Constructing and Using Pearson Symbol Code Indexes (PSCI)

cP7

Introduction

A PSCI can be used for (but is not limited to):

(a) Identifying possible prototype structure types for an unknown material,

(b) Comparing isotypical phases, their

lattice parameters and chemistries.

Notes

- For this, and all metals and alloys problems, please use the empirical formula (it is alphabetized) and the *Crystal Data cell* (ensures that all lattice parameters and axial ratios are from a standard cell).
- In the following search results, the numeric in *Pearson* is the number of atoms in the unit cell and not the number of crystallographic sites. Hence, this is the Pearson Symbol Code (PSC) and not necessarily the Pearson Symbol (PS).

Notes
continued

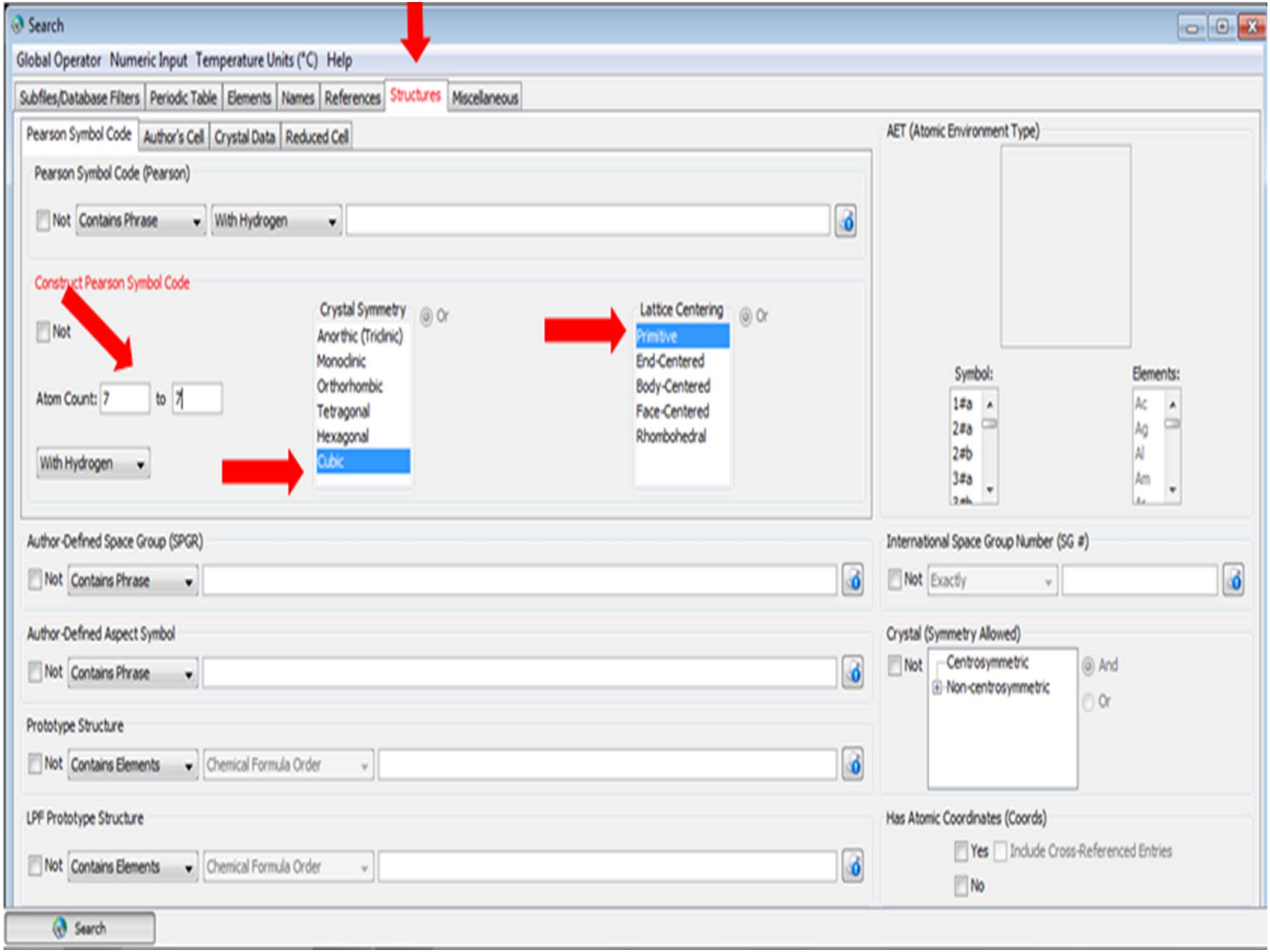
- The *LPF Prototype Translation Table* (reference 2) provides a cross-reference between older and current Metals, Alloys and Related Phases (M&A) Subfile's prototype structures and will be useful to the analyst.
- In each of the following examples, the analyst constructs a PSC index that reflects the requirements of the crystal system, be it as simple as cubic or as complex as anorthic (triclinic).

