# Constructing and Using Pearson Symbol Code Indexes (PSCI)

*mC16 to mC20*

ISO 9001:2008 QUALITY ASSURED COMPANY CERT.NR. 11409.1

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# 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*

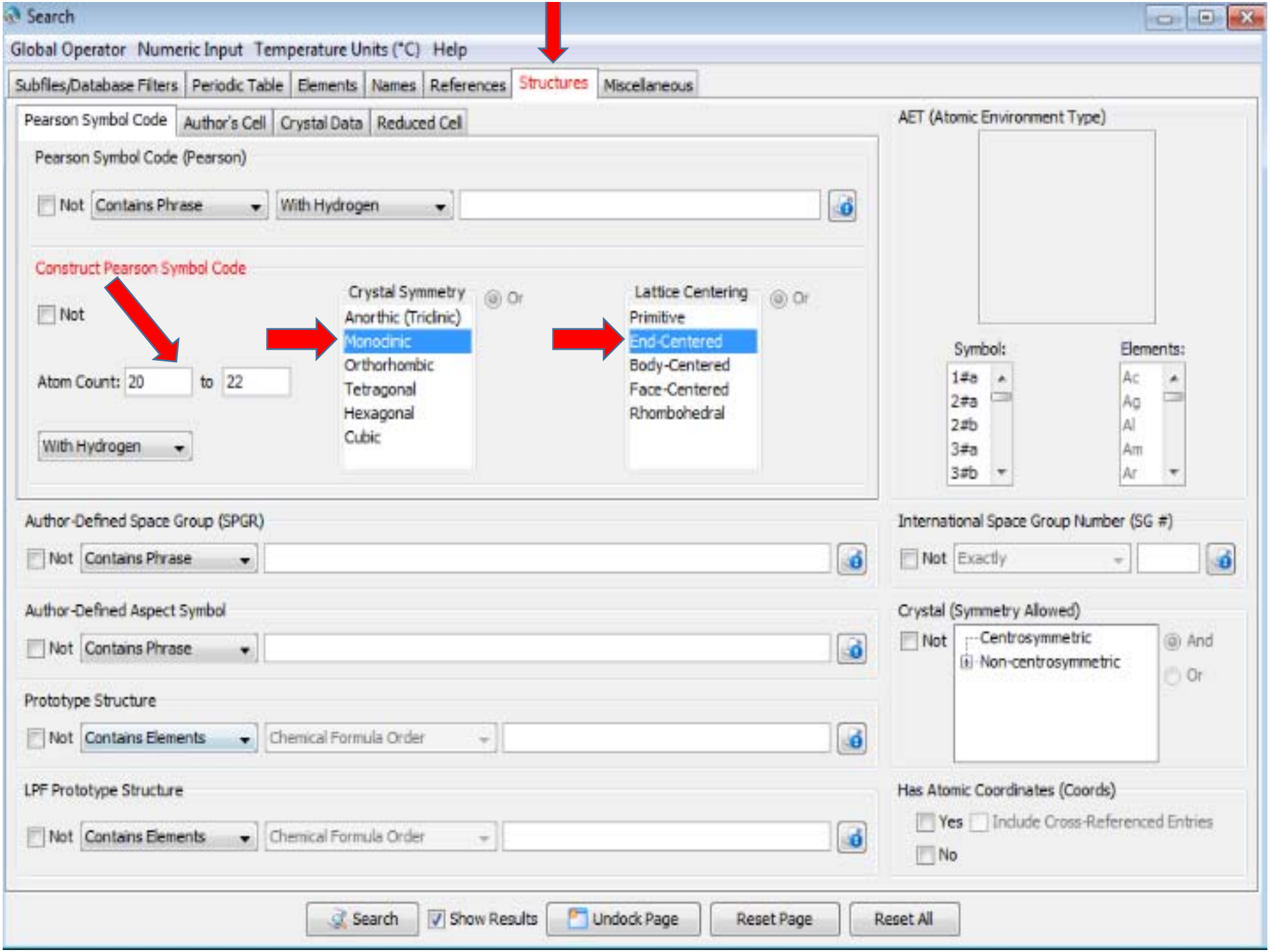
- The *LPF Prototype Translation Table* (reference 2) provides a cross-reference between older and current Metals, Alloys and Related Phases (M&A) Subfile's prototype structures and will be useful to the analyst.
- In each of the following examples, the analyst constructs a PSC index that reflects the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

# Example mC16 to mC20

- Construct a Pearson Symbol Code index for metals and alloys phases having a Pearson Symbol (PS) between mC16 and mC20.

