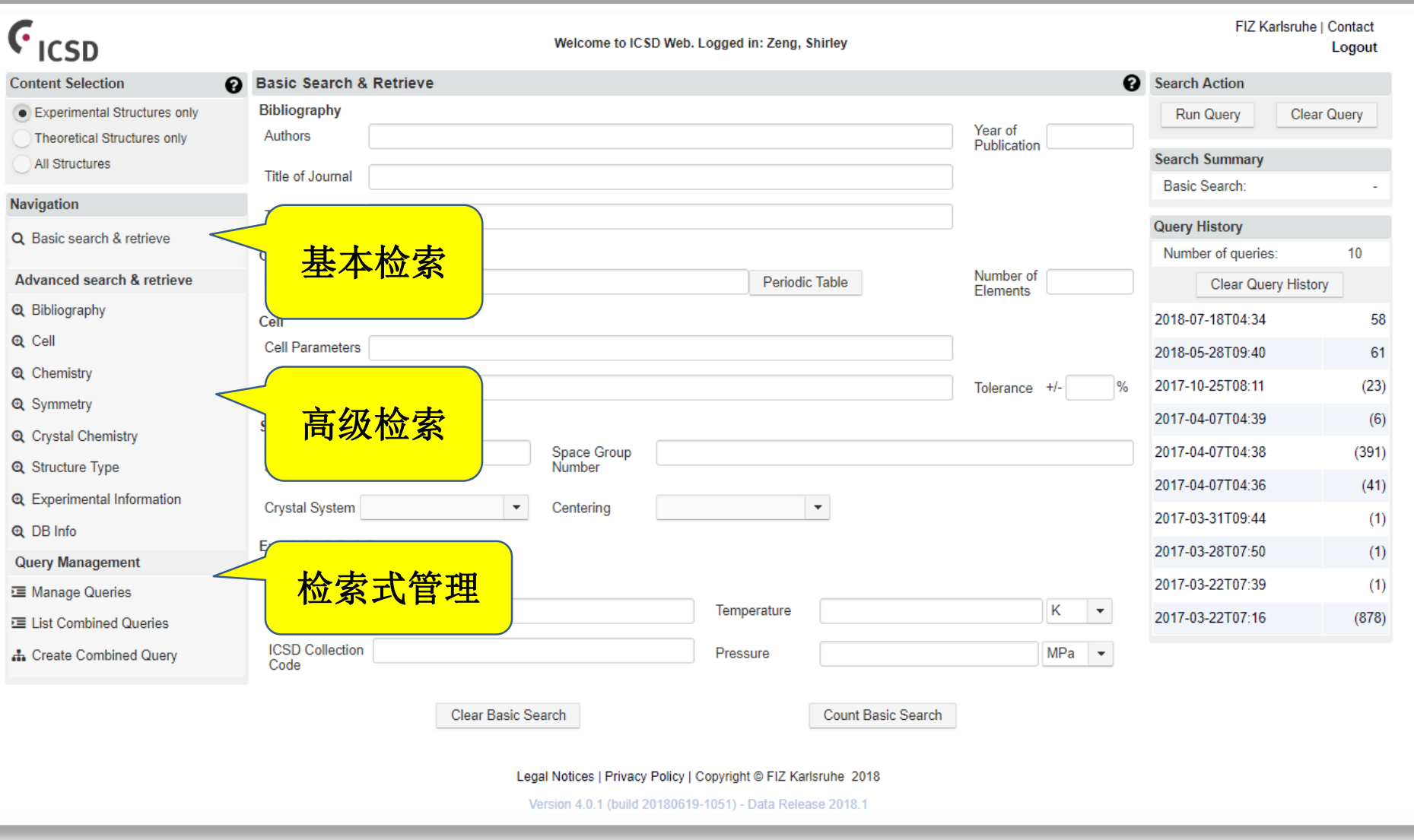
FIZ Karlsruhe
ICSD

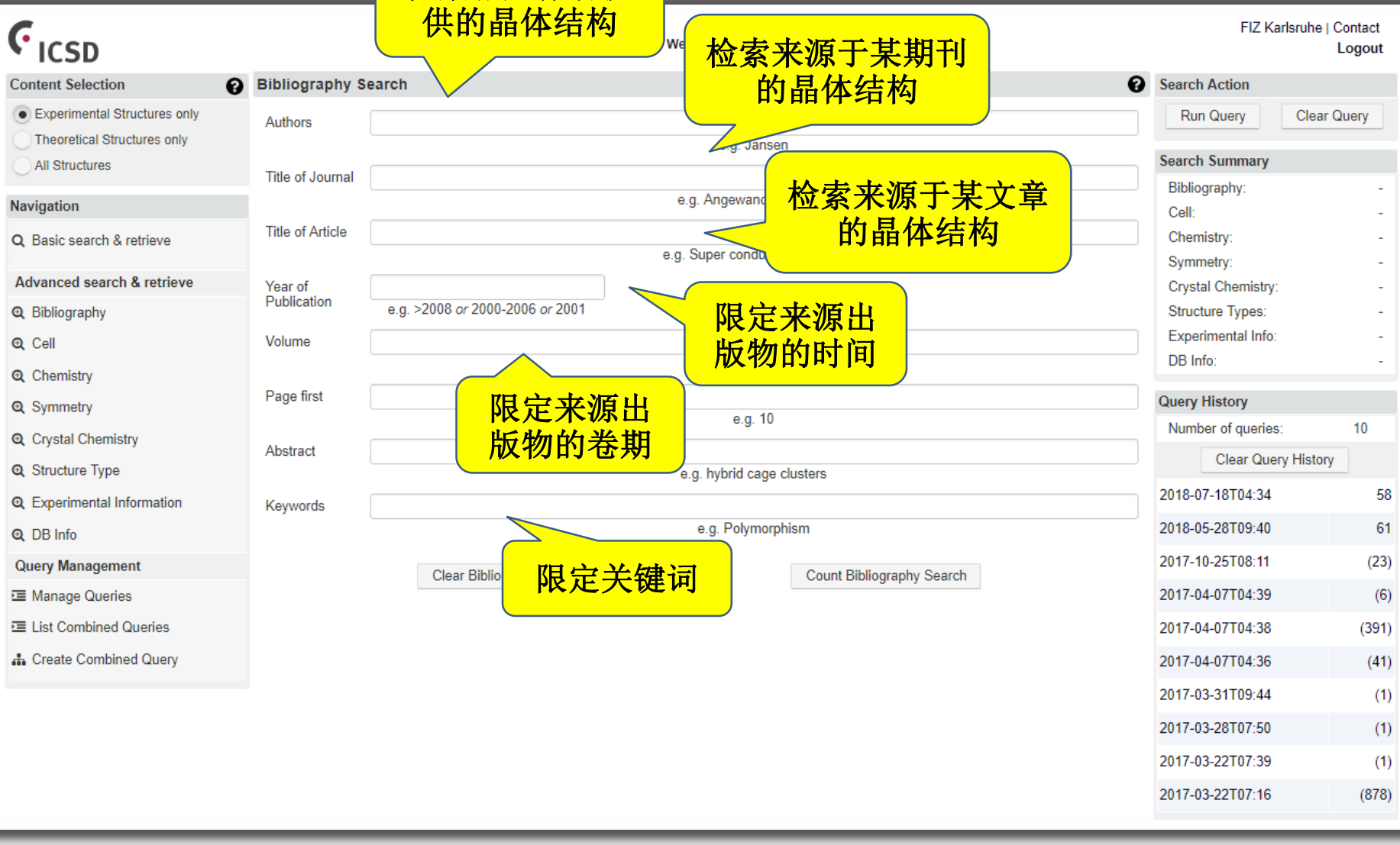
ICSD-无机晶体结构数据库使用指南

iGroup · 上海

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



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
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Logout
Content Selection
Experimental Structures only
Theoretical Structures only
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Advanced search & retrieve
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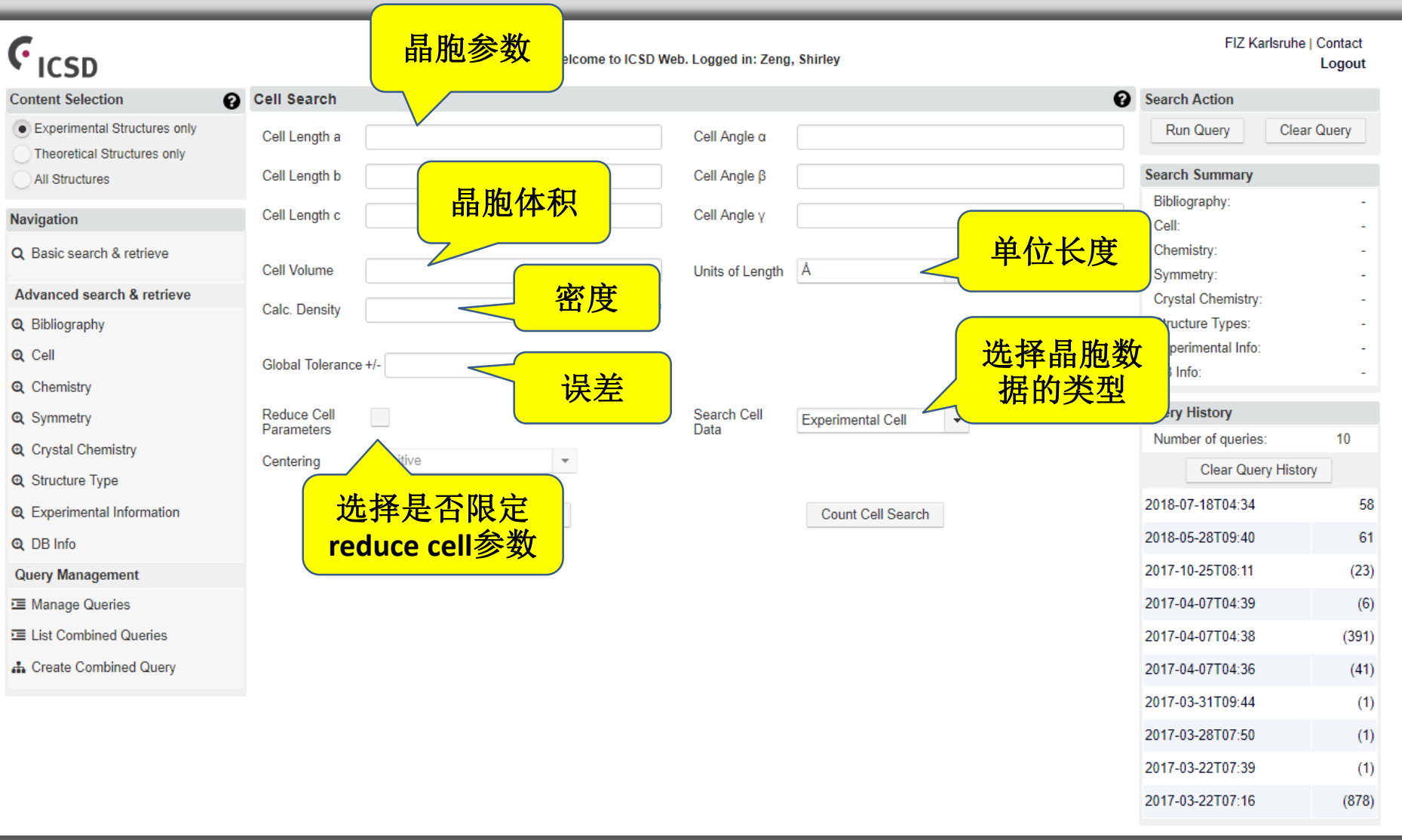
Chemistry
Symmetry
Crystal Chemistry
Structure Type
Experimental Information
DB Info
Query Management
Manage Queries
List Combined Queries
Create Combined Query
Bibliography Search
Authors
e.g. Jansen
Title of Journal
e.g. Angewand
Title of Article
e.g. Super condu
Year of Publication
e.g. >2008 or 2000-2006 or 2001
Volume
Page first
e.g. 10
Abstract
e.g. hybrid cage clusters
Keywords
e.g. Polymorphism
Clear Biblio
Count Bibliography 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-依据晶胞检索