Example cP7

- Construct a Pearson Symbol Code index for metals and alloys phases having a Pearson Symbol Code (PSC) = cP7.

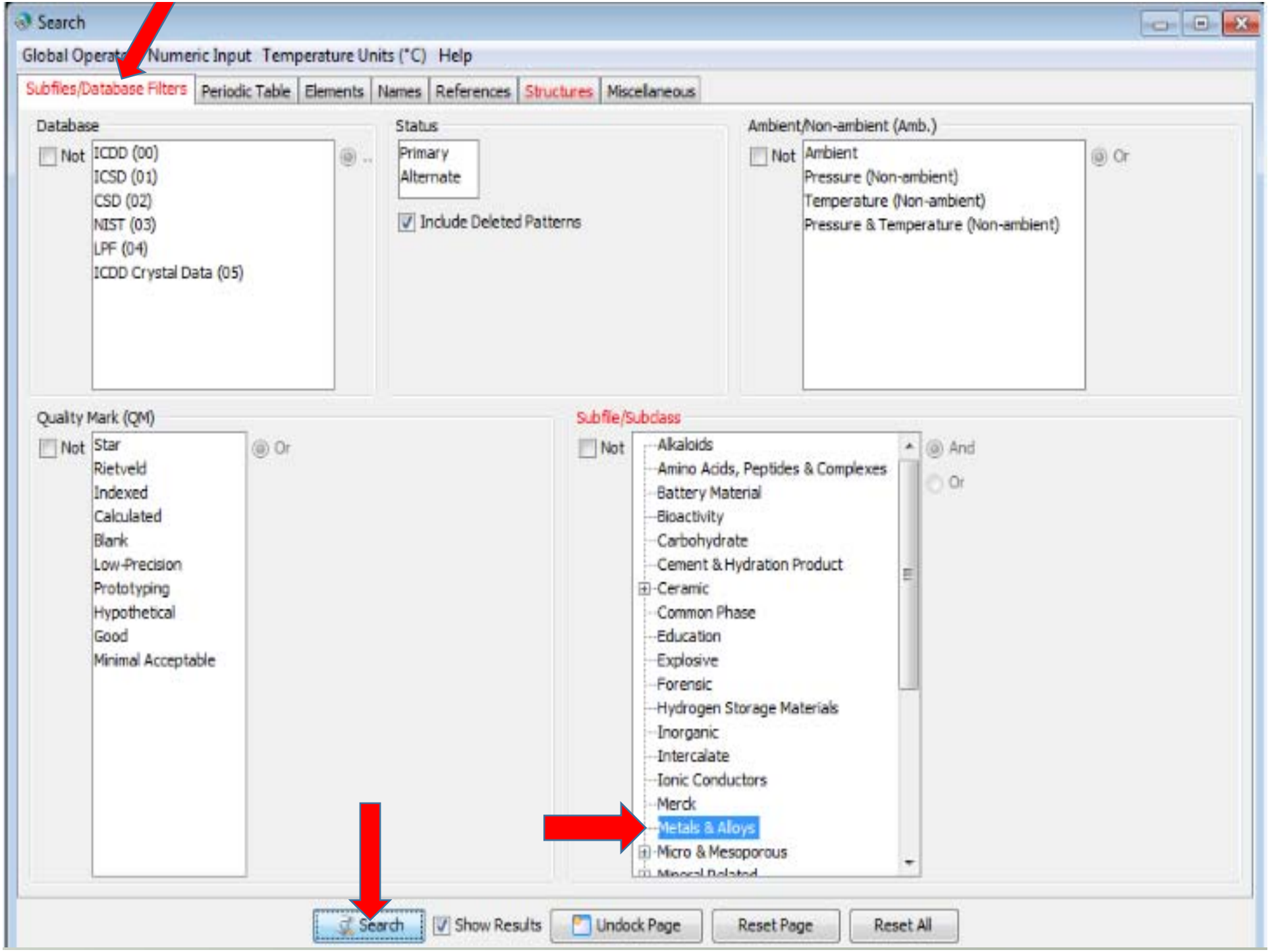
Example cP7
continued

- Click on the *Structures* tab and under *Construct Pearson Symbol Code*, select:
  - *Crystal Symmetry* = Cubic,
  - *Lattice Centering* = Primitive, and
  - *Atom Count* = 7 *to* 7.


Search
Global Operator
Numeric Input
Temperature Units (°C)
Help
Subfiles/Database Filters
Periodic Table
Elements
Names
References
Structures
Miscellaneous
Pearson Symbol Code
Author's Cell
Crystal Data
Reduced Cell
Pearson Symbol Code (Pearson)
Not
Contains Phrase
With Hydrogen
Construct Pearson Symbol Code
Not
Atom Count: 7 to 7
With Hydrogen
Crystal Symmetry
Anorthic (Triclinic)
Monoclinic
Orthorhombic
Tetragonal
Hexagonal
Cubic
Or
Lattice Centering
Primitive
End-Centered
Body-Centered
Face-Centered
Rhombohedral
Or
AET (Atomic Environment Type)
Symbol:
1#a
2#a
2#b
3#a
Elements:
Ac
Ag
Al
Am
Author-Defined Space Group (SPGR)
Not
Contains Phrase
International Space Group Number (SG #)
Not
Exactly
Author-Defined Aspect Symbol
Not
Contains Phrase
Crystal (Symmetry Allowed)
Not
Centrosymmetric
Non-centrosymmetric
And
Or
Prototype Structure
Not
Contains Elements
Chemical Formula Order
LPF Prototype Structure
Not
Contains Elements
Chemical Formula Order
Has Atomic Coordinates (Coords)
Yes
Include Cross-Referenced Entries
No
Search

