Constructing and Using Pearson Symbol Code Indexes (PSCI)

hP20 to hP22

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).

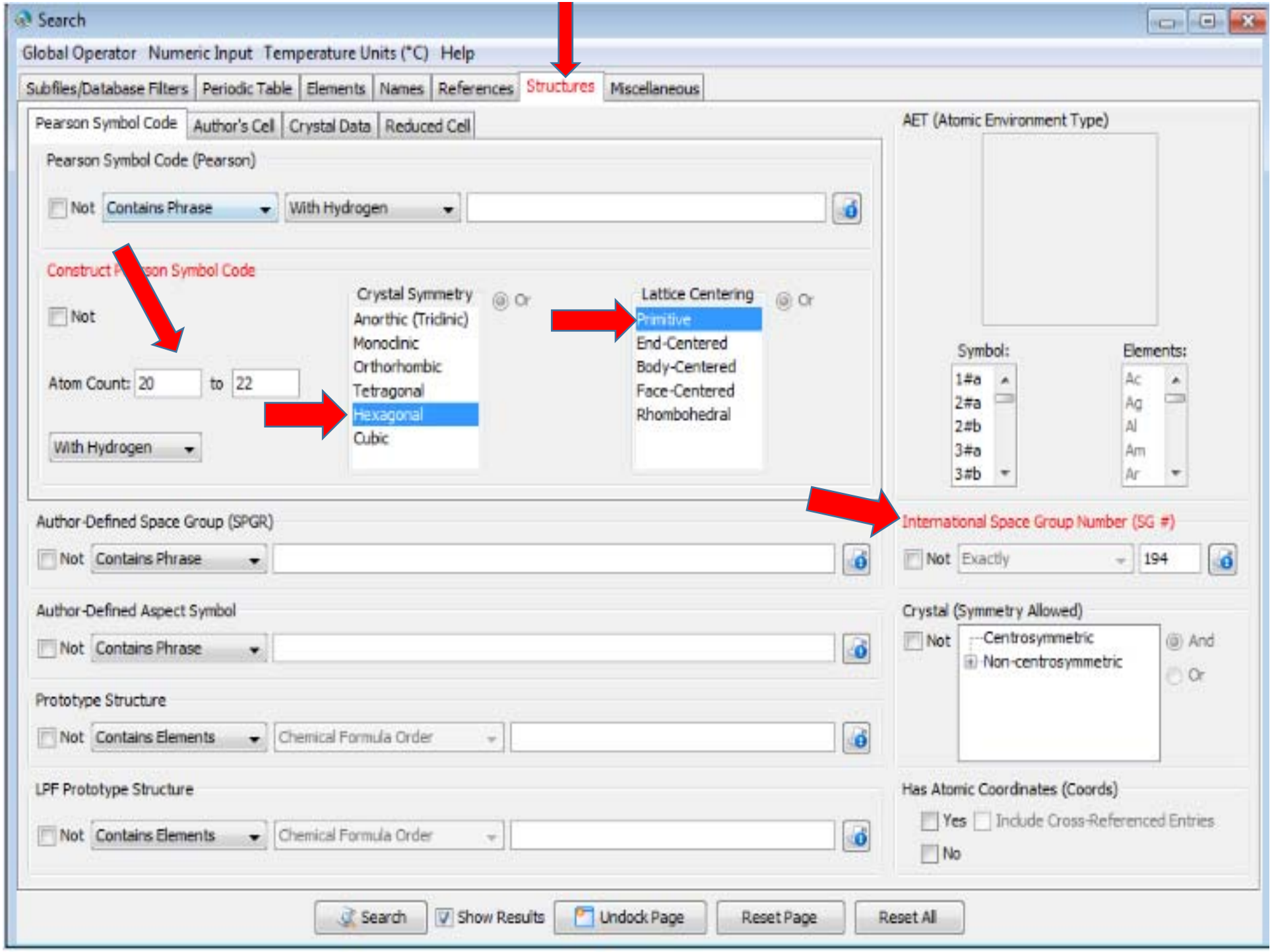
Example hP20 to hP22

Construct a Pearson Symbol Code index for M&A phases having a (a) Pearson Symbol Code (PSC) between hP20 and hP22, and (b) a space group of 194.

Note: The space group is fixed only to limit the size of the output.

