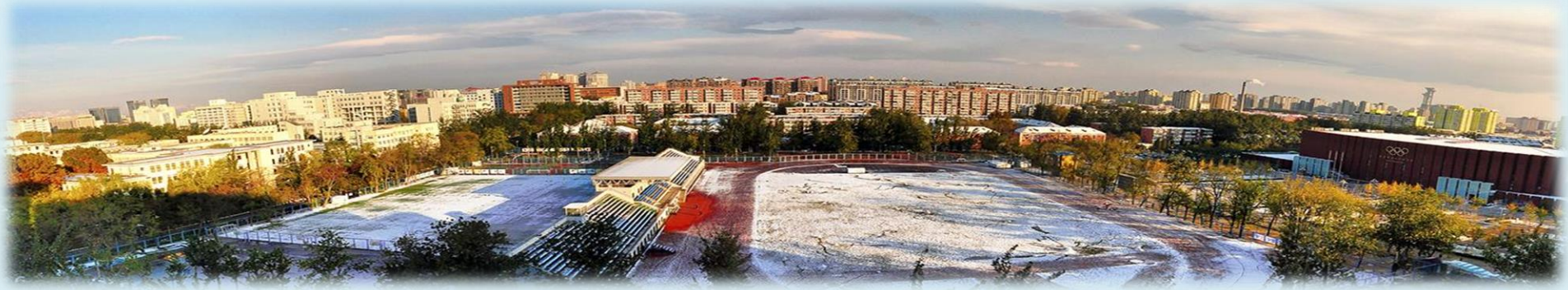


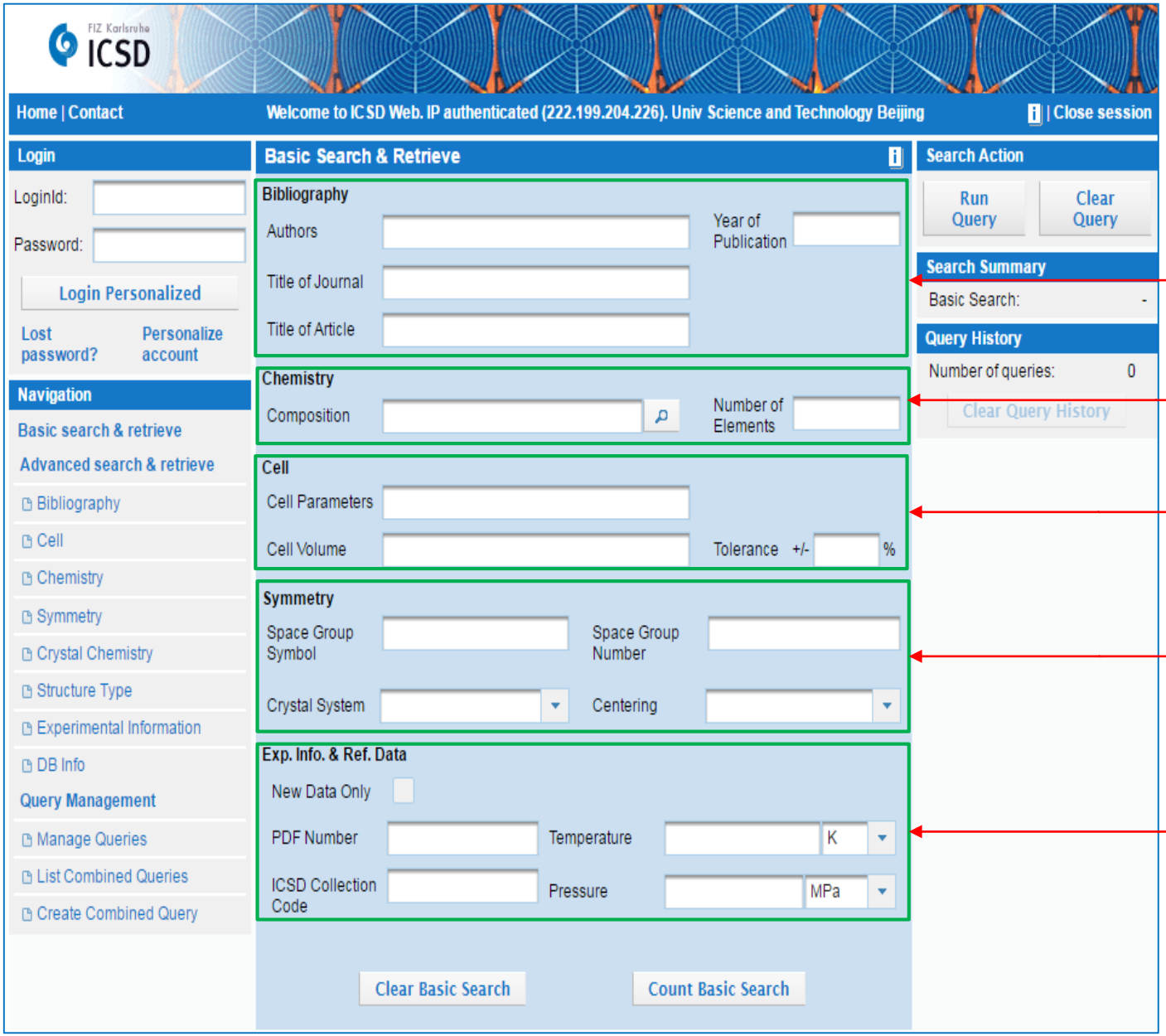
ICSD无机晶体结构数据库使用指南

北京科技大学图书馆

FIZ Karlsruhe
ICSD

1 基本检索

五种检索方式



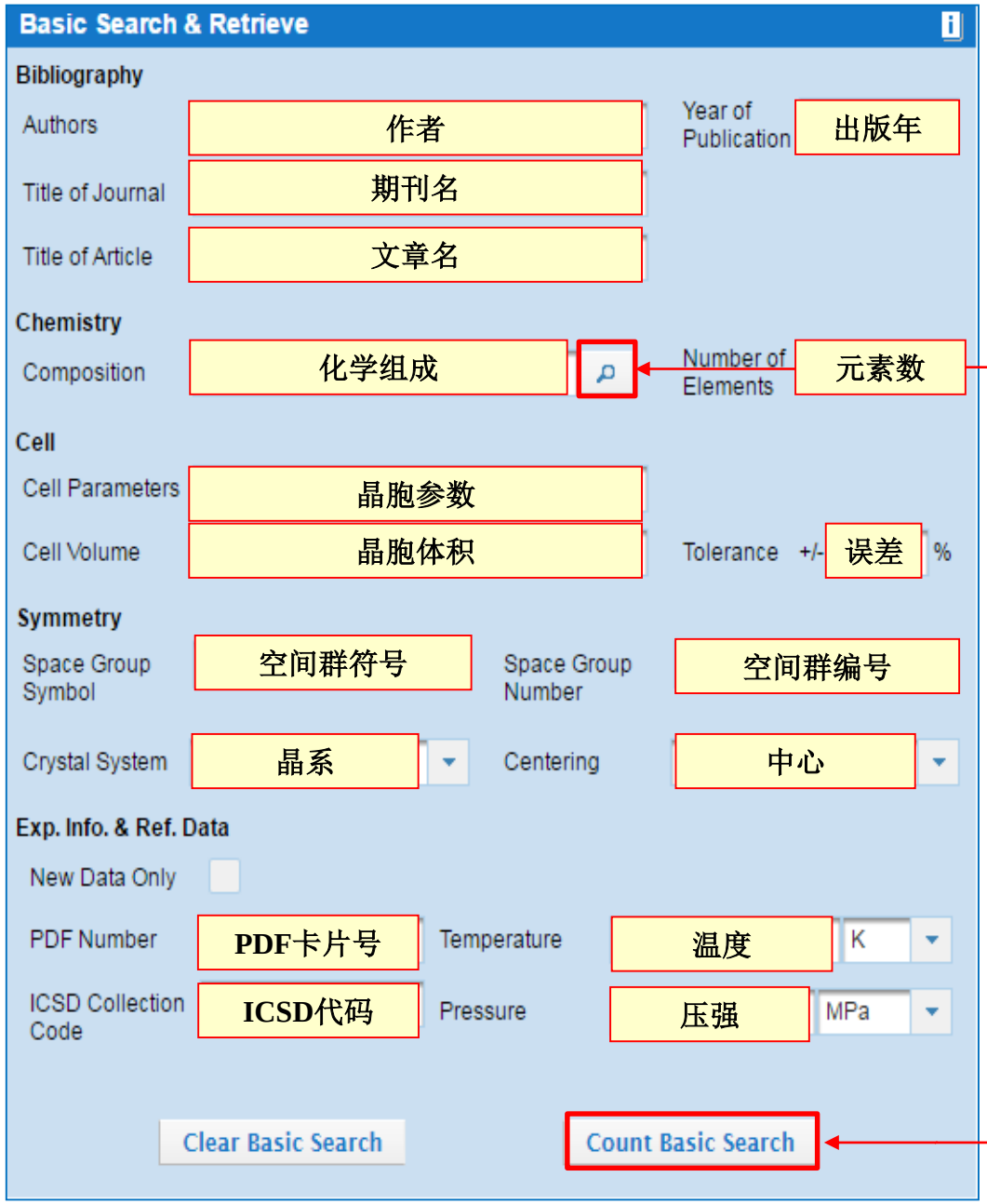
参考文献