# Example mC16 to mC20 *continued*

- Click on the *Structures* tab and under *Construct Pearson Symbol Code*, select:
  - *Crystal Symmetry* = Monoclinic,
  - *Lattice Centering* = End-Centered, and
  - *Atom Count* = 20 *to* 22.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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 (Triclinic)
Monoclinic
Orthorhombic
Tetragonal
Hexagonal
Cubic
Or
Lattice Centering
Primitive
End-Centered
Body-Centered
Face-Centered
Rhombohedral
Or
AET (Atomic Environment Type)
Symbol:
1#e
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
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
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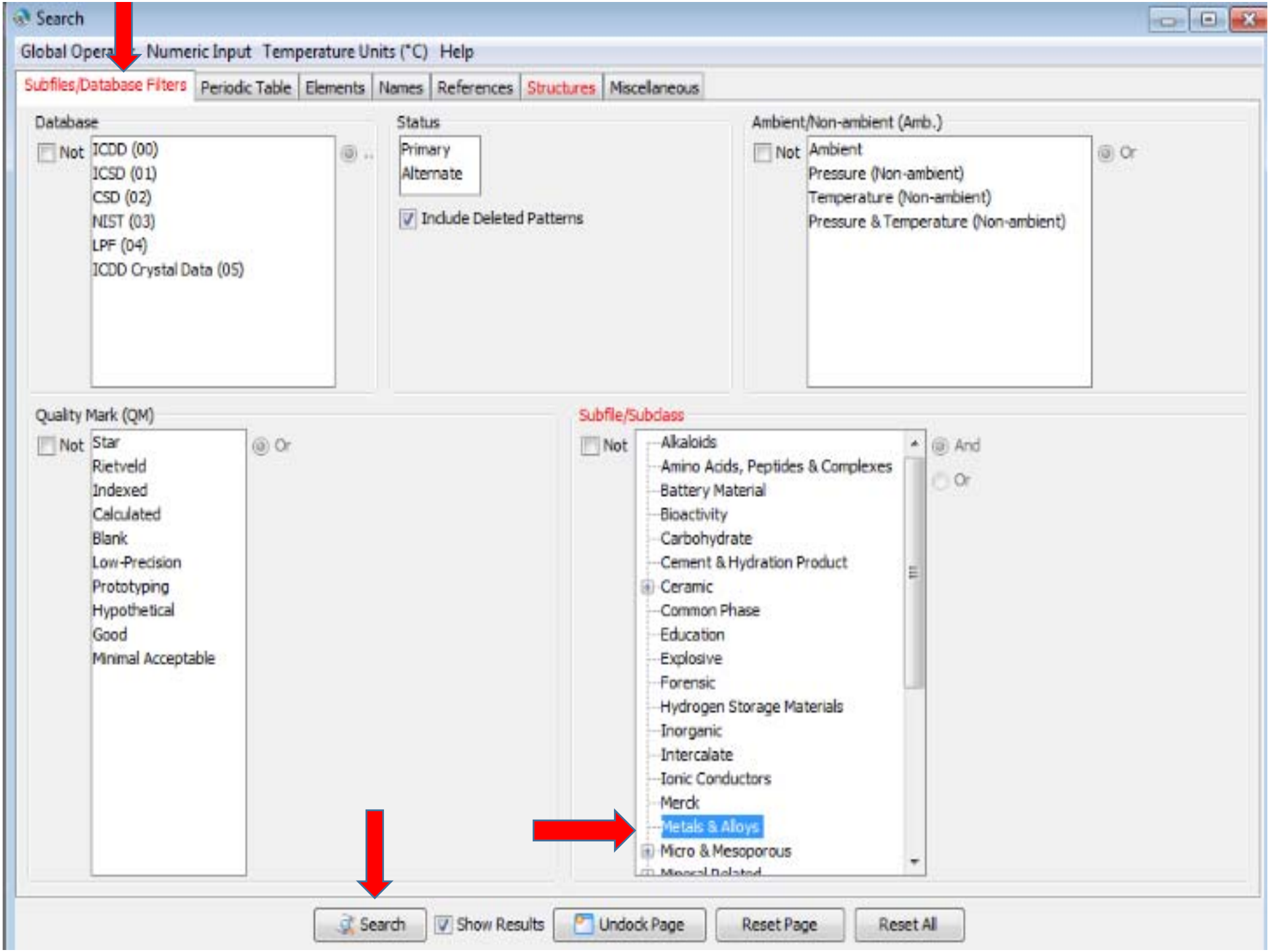
# Example mC16 to mC20 *continued*