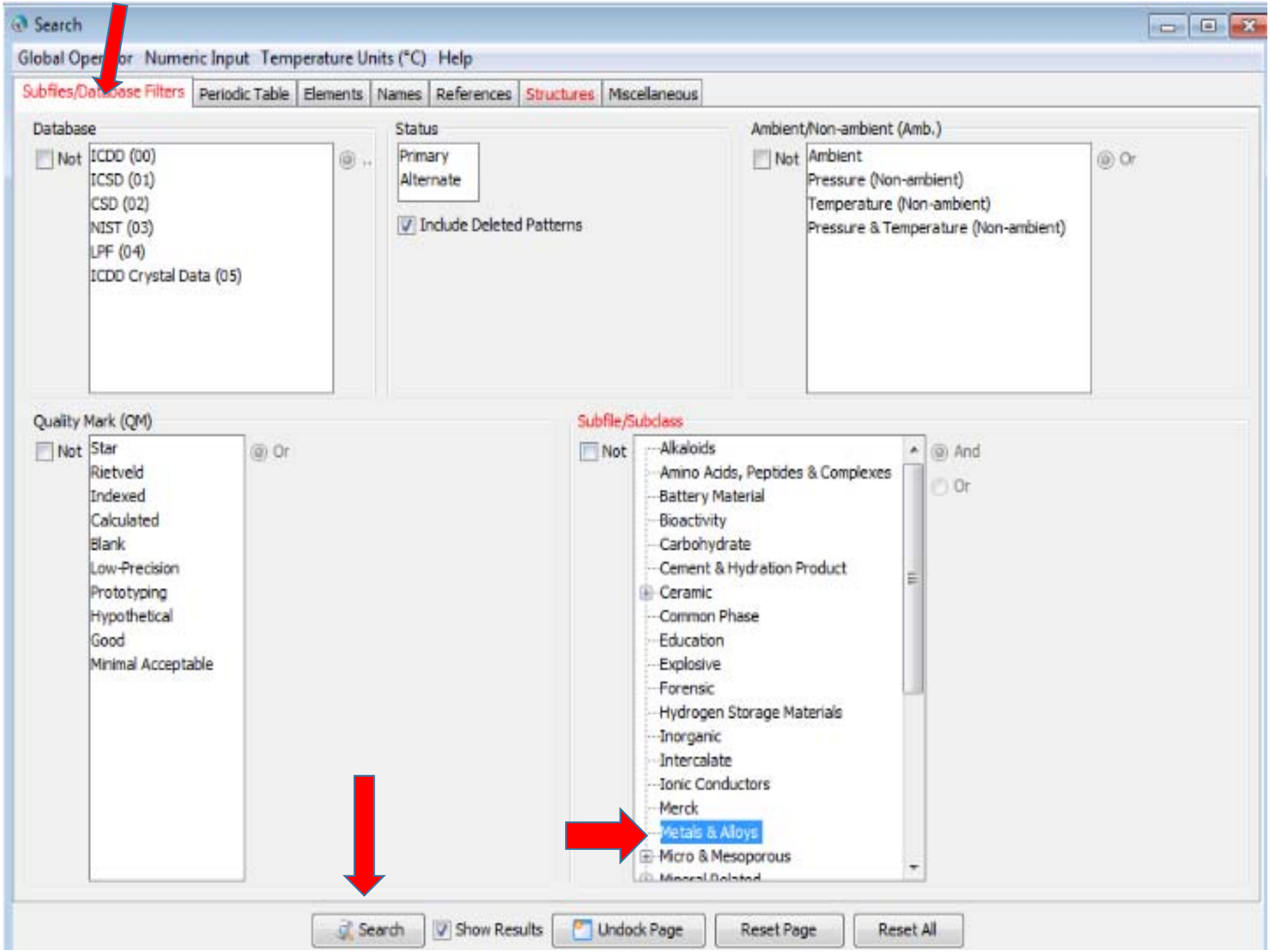
Example hP20 to hP22 *continued*

- Click on the *Structures* tab and under *Construct Pearson Symbol Code*, select:
  - *Crystal Symmetry* = Hexagonal,
  - *Lattice Centering* = Primitive,
  - *Atom Count* = 20 to 22, and
  - *International Space Group Number Exactly 194.*


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:
20
to
22
With Hydrogen
Crystal Symmetry
Anorthic (Tridinic)
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
3#b
Elements:
Ac
Ag
Al
Am
Ar
Author-Defined Space Group (SPGR)
Not
Contains Phrase
International Space Group Number (SG #)
Not
Exactly
194
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
Show Results
Undock Page
Reset Page
Reset All

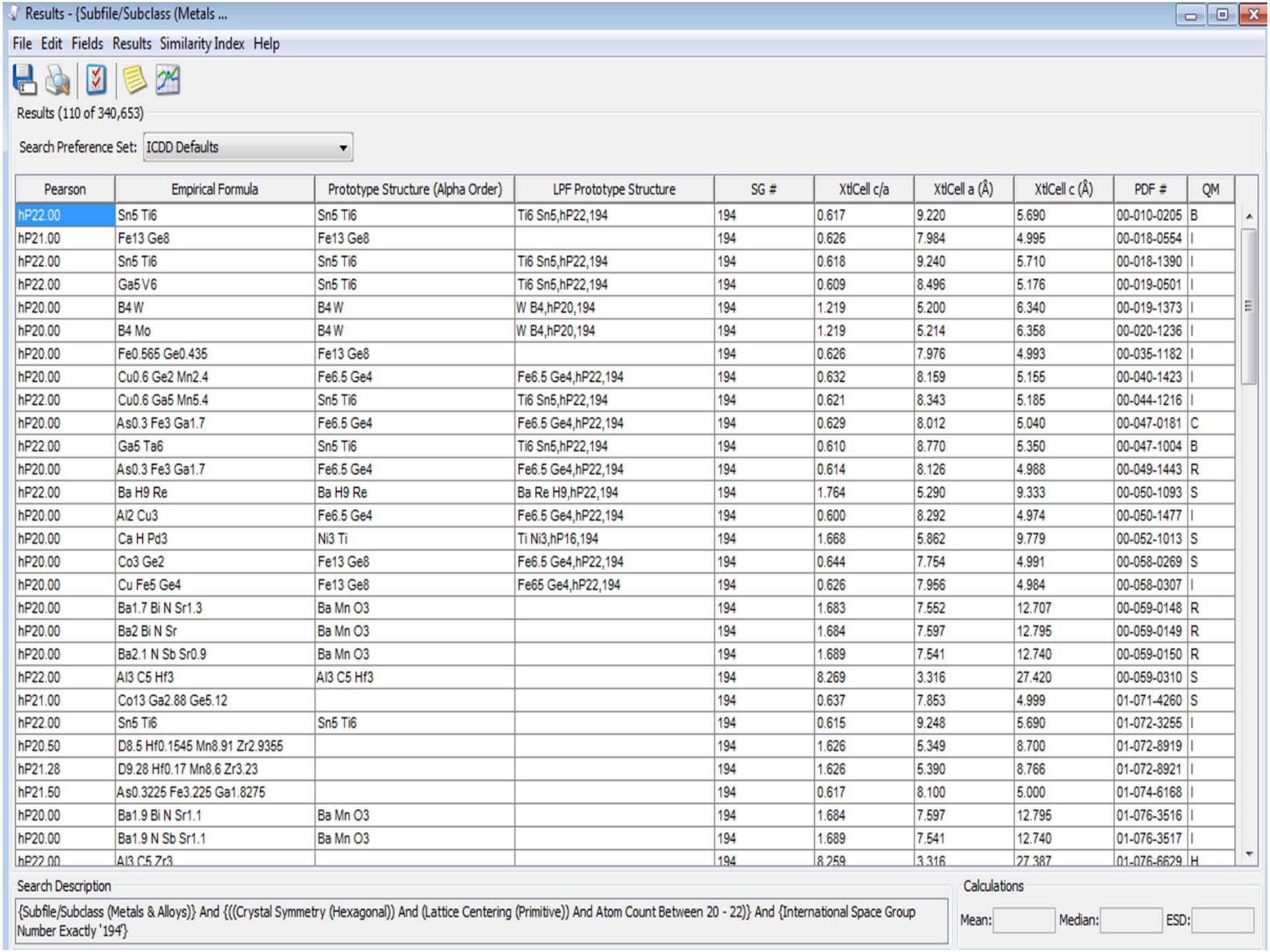
Example hP20 to hP22
continued

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


Search
Global Operator
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 hP20 to hP22 *continued*

