出版物的时间

限定来源出版物的卷期

限定关键词

Search Action
Run Query Clear Query

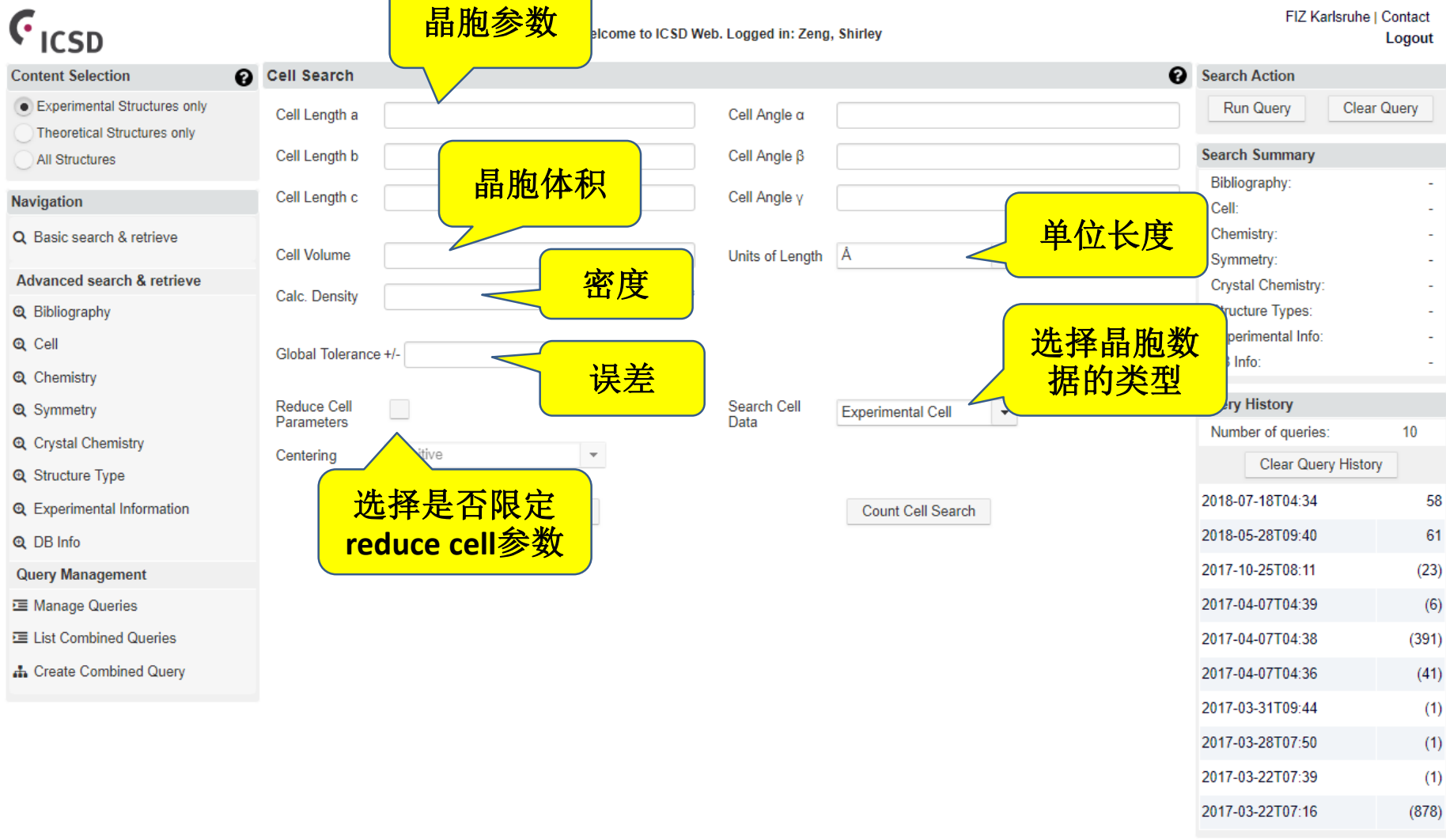
Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-

Query History

Number of queries:	10
Clear Query History	
2018-07-18T04:34	58
2018-05-28T09:40	61
2017-10-25T08:11	(23)
2017-04-07T04:39	(6)
2017-04-07T04:38	(391)
2017-04-07T04:36	(41)
2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