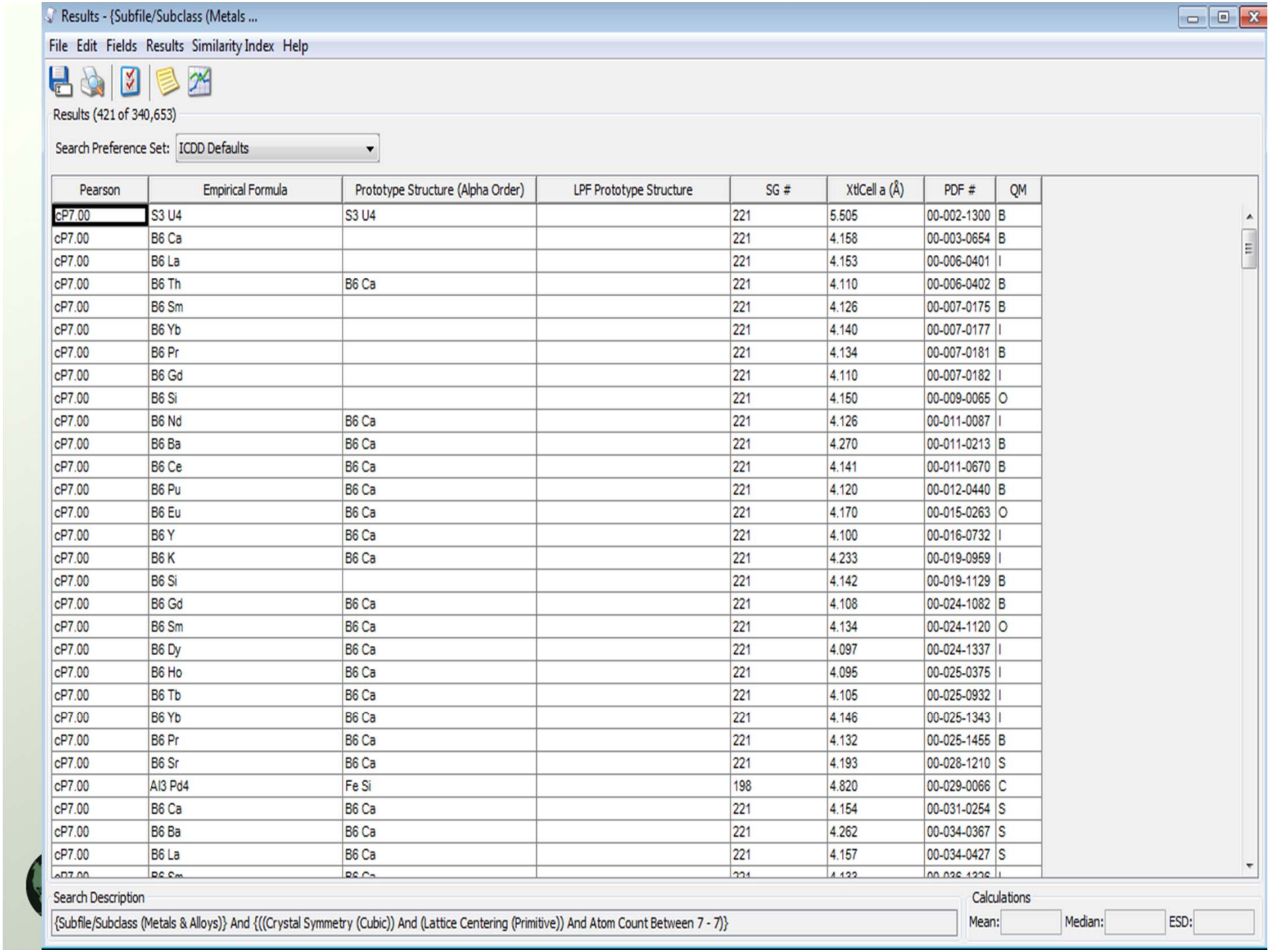
Example cP7
continued

- Click on the *Subfiles/Database Filters* tab and under *Subfile/Subclass* and select *Metals & Alloys*.
- Click on *Search*.


Search
Global Operat
Numeric Input
Temperature Units (°C)
Help
Subfiles/Database Filters
Periodic Table
Elements
Names
References
Structures
Miscellaneous
Database
Not
ICDD (00)
ICSD (01)
CSD (02)
NIST (03)
LPF (04)
ICDD Crystal Data (05)
Status
Primary
Alternate
Include Deleted Patterns
Ambient/Non-ambient (Amb.)
Not
Ambient
Pressure (Non-ambient)
Temperature (Non-ambient)
Pressure & Temperature (Non-ambient)
Or
Quality Mark (QM)
Not
Star
Rietveld
Indexed
Calculated
Blank
Low-Precision
Prototyping
Hypothetical
Good
Minimal Acceptable
Or
Subfile/Subclass
Not
Alkaloids
Amino Acids, Peptides & Complexes
Battery Material
Bioactivity
Carbohydrate
Cement & Hydration Product
Ceramic
Common Phase
Education
Explosive
Forensic
Hydrogen Storage Materials
Inorganic
Intercalate
Ionic Conductors
Merck
Metals & Alloys
Micro & Mesoporous
And
Or
Search
Show Results
Undock Page
Reset Page
Reset All

Example cP7
continued

- Click on *Edit* and then *Preferences* and put the *Results* list in a PSC index form by arranging the columns left-to-right as shown below.
  - *Pearson*
  - *Empirical Formula*
  - *Prototype Structure (Alpha Order)*
  - *LPF Prototype Structure*
  - *SG#*
  - *XtlCell a*
  - *PDF #*
  - *QM*
- Click on *Apply* and then *OK.*