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
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Cell Search
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
Å
Search Cell Data
Experimental Cell
Count Cell Search
Search Action
Run Query
Clear Query
Search Summary
Bibliography:
Cell:
Chemistry:
Symmetry:
Crystal Chemistry:
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Clear Query History
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2018-05-28T09:40 61
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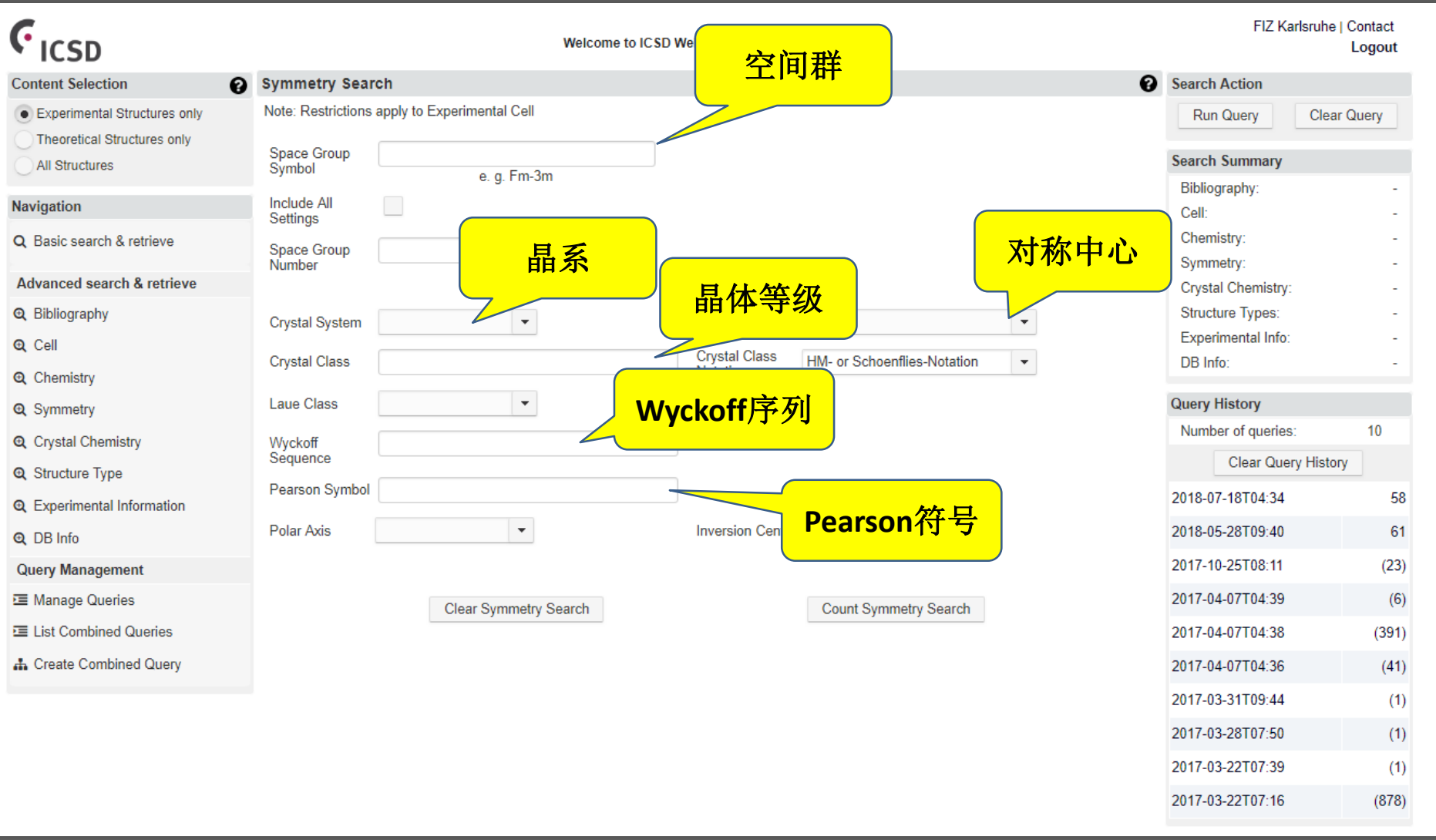
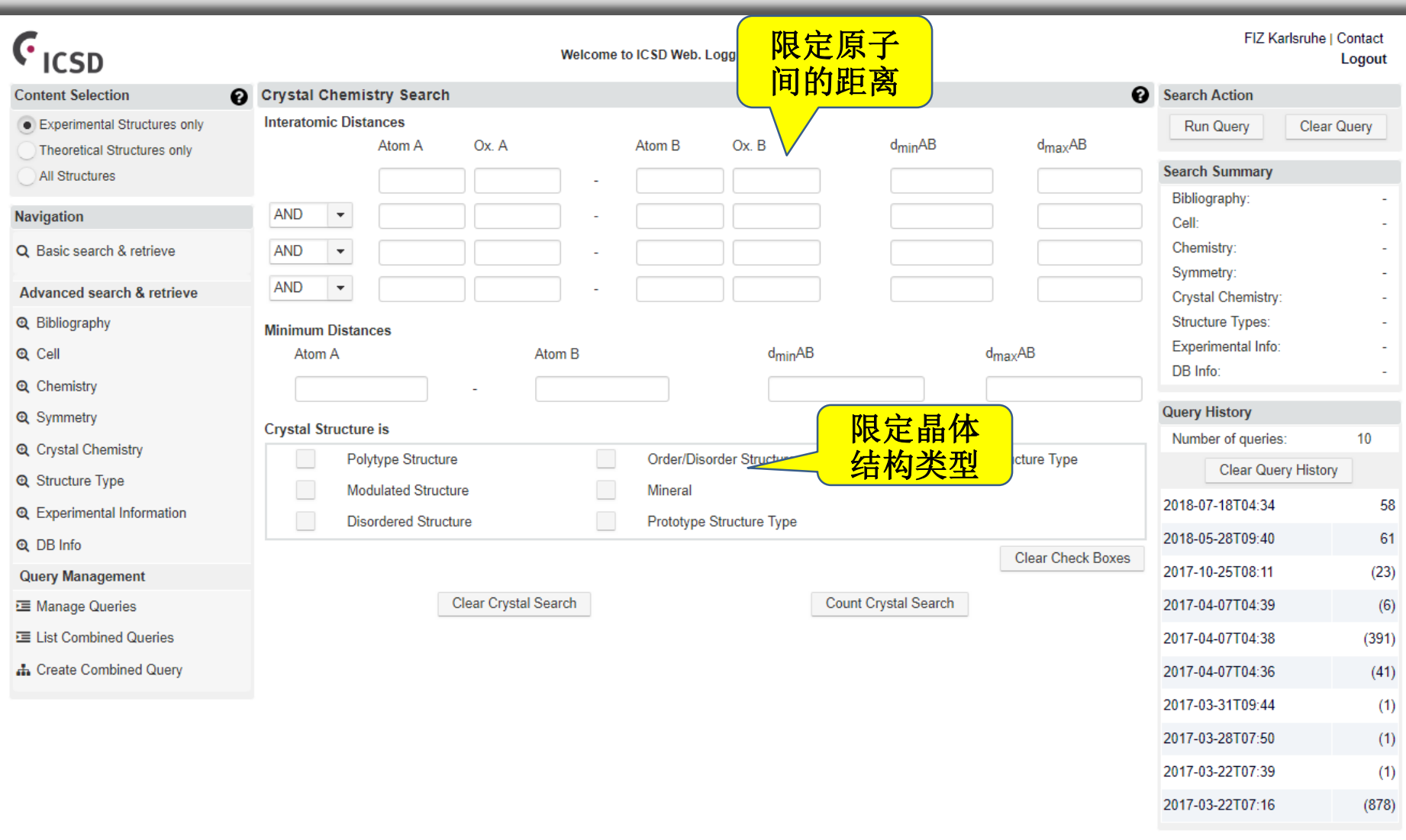
2017-04-07T04:36 (41)
2017-03-31T09:44 (1)
2017-03-28T07:50 (1)
2017-03-22T07:39 (1)
2017-03-22T07:16 (878)