高级检索-依据晶胞检索



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Content Selection

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- Theoretical Structures only
- All Structures

Navigation

- Basic search & retrieve
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Cell Search

晶胞参数

晶胞体积

密度

误差

选择是否限定 reduce cell 参数

Cell Length a

Cell Length b

Cell Length c

Cell Volume

Calc. Density

Global Tolerance +/-

Reduce Cell Parameters

Centering

Cell Angle α

Cell Angle β

Cell Angle γ

Units of Length

单位长度

选择晶胞数据的类型

Search Cell Data

Count Cell Search

Search Action

Run Query Clear Query

Search Summary

Bibliography: -

Cell: -

Chemistry: -

Symmetry: -

Crystal Chemistry: -

Structure Types: -

Experimental Info: -

Info: -

Query History

Number of queries: 10

Clear Query History

Query	Count
2018-07-18T04:34	58
2018-05-28T09:40	61
2017-10-25T08:11	(23)
2017-04-07T04:39	(6)
2017-04-07T04:38	(391)
2017-04-07T04:36	(41)
2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

高级检索-依据化学式检索

Content Selection

Experimental Structures only
 Theoretical Structures only
 All Structures

Navigation

- 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
 - Create Combined Query

Chemistry Search

Composition Number of Elements

Structural Formula

Chemical Name

Mineral Name

Mineral Group

ANX Formula Number of Formula Units

AB Formula

Formula Weight

成分

元素数量

分子式

化学物质名称

矿物群

矿物名称

分子量

Search Action

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-

Query History

Number of queries:	10
<input type="button" value="Clear Query History"/>	
2018-07-18T04:34	58
2018-05-28T09:40	61
2017-10-25T08:11	(23)
2017-04-07T04:39	(6)
2017-04-07T04:38	(391)
2017-04-07T04:36	(41)
2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

高级检索-依据晶体对称性检索

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空间群

晶系

晶体等级

Wyckoff序列

Pearson符号

对称中心

Content Selection

- Experimental Structures only
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Navigation

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Symmetry Search

Note: Restrictions apply to Experimental Cell

Space Group Symbol e. g. Fm-3m

Include All Settings

Space Group Number

Crystal System

Crystal Class Crystal Class HM- or Schoenflies-Notation

Laue Class

Wyckoff Sequence

Pearson Symbol

Polar Axis Inversion Cent

Search Action

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-

Query History

Number of queries: 10

2018-07-18T04:34	58
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2017-10-25T08:11	(23)
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2017-04-07T04:36	(41)
2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

高级检索-依据原子坐标检索



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Navigation

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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"/>

Minimum Distances

Atom A		Atom B	d _{min} AB	d _{max} AB
<input type="text"/>	-	<input type="text"/>	<input type="text"/>	<input type="text"/>

Crystal Structure is

<input type="checkbox"/> Polytype Structure	<input type="checkbox"/> Order/Disorder Structure Type
<input type="checkbox"/> Modulated Structure	<input type="checkbox"/> Mineral
<input type="checkbox"/> Disordered Structure	<input type="checkbox"/> Prototype Structure Type

Clear Check Boxes

Clear Crystal Search Count Crystal Search

Search Action

Run Query Clear Query

Search Summary

- Bibliography: -
- Cell: -
- Chemistry: -
- Symmetry: -
- Crystal Chemistry: -
- Structure Types: -
- Experimental Info: -
- DB Info: -

Query History

Number of queries: 10

Clear Query History

2018-07-18T04:34	58
2018-05-28T09:40	61
2017-10-25T08:11	(23)
2017-04-07T04:39	(6)
2017-04-07T04:38	(391)
2017-04-07T04:36	(41)
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2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

限定原子间的距离

限定晶体结构类型

高级检索-依据晶体结构检索

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Structure Type Search

Pre Defined Structure Types

Structure Type

Search in predefined structure types

Structure Type Descriptors

SpaceGrp Wyck Pearson ANX

结构类型

空间群 **Wyckoff序列** **Pearson符号** **ANX结构**

Search Action

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-

Series: 10

2018-07-18T04:34	58
2018-05-28T09:40	61
2017-10-25T08:11	(23)
2017-04-07T04:39	(6)
2017-04-07T04:38	(391)
2017-04-07T04:36	(41)
2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

高级检索-依据实验信息检索

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Navigation

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Experimental Information Search