- Click on the *Subfiles/Database Filters* tab and under *Subfile/Subclass* and select *Metals & Alloys*.
- Click on *Search*.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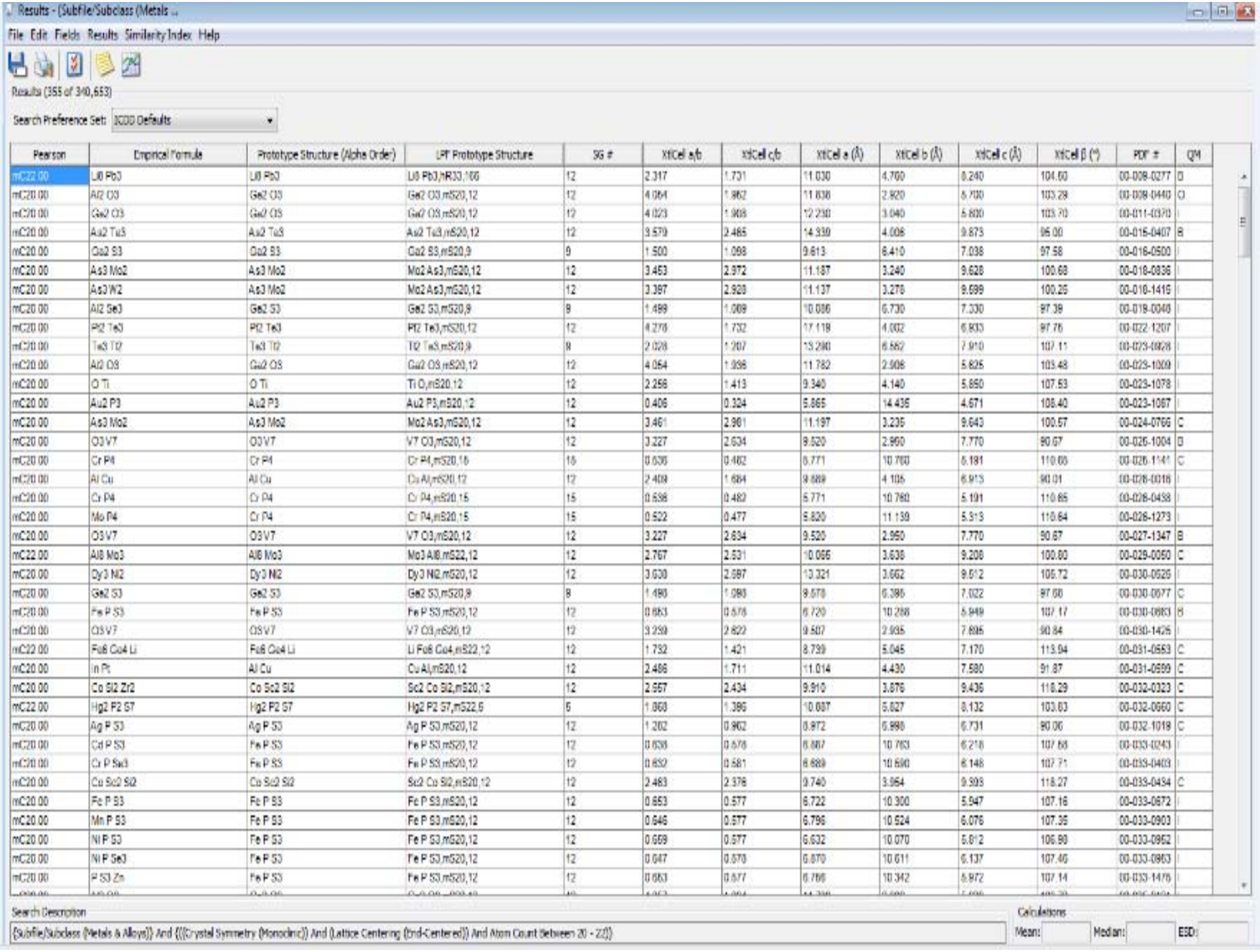
Database
Not
ICDD (00)
ICSD (01)
CSD (02)
NIST (03)
LPF (04)
ICDD Crystal Data (05)
Status
Primary
Alternate
Include Deleted Patterns
Ambient/Non-ambient (Amb.)
Not
Ambient
Pressure (Non-ambient)
Temperature (Non-ambient)
Pressure & Temperature (Non-ambient)
Or
Quality Mark (QM)
Not