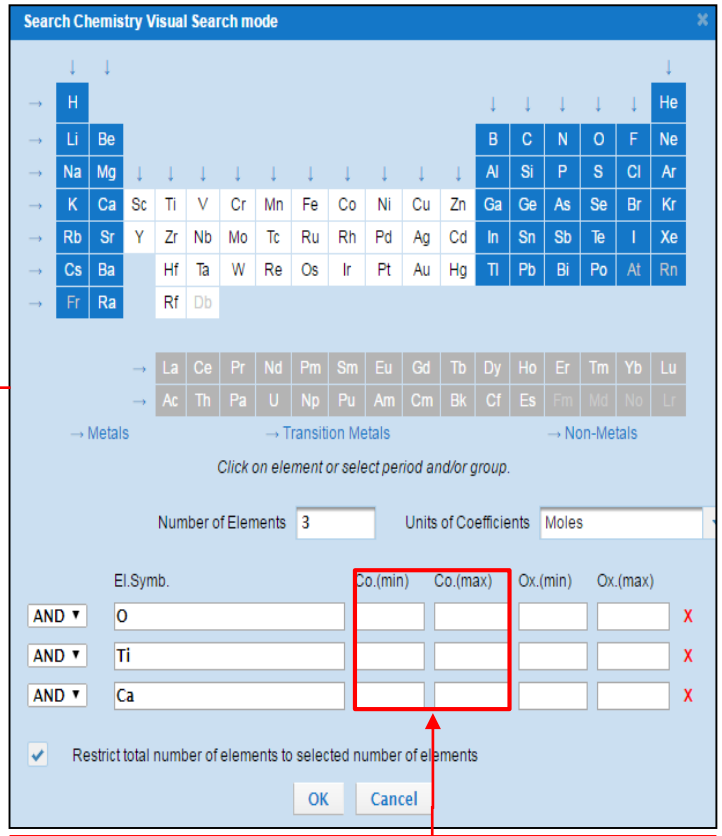
化学组成

晶胞参数

对称性

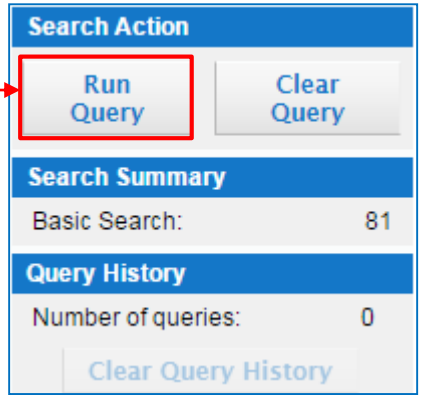
实验和代码信息





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

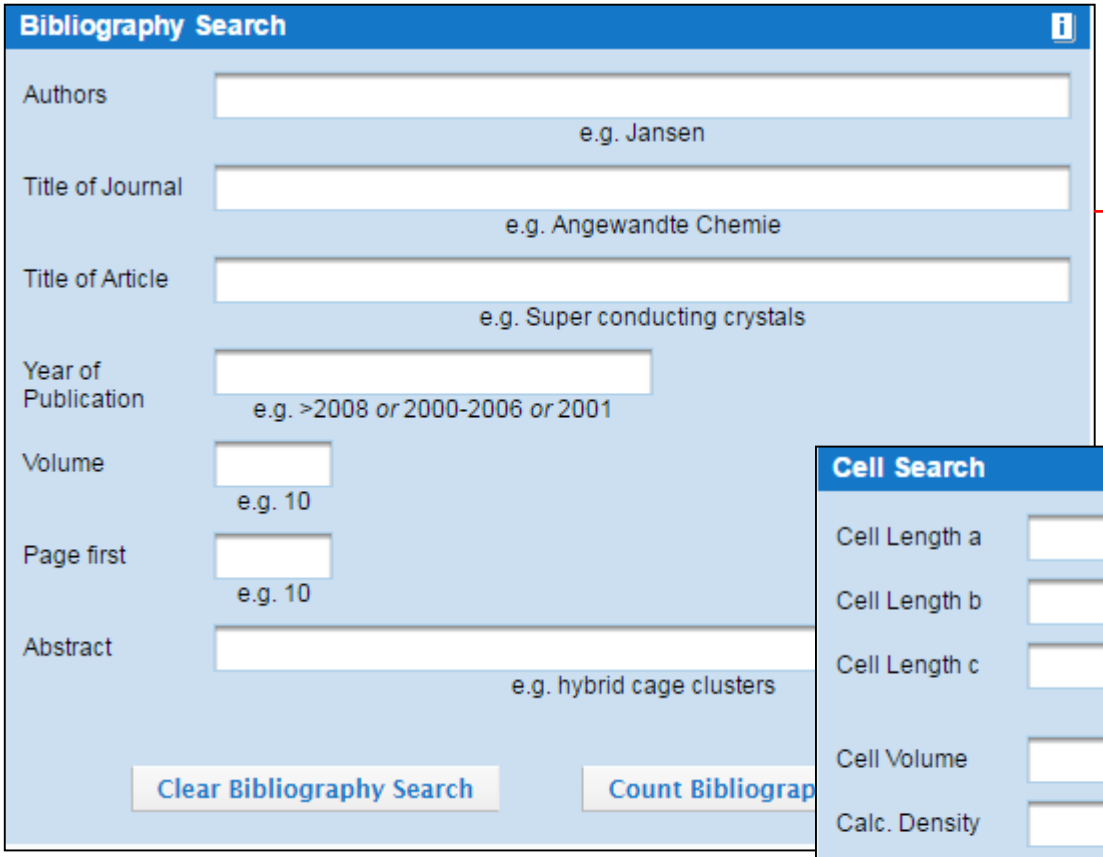
查看具体数据