Temperature K

Pressure MPa

Comments

R-Value

Radiation Type

- X-Ray
- Electrons
- Neutrons
- Synchrotron

Sample Type

- Powder
- Single Crystal

Additional Properties

- Twinned Crystal Data
- Rietveld Refinement employed
- Anharmonic Temperature Factors given
- Absolute Configuration determined
- Experimental PDF number assigned
- Calculated PDF number assigned
- NMR Data available
- Magnetic Structure available
- Earlier work
- Factors available
- Cell Constants without s.d.
- Only Cell and Structure Type determined

Clear Experimental Info Search

Count Experimental Info Search

Search Action

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Chemistry:	-
Types:	-
ental Info:	-
DB Info:	-

Query History

Number of queries: 10

2018-07-18T04:34	58
2018-05-28T09:40	61
2017-10-25T08:11	(23)
2017-04-07T04:39	(6)
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2017-04-07T04:36	(41)
2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

温度

压力

注释

射线类型

R值

样本类型

其他属性

高级检索-依据数据库记录信息检索

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ICSD

Content Selection ? **DB Info Search**

- Experimental Structures only
- Theoretical Structures only
- All Structures

Navigation

- Basic search & retrieve
- Advanced search & retrieve
 - Bibliography
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 - Chemistry
 - Symmetry
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 - DB Info
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 - List Combined Queries
 - Create Combined Query

DB Info Search

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

PDF Number e.g. 47-1360 **PDF文档号码**

Release Tag e.g. 2007.1 or 2005.1-2007.1 **发布时间**

Recording Date yyyy-mm-dd, e.g. 1998-06-26 **修改日期**

Modification Date yyyy-mm-dd, e.g. 2006-04-01 **收录日期**

New Data Only

Clear DB Info Search Count DB Info Search

Search Action

Run Query Clear Query

Chemistry: -

Symmetry: -

Crystal Chemistry: -

Structure Types: -

Experimental Info: -

DB Info: -

Query History

Number of queries: 10

Clear Query History

2018-07-18T04:34	58
2018-05-28T09:40	61
2017-10-25T08:11	(23)
2017-04-07T04:39	(6)
2017-04-07T04:38	(391)
2017-04-07T04:36	(41)
2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

限定来源仅为新数据

检索结果显示



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Results: List View # of Hits: 34

Buttons: Back to Query, Show Detailed View, Export Data, Report, Compare Structures, Compare Powder Pattern, Column Selection, Filter

<input type="checkbox"/>	Coll. Code ^	HMS ^	Struct. Form.	Title ^	Authors ^	Reference ^	☆
<input type="checkbox"/>	5319	I-4 2 m	(Ag _{0.88} Cu _{1.12}) ₂	Mercury-arsenic sulfide	Biagioni, c.; Bonaccorsi, R.	Mineralogical Magazine	☆
<input type="checkbox"/>	37160	C 1 c 1	Zn (Ag (S C N) ₂) ₂				☆
<input type="checkbox"/>	39691	I-4 3 m	Cu _{9.9} Ag _{0.06} Zn _{1.8} La ₆ Ni ₆ P ₁₇				☆
<input type="checkbox"/>	39692	I-4 3 m	Cu _{7.02} Ag _{2.88} Zn _{1.1} La ₆ Ni ₆ P ₁₇	Crystal structure feature	Rozhdestvenskaya, I.	Mineralogicheskii Zhurnal	☆
<input type="checkbox"/>	39693	I-4 3 m	Cu _{6.3} Ag _{3.54} Zn _{1.4} Cu _{11+x} Sb ₄ S ₁₃	Crystal structure feature	Rozhdestvenskaya, I.	Mineralogicheskii Zhurnal	☆
<input type="checkbox"/>	39694	I-4 3 m	Cu _{4.44} Ag ₆ Zn _{0.6} F (Cu,Zn) ₅ Ag ₆ FeSb ₄ S ₁₃	Crystal structure feature	Rozhdestvenskaya, I.	Mineralogicheskii Zhurnal	☆
<input type="checkbox"/>	48197	P n a 21	Zn Ag P S ₄ KNiPO ₄	Structure du Tetrathionate	Toffoli, P.; Rouland, J.	Acta Crystallographica	☆
<input type="checkbox"/>	71563	C 1 2/c 1	Zn (Ag (S C N) ₂) ₂	Redetermination of structure	Jones, P.G.; Bember, J.	Acta Crystallographica	☆
<input type="checkbox"/>	72719	C 1 2/c 1	Ag ₂ Zn (P ₂ S ₆)	Synthesis and structure	Boucher, F.; Evain, M.	European Journal of Mineralogy	☆
<input type="checkbox"/>	154404	P m n 21	Ag (Cd _{0.5} Zn _{1.5}) (G Enargite-Cu ₃ As ₄	Synthesis and X-ray	Parasyuk, O.V.; Olek, S.	Crystal Research and Technology	☆

