FIZ Karlsruhe
ICSD

ICSD-无机晶体结构数据库使用指南

iGroup · 上海

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Pearson Symbol
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Number of Elements
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AB Formula Chem. Comp.
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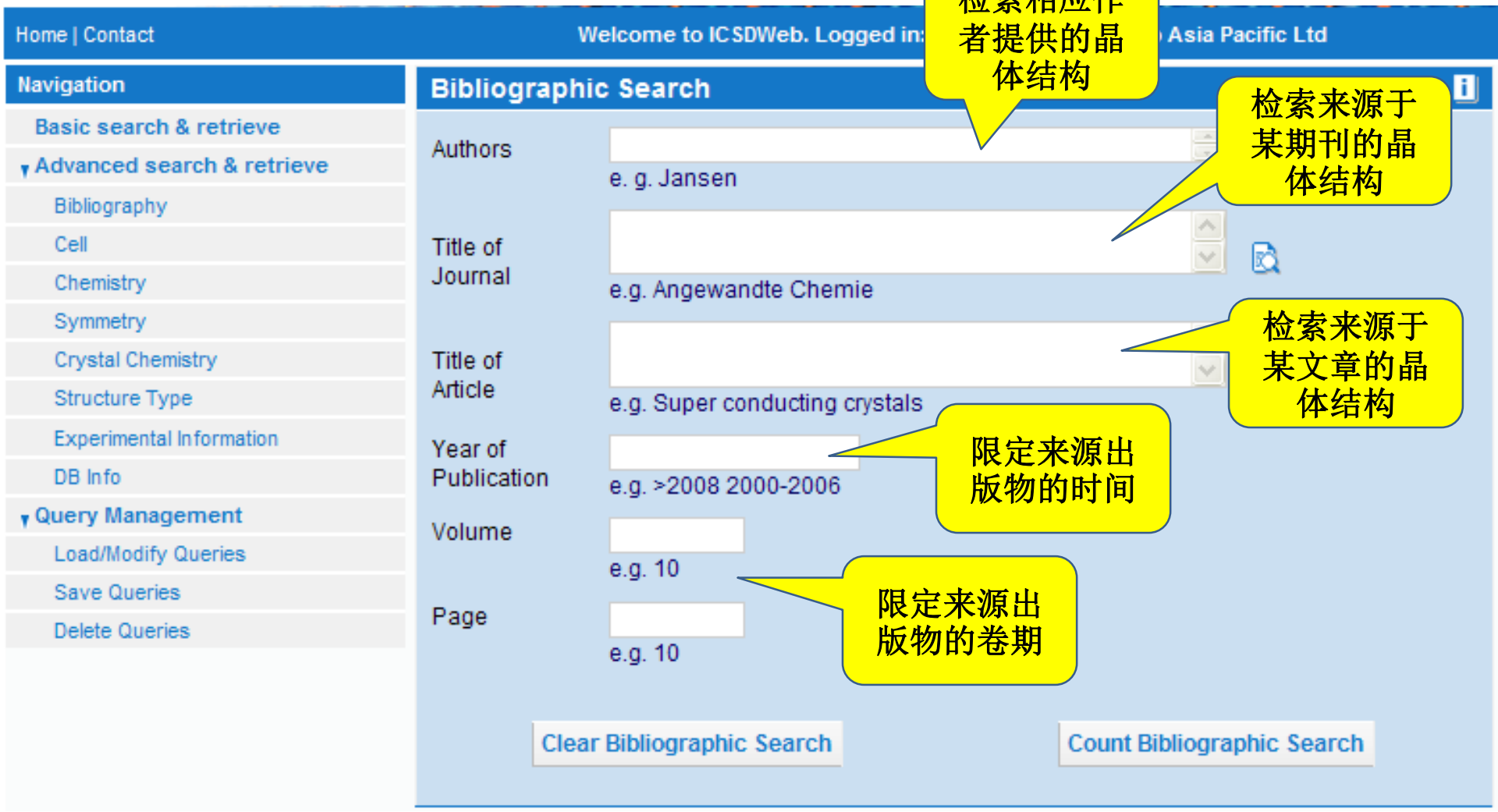
Number of queries: 19
Clear Query History
2012-08-06T17:43 CHEM,STYPE 3
2012-07-25T13:28 CHEM,STYPE,EXP,... 1
2012-07-25T13:25 CHEM,STYPE 3
2012-07-25T13:22 STYPE 707
2012-07-25T13:21 STYPE 0
2012-07-03T10:09 BIB,CELL 0