高级检索-依据化学式检索

高级检索-依据晶体对称性检索

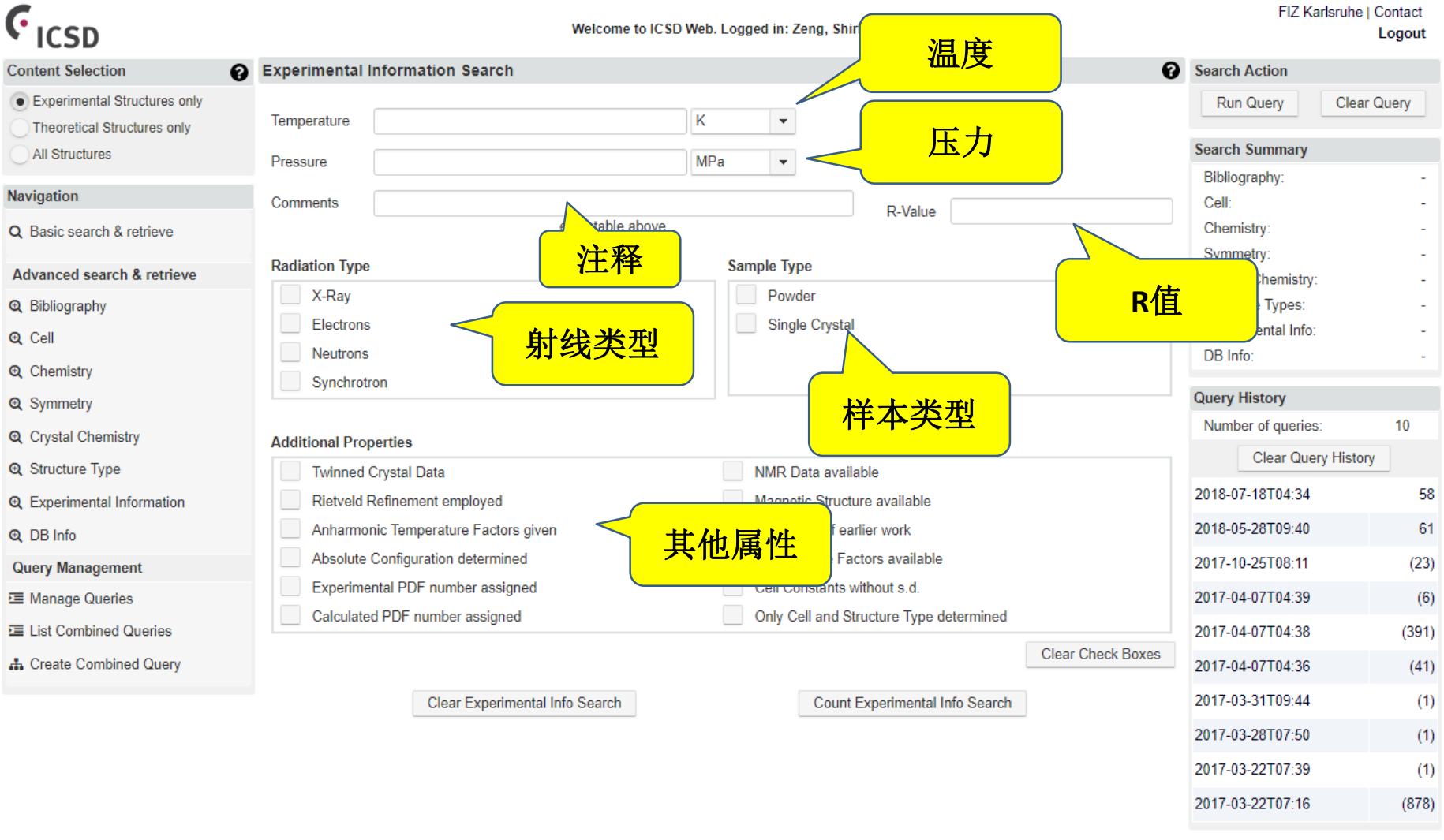


高级检索-依据原子坐标检索

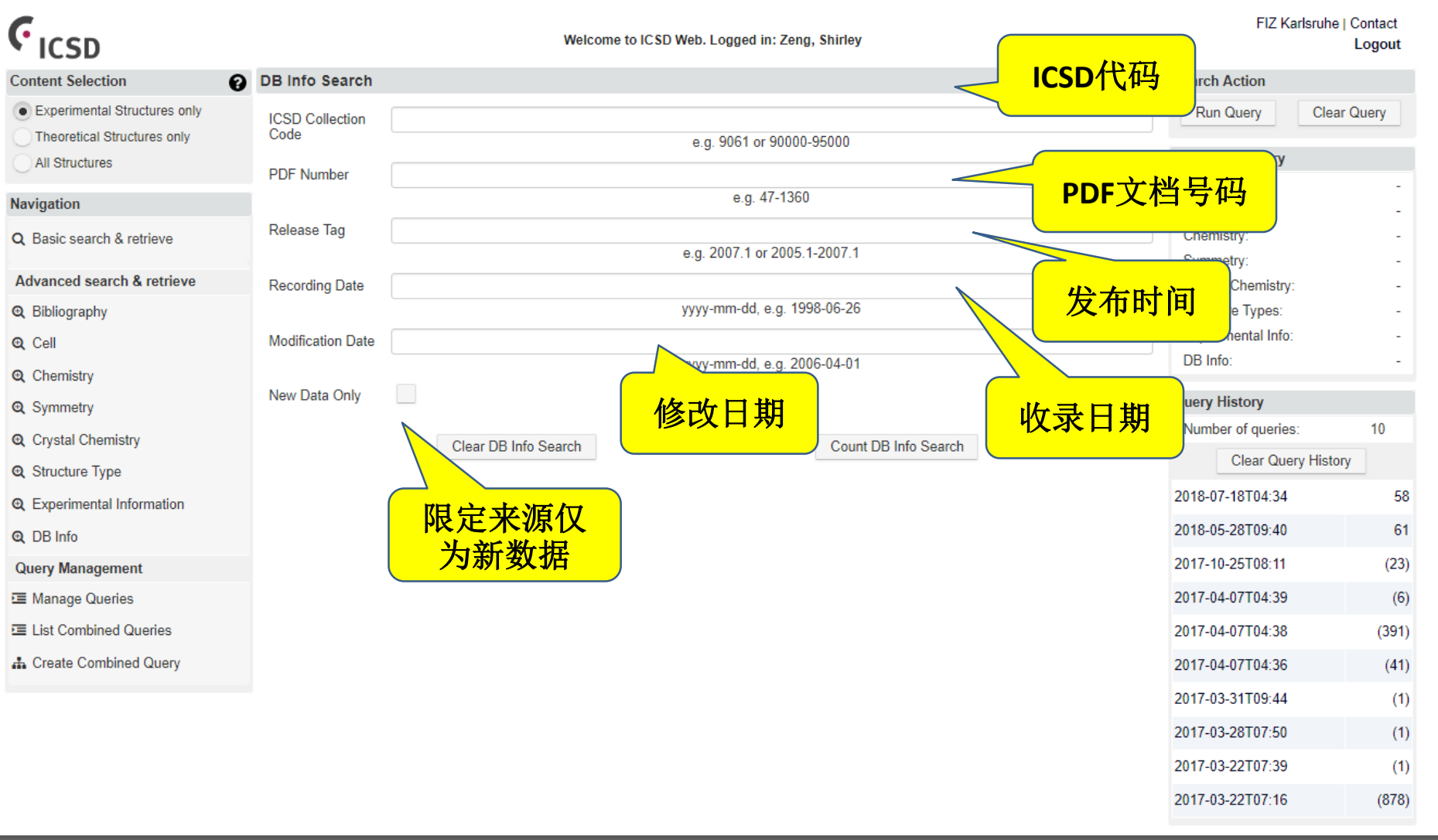


高级检索-依据晶体结构检索

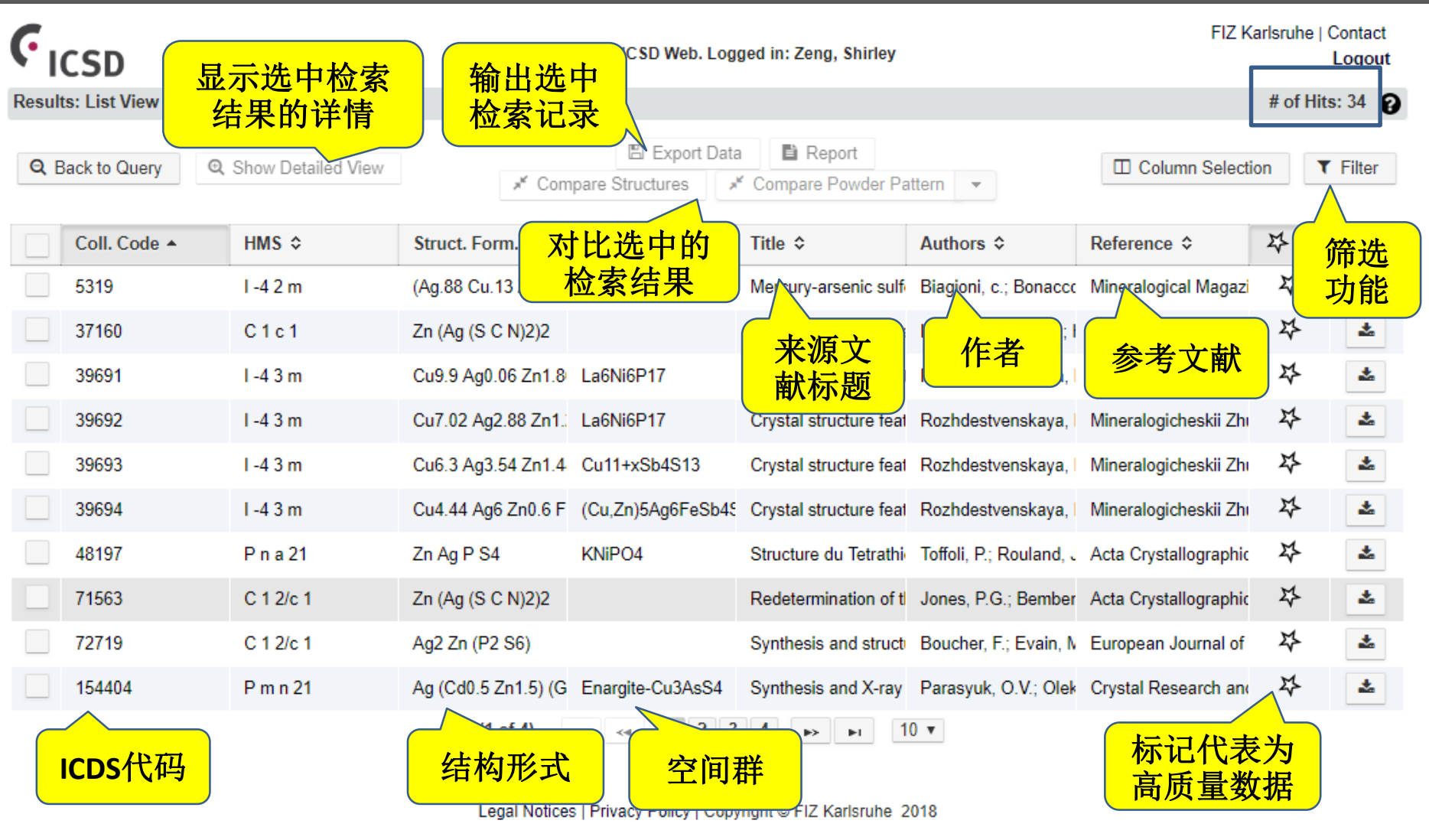
高级检索-依据实验信息检索



高级检索-依据数据库记录信息检索



检索结果显示


ICSD
CSD Web. Logged in: Zeng, Shirley
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Logout
Results: List View
# 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
Compare Structures
Compare Powder Pattern
Column Selection
Filter
对比选中的检索结果
筛选功能
来源文献标题
作者
参考文献
Coll. Code
HMS
Struct. Form.