Navigation: 1 of 4, <<, <, >, >>, 10

显示选中检索结果的详情

输出选中检索记录

对比选中的检索结果

来源文献标题

作者

参考文献

筛选功能

ICDS代码

结构形式

空间群

标记代表为高质量数据

检索结果的详细信息： 一条完整的记录



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Detailed View

Entry 1 of 1 ?

Back to Query

Back to List



Export Cif

Report

Feedback to Editor

Summary

Collection Code 5319

Struct.formula (Ag.88 Cu.13 Zn.08) Hg1.91 Tl (As.79 Sb.21)2 S6

Author Biagioni, c.; Bonaccorsi, E.; Moelo, Y.; Orlandi, P.; Bindi, L.; D'Orazio, M.; Vezzoni, S.

Space Group I-4 2 m (121)

Title of Article Mercury-arsenic sulfosalts from the Apuan Alps (Tuscany, Italy). II. Arsiccioite, AgHg₂TlAs₂S₆, a new mineral from the Monte Arsiccio mine: occurrence, crystal structure and crystal chemistry of the routhierite isotopic series

Unit Cell 10.1386(6) 10.1386(6) 11.3441(5) 90. 90. 90.

Reference Mineralogical Magazine (2014) 78, (1) p101-p117

Cell Volume 1166.07 Å³ Formula Units per Cell 4

Warnings & Comments 0 Warnings / 0 Comments

Temperature room temperature Pressure atmospheric

PDF-Numbers R-Value 0.0304

Remark High Quality Data

Details ?

Expand all / Close all

Visualization

Chemistry

Published Crystal Structure Data

Standardized Crystal Structure Data

Distances and Angles

Bibliography

Experimental

Warnings and Comments

Compare Published and Standardized Structure

检索结果的详细信息： 一条完整的记录

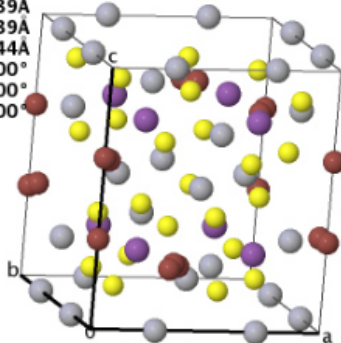
Details ?

Expand all / Close all

Visualization

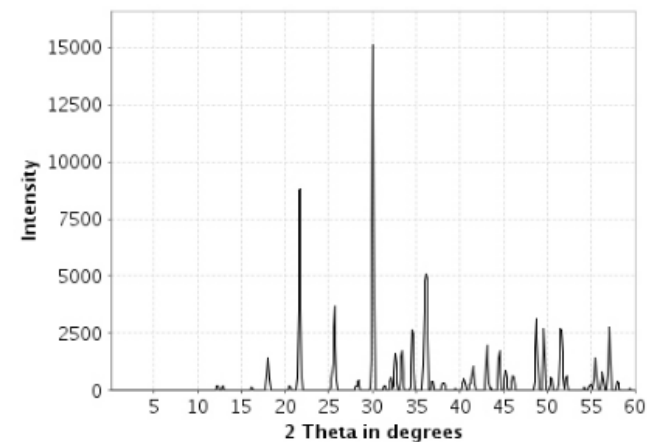
Published Crystal Structure


HM:I -4 2 m
a=10.139Å
b=10.139Å
c=11.344Å
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=90.000^\circ$



 Interactive Visualization

Powder Pattern



 Interactive Visualization

Chemistry

Sum Formula

Struct. Form

Chemical Name

Mineral Name

Mineral Group

Number of Formula Units

ANX Formula
Cryst. Comp.

AB Formula
Chem. Comp.