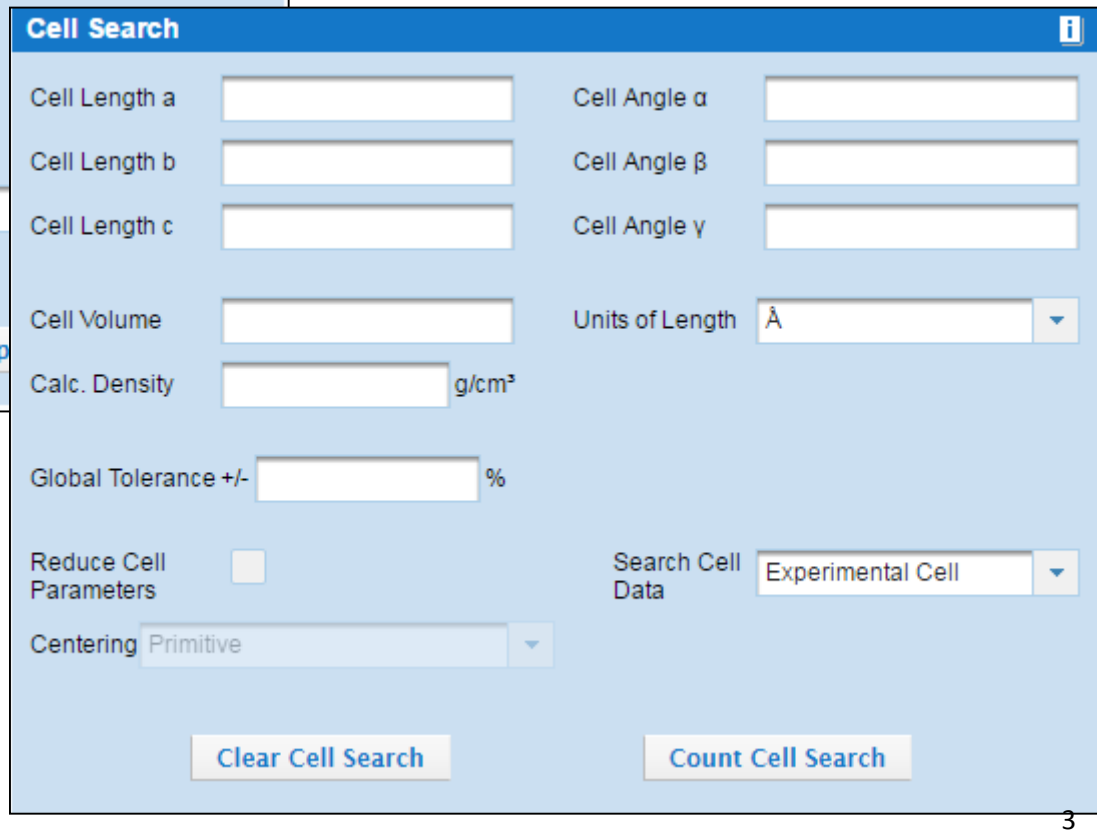
开始搜寻

主要是通过化学组成来搜寻晶体结构数据

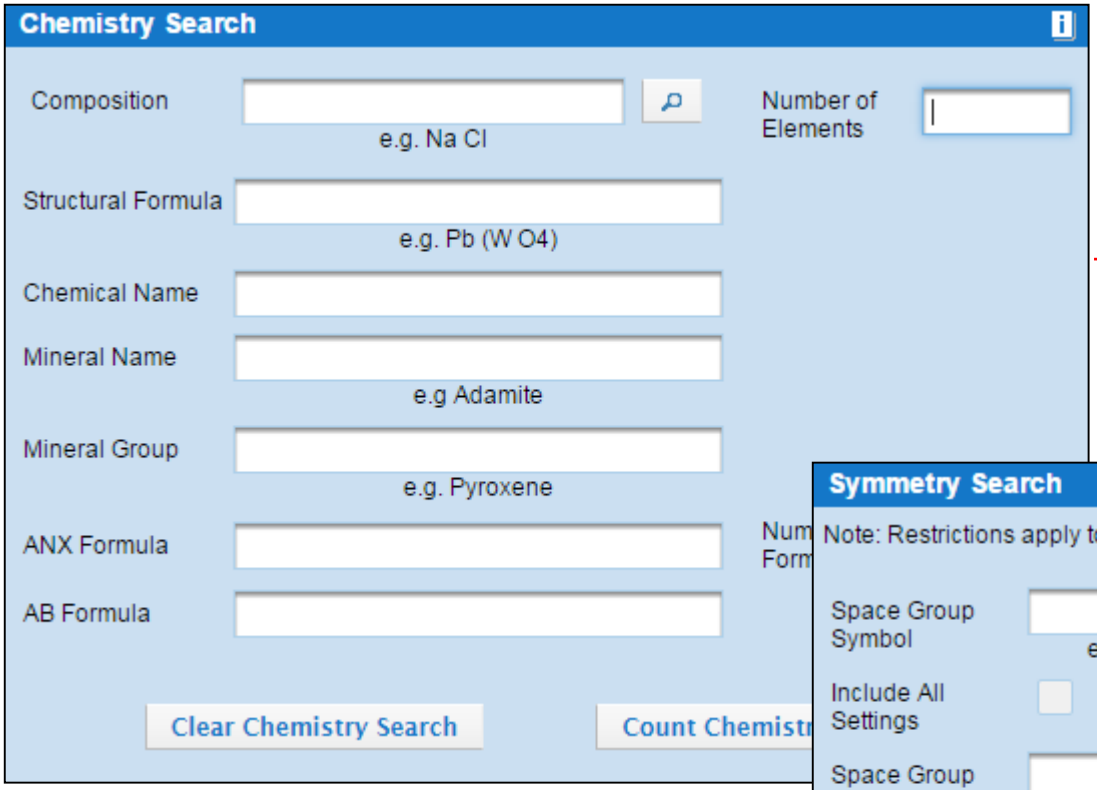
2 高级检索（很少用）



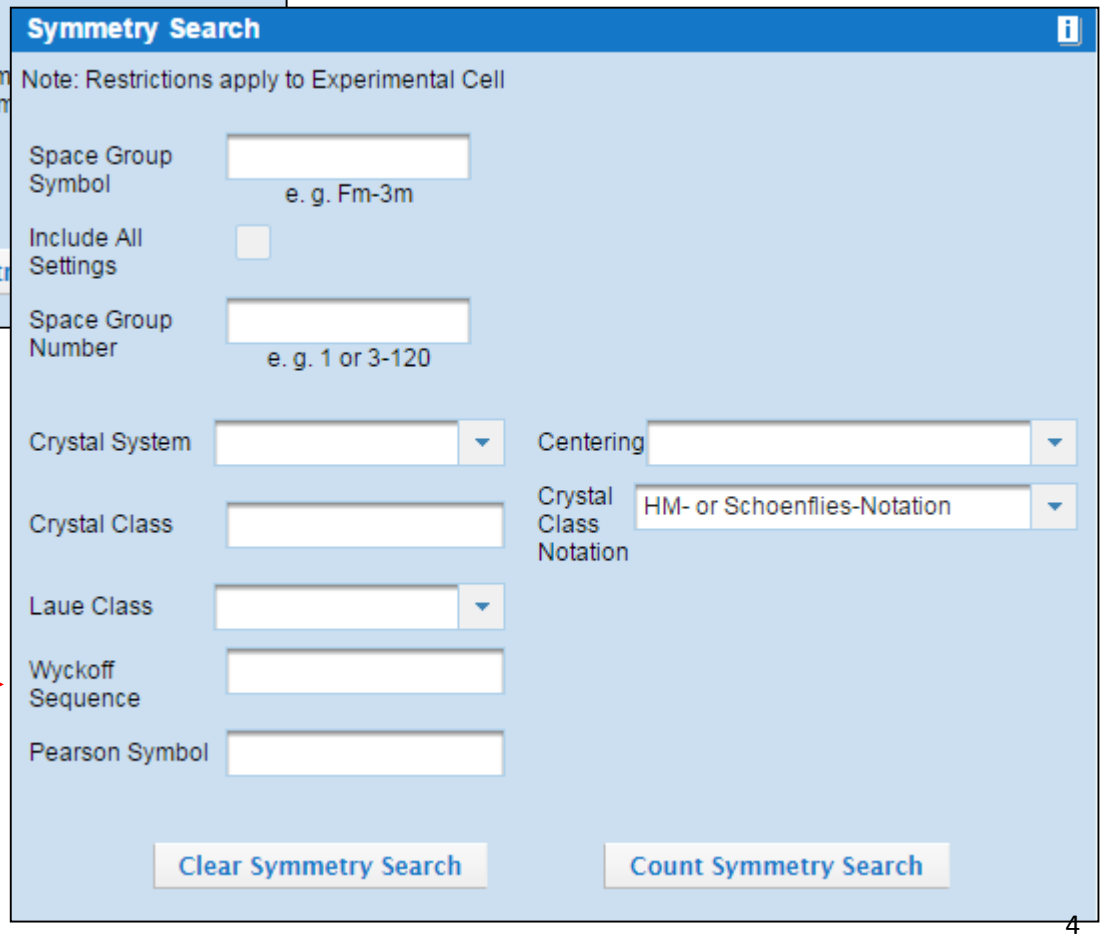
输入文献信息检索



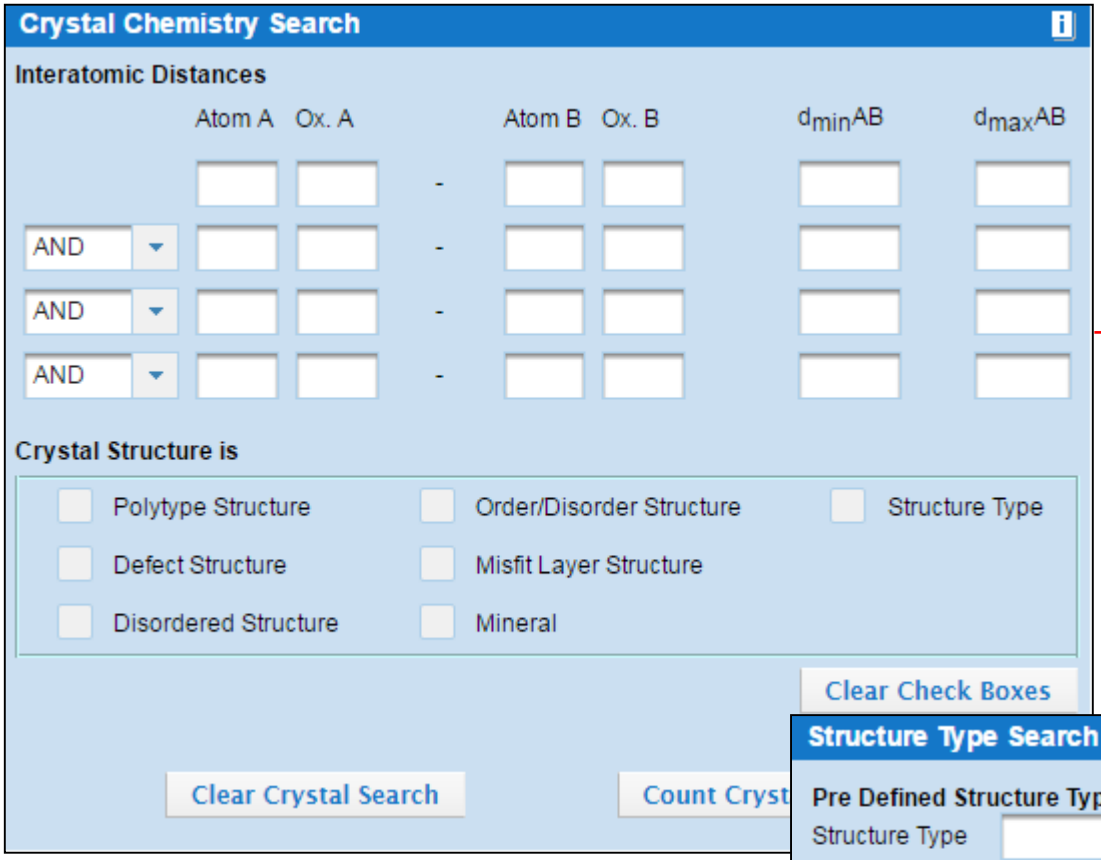