Star
Rietveld
Indexed
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 mC16 to mC20 *continued*

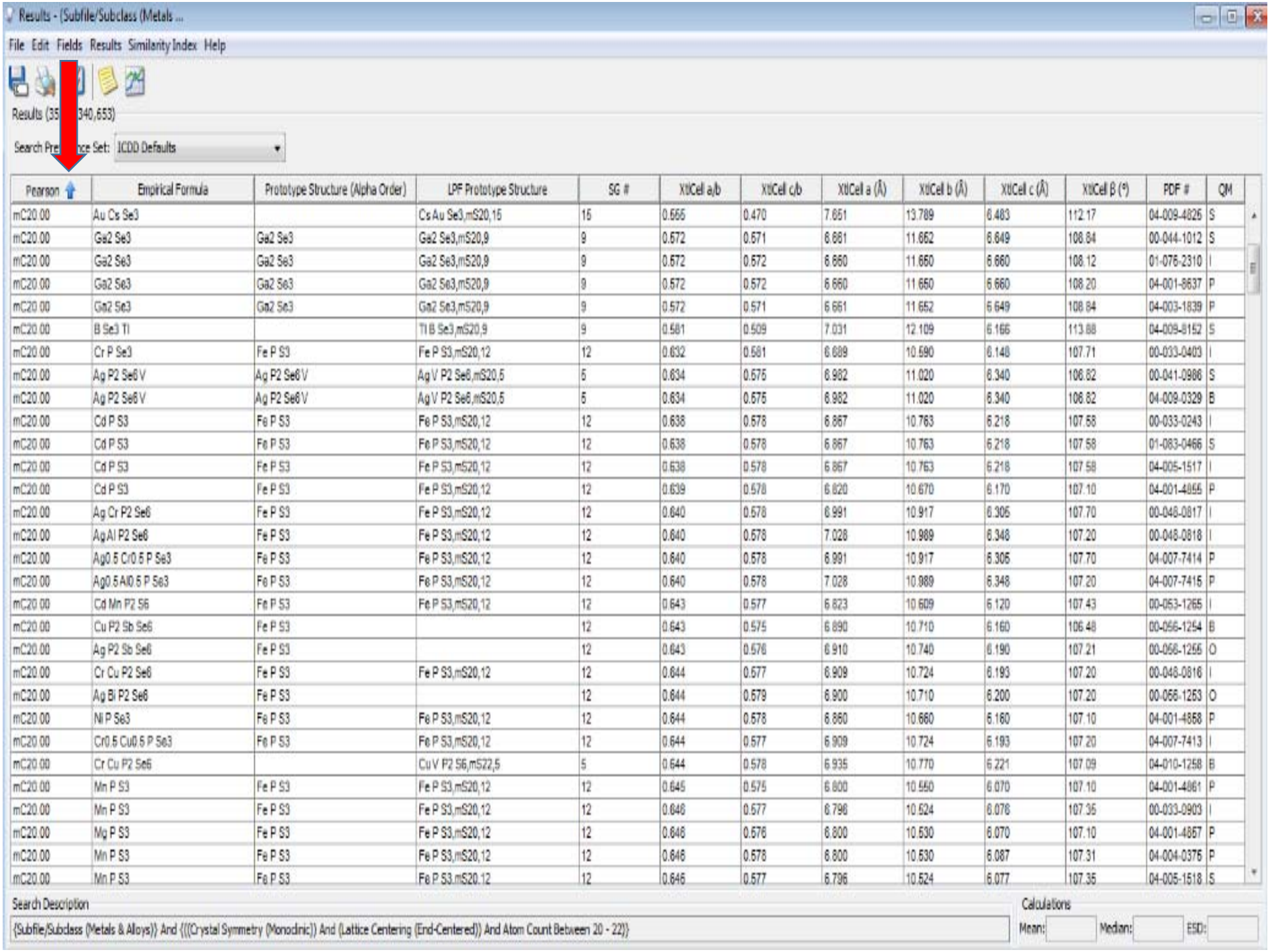
- Click on *Edit* and then *Preferences* and put the *Results* list in a PSC index form by arranging the columns left-to-right as shown below.
  - *Pearson*
  - *Empirical Formula*
  - *Prototype Structure (Alpha Order)*
  - *LPF Prototype Structure*
  - *SG#*
  - *XtlCell a/b*
  - *XtlCell c/b*
  -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