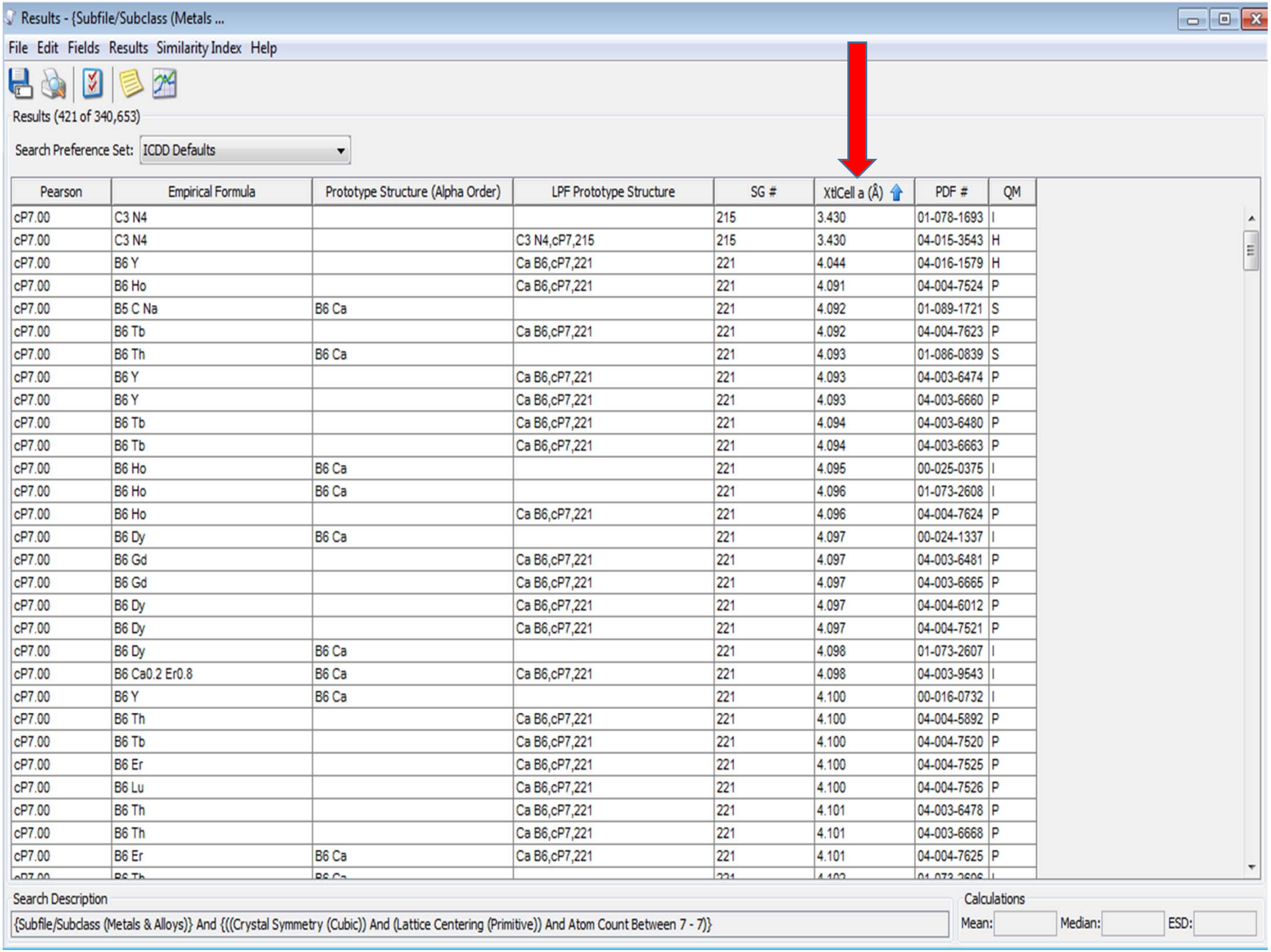
Pearson	Empirical Formula	Prototype Structure (Alpha Order)	LPF Prototype Structure	SG #	XtlCell a (Å)	PDF #	QM
cP7.00	S3 U4	S3 U4		221	5.505	00-002-1300	B
cP7.00	B6 Ca			221	4.158	00-003-0654	B
cP7.00	B6 La			221	4.153	00-006-0401	I
cP7.00	B6 Th	B6 Ca		221	4.110	00-006-0402	B
cP7.00	B6 Sm			221	4.126	00-007-0175	B
cP7.00	B6 Yb			221	4.140	00-007-0177	I
cP7.00	B6 Pr			221	4.134	00-007-0181	B
cP7.00	B6 Gd			221	4.110	00-007-0182	I
cP7.00	B6 Si			221	4.150	00-009-0065	O
cP7.00	B6 Nd	B6 Ca		221	4.126	00-011-0087	I
cP7.00	B6 Ba	B6 Ca		221	4.270	00-011-0213	B
cP7.00	B6 Ce	B6 Ca		221	4.141	00-011-0670	B
cP7.00	B6 Pu	B6 Ca		221	4.120	00-012-0440	B