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
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限定来源出版物的卷期
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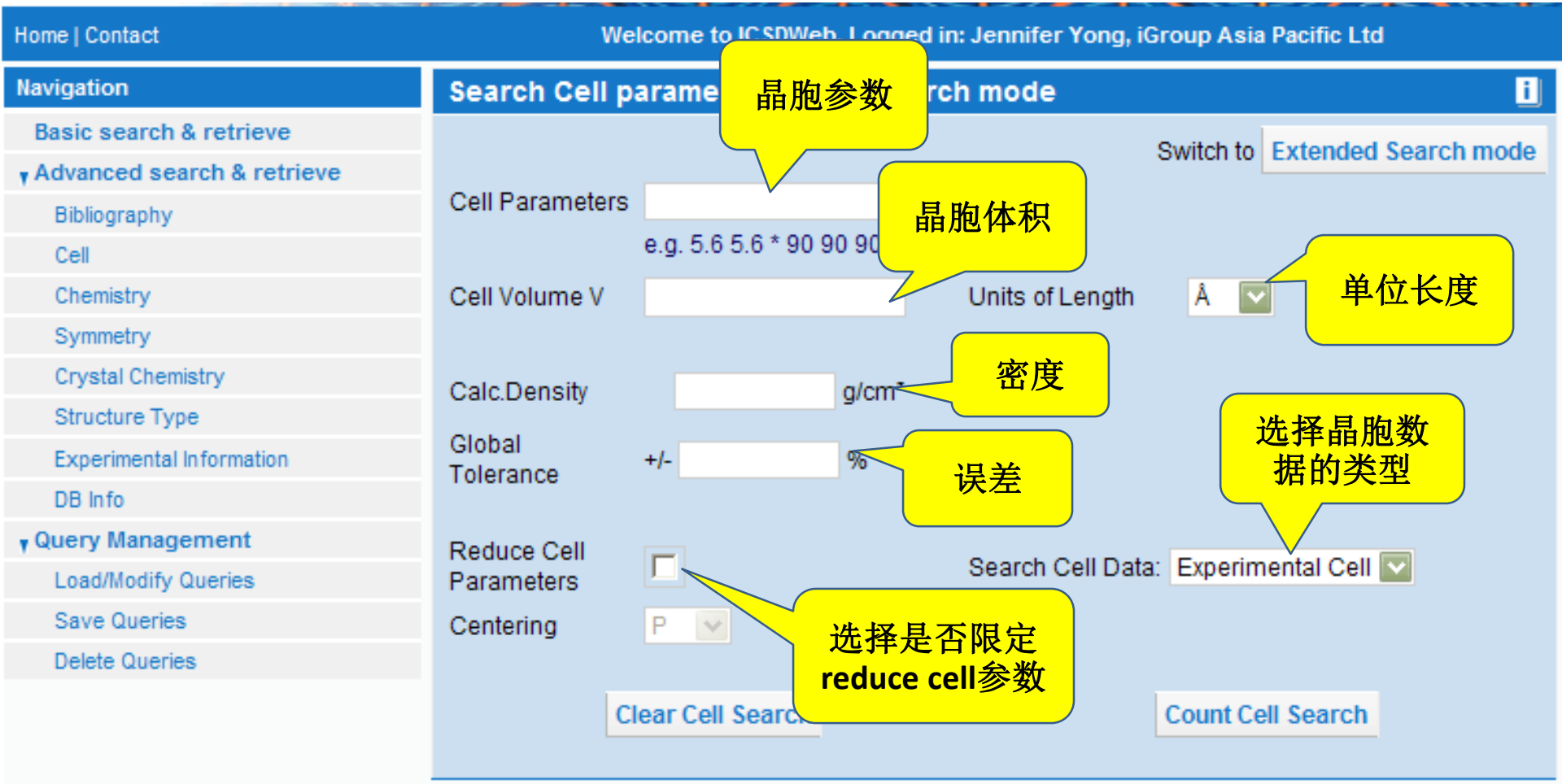
Authors
e. g. Jansen
Title of Journal
e.g. Angewandte Chemie
Title of Article
e.g. Super conducting crystals
Year of Publication
e.g. >2008 2000-2006
Volume
e.g. 10
Page
e.g. 10
Clear Bibliographic Search
Count Bibliographic Search