| Pearson | Empirical Formula | Prototype Structure (Alpha Order) | LPT Prototype Structure | SG # | XtlCell a/b | XtlCell c/b | XtlCell a (Å) | XtlCell b (Å) | XtlCell c (Å) | XtlCell β (°) | PDF # | QM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| mC22.00 | Li0 Pb3 | Li0 Pb3 | Li0 Pb3,hR30,166 | 12 | 2.317 | 1.731 | 11.030 | 4.760 | 8.240 | 104.60 | 00-008-0277 | D |
| mC20.00 | Al2 O3 | Ge2 O3 | Ge2 O3,mS20,12 | 12 | 4.064 | 1.962 | 11.836 | 2.920 | 5.730 | 103.28 | 00-008-0440 | D |
| mC20.00 | Ga2 O3 | Ge2 O3 | Ge2 O3,mS20,12 | 12 | 4.023 | 1.908 | 12.230 | 3.040 | 5.800 | 103.70 | 00-011-0370 | I |
| mC20.00 | As2 Te3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.579 | 2.485 | 14.339 | 4.008 | 9.873 | 96.00 | 00-015-0407 | B |
| mC20.00 | Ga2 S3 | Ga2 S3 | Ga2 S3,mS20,9 | 9 | 1.500 | 1.098 | 9.613 | 6.410 | 7.038 | 97.58 | 00-016-0500 | I |
| mC20.00 | As3 Mo2 | As3 Mo2 | Mo2 As3,mS20,12 | 12 | 3.453 | 2.972 | 11.187 | 3.240 | 9.628 | 100.68 | 00-018-0836 | I |
| mC20.00 | As3 W2 | As3 Mo2 | Mo2 As3,mS20,12 | 12 | 3.397 | 2.928 | 11.137 | 3.278 | 9.599 | 100.25 | 00-018-1415 | I |
| mC20.00 | Al2 Se3 | Ga2 S3 | Ga2 S3,mS20,9 | 9 | 1.499 | 1.089 | 10.086 | 6.730 | 7.330 | 97.39 | 00-019-0040 | I |
| mC20.00 | Pt2 Te3 | Pt2 Te3 | Pt2 Te3,mS20,12 | 12 | 4.276 | 1.732 | 17.118 | 4.002 | 6.933 | 97.76 | 00-022-1207 | I |
| mC20.00 | Te3 Ti2 | Te3 Ti2 | Ti2 Te3,mS20,9 | 9 | 2.028 | 1.207 | 13.290 | 6.552 | 7.910 | 107.11 | 00-023-0628 | I |
| mC20.00 | Al2 O3 | Ga2 O3 | Ga2 O3,mS20,12 | 12 | 4.064 | 1.998 | 11.782 | 2.906 | 5.825 | 103.48 | 00-023-1009 | I |
| mC20.00 | O Ti | O Ti | Ti O,mS20,12 | 12 | 2.256 | 1.413 | 9.340 | 4.140 | 5.850 | 107.53 | 00-023-1078 | I |
| mC20.00 | Au2 P3 | Au2 P3 | Au2 P3,mS20,12 | 12 | 0.406 | 0.324 | 5.865 | 14.435 | 4.671 | 108.40 | 00-023-1067 | I |
| mC20.00 | As3 Mo2 | As3 Mo2 | Mo2 As3,mS20,12 | 12 | 3.461 | 2.981 | 11.197 | 3.235 | 9.643 | 100.57 | 00-024-0766 | C |
| mC20.00 | O3 V7 | O3 V7 | V7 O3,mS20,12 | 12 | 3.227 | 2.634 | 9.520 | 2.950 | 7.770 | 90.67 | 00-025-1004 | D |
| mC20.00 | Cr P4 | Cr P4 | Cr P4,mS20,15 | 15 | 0.636 | 0.482 | 5.771 | 10.760 | 5.191 | 110.65 | 00-026-1141 | C |
| mC20.00 | Al Cu | Al Cu | Cu Al,mS20,12 | 12 | 2.408 | 1.684 | 9.889 | 4.106 | 6.913 | 90.01 | 00-028-0016 | I |
| mC20.00 | Cr P4 | Cr P4 | Cr P4,mS20,15 | 15 | 0.638 | 0.482 | 5.771 | 10.760 | 5.191 | 110.65 | 00-028-0438 | I |
| mC20.00 | Mo P4 | Cr P4 | Cr P4,mS20,15 | 15 | 0.522 | 0.477 | 5.820 | 11.139 | 5.313 | 110.64 | 00-028-1273 | I |
| mC20.00 | O3 V7 | O3 V7 | V7 O3,mS20,12 | 12 | 3.227 | 2.634 | 9.520 | 2.950 | 7.770 | 90.67 | 00-027-1347 | B |
| mC22.00 | Al8 Mo3 | Al8 Mo3 | Mo3 Al8,mS22,12 | 12 | 2.767 | 2.531 | 10.066 | 3.638 | 9.206 | 100.80 | 00-029-0060 | C |
| mC20.00 | Dy3 Ni2 | Dy3 Ni2 | Dy3 Ni2,mS20,12 | 12 | 3.630 | 2.587 | 13.321 | 3.662 | 9.512 | 105.72 | 00-030-0525 | I |
| mC20.00 | Ge2 S3 | Ge2 S3 | Ge2 S3,mS20,9 | 9 | 1.490 | 1.080 | 9.578 | 6.386 | 7.022 | 97.66 | 00-030-0677 | C |
| mC20.00 | Fe P S3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.663 | 0.578 | 6.720 | 10.288 | 5.949 | 107.17 | 00-030-0663 | B |
| mC20.00 | O3 V7 | O3 V7 | V7 O3,mS20,12 | 12 | 3.259 | 2.622 | 9.507 | 2.935 | 7.695 | 90.84 | 00-030-1426 | I |
| mC22.00 | Fe8 Co4 Li | Fe8 Co4 Li | Li Fe8 Co4,mS22,12 | 12 | 1.732 | 1.421 | 8.739 | 5.045 | 7.170 | 113.94 | 00-031-0653 | C |
| mC20.00 | In Pt | Al Cu | Cu Al,mS20,12 | 12 | 2.486 | 1.711 | 11.014 | 4.430 | 7.580 | 91.87 | 00-031-0699 | C |
| mC20.00 | Co Si2 Zr2 | Co Sc2 Si2 | Sc2 Co Si2,mS20,12 | 12 | 2.957 | 2.434 | 9.910 | 3.676 | 9.436 | 118.29 | 00-032-0323 | C |
| mC22.00 | Hg2 F2 S7 | Hg2 F2 S7 | Hg2 F2 S7,mS22,6 | 6 | 1.868 | 1.386 | 10.087 | 5.627 | 8.132 | 103.63 | 00-032-0660 | C |
| mC20.00 | Ag P S3 | Ag P S3 | Ag P S3,mS20,12 | 12 | 1.202 | 0.962 | 8.972 | 6.998 | 6.731 | 90.06 | 00-032-1019 | C |
| mC20.00 | Cd P S3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.638 | 0.578 | 6.867 | 10.763 | 6.218 | 107.66 | 00-033-0243 | I |
| mC20.00 | Cr P Se3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.652 | 0.581 | 6.689 | 10.690 | 6.148 | 107.71 | 00-033-0403 | I |
| mC20.00 | Co Sc2 Si2 | Co Sc2 Si2 | Sc2 Co Si2,mS20,12 | 12 | 2.483 | 2.378 | 9.740 | 3.954 | 9.393 | 118.27 | 00-033-0434 | C |
| mC20.00 | Fe P S3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.653 | 0.577 | 6.722 | 10.300 | 5.947 | 107.16 | 00-033-0672 | I |
| mC20.00 | Mn P S3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.646 | 0.577 | 6.796 | 10.524 | 6.076 | 107.35 | 00-033-0903 | I |
| mC20.00 | Ni P S3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.659 | 0.577 | 6.632 | 10.070 | 5.812 | 106.80 | 00-033-0952 | I |
| mC20.00 | Ni P Se3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.647 | 0.570 | 6.870 | 10.611 | 6.137 | 107.46 | 00-033-0963 | I |
| mC20.00 | P S3 Zn | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.663 | 0.577 | 6.766 | 10.342 | 5.972 | 107.14 | 00-033-1476 | I |