检索结果的详细信息： 一条完整的记录



Published Crystal Structure Data

Cell Parameters	10.1386(6) 10.1386(6) 11.3441(5) 90. 90. 90.		
Volume	1166.07	Formula Units per Cell	4
Space Group	I -4 2 m (121)	Pearson Symbol	tl48
Crystal System	tetragonal	Crystal Class	-42m
Wyckoff Sequence	j i3 f e d	Structure Type	
Axis Ratios	a/b 1.0000	b/c 0.8937	c/a 1.1189
Remark			

EL	Lbl	OxState	Wyck Symb	X	Y	Z	U	SOF	H
Tl	1	+1.00	4 e	0	0	0.345(1)	.043(1)	0.360000	.36
Tl	2	+1.00	8 i	.026(1)	-.026(1)	0.3588(3)	.043(1)	0.320000	.32
Hg	1	+2.00	4 d	0	0.5	0.75	.0386(3)	0.650000	.65
Ag	1	+1.00	4 d	0	0.5	0.75	.0386(3)	0.140000	.14
Cu	1	+1.00	4 d	0	0.5	0.75	.0386(3)	0.130000	.13
Zn	1	+2.00	4 d	0	0.5	0.75	.0386(3)	0.080000	.08
Hg	2	+2.00	8 f	0.22008(6)	0.5	0.5	.0339(2)	0.630000	.63
Ag	2	+1.00	8 f	0.22008(6)	0.5	0.5	.0339(2)	0.370000	.37
As	1	+3.00	8 i	0.25816(7)	0.25816(7)	0.25354(13)	.0225(3)	0.790000	.79
Sb	1	+3.00	8 i	0.25816(7)	0.25816(7)	0.25354(13)	.0225(3)	0.210000	.21
S	1	-2.00	16 j	0.0949(2)	0.3284(2)	0.3797(2)	.0244(3)		
S	2	-2.00	8 i	0.1232(2)	0.1232(2)	0.1428(2)	.0220(5)		

检索结果的详细信息— 一条完整的记录



Standardized Crystal Structure Data

Cell Parameters	10.1386 10.1386 11.3441 90.000 90.000 90.000				
Volume	1166.07	Formula Units per Cell	4	Calc. Dens.	6.03
Space Group	I -4 2 m(121)	Pearson Symbol	tl48		
Crystal System	tetragonal	Crystal Class	-42m	Laue Class	4/mmm
Wyckoff Sequence	j i3 g e d				
Axis Ratios	a/b 1.0000	b/c 0.8937	c/a 1.1189		
Transformation Method	Tidy				
Transformation Info	TRANS Origin 0 0 1/2				
Remark					

EL	Lbl	OxState	Wyck Symb	X	Y	Z	U	SOF
Tl	1	+1.00	4 e	0.0000	0.0000	0.1550	0.0430	0.3600
Tl	2	+1.00	8 i	0.0260	0.0260	0.1412	0.0430	0.3200
Hg	1	+2.00	4 d	0.0000	0.5000	0.2500	0.0386	0.6500
Ag	1	+1.00	4 d	0.0000	0.5000	0.2500	0.0386	0.1400
Cu	1	+1.00	4 d	0.0000	0.5000	0.2500	0.0386	0.1300
Zn	1	+2.00	4 d	0.0000	0.5000	0.2500	0.0386	0.0800
Hg	2	+2.00	8 g	0.2799	0.0000	0.5000	0.0339	0.6300
Ag	2	+1.00	8 g	0.2799	0.0000	0.5000	0.0339	0.3700
As	1	+3.00	8 i	0.2418	0.2418	0.2535	0.0225	0.7900
Sb	1	+3.00	8 i	0.2418	0.2418	0.2535	0.0225	0.2100
S	1	-2.00	16 j	0.1716	0.4051	0.3797	0.0244	
S	2	-2.00	8 i	0.3768	0.3768	0.1428	0.0220	

检索结果的详细信息： 一条完整的记录



Distances and Angles

Select pairs of elements

Select from atom position

Atom A

Ag
 As
 Cu
 Hg

✓ (un)select all

Atom B

Ag
 As
 Cu
 Hg

✓ (un)select all

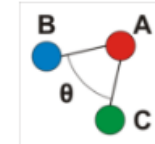
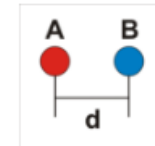
Atom C