高级检索-依据晶胞检索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Search Cell parame rch mode
Switch to Extended Search mode
Cell Parameters
e.g. 5.6 5.6 * 90 90 90
Cell Volume V
Units of Length
Å
Calc.Density
g/cm
Global Tolerance
+/-
%
Reduce Cell Parameters
Centering
P
Search Cell Data:
Experimental Cell
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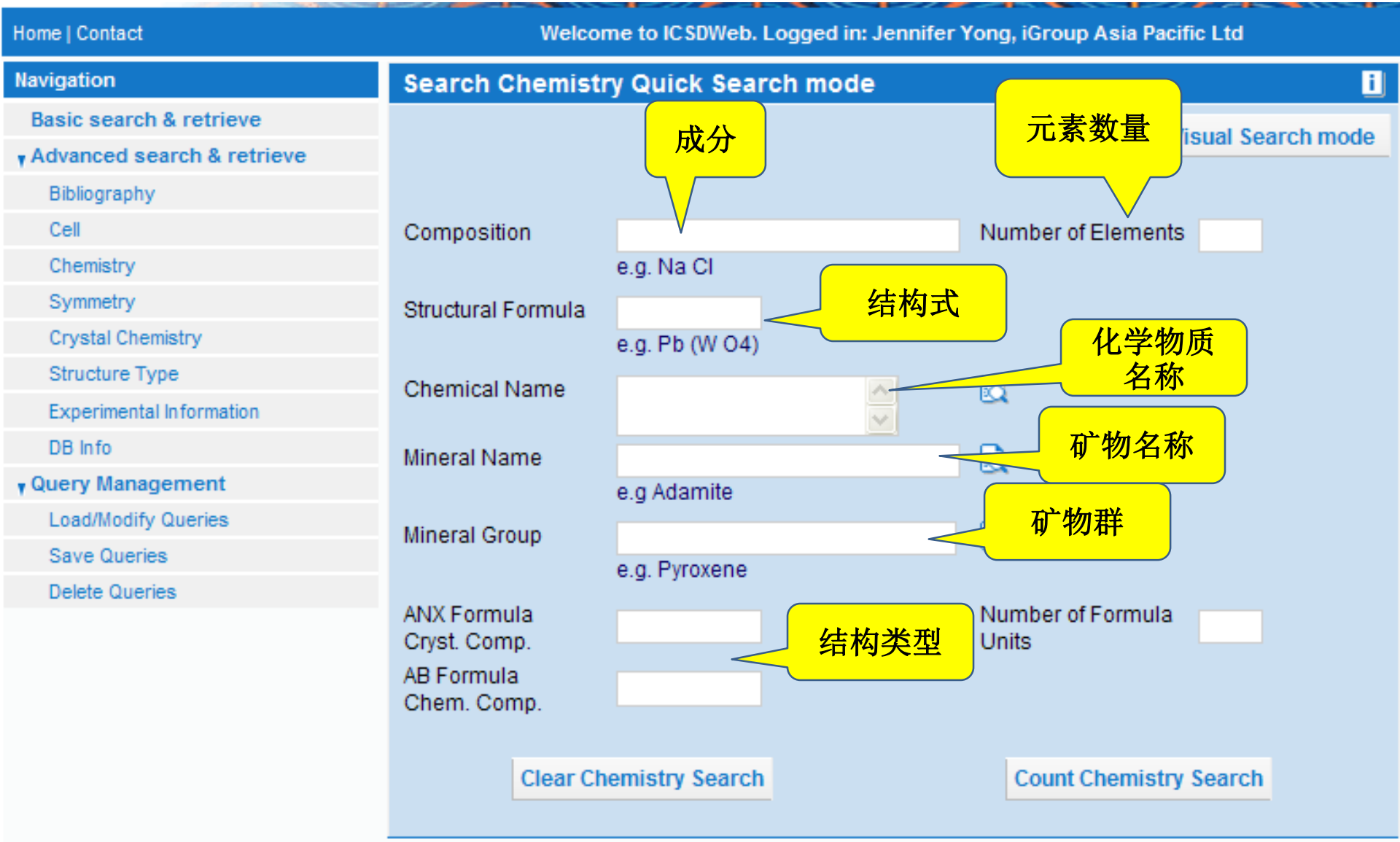
晶胞参数
晶胞体积
单位长度
密度
误差
选择晶胞数据的类型
选择是否限定reduce cell参数