# Example mC16 to mC20
## *continued*

- Many sorting options are used here. For example, sorting on *Pearson*, *XtlCell a/b*, *SG#*, or *LPF Prototype Structure* will produce useful results.
- For this example, the analyst will want to try many different sorts to determine which is more effective for his/her interests.


Results - (Subfile/Subclass (Metals ...
File Edit Fields Results Similarity Index Help
Results (35 340,653)
Search Pre nce Set: ICDD Defaults
Pearson
Empirical Formula
Prototype Structure (Alpha Order)
LPF Prototype Structure
SG #
XtlCell a/b
XtlCell c/b
XtlCell a (Å)
XtlCell b (Å)
XtlCell c (Å)
XtlCell β (°)
PDF #
QM
mC20.00 Au Cs Se3 Cs Au Se3,mS20,15 15 0.666 0.470 7.651 13.789 6.483 112.17 04-009-4825 S
mC20.00 Ga2 Se3 Ga2 Se3 Ga2 Se3,mS20,9 9 0.672 0.671 6.681 11.652 6.649 108.84 00-044-1012 S
mC20.00 Ga2 Se3 Ga2 Se3 Ga2 Se3,mS20,9 9 0.672 0.672 6.660 11.650 6.660 108.12 01-076-2310 I
mC20.00 Ga2 Se3 Ga2 Se3 Ga2 Se3,mS20,9 9 0.672 0.672 6.660 11.650 6.660 108.20 04-001-8637 P
mC20.00 Ga2 Se3 Ga2 Se3 Ga2 Se3,mS20,9 9 0.672 0.671 6.661 11.652 6.649 108.84 04-003-1839 P
mC20.00 B Se3 Tl Tl B Se3,mS20,9 9 0.681 0.609 7.031 12.109 6.166 113.88 04-009-8152 S
