

ICSD-无机晶体结构数据库 使用指南

iGroup · 上海

ICSD数据库

访问链接: <https://icsd.fiz-karlsruhe.de>

备用访问链接: <https://141.66.193.6/>



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Logout

Content Selection

- ☒ Experimental Structures only
- ☐ Theoretical Structures only
- ☐ All Structures

Navigation

Basic search & retrieve

基本检索

Advanced search & retrieve

高级检索

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

Title of Journal

Year of
Publication

Cell

Cell Parameters

Periodic Table

Number of
Elements

Tolerance +/- %

Space Group
Number

Crystal System

Centering

E

ICSD Collection
Code

Temperature

Pressure

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)

高级检索-依据文献检索



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

Bibliography Search

Authors

Title of Journal

Title of Article

Year of Publication

Volume

Page first

Abstract

Keywords

Clear Bibliography Search

Count Bibliography Search

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Logout

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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2017-10-25T08:11	(23)
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2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

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

高级检索-依据晶胞检索



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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

Cell Search

Cell Length a Cell Angle α
Cell Length b Cell Angle β
Cell Length c Cell Angle γ
Cell Volume Units of Length
Calc. Density
Global Tolerance +/-
Reduce Cell Parameters ☐
Centering

Search Cell Data

Search Action

Search Summary

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

晶胞参数

晶胞体积

密度

误差

选择是否限定
reduce cell参数

单位长度

选择晶胞数
据的类型

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 Periodic Table Number of Elements
e.g. Na Cl

Structural Formula
e.g. Pb (W O4)

Chemical Name

Mineral Name

Mineral Group
e.g. Pyroxene

ANX Formula Number of Formula Units

AB Formula

Formula Weight

Clear Chemistry Search

Count Chemistry Search

成分

元素数量

分子式

化学物质名称

矿物名称

矿物群

分子量

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Logout

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)

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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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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

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

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
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2017-03-31T09:44	(1)
2017-03-28T07:50	(1)
2017-03-22T07:39	(1)
2017-03-22T07:16	(878)

空间群

晶系

晶体等级

Wyckoff序列

Pearson符号

对称中心

高级检索-依据原子坐标检索



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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

Crystal Chemistry Search

Interatomic Distances

	Atom A	Ox. A		Atom B	Ox. B	d _{min} AB	d _{max} AB
			-				
AND			-				
AND			-				
AND			-				

Minimum Distances

Atom A		Atom B	d _{min} AB	d _{max} AB
	-			

Crystal Structure is

☐ Polytype Structure	☐ Order/Disorder Structure Type
☐ Modulated Structure	☐ Mineral
☐ Disordered Structure	☐ Prototype Structure Type

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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2017-03-28T07:50	(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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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

Structure Type Search

Pre Defined Structure Types

Structure Type

☐ Search in predefined structure types

Structure Type Descriptors

☐ SpaceGrp ☐ Wyck ☐ Pearson ☐ ANX

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)

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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☐ 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

Experimental Information Search

Temperature K
Pressure MPa
Comments
R-Value

温度
压力

注释
射线类型

样本类型

R值

其他属性

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)
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-依据数据库记录信息检索

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Content Selection

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☐ 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

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 ☐

Clear DB Info Search

Count DB Info Search

ICSD代码

PDF文档号码

发布时间

收录日期

修改日期

限定来源仅为新数据

Search Action

Run Query Clear Query

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

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Results: List View

of Hits: 34

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

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

ICDS代码

结构形式

空间群

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

标记代表为高质量数据

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检索结果的详细信息： 一条完整的记录

Detailed View

Entry 1 of 1 ?

[Back to Query](#)

[Back to List](#)

[Previous](#) [First](#) [Next](#) [Last](#)

[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

Space Group I-4 2 m (121)

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

Cell Volume 1166.07 Å³ Formula Units per Cell 4

Temperature room temperature Pressure atmospheric

PDF-Numbers R-Value 0.0304

Remark  High Quality Data

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

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 isotypic series

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

Warnings & Comments 0 Warnings / 0 Comments

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

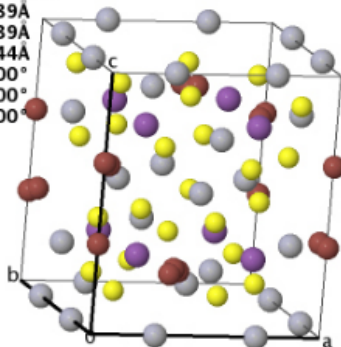
Details

Expand all / Close all

Visualization

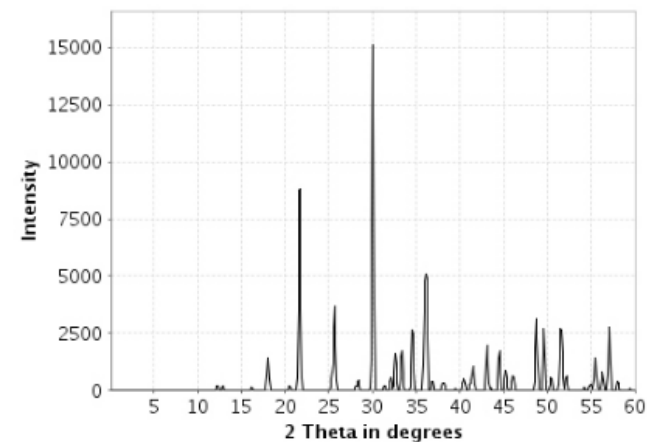
Published Crystal Structure

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 Ag_{0.88} As_{1.58} Cu_{0.13} Hg_{1.91} S₆ Sb_{0.42} Tl₁ Zn_{0.08}

Struct. Form (Ag_{0.88} Cu_{0.13} Zn_{0.08}) Hg_{1.91} Tl (As_{0.79} Sb_{0.21})₂ S₆

Chemical Name Silver mercury thallium arsenosulfide

Mineral Name Arsiccioite

Mineral Group

Number of Formula Units 4

ANX Formula
Cryst. Comp.

AB₂C₃X₆

AB Formula
Chem. Comp.

ABC₂D₂E₆

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

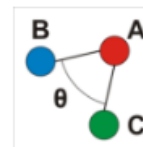
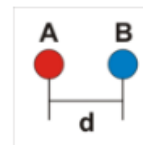
Atom C

☐ 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 isotypic 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

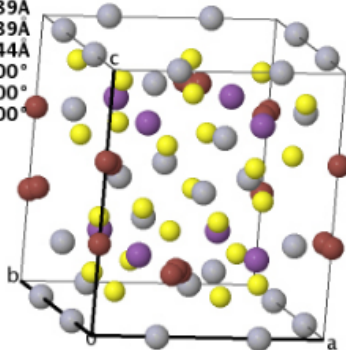
Comments

检索结果的详细信息： 一条完整的记录

▼ Compare Published and Standardized Structure

Published Crystal Structure

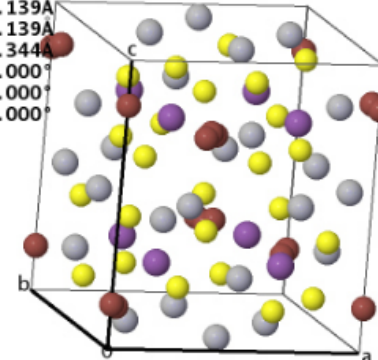
HM:I -4 2 m
a=10.139Å
b=10.139Å
c=11.344Å
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=90.000^\circ$



Standardized Crystal Structure

★ 收藏

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

检索式管理

ICSD

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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:

Chemical Name:

Mineral Name:

Mineral Group:

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



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THANK YOU !