高级检索-依据化学式检索



高级检索-依据晶体对称性检索

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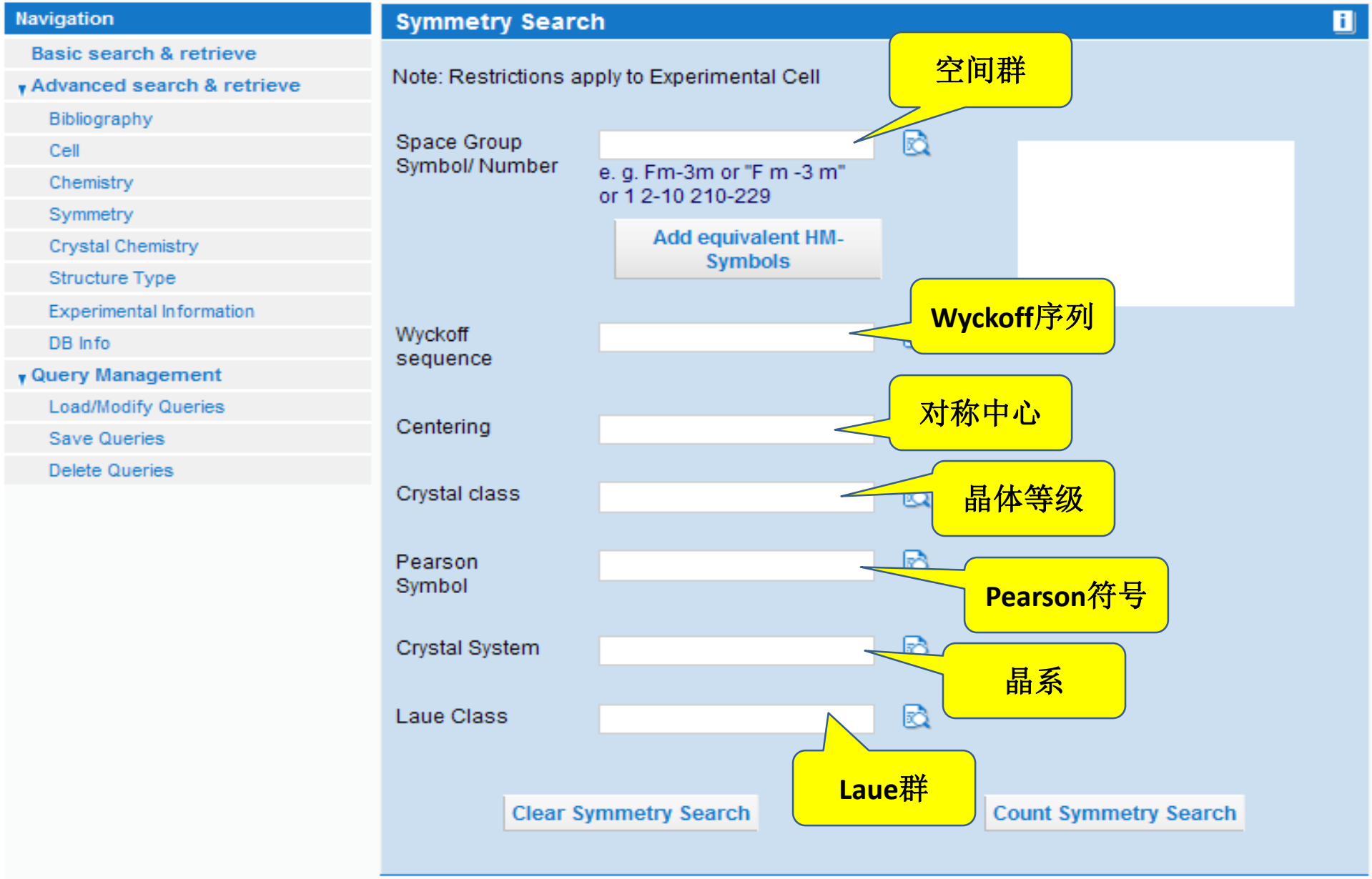