Title
Authors
Reference
5319 I -4 2 m (Ag.88 Cu.13 Mercury-arsenic sulf Biagioni, c.; Bonacc Mineralogical Magazi
37160 C 1 c 1 Zn (Ag (S C N)2)2
39691 I -4 3 m Cu9.9 Ag0.06 Zn1.8 La6Ni6P17
39692 I -4 3 m Cu7.02 Ag2.88 Zn1. La6Ni6P17 Crystal structure feat Rozhdestvenskaya, Mineralogicheskii Zh
39693 I -4 3 m Cu6.3 Ag3.54 Zn1.4 Cu11+xSb4S13 Crystal structure feat Rozhdestvenskaya, Mineralogicheskii Zh
39694 I -4 3 m Cu4.44 Ag6 Zn0.6 F (Cu,Zn)5Ag6FeSb4 Crystal structure feat Rozhdestvenskaya, Mineralogicheskii Zh
48197 P n a 21 Zn Ag P S4 KNiPO4 Structure du Tetrathi Toffoli, P.; Rouland, Acta Crystallographic
71563 C 1 2/c 1 Zn (Ag (S C N)2)2 Redetermination of t Jones, P.G.; Bember Acta Crystallographic
72719 C 1 2/c 1 Ag2 Zn (P2 S6) Synthesis and struct Boucher, F.; Evain, M European Journal of
154404 P m n 21 Ag (Cd0.5 Zn1.5) (G Enargite-Cu3AsS4 Synthesis and X-ray Parasyuk, O.V.; Olek Crystal Research an
10
ICDS代码
结构形式
空间群
标记代表为高质量数据
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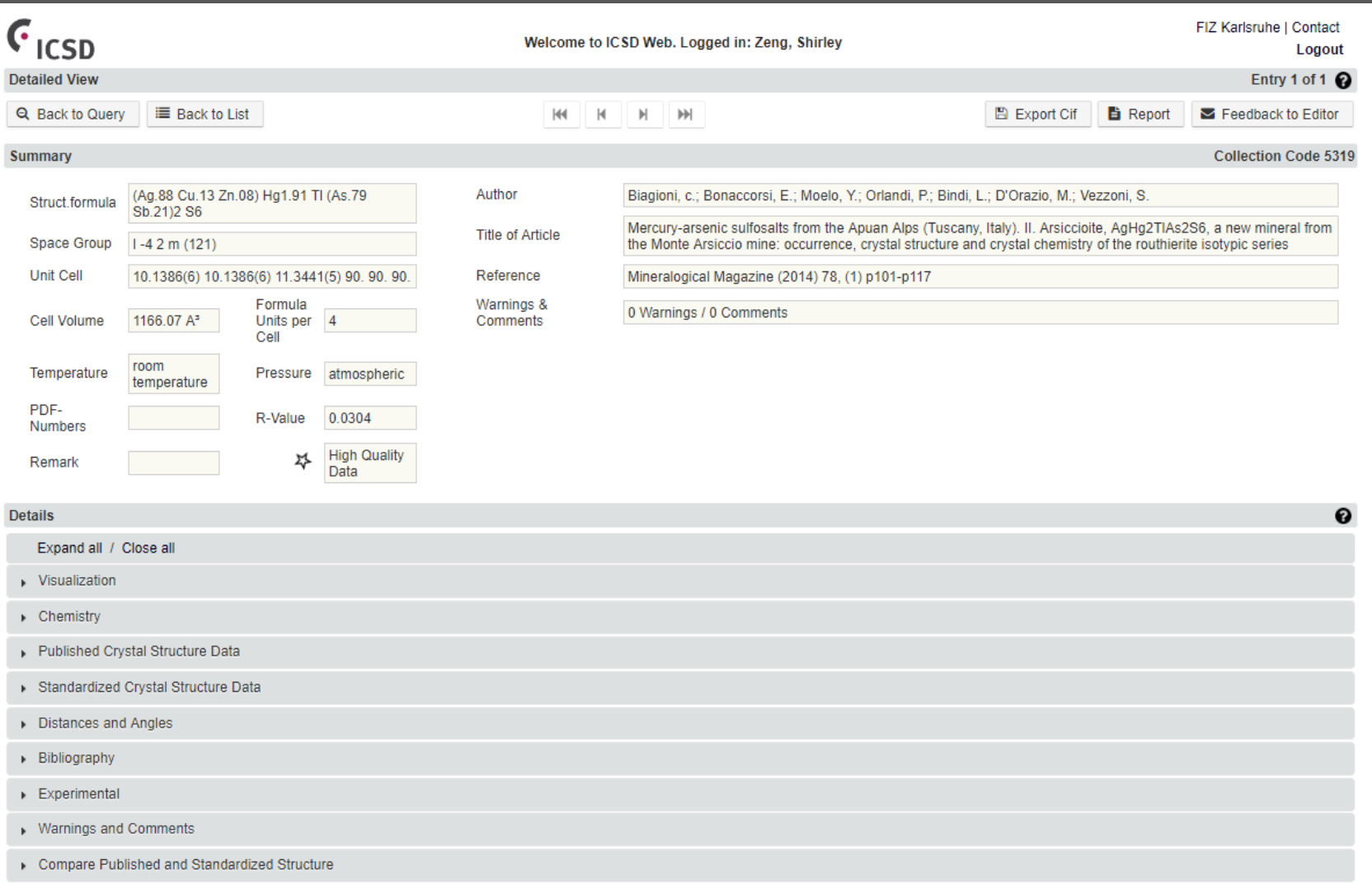
检索结果的详细信息：一条完整的记录