mC20.00 Cr P Se3 Fe P S3 Fe P S3,mS20,12 12 0.632 0.681 6.689 10.590 6.148 107.71 00-033-0403 I
mC20.00 Ag P2 Se6 V Ag P2 Se6 V Ag V P2 Se6,mS20,5 5 0.634 0.675 6.982 11.020 6.340 106.82 00-041-0986 S
mC20.00 Ag P2 Se6 V Ag P2 Se6 V Ag V P2 Se6,mS20,5 5 0.634 0.675 6.982 11.020 6.340 106.82 04-009-0329 B
mC20.00 Cd P S3 Fe P S3 Fe P S3,mS20,12 12 0.638 0.678 6.867 10.763 6.218 107.58 00-033-0243 I
mC20.00 Cd P S3 Fe P S3 Fe P S3,mS20,12 12 0.638 0.678 6.867 10.763 6.218 107.58 01-083-0466 S
mC20.00 Cd P S3 Fe P S3 Fe P S3,mS20,12 12 0.638 0.678 6.867 10.763 6.218 107.58 04-005-1517 I
mC20.00 Cd P S3 Fe P S3 Fe P S3,mS20,12 12 0.639 0.678 6.820 10.670 6.170 107.10 04-001-4855 P
mC20.00 Ag Cr P2 Se6 Fe P S3 Fe P S3,mS20,12 12 0.640 0.678 6.991 10.917 6.305 107.70 00-048-0817 I
mC20.00 Ag Al P2 Se6 Fe P S3 Fe P S3,mS20,12 12 0.640 0.678 7.028 10.989 6.348 107.20 00-048-0818 I
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mC20.00 Cd Mn P2 S6 Fe P S3 Fe P S3,mS20,12 12 0.643 0.677 6.823 10.609 6.120 107.43 00-053-1265 I
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mC20.00 Ni P Se3 Fe P S3 Fe P S3,mS20,12 12 0.644 0.678 6.860 10.660 6.160 107.10 04-001-4858 P