高级检索-依据原子坐标检索

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Crystal Chemistry Search

限定原子间的距离

Interatomic Distances

	Atom A	Ox. A		Atom B	Ox. B	d_{min}^{AB}	d_{max}^{AB}
			-				
AND			-				
AND			-				
AND			-				

限定晶体结构类型

Crystal Structure is

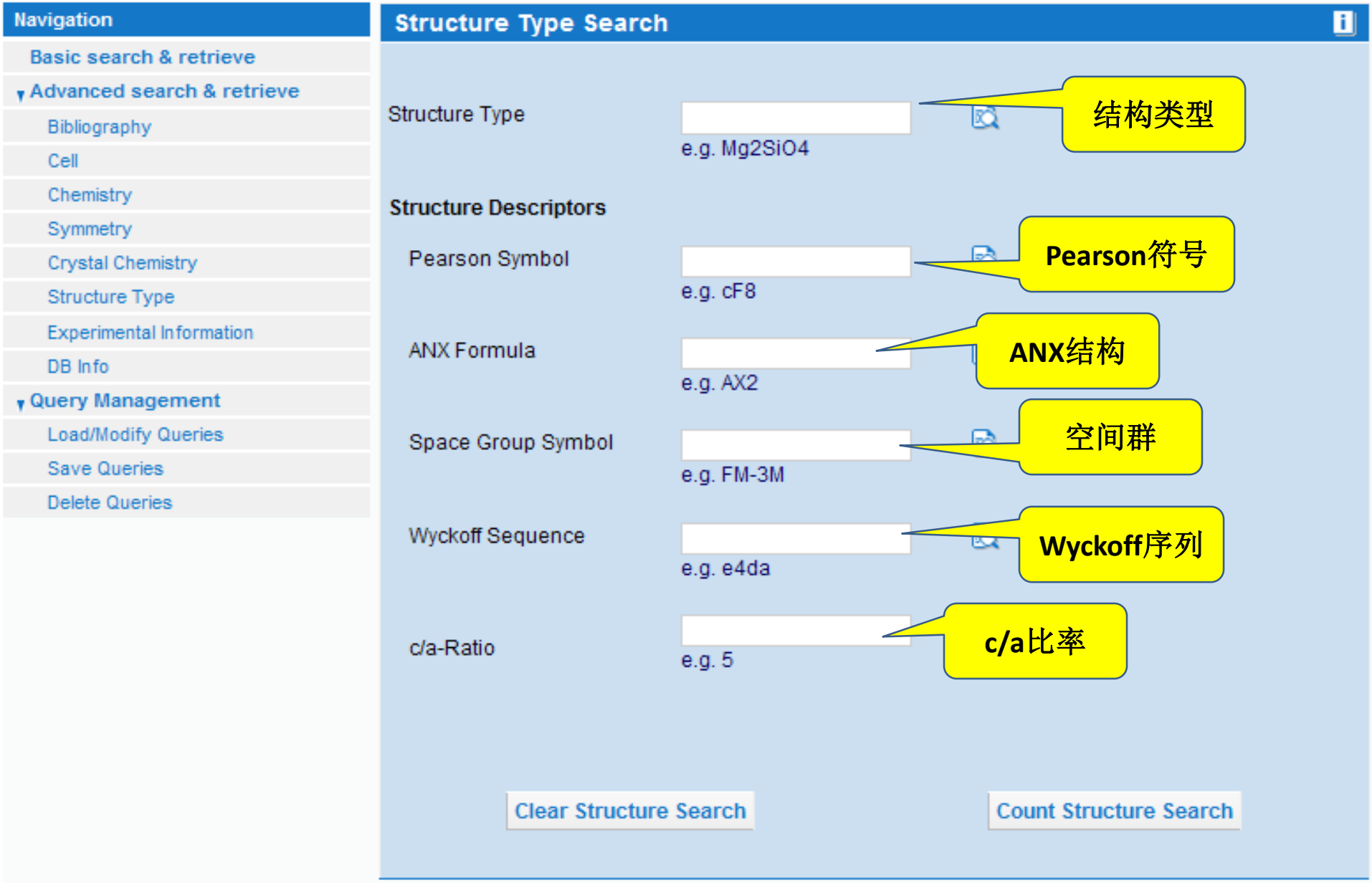
- ☐ Polytype Structure
- ☐ Order/Disorder Structure
- ☐ Structure Type
- ☐ Defect Structure
- ☐ Misfit Layer Structure
- ☐ Disordered Structure
- ☐ Mineral