cP7.00	B6 Eu	B6 Ca		221	4.170	00-015-0263	O
cP7.00	B6 Y	B6 Ca		221	4.100	00-016-0732	I
cP7.00	B6 K	B6 Ca		221	4.233	00-019-0959	I
cP7.00	B6 Si			221	4.142	00-019-1129	B
cP7.00	B6 Gd	B6 Ca		221	4.108	00-024-1082	B
cP7.00	B6 Sm	B6 Ca		221	4.134	00-024-1120	O
cP7.00	B6 Dy	B6 Ca		221	4.097	00-024-1337	I
cP7.00	B6 Ho	B6 Ca		221	4.095	00-025-0375	I
cP7.00	B6 Tb	B6 Ca		221	4.105	00-025-0932	I
cP7.00	B6 Yb	B6 Ca		221	4.146	00-025-1343	I
cP7.00	B6 Pr	B6 Ca		221	4.132	00-025-1455	B
cP7.00	B6 Sr	B6 Ca		221	4.193	00-028-1210	S
cP7.00	Al3 Pd4	Fe Si		198	4.820	00-029-0066	C
cP7.00	B6 Ca	B6 Ca		221	4.154	00-031-0254	S
cP7.00	B6 Ba	B6 Ca		221	4.262	00-034-0367	S
cP7.00	B6 La	B6 Ca		221	4.157	00-034-0427	S

