

ICSD-无机晶体结构数据库 使用指南

iGroup · 上海

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

Crystal System Space Group Number

Cell

Cell Parameters

Temperature Tolerance +/- %

Crystal System Centering

ICSD Collection Code

Temperature K

Pressure MPa

ICSD Collection Code

Temperature K

Pressure MPa

Clear Basic Search

Count Basic Search

Search Action

Run Query Clear Query

Search Summary

Basic Search: -

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)

基本检索

高级检索

检索式管理

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

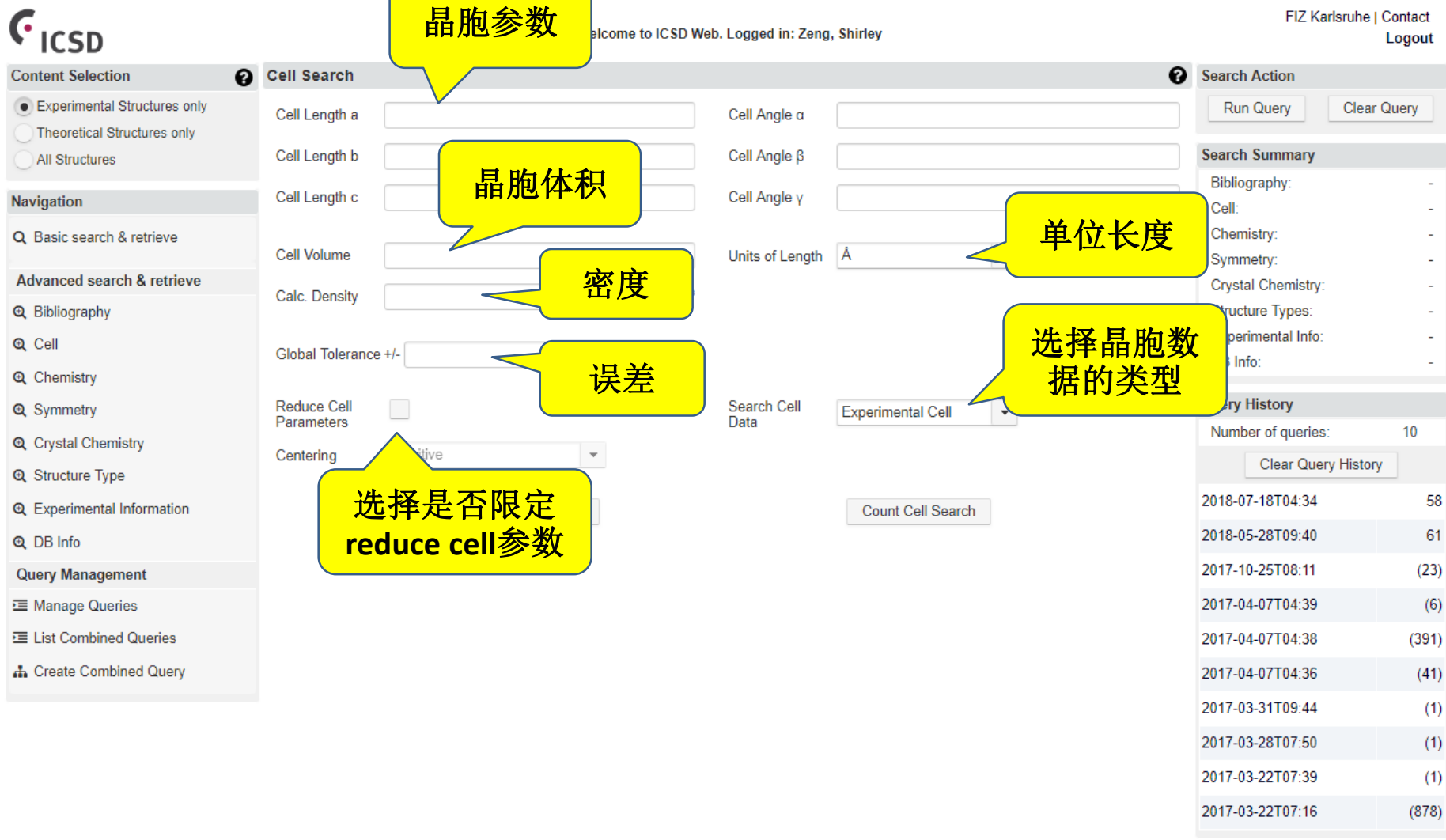
Search Summary

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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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

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

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Content Selection

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Chemistry Search

Composition Number of Elements

Structural Formula **分子式**

Chemical Name **化学物质名称**

Mineral Name **矿物名称**

Mineral Group **矿物群**

ANX Formula Number of Formula Units

AB Formula

Formula Weight **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

Content Selection

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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 Cen

晶系

晶体等级

Wyckoff序列

Pearson符号

对称中心

Clear Symmetry Search

Count Symmetry 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)
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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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
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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