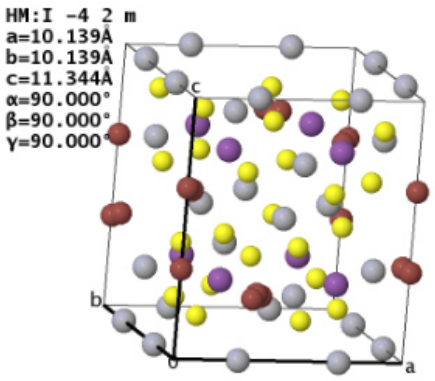
检索结果的详细信息：一条完整的记录

Details

Expand all / Close all

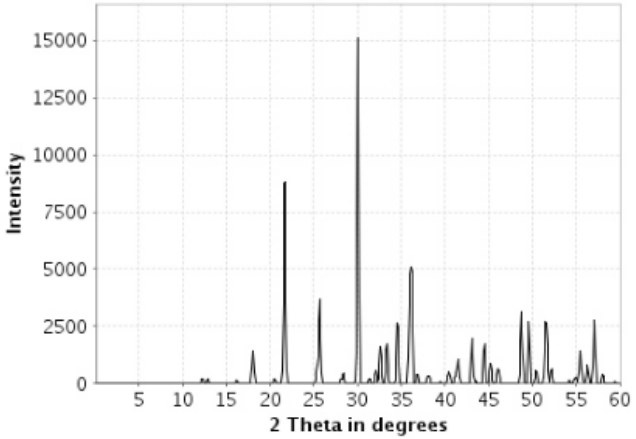
Visualization

Published Crystal Structure



Interactive Visualization

Powder Pattern



Interactive Visualization

Chemistry

Sum Formula	Ag0.88 As1.58 Cu0.13 Hg1.91 S6 Sb0.42 Tl1 Zn0.08
Struct. Form	(Ag.88 Cu.13 Zn.08) Hg1.91 Tl (As.79 Sb.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

FIZ Karlsruhe ICSD

▾ 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	tI48		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

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▾ 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	tI48		
Crystal System	tetragonal	Crystal Class	-42m	Laue Class	4/mmm
Wyckoff Sequence	j i3 g e d				

Axis Ratios	a/b	b/c	c/a
	1.0000	0.8937	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

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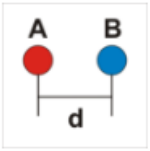
▾ Distances and Angles

Select pairs of elements | Select from atom position

Atom A	Atom B	Atom C
Ag	Ag	Ag
As	As	As
Cu	Cu	Cu
Hg	Hg	Hg
✔ (un)select all	✔ (un)select all	✔ (un)select all

Histograms

Calculate



▾ Bibliography

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
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

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Experimental

External Conditions

Temperature: room temperature

Pressure: atmospheric

Radiation Type

- [x] Xray
- [ ] Electrons
- [ ] Neutrons
- [ ] Synchroton

Sample Type

- [ ] Powder
- [x] Single Crystal

R-value: 0.0304

Additional Information

- [ ] Twinned Crystal Data
- [x] 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
- [x] Mineral
- [ ] Structure Prototype