Ag
 As
 Cu
 Hg

✓ (un)select all

Histograms

Calculate



Bibliography

Title of Article	Mercury-arsenic sulfosalts from the Apuan Alps (Tuscany, Italy). II. Arsiccioite, AgHg ₂ TlAs ₂ S ₆ , a new mineral from the Monte Arsiccio mine: occurrence, crystal structure and crystal chemistry of the routhierite isotopic series
1st Reference	Mineralogical Magazine (2014) 78, (1) p101-p117 DOI: 10.1180/minmag.2014.078.1.08 Get full text by: Google
Keywords	
2nd Reference	
3rd Reference	

检索结果的详细信息： 一条完整的记录



▼ Experimental

External Conditions

Temperature

room temperature

Pressure

atmospheric

Radiation Type

- Xray Electrons Neutrons Synchrotron

Sample Type

- Powder Single Crystal

R-value

0.0304

Additional Information

- | | | |
|--|---|--|
| <input type="checkbox"/> Twinned Crystal Data | <input checked="" type="checkbox"/> Temperature Factors available | <input type="checkbox"/> NMR Data available |
| <input type="checkbox"/> Rietveld Refinement employed | <input type="checkbox"/> Magnetic Structure Available | <input type="checkbox"/> Correction of Earlier Work |
| <input type="checkbox"/> Absolute Configuration Determined | <input type="checkbox"/> Anharmonic temperature factors given | <input type="checkbox"/> Cell Constants without s.d. |
| <input type="checkbox"/> Experimental PDF Number assigned | <input type="checkbox"/> Calculated PDF Number assigned | <input type="checkbox"/> Only Cell and Structure Type determined |

Properties of Structure

- | | | |
|---|---|---|
| <input type="checkbox"/> Polytype Structure | <input type="checkbox"/> Order/Disorder Structure | <input type="checkbox"/> Disordered Structure |
| <input type="checkbox"/> Prototype Structure Type | <input type="checkbox"/> Modulated Structure | <input checked="" type="checkbox"/> Mineral |
| <input type="checkbox"/> Structure Prototype | | |

▼ Warnings and Comments

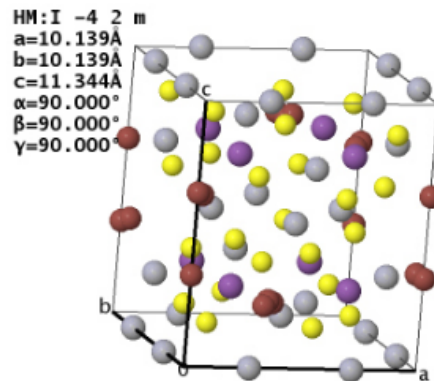
Warnings

Comments

检索结果的详细信息： 一条完整的记录

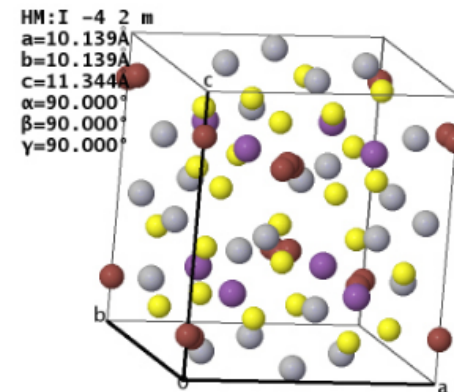
▼ Compare Published and Standardized Structure

Published Crystal Structure



Standardized Crystal Structure

★ 收藏



Interactive Visualization

检索式管理

Welcome to ICSD Web. Logged in: Zeng, Shirley

FIZ Karlsruhe | Contact
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Content Selection

- Experimental Structures only
- Theoretical Structures only
- All Structures

Navigation

- 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
 - Create Combined Query

Chemistry Search

Composition: Number of Elements:

Structural Formula: e.g. Pb (W O4)

Chemical Name:

Mineral Name: e.g. Adamite

Mineral Group: e.g. Pyroxene

ANX Formula:

Number of Formula Units:

Search Action

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	34
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Combined Results:	34

Query History

Number of queries: 12

2018-08-07T08:46	34
2018-08-07T08:45	882
2018-07-18T04:34	58
2018-05-28T09:40	61
2017-10-25T08:11	(23)
2017-04-07T04:39	(6)
2017-04-07T04:38	(391)

检索式管理

联合检索式列表

创建联合检索式

检索历史列表

谢谢！