Clear Check Boxes

Clear Crystal Search

Count Crystal Search

高级检索-依据晶体结构检索



高级检索-依据实验信息检索

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Experimental Information Search

Temperature
e.g. 200K 200-300K
温度

Pressure
e.g. 2MPa 5-7GPa
压力

Comments
e.g. s[illegible]e above
注释

R-Value
R值

Radiation Type
- X-Ray
- Electrons
- Neutrons
- Synchroton

射线类型

Sample Type
- Powder
- Single Crystal

样本类型

ear Check Boxes

Additional Properties

其他属性

- Twinned Crystal Data
- Rietveld Refinement employed
- Anharmonic Temperature Factors given
- Absolute Configuration determined
- Theoretically calculated structures
- NMR Data available
- Magnetic Structure available
- Correction of earlier work

Clear Check Boxes

高级检索-依据数据库记录信息检索

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DB Info Search

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

PDF Number
e.g. 01-077-1145 or 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
收录日期

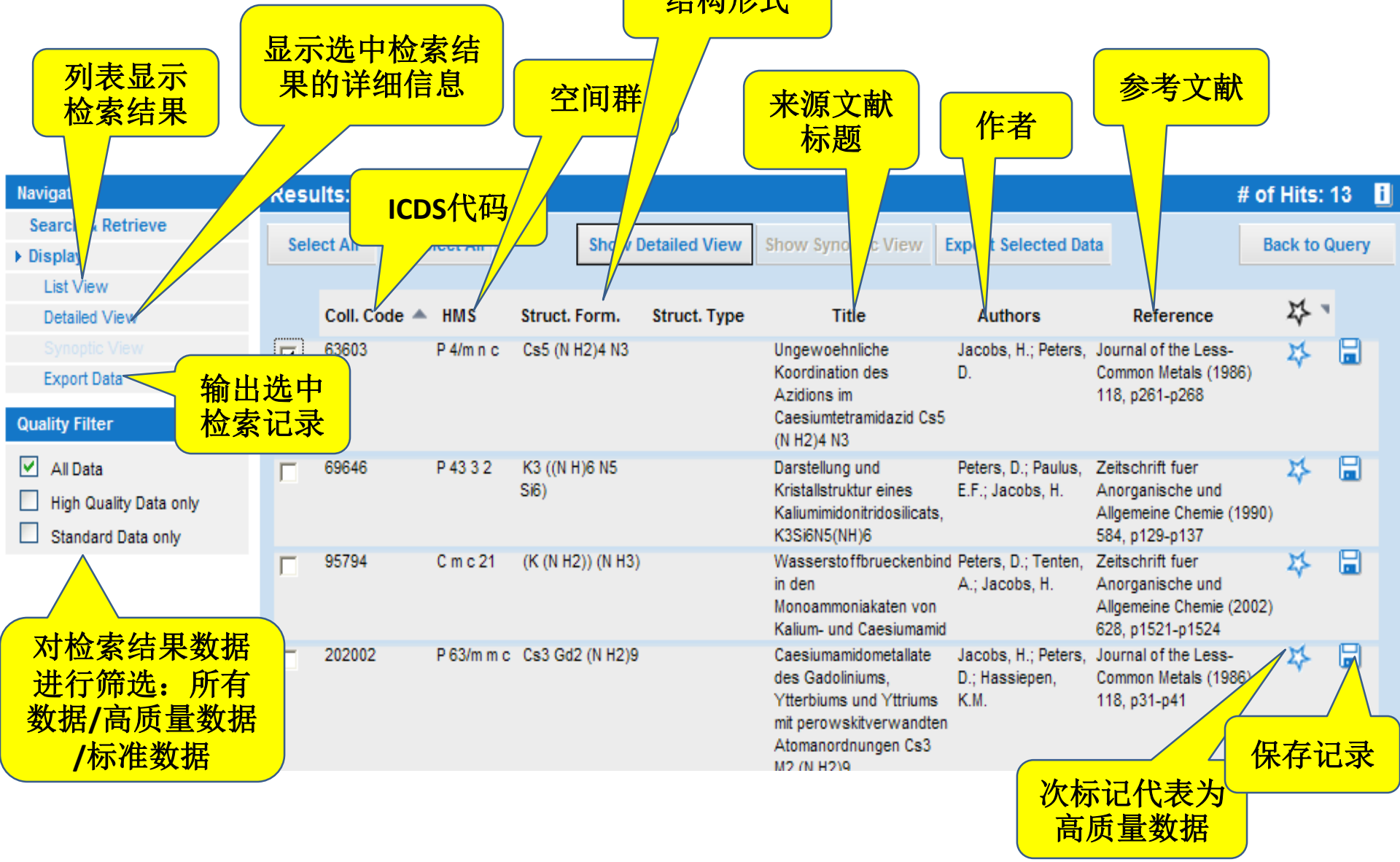
Modification Date
yyyy-mm-dd, e.g. 2006-04-01
修改日期