Example cP7
continued

- Various sorting options may be used here.
- For example, sorting on *XtlCell a*, *Pearson*, *LPF Prototype Structure* or *SG#* will produce useful results. When the Pearson Symbol is constant (the case here), an *XtlCell a* search is recommended first.

Example cP7
continued

- Clicking on the *XtlCell a* column resorts the list in order of lattice parameter. The result is a sort that often groups entries together that have the same or similar cell size.


Results - {Subfile/Subclass (Metals ...
File Edit Fields Results Similarity Index Help
Results (421 of 340,653)
Search Preference Set: ICDD Defaults
Pearson | Empirical Formula | Prototype Structure (Alpha Order) | LPF Prototype Structure | SG # | XtlCell a (Å) | PDF # | QM
cP7.00 | C3 N4 | | | 215 | 3.430 | 01-078-1693 | I
cP7.00 | C3 N4 | | C3 N4,cP7,215 | 215 | 3.430 | 04-015-3543 | H
cP7.00 | B6 Y | | Ca B6,cP7,221 | 221 | 4.044 | 04-016-1579 | H
cP7.00 | B6 Ho | | Ca B6,cP7,221 | 221 | 4.091 | 04-004-7524 | P
cP7.00 | B5 C Na | B6 Ca | | 221 | 4.092 | 01-089-1721 | S
cP7.00 | B6 Tb | | Ca B6,cP7,221 | 221 | 4.092 | 04-004-7623 | P
cP7.00 | B6 Th | B6 Ca | | 221 | 4.093 | 01-086-0839 | S
cP7.00 | B6 Y | | Ca B6,cP7,221 | 221 | 4.093 | 04-003-6474 | P
cP7.00 | B6 Y | | Ca B6,cP7,221 | 221 | 4.093 | 04-003-6660 | P
cP7.00 | B6 Tb | | Ca B6,cP7,221 | 221 | 4.094 | 04-003-6480 | P
cP7.00 | B6 Tb | | Ca B6,cP7,221 | 221 | 4.094 | 04-003-6663 | P
cP7.00 | B6 Ho | B6 Ca | | 221 | 4.095 | 00-025-0375 | I
cP7.00 | B6 Ho | B6 Ca | | 221 | 4.096 | 01-073-2608 | I
cP7.00 | B6 Ho | | Ca B6,cP7,221 | 221 | 4.096 | 04-004-7624 | P
cP7.00 | B6 Dy | B6 Ca | | 221 | 4.097 | 00-024-1337 | I
cP7.00 | B6 Gd | | Ca B6,cP7,221 | 221 | 4.097 | 04-003-6481 | P
cP7.00 | B6 Gd | | Ca B6,cP7,221 | 221 | 4.097 | 04-003-6665 | P
cP7.00 | B6 Dy | | Ca B6,cP7,221 | 221 | 4.097 | 04-004-6012 | P
cP7.00 | B6 Dy | | Ca B6,cP7,221 | 221 | 4.097 | 04-004-7521 | P
cP7.00 | B6 Dy | B6 Ca | | 221 | 4.098 | 01-073-2607 | I
cP7.00 | B6 Ca0.2 Er0.8 | B6 Ca | Ca B6,cP7,221 | 221 | 4.098 | 04-003-9543 | I
cP7.00 | B6 Y | B6 Ca | | 221 | 4.100 | 00-016-0732 | I
cP7.00 | B6 Th | | Ca B6,cP7,221 | 221 | 4.100 | 04-004-5892 | P
cP7.00 | B6 Tb | | Ca B6,cP7,221 | 221 | 4.100 | 04-004-7520 | P
cP7.00 | B6 Er | | Ca B6,cP7,221 | 221 | 4.100 | 04-004-7525 | P
cP7.00 | B6 Lu | | Ca B6,cP7,221 | 221 | 4.100 | 04-004-7526 | P
cP7.00 | B6 Th | | Ca B6,cP7,221 | 221 | 4.101 | 04-003-6478 | P
cP7.00 | B6 Th | | Ca B6,cP7,221 | 221 | 4.101 | 04-003-6668 | P
cP7.00 | B6 Er | B6 Ca | Ca B6,cP7,221 | 221 | 4.101 | 04-004-7625 | P
Search Description
{Subfile/Subclass (Metals & Alloys)} And {((Crystal Symmetry (Cubic)) And (Lattice Centering (Primitive)) And Atom Count Between 7 - 7)}
Calculations
Mean:
Median:
ESD:

Example cP7
Search Results

What do your search results show?

1. How many entries do you have?
2. What space groups are present?
3. What are the main prototype structures you see?
4. Is there a dominant one?
5. What is the range of lattice parameter (*XtlCell a*) for the dominant prototype structure?
6. Compare your results with the following discussion.

Example cP7
Search Results, continued

- More than 400 entries fit the search criteria.
- The following LPF prototype structures are present, and most (but not all) of the PDF entries have been identified as having one of these.
  - CaB_6,cP7,221
  - C_3N_4,cP7,215
  - $Ga[CN]_3$,cP7,221
  - U_4S_3,cP7,221
- All assigned LPF prototype structures have either a space group of 215 or 221.

Example cP7
Search Results, continued

- Space groups 195 and 198 are also present.
- [Note: The space group 195 entry could be corrected to space group 221 since it likely is the U_4S_3,cP7,221 type. The space group 198 entry is probably the FeSi,cP8,198 type.]
- Most entries are the CaB_6,cP7,221 type.

Example cP7
Search Results, continued

- For entries having the CaB_6,cP7,221 prototype structure, the
  - Lattice parameter (*XtlCell a*) varies from about 4.044 angstroms to 4.410 angstroms.
  - Anions include boron for all entries, though a few entries have small amounts of carbon replacing some of the boron.
  - Cations include Periodic Table group 1a metals, group 2a metals, rare earths, and actinides.

Example cP7

Thus, both the cell size and the chemistry are limited, and if a new material is thought to have this structure, it likely will conform to this description.

References

General References

1.) The *Strukturbericht Symbol Index* provides a cross-reference between metals, alloys and related phases' Strukturbericht symbols and PDF entries.
http://www.icdd.com/subcommittees/metalsalloys/files/III%201%20b%20Strukturbericht%20Symbol%20Index%2008-19-10.xls

2.) The *LPF Prototype Translation Table for Metallic Structures* provides a cross-reference between older and current metals, alloys and related phases' prototype structures.
http://www.icdd.com/subcommittees/metalsalloys/files/LPF%20Prototype%20Translation%20Tables%20V-2.1%2010-21-13.xlsx

3.) A chemical electronegativity table.
http://www.icdd.com/subcommittees/metalsalloys/files/VI%207%20M&A%20Electronegativity%20Table%2011-24-11.xls

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