Warnings and Comments

Warnings

Comments

检索结果的详细信息：
一条完整的记录

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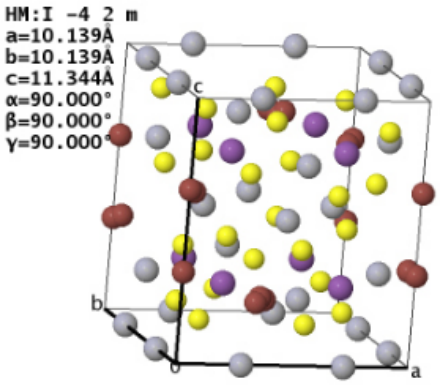
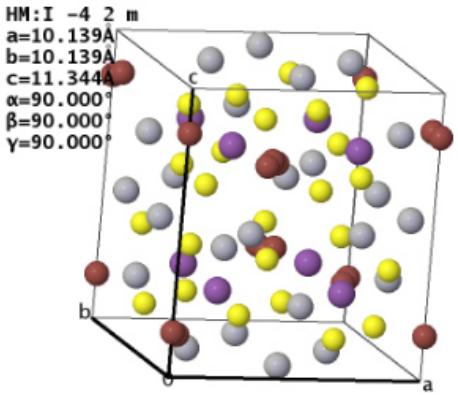
Compare Published and Standardized Structure

Published Crystal Structure



Standardized Crystal Structure

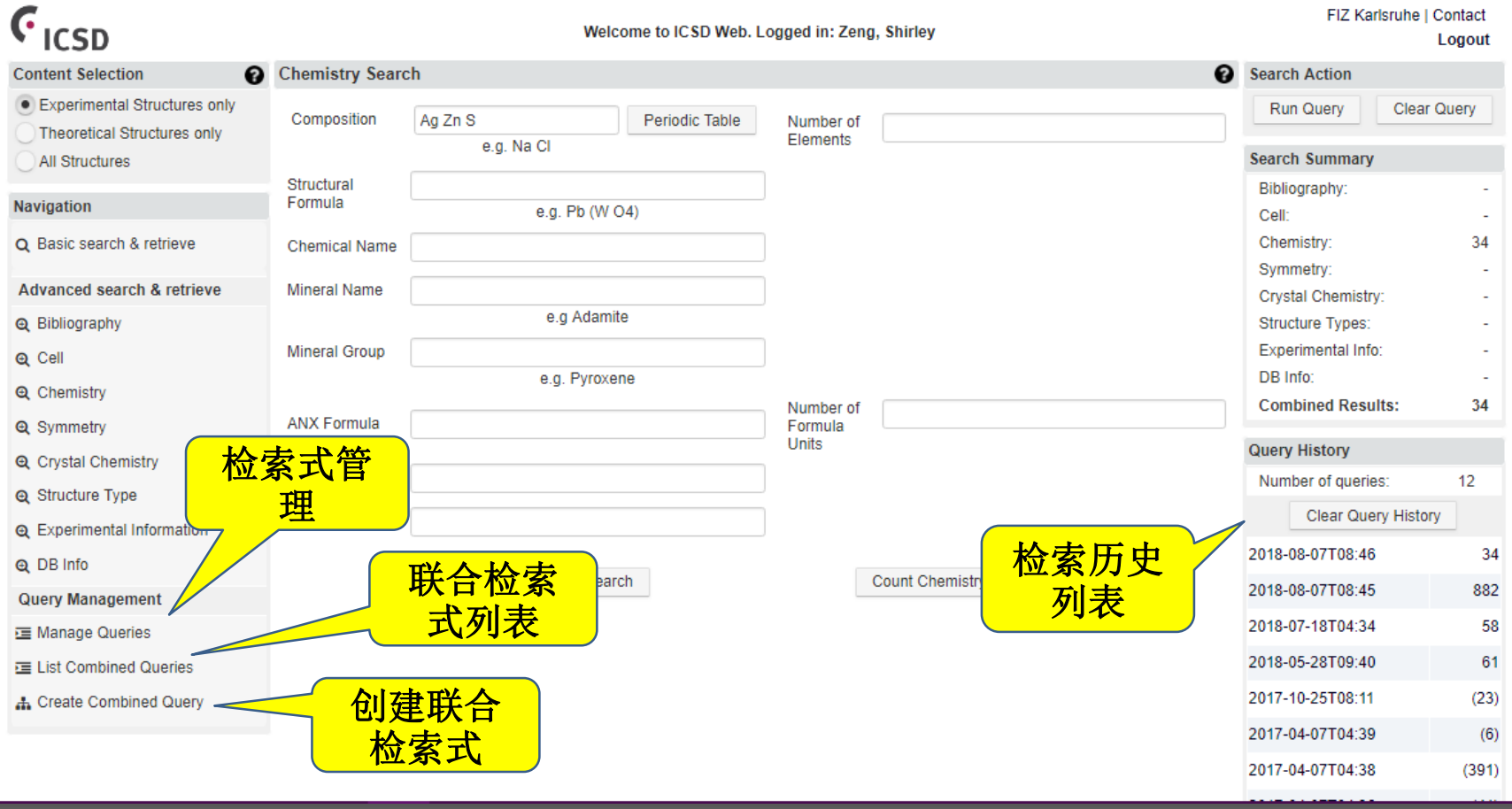
★ 收藏



Interactive Visualization

Version 4.0.1 (build 20180619-1051) - Data Release 2018.1

检索式管理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Chemistry Search
Composition
Ag Zn S
Periodic Table
e.g. Na Cl
Structural Formula
e.g. Pb (W O4)
Chemical Name
Mineral Name
e.g Adamite
Mineral Group
e.g. Pyroxene
ANX Formula
Number of Elements
Number of Formula Units
Count Chemistry
Search Action
Run Query
Clear Query
Search Summary
Bibliography: -
Cell: -
Chemistry: 34
Symmetry: -
Crystal Chemistry: -
Structure Types: -
Experimental Info: -
DB Info: -
Combined Results: 34
Query History
Number of queries: 12
Clear Query History
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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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谢谢！