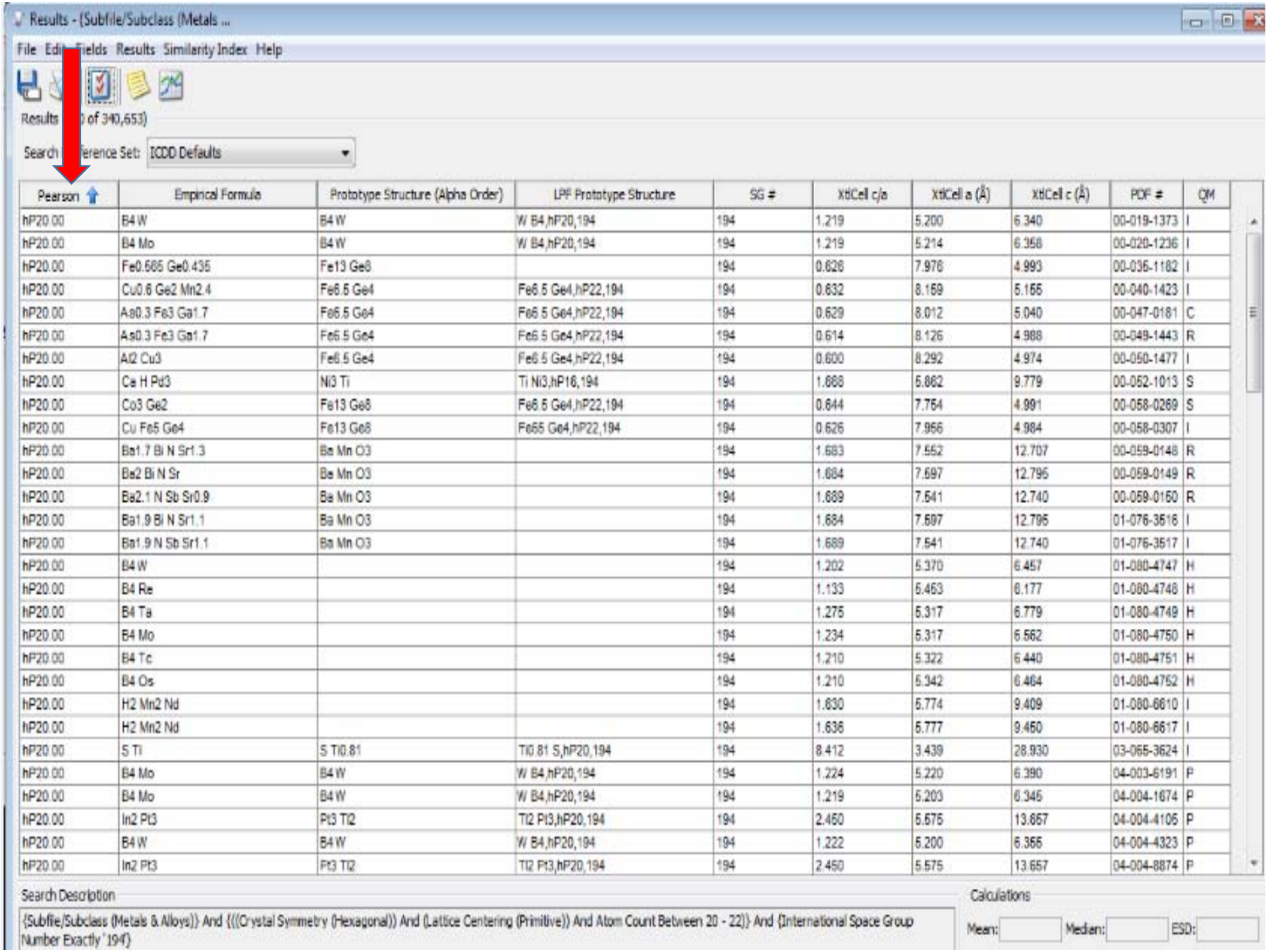
- Click on *Edit* and then *Preferences* and put the *Results* list in a PSC index form by arranging the columns left-to-right as shown below.
  - *Pearson*
  - *Empirical Formula*
  - *Prototype Structure (Alpha Order)*
  - *LPF Prototype Structure*
  - *SG#*
  - *XtlCell c/a*
  - *XtlCell a*
  - *XtlCell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