输入晶胞参数信息检索



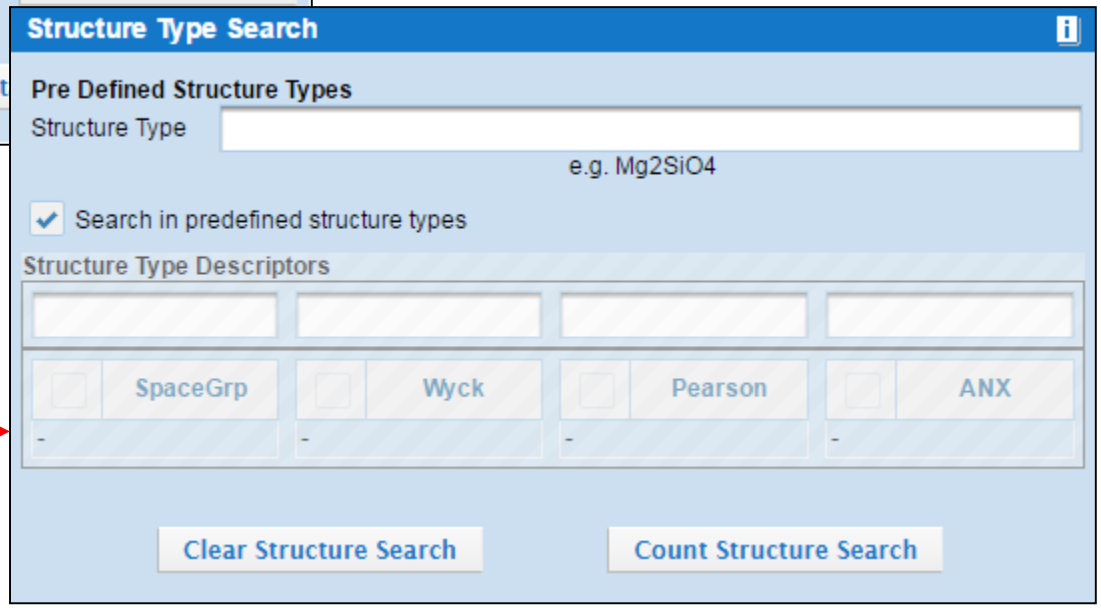
输入化学信息检索



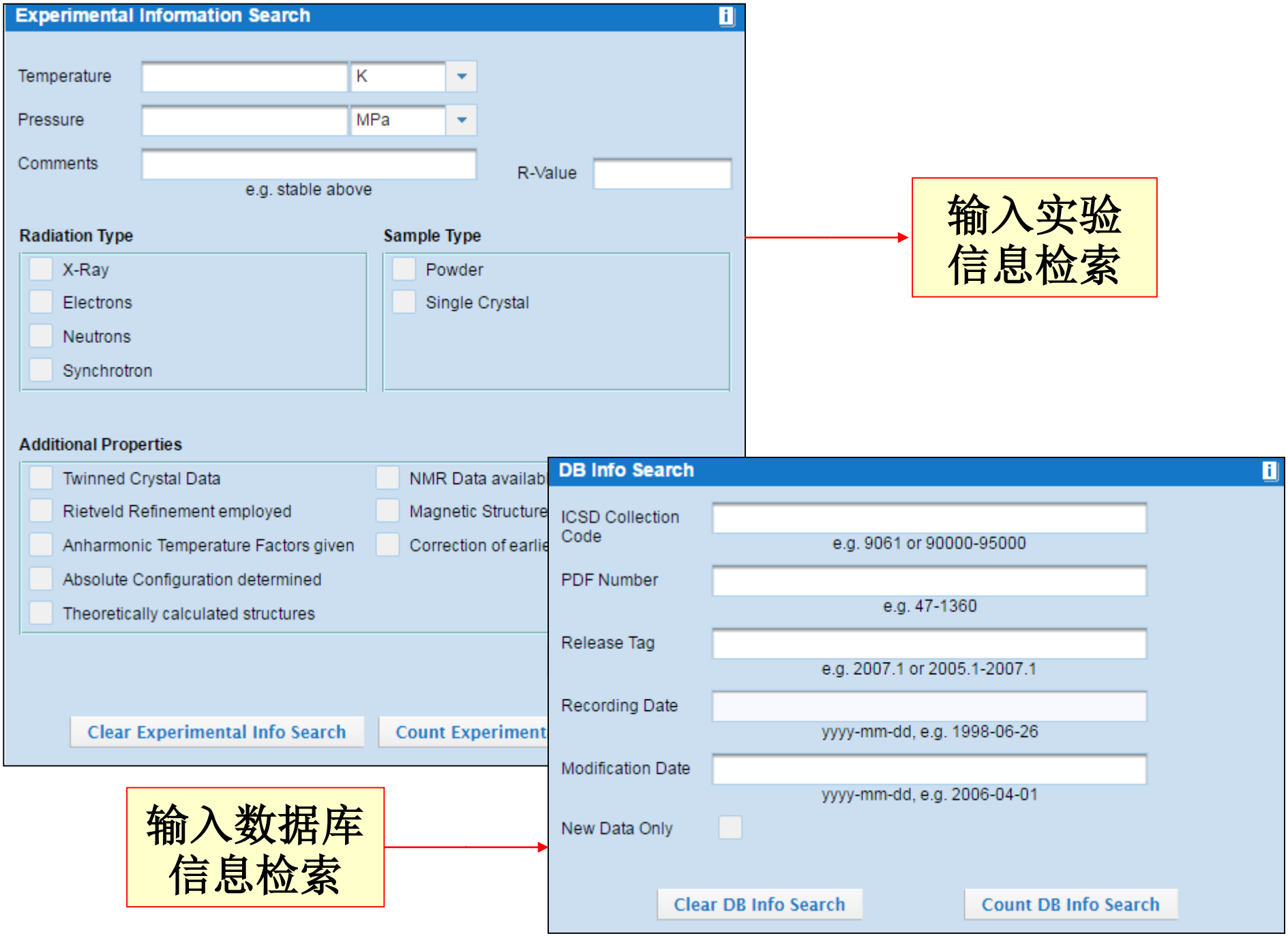
输入对称性信息检索



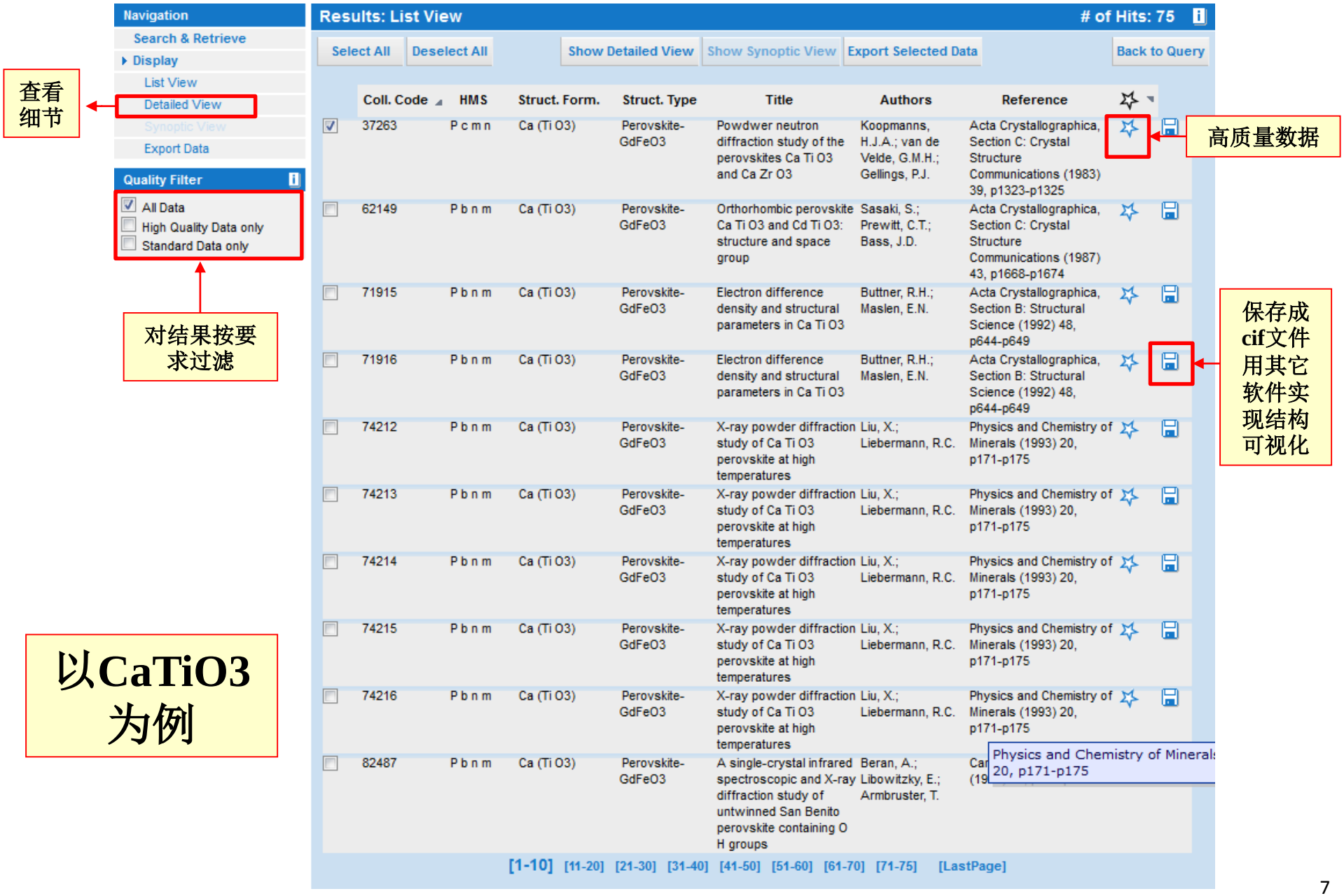
输入晶体化学信息检索



输入结构类型信息检索


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
Additional Properties
Twinned Crystal Data
Rietveld Refinement employed
Anharmonic Temperature Factors given
Absolute Configuration determined
Theoretically calculated structures
NMR Data availab
Magnetic Structure
Correction of earlie
Clear Experimental Info Search
Count Experiment
输入实验信息检索
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
Clear DB Info Search
Count DB Info Search
输入数据库信息检索