New Data Only
限定来源仅为新数据

Clear DB Info Search

Count DB Info Search

检索结果显示


列表显示检索结果
显示选中检索结果的详细信息
空间群
结构形式
来源文献标题
作者
参考文献
ICDS代码
输出选中检索记录
对检索结果数据进行筛选：所有数据/高质量数据/标准数据
次标记代表为高质量数据
保存记录
Navigat
Search & Retrieve
Display
List View
Detailed View
Synoptic View
Export Data
Quality Filter
All Data
High Quality Data only
Standard Data only
Results:
# of Hits: 13
Select All
Show Detailed View
Show Synoptic View
Export Selected Data
Back to Query
Coll. Code
HMS
Struct. Form.
Struct. Type
Title
Authors
Reference
63603
P 4/m n c
Cs5 (N H2)4 N3
Ungewoehnliche Koordination des Azidions im Caesiumtetramidazid Cs5 (N H2)4 N3
Jacobs, H.; Peters, D.
Journal of the Less-Common Metals (1986) 118, p261-p268
69646
P 43 3 2
K3 ((N H)6 N5 Si6)
Darstellung und Kristallstruktur eines Kaliumimidonitridosilicats, K3Si6N5(NH)6
Peters, D.; Paulus, E.F.; Jacobs, H.
Zeitschrift fuer Anorganische und Allgemeine Chemie (1990) 584, p129-p137
95794
C m c 21
(K (N H2)) (N H3)
Wasserstoffbrueckenbind in den Monoammoniakaten von Kalium- und Caesiumamid
Peters, D.; Tenten, A.; Jacobs, H.
Zeitschrift fuer Anorganische und Allgemeine Chemie (2002) 628, p1521-p1524
202002
P 63/m m c
Cs3 Gd2 (N H2)9
Caesiumamidometallate des Gadoliniums, Ytterbiums und Yttriums mit perowskitverwandten Atomanordnungen Cs3 M2 (N H2)9
Jacobs, H.; Peters, D.; Hassiepen, K.M.
Journal of the Less-Common Metals (1986) 118, p31-p41

检索结果的详细信息

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Summary

Collection Code 63603

Struct.formula	Cs5 (N H2)4 N3		
Space Group	P 4/m n c(128)		
Unit Cell	8.918(2) 8.918(2) 8.807(2) 90. 90. 90.		
Cell Volume	700.43 A^3	Formula Units per Cell	2
Temperature	room temperature	Pressure	atmospheric
PDF-numbers	01-078-2385 38-671	R-value	0.036
Remark		High Quality Data	

Export CIF File | MyBaseFileName

Author	Jacobs, H.; Peters, D.
Title of Article	Ungewoehnliche Koordination des Azidions im Caesiumtetramidazid Cs5 (N H2)4 N3
Reference	Journal of the Less-Common Metals (1986) 118, p261-p268
Warnings & Comments	1 Warnings / 0 Comments