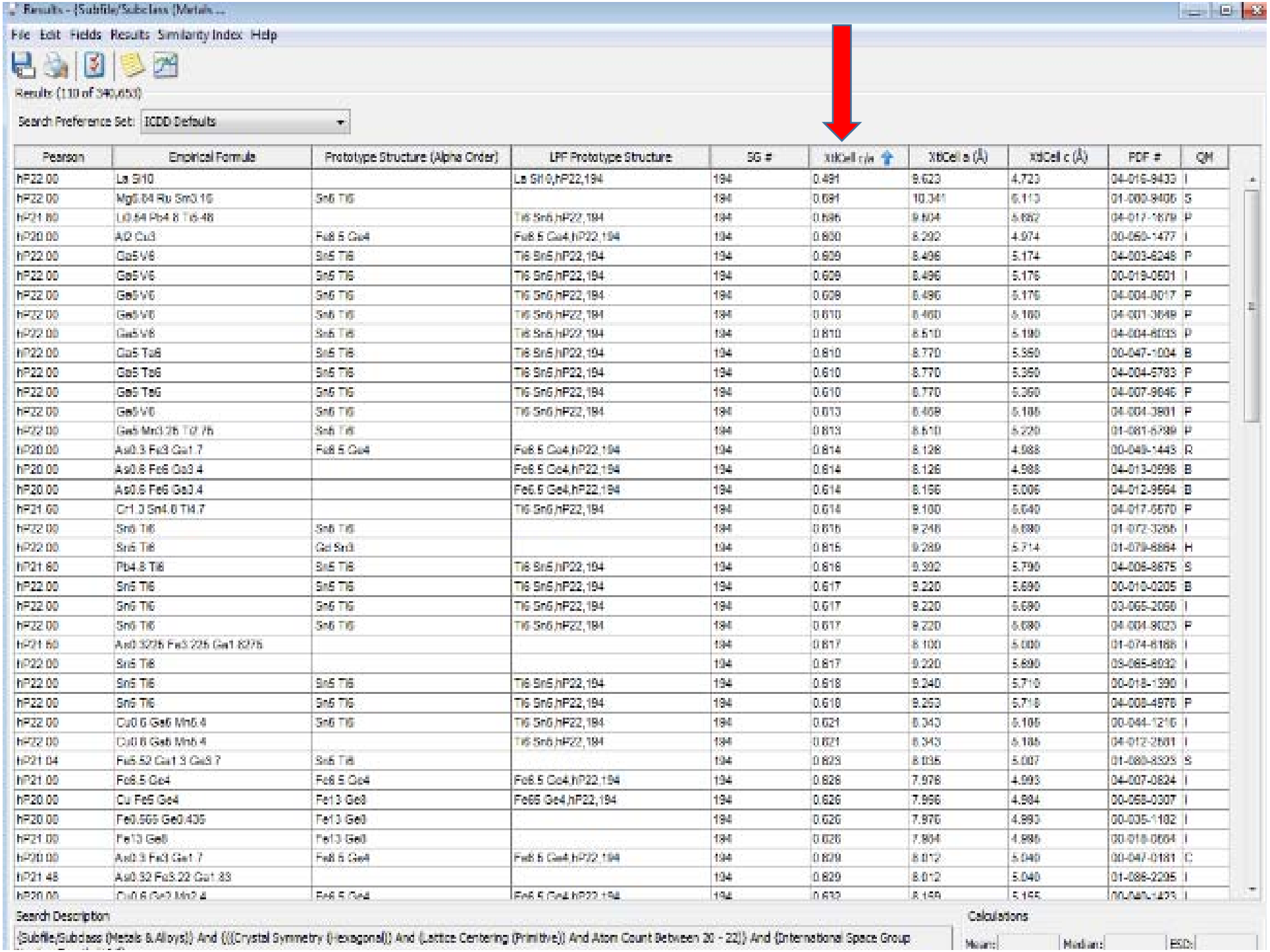

Results - {Subfile/Subclass (Metals ...
File Edit Fields Results Similarity Index Help
Results (110 of 340,653)
Search Preference Set: ICDD Defaults
Pearson | Empirical Formula | Prototype Structure (Alpha Order) | LPF Prototype Structure | SG # | XtlCell c/a | XtlCell a (Å) | XtlCell c (Å) | PDF # | QM
hP22.00 | Sn5 Ti6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.617 | 9.220 | 5.690 | 00-010-0205 | B
hP21.00 | Fe13 Ge8 | Fe13 Ge8 | | 194 | 0.626 | 7.984 | 4.995 | 00-018-0554 | I
hP22.00 | Sn5 Ti6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.618 | 9.240 | 5.710 | 00-018-1390 | I
hP22.00 | Ga5 V6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.609 | 8.496 | 5.176 | 00-019-0501 | I
hP20.00 | B4 W | B4 W | W B4,hP20,194 | 194 | 1.219 | 5.200 | 6.340 | 00-019-1373 | I
hP20.00 | B4 Mo | B4 W | W B4,hP20,194 | 194 | 1.219 | 5.214 | 6.358 | 00-020-1236 | I
hP20.00 | Fe0.565 Ge0.435 | Fe13 Ge8 | | 194 | 0.626 | 7.976 | 4.993 | 00-035-1182 | I
hP20.00 | Cu0.6 Ge2 Mn2.4 | Fe6.5 Ge4 | Fe6.5 Ge4,hP22,194 | 194 | 0.632 | 8.159 | 5.155 | 00-040-1423 | I
hP22.00 | Cu0.6 Ga5 Mn5.4 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.621 | 8.343 | 5.185 | 00-044-1216 | I
hP20.00 | As0.3 Fe3 Ga1.7 | Fe6.5 Ge4 | Fe6.5 Ge4,hP22,194 | 194 | 0.629 | 8.012 | 5.040 | 00-047-0181 | C
hP22.00 | Ga5 Ta6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.610 | 8.770 | 5.350 | 00-047-1004 | B
hP20.00 | As0.3 Fe3 Ga1.7 | Fe6.5 Ge4 | Fe6.5 Ge4,hP22,194 | 194 | 0.614 | 8.126 | 4.988 | 00-049-1443 | R
hP22.00 | Ba H9 Re | Ba H9 Re | Ba Re H9,hP22,194 | 194 | 1.764 | 5.290 | 9.333 | 00-050-1093 | S
hP20.00 | Al2 Cu3 | Fe6.5 Ge4 | Fe6.5 Ge4,hP22,194 | 194 | 0.600 | 8.292 | 4.974 | 00-050-1477 | I
hP20.00 | Ca H Pd3 | Ni3 Ti | Ti Ni3,hP16,194 | 194 | 1.668 | 5.862 | 9.779 | 00-052-1013 | S
hP20.00 | Co3 Ge2 | Fe13 Ge8 | Fe6.5 Ge4,hP22,194 | 194 | 0.644 | 7.754 | 4.991 | 00-058-0269 | S
hP20.00 | Cu Fe5 Ge4 | Fe13 Ge8 | Fe65 Ge4,hP22,194 | 194 | 0.626 | 7.956 | 4.984 | 00-058-0307 | I
hP20.00 | Ba1.7 Bi N Sr1.3 | Ba Mn O3 | | 194 | 1.683 | 7.552 | 12.707 | 00-059-0148 | R
hP20.00 | Ba2 Bi N Sr | Ba Mn O3 | | 194 | 1.684 | 7.597 | 12.795 | 00-059-0149 | R
hP20.00 | Ba2.1 N Sb Sr0.9 | Ba Mn O3 | | 194 | 1.689 | 7.541 | 12.740 | 00-059-0150 | R
hP22.00 | Al3 C5 Hf3 | Al3 C5 Hf3 | | 194 | 8.269 | 3.316 | 27.420 | 00-059-0310 | S
hP21.00 | Co13 Ga2.88 Ge5.12 | | | 194 | 0.637 | 7.853 | 4.999 | 01-071-4260 | S
hP22.00 | Sn5 Ti6 | Sn5 Ti6 | | 194 | 0.615 | 9.248 | 5.690 | 01-072-3255 | I
hP20.50 | D8.5 Hf0.1545 Mn8.91 Zr2.9355 | | | 194 | 1.626 | 5.349 | 8.700 | 01-072-8919 | I
hP21.28 | D9.28 Hf0.17 Mn8.6 Zr3.23 | | | 194 | 1.626 | 5.390 | 8.766 | 01-072-8921 | I
hP21.50 | As0.3225 Fe3.225 Ga1.8275 | | | 194 | 0.617 | 8.100 | 5.000 | 01-074-6168 | I
hP20.00 | Ba1.9 Bi N Sr1.1 | Ba Mn O3 | | 194 | 1.684 | 7.597 | 12.795 | 01-076-3516 | I
hP20.00 | Ba1.9 N Sb Sr1.1 | Ba Mn O3 | | 194 | 1.689 | 7.541 | 12.740 | 01-076-3517 | I
hP22.00 | Al3 C5 Zr3 | | | 194 | 8.259 | 3.316 | 27.387 | 01-076-6629 | H
Search Description
{Subfile/Subclass (Metals & Alloys)} And {{{(Crystal Symmetry (Hexagonal)) And (Lattice Centering (Primitive)) And Atom Count Between 20 - 22)} And {International Space Group Number Exactly '194'}
Calculations
Mean:
Median:
ESD:

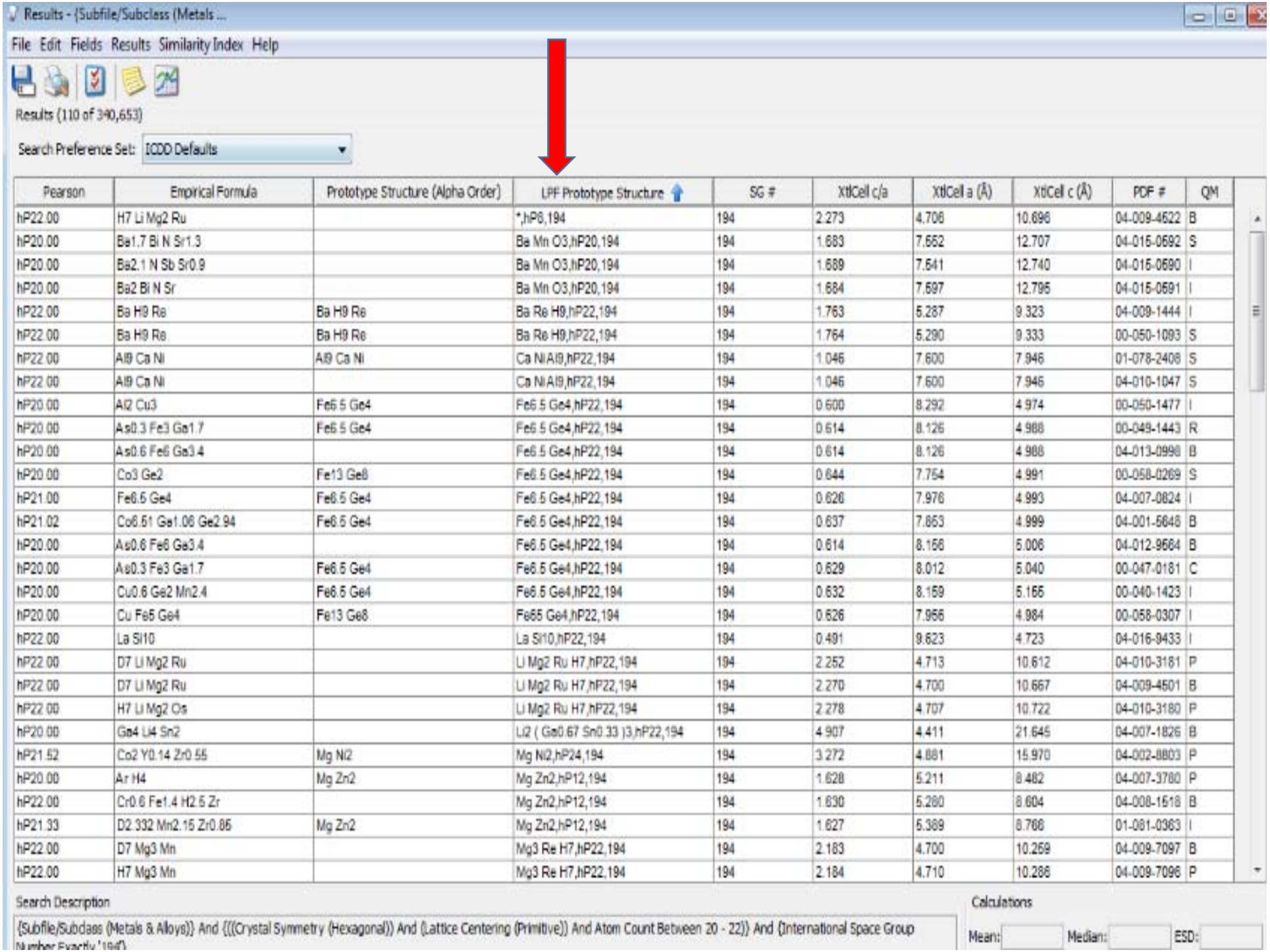
Example hP20 to hP22 *continued*

- Various sorting options may be used here.
- For example, sorting on *Pearson*, *XtlCell c/a* (the axial ratio), or *LPF Prototype Structure* will produce useful results.

Note: For this example, the analyst will want to try all three sorts to determine which is more effective for his/her interests.