Clear Structure Search

Clear Query

Search Action

Run Query

Search Summary

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

Series: 10

Clear Query History

2018-07-18T04:34	58
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2017-10-25T08:11	(23)
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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)

结构类型

空间群

Wyckoff序列

Pearson符号

ANX结构

高级检索-依据实验信息检索

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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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Content Selection **?** DB Info Search

- 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
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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 **限定来源仅为新数据**

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)

检索结果显示



Results: List View

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of Hits: 34

显示选中检索结果的详情

输出选中检索记录

Back to Query

Show Detailed View

Export Data

Report

Column Selection

Filter

Compare Structures

Compare Powder Pattern

<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	☆

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

ICSD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 Å ³	Warnings & Comments	0 Warnings / 0 Comments
	Formula Units per Cell 4		
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

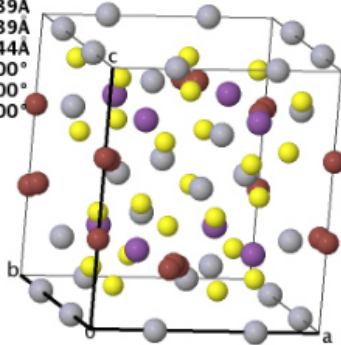
Details ?


Expand all / Close all

Visualization

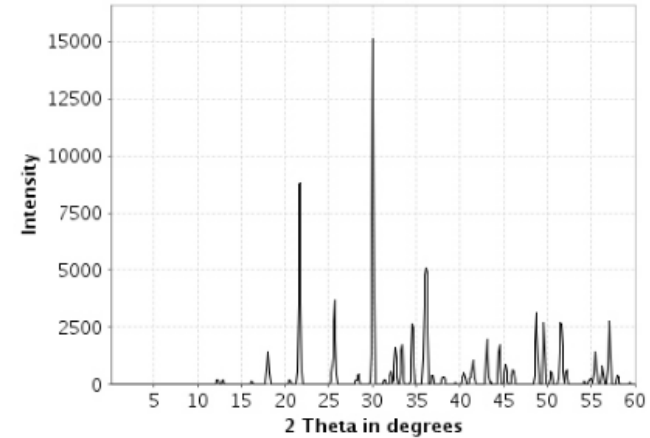
Published Crystal Structure


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	Calc. Dens.	6.03
Space Group	I -4 2 m (121)	Pearson Symbol	tl48	Meas. Dens.	
Crystal System	tetragonal	Crystal Class	-42m	Laue Class	4/mmm
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

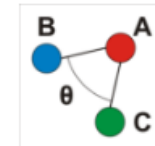
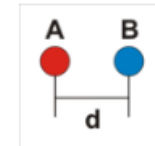
Atom C

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

Twinned Crystal Data

Temperature Factors available

NMR Data available

Rietveld Refinement employed

Magnetic Structure Available

Correction of Earlier Work

Absolute Configuration Determined

Anharmonic temperature factors given

Cell Constants without s.d.

Experimental PDF Number assigned

Calculated PDF Number assigned

Only Cell and Structure Type determined

Properties of Structure

Polytype Structure

Order/Disorder Structure

Disordered Structure

Prototype Structure Type

Modulated Structure

Mineral

Structure Prototype

▼ Warnings and Comments

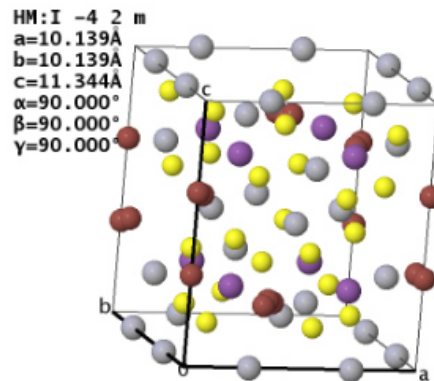
Warnings

Comments

检索结果的详细信息： 一条完整的记录

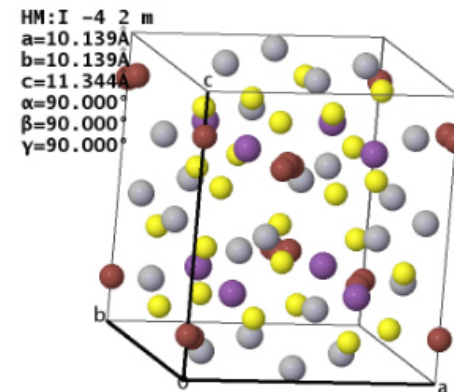
▼ Compare Published and Standardized Structure

Published Crystal Structure



Standardized Crystal Structure

★ 收藏



Interactive Visualization

检索式管理

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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

Chemistry Search

Composition: Number of Elements:

Structural Formula:

Chemical Name:

Mineral Name:

Mineral Group:

ANX Formula:

Number of Formula Units:

Search Action

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	34
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Structure Types:	-
Experimental Info:	-
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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！