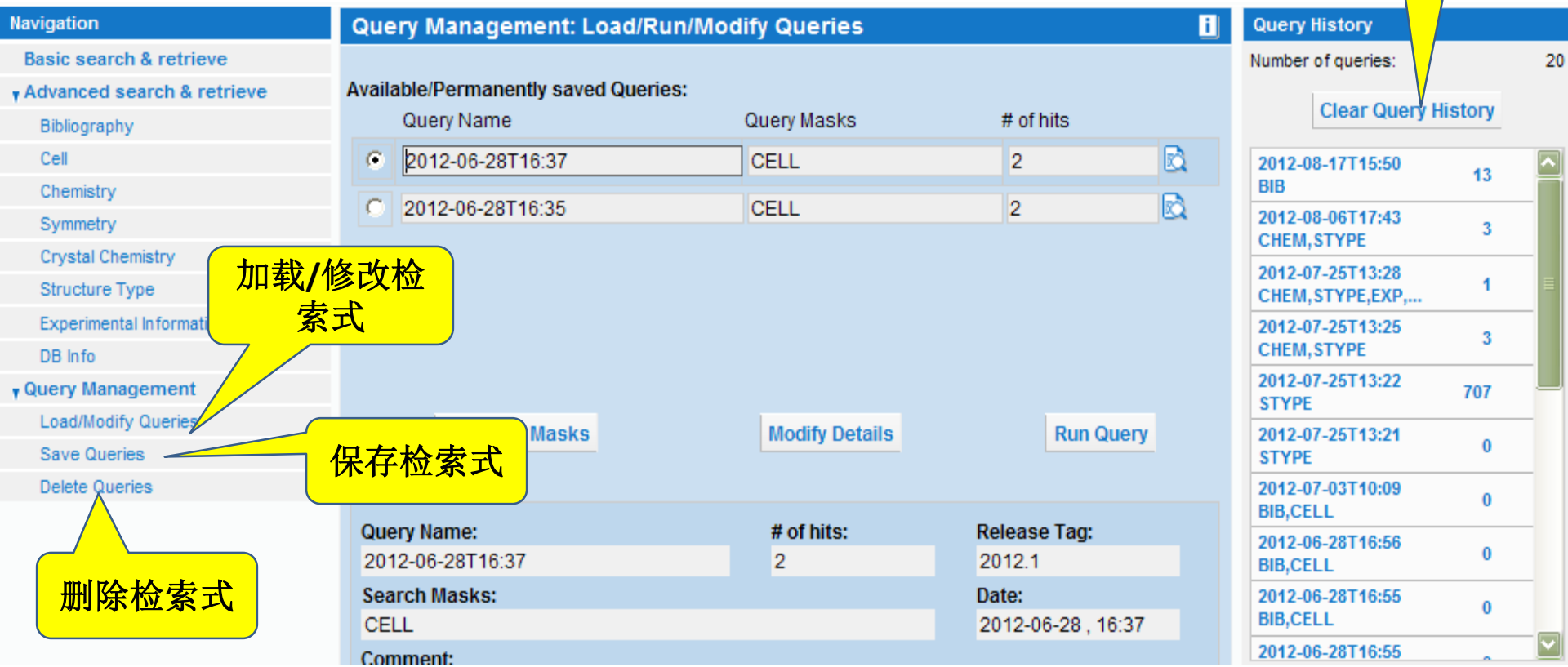
Feedback to the ICSD Editor

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

检索式管理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保存检索式
删除检索式
Query Management: Load/Run/Modify Queries
Available/Permanently saved Queries:
Query Name
Query Masks
# of hits
2012-06-28T16:37
CELL
2
2012-06-28T16:35
CELL
2
Masks
Modify Details
Run Query
Query Name:
2012-06-28T16:37
# of hits:
2
Release Tag:
2012.1
Search Masks:
CELL
Date:
2012-06-28 , 16:37
Comment:
Query History
Number of queries:
20
Clear Query History
2012-08-17T15:50
BIB
13
2012-08-06T17:43
CHEM,STYPE
3
2012-07-25T13:28
CHEM,STYPE,EXP,...
1
2012-07-25T13:25
CHEM,STYPE
3
2012-07-25T13:22
STYPE
707
2012-07-25T13:21
STYPE
0
2012-07-03T10:09
BIB,CELL
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2012-06-28T16:56
BIB,CELL
0
2012-06-28T16:55
BIB,CELL
0
2012-06-28T16:55

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谢谢！