Results - (Subfile/Subclass (Metals ...
File Edit Fields Results Similarity Index Help
Results (of 340,653)
Search Reference Set: ICDD Defaults
Pearson | Empirical Formula | Prototype Structure (Alpha Order) | LPF Prototype Structure | SG # | XtlCell c/a | XtlCell a (Å) | XtlCell c (Å) | PDF # | QM
hP20.00 | B4 W | B4 W | W B4,hP20,194 | 194 | 1.219 | 5.200 | 6.340 | 00-019-1373 | I
hP20.00 | B4 Mo | B4 W | W B4,hP20,194 | 194 | 1.219 | 5.214 | 6.358 | 00-020-1236 | I
hP20.00 | Fe0.565 Ge0.435 | Fe13 Ge8 | | 194 | 0.626 | 7.976 | 4.993 | 00-035-1182 | I
hP20.00 | Cu0.6 Ge2 Mn2.4 | Fe6.5 Ge4 | Fe6.5 Ge4,hP22,194 | 194 | 0.632 | 8.159 | 5.156 | 00-040-1423 | I
hP20.00 | As0.3 Fe3 Ga1.7 | Fe6.5 Ge4 | Fe6.5 Ge4,hP22,194 | 194 | 0.629 | 8.012 | 5.040 | 00-047-0181 | C
hP20.00 | As0.3 Fe3 Ga1.7 | Fe6.5 Ge4 | Fe6.5 Ge4,hP22,194 | 194 | 0.614 | 8.126 | 4.988 | 00-049-1443 | R
hP20.00 | Al2 Cu3 | Fe6.5 Ge4 | Fe6.5 Ge4,hP22,194 | 194 | 0.600 | 8.292 | 4.974 | 00-050-1477 | I
hP20.00 | Ca H Pd3 | Ni3 Ti | Ti Ni3,hP16,194 | 194 | 1.668 | 5.862 | 9.779 | 00-052-1013 | S
hP20.00 | Co3 Ge2 | Fe13 Ge8 | Fe6.5 Ge4,hP22,194 | 194 | 0.644 | 7.764 | 4.991 | 00-058-0269 | S
hP20.00 | Cu Fe5 Ge4 | Fe13 Ge8 | Fe65 Ge4,hP22,194 | 194 | 0.626 | 7.956 | 4.984 | 00-058-0307 | I
hP20.00 | Ba1.7 Bi N Sr1.3 | Ba Mn O3 | | 194 | 1.683 | 7.552 | 12.707 | 00-059-0148 | R
hP20.00 | Ba2 Bi N Sr | Ba Mn O3 | | 194 | 1.684 | 7.597 | 12.795 | 00-059-0149 | R
hP20.00 | Ba2.1 N Sb Sr0.9 | Ba Mn O3 | | 194 | 1.689 | 7.541 | 12.740 | 00-059-0150 | R
hP20.00 | Ba1.9 Bi N Sr1.1 | Ba Mn O3 | | 194 | 1.684 | 7.597 | 12.795 | 01-076-3516 | I
hP20.00 | Ba1.9 N Sb Sr1.1 | Ba Mn O3 | | 194 | 1.689 | 7.541 | 12.740 | 01-076-3517 | I
hP20.00 | B4 W | | | 194 | 1.202 | 5.370 | 6.457 | 01-080-4747 | H
hP20.00 | B4 Re | | | 194 | 1.133 | 5.453 | 6.177 | 01-080-4748 | H
hP20.00 | B4 Ta | | | 194 | 1.275 | 5.317 | 6.779 | 01-080-4749 | H
hP20.00 | B4 Mo | | | 194 | 1.234 | 5.317 | 6.562 | 01-080-4750 | H
hP20.00 | B4 Tc | | | 194 | 1.210 | 5.322 | 6.440 | 01-080-4751 | H
hP20.00 | B4 Os | | | 194 | 1.210 | 5.342 | 6.464 | 01-080-4752 | H
hP20.00 | H2 Mn2 Nd | | | 194 | 1.630 | 5.774 | 9.409 | 01-080-6610 | I
hP20.00 | H2 Mn2 Nd | | | 194 | 1.636 | 5.777 | 9.460 | 01-080-6617 | I
hP20.00 | S Ti | S Ti0.81 | Ti0.81 S,hP20,194 | 194 | 8.412 | 3.439 | 28.930 | 03-065-3624 | I
hP20.00 | B4 Mo | B4 W | W B4,hP20,194 | 194 | 1.224 | 5.220 | 6.390 | 04-003-6191 | P
hP20.00 | B4 Mo | B4 W | W B4,hP20,194 | 194 | 1.219 | 5.203 | 6.345 | 04-004-1674 | P
hP20.00 | In2 Pt3 | Pt3 Ti2 | Ti2 Pt3,hP20,194 | 194 | 2.460 | 5.675 | 13.657 | 04-004-4105 | P
hP20.00 | B4 W | B4 W | W B4,hP20,194 | 194 | 1.222 | 5.200 | 6.356 | 04-004-4323 | P
hP20.00 | In2 Pt3 | Pt3 Ti2 | Ti2 Pt3,hP20,194 | 194 | 2.460 | 5.575 | 13.657 | 04-004-8874 | P
Search Description
{Subfile/Subclass (Metals & Alloys)} And {((Crystal Symmetry (Hexagonal)) And (Lattice Centering (Primitive)) And Atom Count Between 20 - 22)} And {International Space Group Number Exactly '194'}
Calculations
Mean:
Median:
ESD:


Results - (Subfile/Subclass (Metals ...
File Edit Fields Results Similarity Index Help
Results (110 of 340,650)
Search Preference Set: ICDD Defaults
Pearson | Empirical Formula | Prototype Structure (Alpha Order) | LPF Prototype Structure | SG # | XdCell c/a | XdCell a (Å) | XdCell c (Å) | PDF # | QM
hP22.00 | La Si10 | | La Si10,hP22,194 | 194 | 0.491 | 8.623 | 4.723 | 04-016-9433 | I
hP22.00 | Mg5.64 Ru Sm3.16 | Sn5 Ti6 | | 194 | 0.691 | 10.341 | 6.113 | 01-000-9400 | S
hP21.80 | La0.64 Pb4.8 Ti6.48 | | Ti6 Sn5,hP22,194 | 194 | 0.686 | 9.604 | 6.592 | 04-017-1679 | P
hP20.00 | Al2 Cu3 | Fe8.5 Ge4 | Fe8.5 Ge4,hP22,194 | 194 | 0.630 | 8.292 | 4.974 | 00-050-1477 | I
hP22.00 | Ga5 V6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.609 | 8.496 | 5.174 | 04-003-6248 | P
hP22.00 | Ga5 V6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.609 | 8.496 | 5.176 | 00-019-0501 | I
hP22.00 | Ga5 V6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.609 | 8.496 | 5.176 | 04-004-0017 | P
hP22.00 | Ga5 V6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.610 | 8.460 | 5.160 | 04-001-3649 | P
hP22.00 | Ga5 V6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.610 | 8.510 | 5.190 | 04-004-6035 | P
hP22.00 | Ga5 Ta6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.610 | 8.770 | 5.350 | 00-047-1004 | B
hP22.00 | Ga5 Ta6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.610 | 8.770 | 5.350 | 04-004-5783 | P
hP22.00 | Ga5 Ta6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.610 | 8.770 | 5.350 | 04-007-9646 | P
hP22.00 | Ga5 V6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.613 | 8.468 | 5.186 | 04-004-3801 | P
hP22.00 | Ga5 Mn0.25 Ti7.75 | Sn5 Ti6 | | 194 | 0.613 | 8.510 | 5.220 | 01-081-6789 | P
hP20.00 | As0.3 Fe3 Ga1.7 | Fe8.5 Ge4 | Fe8.5 Ge4,hP22,194 | 194 | 0.614 | 8.128 | 4.988 | 00-049-1445 | R
hP20.00 | As0.8 Fe6 Ga3.4 | | Fe8.5 Ge4,hP22,194 | 194 | 0.614 | 8.126 | 4.988 | 04-013-0998 | B
hP20.00 | As0.8 Fe6 Ga3.4 | | Fe8.5 Ge4,hP22,194 | 194 | 0.614 | 8.156 | 5.006 | 04-012-9564 | B
hP21.60 | Cr1.3 Sn4.8 Ti4.7 | | Ti6 Sn5,hP22,194 | 194 | 0.614 | 8.100 | 5.040 | 04-017-5570 | P
hP22.00 | Sn5 Ti6 | Sn5 Ti6 | | 194 | 0.616 | 9.246 | 5.690 | 01-072-3266 | I
hP22.00 | Sn5 Ti6 | Cd Sn3 | | 194 | 0.616 | 9.289 | 5.714 | 01-079-6864 | H
hP21.60 | Pb4.8 Ti6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.616 | 9.392 | 5.790 | 04-006-8675 | S
hP22.00 | Sn5 Ti6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.617 | 9.220 | 5.690 | 00-010-0205 | B
hP22.00 | Sn5 Ti6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.617 | 9.220 | 5.690 | 03-065-2050 | I
hP22.00 | Sn5 Ti6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.617 | 9.220 | 5.690 | 04-004-9023 | P
hP21.60 | As0.3225 Fe3.225 Ge1.6275 | | | 194 | 0.617 | 8.100 | 5.000 | 01-074-6166 | I
hP22.00 | Sn5 Ti6 | | | 194 | 0.617 | 9.220 | 5.690 | 03-065-9032 | I
hP22.00 | Sn5 Ti6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.618 | 9.240 | 5.710 | 00-018-1390 | I
hP22.00 | Sn5 Ti6 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.618 | 9.253 | 5.718 | 04-008-4978 | P
hP22.00 | Cu0.6 Ge6 Mn5.4 | Sn5 Ti6 | Ti6 Sn5,hP22,194 | 194 | 0.621 | 8.343 | 5.185 | 00-044-1216 | I
hP22.00 | Cu0.6 Ge6 Mn5.4 | | Ti6 Sn5,hP22,194 | 194 | 0.621 | 8.343 | 5.185 | 04-012-2681 | I
hP21.04 | Fe5.52 Ge1.3 Ge9.7 | Sn5 Ti6 | | 194 | 0.623 | 8.035 | 5.007 | 01-080-8525 | S
hP21.00 | Fe8.5 Ge4 | Fe8.5 Ge4 | Fe8.5 Ge4,hP22,194 | 194 | 0.626 | 7.978 | 4.993 | 04-007-0824 | I
hP20.00 | Cu Fe5 Ge4 | Fe13 Ge8 | Fe65 Ge4,hP22,194 | 194 | 0.626 | 7.956 | 4.984 | 00-058-0307 | I
hP20.00 | Fe9.569 Ge0.435 | Fe13 Ge8 | | 194 | 0.626 | 7.976 | 4.993 | 00-035-1102 | I
hP21.00 | Fe13 Ge8 | Fe13 Ge8 | | 194 | 0.626 | 7.984 | 4.996 | 00-018-0604 | I
hP20.00 | As0.3 Fe3 Ge1.7 | Fe8.5 Ge4 | Fe8.5 Ge4,hP22,194 | 194 | 0.629 | 8.012 | 5.040 | 00-047-0181 | C
hP21.48 | As0.52 Fe3.22 Cu1.83 | | | 194 | 0.629 | 8.012 | 5.040 | 01-088-2295 | I
Search Description
(Subfile/Subclass (Metals & Alloys)) And (((Crystal Symmetry (Hexagonal)) And (Lattice Centering (Primitive)) And Atom Count Between 20 - 22)) And (International Space Group
Calculations
Mean: Median: FSD:



Pearson	Empirical Formula	Prototype Structure (Alpha Order)	LPF Prototype Structure	SG #	XtlCell c/a	XtlCell a (Å)	XtlCell c (Å)	PDF #	QM
hP22.00	H7 Li Mg2 Ru		*,hP6,194	194	2.273	4.706	10.696	04-009-4622	B
hP20.00	Ba1.7 Bi N Sr1.3		Ba Mn O3,hP20,194	194	1.683	7.652	12.707	04-015-0592	S
hP20.00	Ba2.1 N Sb Sr0.9		Ba Mn O3,hP20,194	194	1.689	7.641	12.740	04-015-0690	I
hP20.00	Ba2 Bi N Sr		Ba Mn O3,hP20,194	194	1.684	7.697	12.795	04-015-0691	I
hP22.00	Ba H9 Re	Ba H9 Re	Ba Re H9,hP22,194	194	1.763	5.287	9.323	04-009-1444	I
hP22.00	Ba H9 Re	Ba H9 Re	Ba Re H9,hP22,194	194	1.764	5.290	9.333	00-050-1093	S
hP22.00	Al9 Ca Ni	Al9 Ca Ni	Ca Ni Al9,hP22,194	194	1.046	7.600	7.946	01-078-2408	S
hP22.00	Al9 Ca Ni		Ca Ni Al9,hP22,194	194	1.046	7.600	7.946	04-010-1047	S
hP20.00	Al2 Cu3	Fe6.5 Ge4	Fe6.5 Ge4,hP22,194	194	0.600	8.292	4.974	00-050-1477	I
hP20.00	As0.3 Fe3 Ga1.7	Fe6.5 Ge4	Fe6.5 Ge4,hP22,194	194	0.614	8.126	4.988	00-048-1443	R
hP20.00	As0.6 Fe6 Ga3.4		Fe6.5 Ge4,hP22,194	194	0.614	8.126	4.988	04-013-0998	B
hP20.00	Co3 Ge2	Fe13 Ge8	Fe6.5 Ge4,hP22,194	194	0.644	7.754	4.991	00-058-0269	S
hP21.00	Fe6.5 Ge4	Fe6.5 Ge4	Fe6.5 Ge4,hP22,194	194	0.626	7.976	4.993	04-007-0824	I
hP21.02	Co6.51 Ge1.06 Ge2.94	Fe6.5 Ge4	Fe6.5 Ge4,hP22,194	194	0.637	7.853	4.999	04-001-5648	B
hP20.00	As0.6 Fe6 Ga3.4		Fe6.5 Ge4,hP22,194	194	0.614	8.156	5.006	04-012-9564	B
hP20.00	As0.3 Fe3 Ga1.7	Fe6.5 Ge4	Fe6.5 Ge4,hP22,194	194	0.629	8.012	5.040	00-047-0181	C
hP20.00	Cu0.6 Ge2 Mn2.4	Fe6.5 Ge4	Fe6.5 Ge4,hP22,194	194	0.632	8.159	5.166	00-040-1423	I
hP20.00	Cu Fe5 Ge4	Fe13 Ge8	Fe65 Ge4,hP22,194	194	0.626	7.966	4.984	00-058-0307	I
hP22.00	La Si10		La Si10,hP22,194	194	0.491	9.623	4.723	04-016-9433	I
hP22.00	D7 Li Mg2 Ru		Li Mg2 Ru H7,hP22,194	194	2.252	4.713	10.612	04-010-3181	P
hP22.00	D7 Li Mg2 Ru		Li Mg2 Ru H7,hP22,194	194	2.270	4.700	10.667	04-009-4501	B
hP22.00	H7 Li Mg2 Os		Li Mg2 Ru H7,hP22,194	194	2.278	4.707	10.722	04-010-3180	P
hP20.00	Ga4 Li4 Sn2		Li2 (Ga0.67 Sn0.33)3,hP22,194	194	4.907	4.411	21.645	04-007-1826	B
hP21.52	Co2 Y0.14 Zr0.55	Mg Ni2	Mg Ni2,hP24,194	194	3.272	4.881	15.970	04-002-8803	P
hP20.00	Ar H4	Mg Zn2	Mg Zn2,hP12,194	194	1.628	5.211	8.482	04-007-3780	P
hP22.00	Cr0.6 Fe1.4 H2.5 Zr		Mg Zn2,hP12,194	194	1.630	5.260	8.604	04-008-1518	B
hP21.33	D2.332 Mn2.15 Zr0.85	Mg Zn2	Mg Zn2,hP12,194	194	1.627	5.389	8.766	01-081-0363	I
hP22.00	D7 Mg3 Mn		Mg3 Re H7,hP22,194	194	2.183	4.700	10.259	04-009-7097	B
hP22.00	H7 Mg3 Mn		Mg3 Re H7,hP22,194	194	2.184	4.710	10.286	04-009-7096	P

Example hP20 to hP22
Search Results

What do your search results show?

1.) How many entries do you have?
2.) What are the main LPF prototype structures you see?
3.) Is there a dominant one?
4.) What is the range of lattice parameter (*XtlCell a*) for the dominant prototype structure?
5.) Look at entries 01-071-4260 and 01-086-2295. What LPF prototype structure do you think these entries should have? Why?
6.) What prototype structure would $Co_{6.51}Al_{1.1}Ge_{2.9}$ have? Hint: Look for a similar chemistry; perhaps one with gallium instead of the aluminum in this example.

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Example hP20 to hP22
Search Results, continued

Compare your results with the following discussion.

Example hP20 to hP22
Search Results, continued

- These sorts show (among other things) that:
  - More than 100 entries fit the search criteria,
  - At least 22 LPF prototype structures are present,
  - Both the *Pearson* and *XtlCell c/a* sorts easily separating most of these types,
  - The *LPF Prototype Structure* sort lists the prototype structures within the search criteria, and
  - It would be relatively easy to assign prototype structures to many PDF phases where they are missing as well as an analyst's unknown metallic phase that fits into the search criteria.

Example hP20 to hP22
Search Results, continued

- For example, using the *XtlCell c/a* sort, two prototype structures with similar c/a values are found. Please concentrate on range in c/a of 0.591 to 0.644.
  - The $Fe_{6.5}Ge_4$,hP22,194 type has 15 entries with c/a between 0.600 and 0.644 and *Pearson* = hP20 to hP21.50, though not all are marked with the type.
  - The Ti_6Sn_5,hP22,194 type has 25 entries with c/a between 0.591 and 0.623 and *Pearson* = hP21.04 to hP22, though not all are marked with the type.

Example hP20 to hP22
Search Results, continued

- Thus, if the analyst has an unknown metallic phase in space group 194 and has a c/a of about 0.62, these two structures would be of interest. There are several approaches that would help in choosing which structure is more likely. Some are listed below.
  - Compare the d's and I's of the unknown versus each of the prototype structures and their examples. This helps most when the prototype structures have d's and I's that are significantly different.
  - Look at the crystal chemistry of the examples of each prototype structure. That is, are the elements in the unknown material more similar to those in the examples of one prototype structure than the other?
  - Calculate hypothetical powder patterns for the analyst's material using (a) his/her material's chemistry and (b) the atom positions for each prototype structure in turn. The resultant patterns could then be compared to the unknown material's experimental pattern

Example hP20 to hP22
Search Results, continued

The answer to questions 5 and 6, above, is $Fe_{6.5}Ge_4$,hP22,194. The analyst is encouraged to study the various sort results, since they have many uses. For example, in an ongoing project, the ICDD M&A Subcommittee is using such sorts to update assigned prototype structures in the M&A Subfile.

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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