3 检索结果


查看细节
高质量数据
保存成cif文件用其它软件实现结构可视化
对结果按要求过滤
以CaTiO3为例
Navigation
Search & Retrieve
Display
List View
Detailed View
Synoptic View
Export Data
Quality Filter
All Data
High Quality Data only
Standard Data only
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
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
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
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
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
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
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
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
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
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
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 Mineral
20, p171-p175
[1-10] [11-20] [21-30] [31-40] [41-50] [51-60] [61-70] [71-75] [LastPage]

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.		
Cell Volume	224.12 A^3	Formula Units per Cell	4
Temperature	room temperature	Pressure	atmospheric
PDF-numbers	01-076-2400 22-153	R-value	0.0452
		Reference	Acta Crystallographica, Section C: Crystal Structure Communications (1983) 39,
		Warnings & Comments	0 Warnings / 1 Comments
Remark		High Quality Data	

Export CIF File | 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

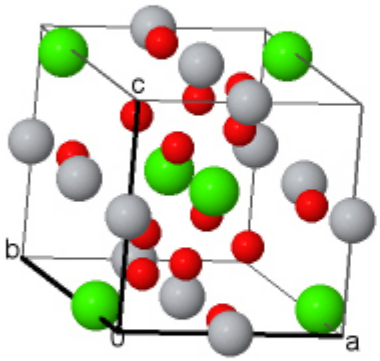
- 结构可视化
- 化学信息
- 出版的晶体结构数据
- 标准化的晶体结构数据
- 键长和键角
- 参考文献
- 实验信息
- 警告和评论
- 出版和标准化的结构比较

Visualization

可视化

Published Crystal Structure

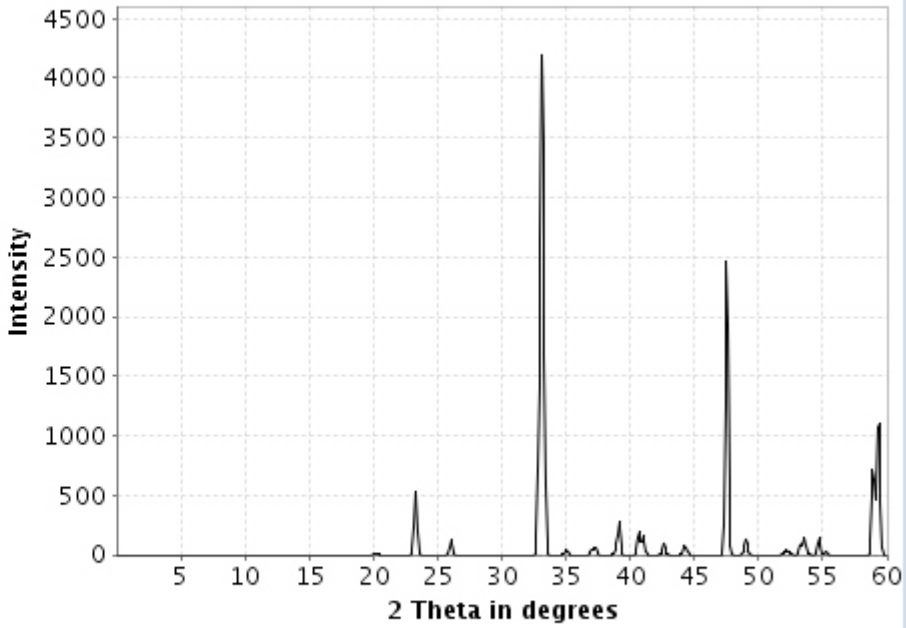
HM: P c m n
a=5.383Å
b=7.645Å
c=5.446Å
α=90.000°
β=90.000°
γ=90.000°



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	Number of Formula Units	4
Struct.Form.	Ca (Ti O3)	ANX Formula Cryst.Comp.	ABX3
Chemical Name	Calcium titanate	AB Formula Chem.Comp.	ABC3
Mineral Name	Perovskite		
Mineral Group	Perovskite		

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 c2 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	-.0173(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)		

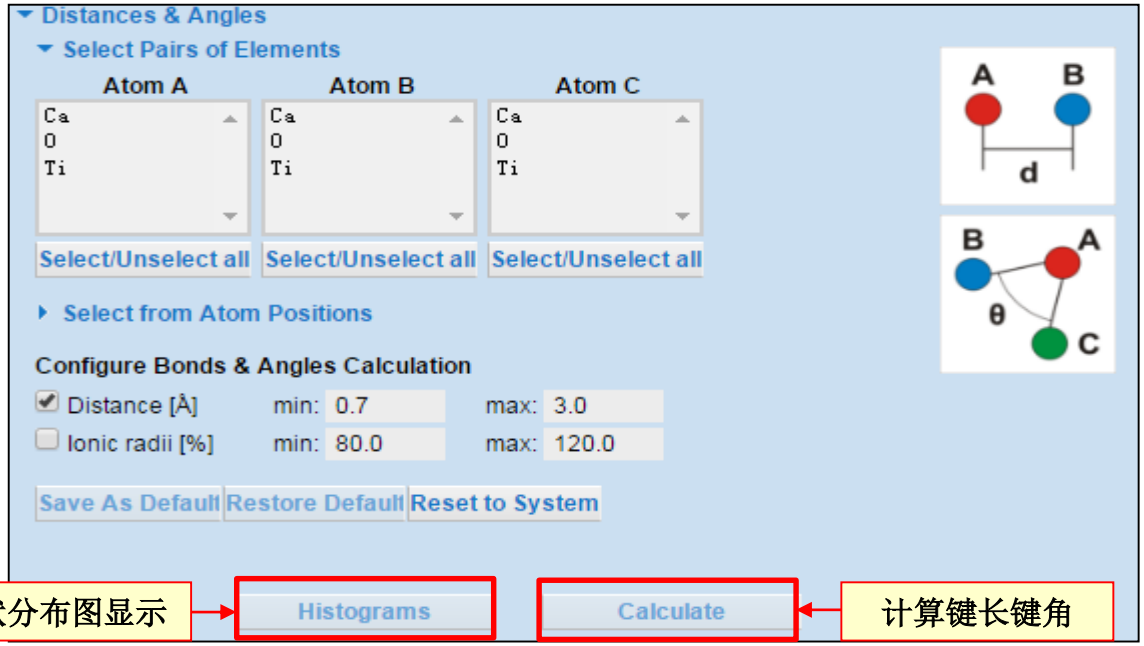
Standardized Crystal Structure Data

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 c2 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					

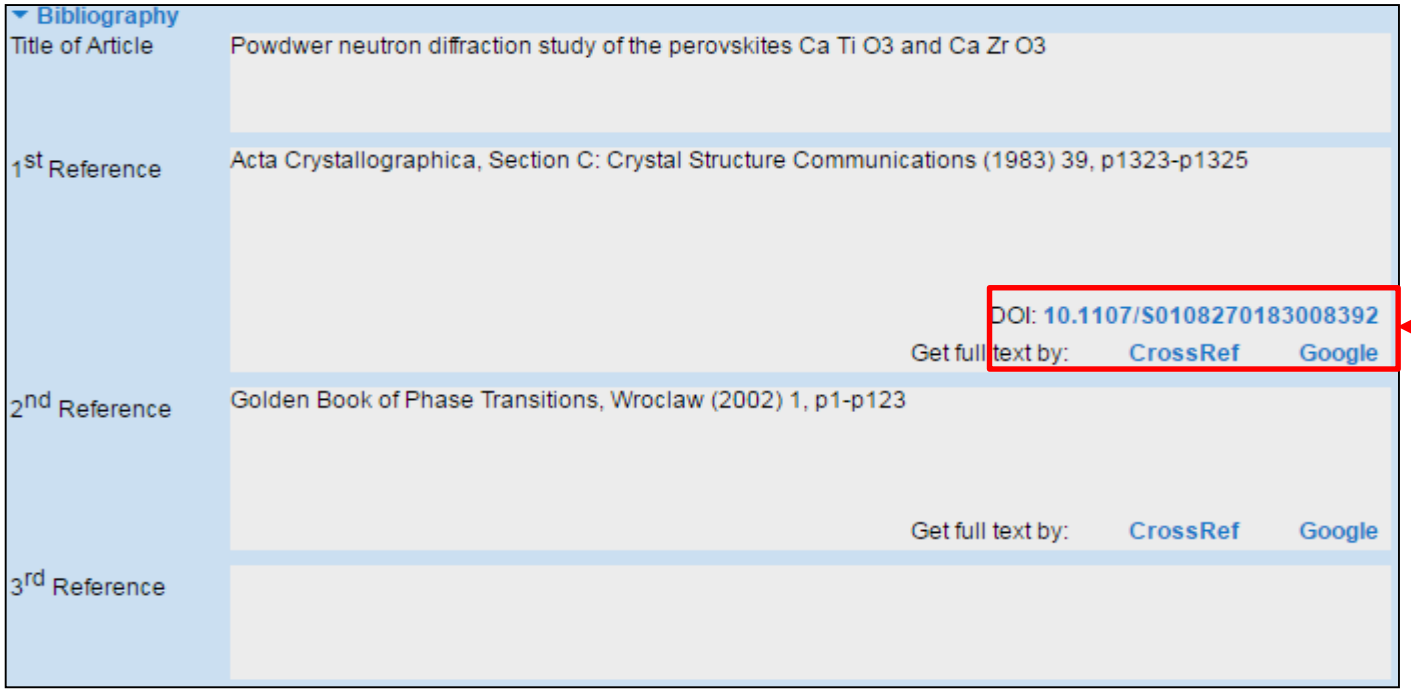
EL	Lbl	Ox State	Wyck Symb	X	Y	Z	B	SOF
Ca	1	+2.00	4c	0.4640	0.2500	0.0083	1.0100	
O	1	-2.00	4c	0.5173	0.2500	0.5726	0.9400	
O	2	-2.00	8d	0.2123	0.0369	0.2901	0.9400	
Ti	1	+4.00	4a	0.0000	0.0000	0.0000	0.5900	

出版的和标准化的晶体结构数据比较

键长和键角计算



参考文献



实验信息

Experimental Information

External Conditions

Temperature: room temperature

Pressure: atmospheric

Radiation Type

- [ ] X-ray
- [ ] Electrons
- [x] Neutrons
- [ ] Synchrotron

Sample Type

- [x] Powder
- [ ] Single Crystal

R-Value: 0.0452

Additional Information

- [ ] Twinned Crystal Data
- [ ] Theoretically calculated structures
- [ ] NMR Data available
- [x] 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
- [x] Mineral
- [ ] Structure Prototype

相关评论

Warnings & Comments

Warnings

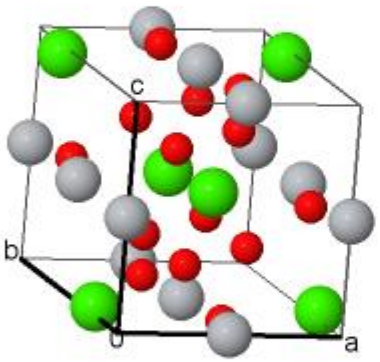
Comments

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

Compare Published & Standardized Structure

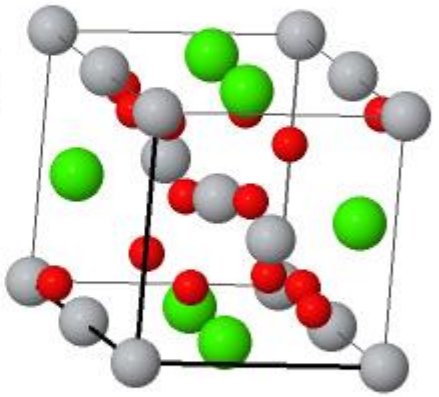
Published Structure

HM:P c m n
a=5.383Å
b=7.645Å
c=5.446Å
α=90.000°
β=90.000°
γ=90.000°



Standardized Structure

HM:P n m a
a=5.446Å
b=7.645Å
c=5.383Å
α=90.000°
β=90.000°
γ=90.000°



Interactive Visualization

出版的和标准化的晶体结构数据比较


Thanks for your attention