mC20.00 Cr0.5 Cu0.5 P Se3 Fe P S3 Fe P S3,mS20,12 12 0.644 0.677 6.909 10.724 6.193 107.20 04-007-7413 I
mC20.00 Cr Cu P2 Se6 Cu V P2 S6,mS22,5 5 0.644 0.678 6.935 10.770 6.221 107.09 04-010-1258 B
mC20.00 Mn P S3 Fe P S3 Fe P S3,mS20,12 12 0.645 0.675 6.800 10.550 6.070 107.10 04-001-4861 P
mC20.00 Mn P S3 Fe P S3 Fe P S3,mS20,12 12 0.646 0.677 6.796 10.524 6.076 107.35 00-033-0903 I
mC20.00 Mg P S3 Fe P S3 Fe P S3,mS20,12 12 0.646 0.676 6.800 10.530 6.070 107.10 04-001-4857 P
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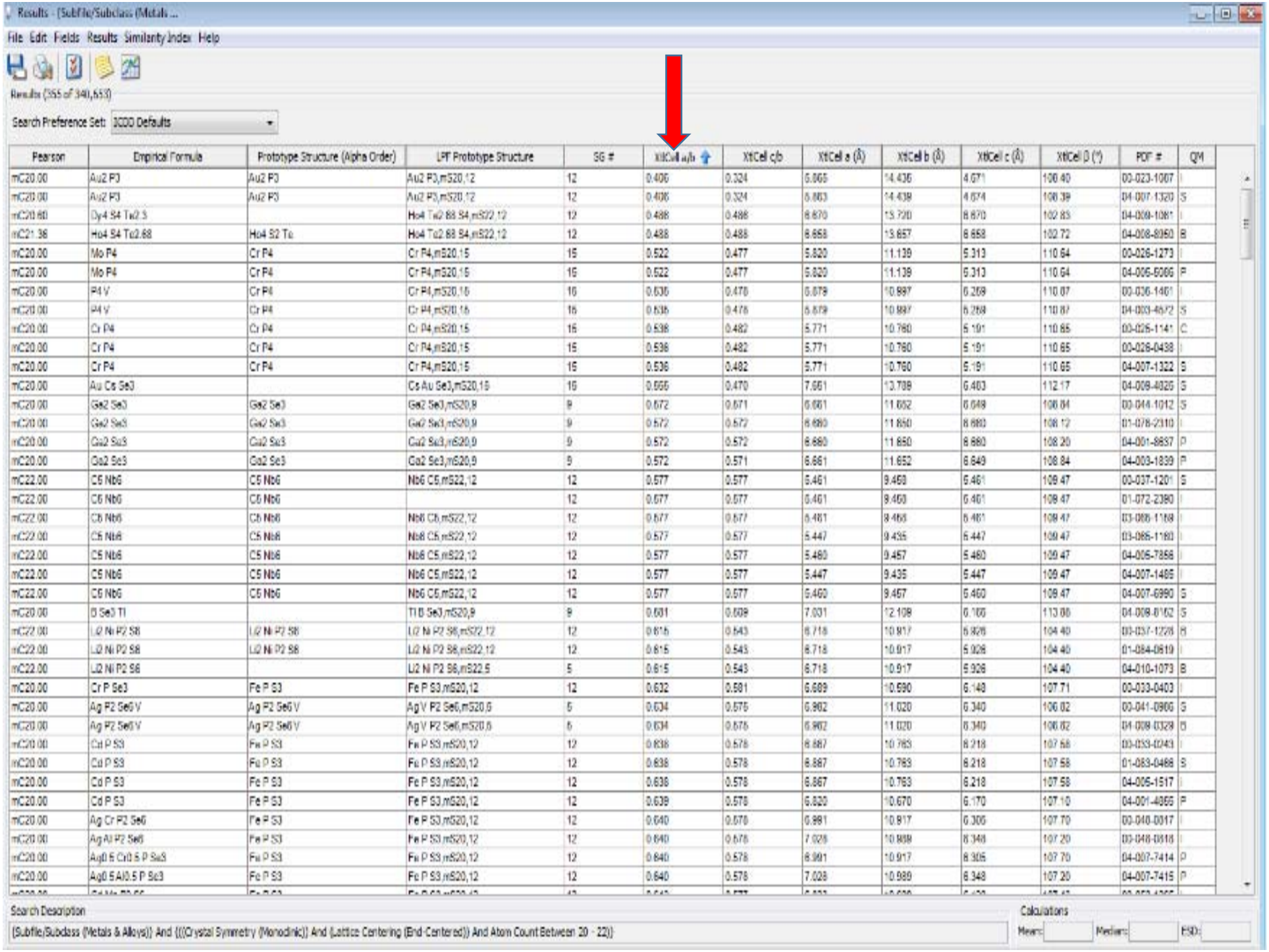
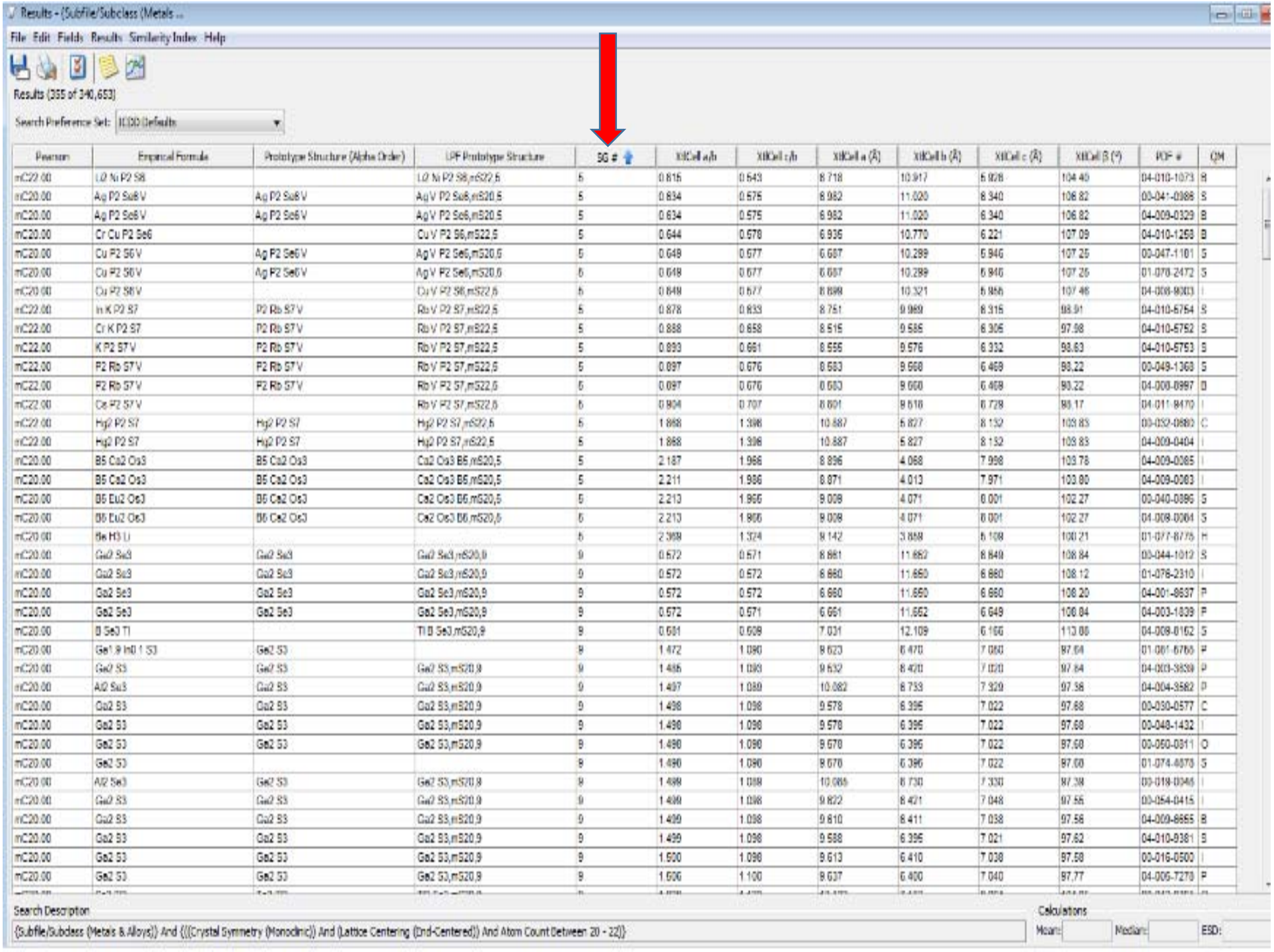
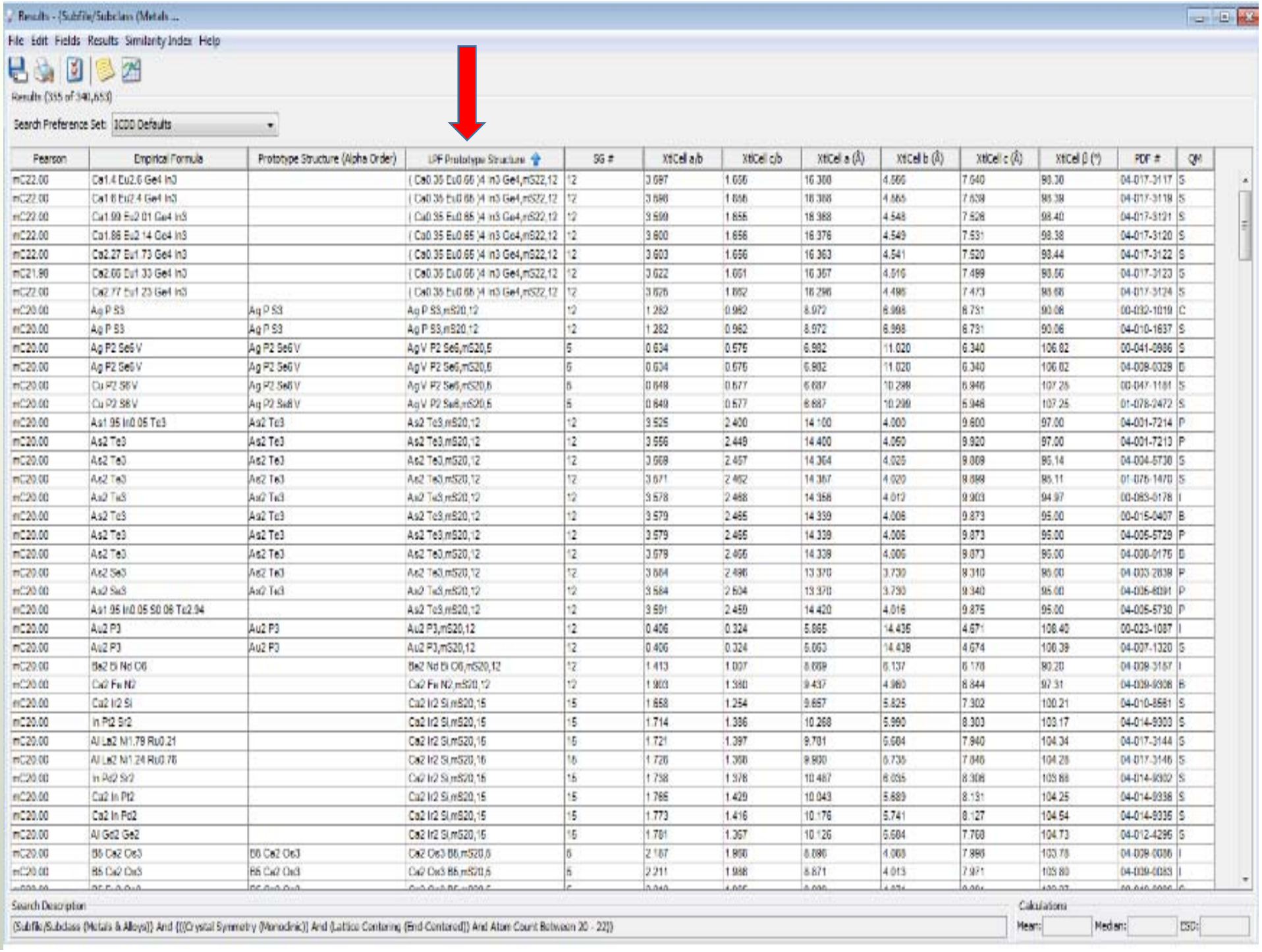
Calculations
Mean:
Median:
ESD:




| Pearson | Empirical Formula | Prototype Structure (Alpha Order) | LPF Prototype Structure | SG # | XtlCell a/b | XtlCell c/b | XtlCell a (Å) | XtlCell b (Å) | XtlCell c (Å) | XtlCell β (°) | PDF # | QM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| mC20.00 | Au2 P3 | Au2 P3 | Au2 P3,mS20,12 | 12 | 0.406 | 0.324 | 5.865 | 14.436 | 4.671 | 100.40 | 00-023-1007 | I |
| mC20.00 | Au2 P3 | Au2 P3 | Au2 P3,mS20,12 | 12 | 0.406 | 0.324 | 5.863 | 14.439 | 4.674 | 100.39 | 04-007-1320 | S |
| mC20.60 | Dy4 S4 Te2.3 | | Ho4 Te2.88 S4,mS22,12 | 12 | 0.488 | 0.488 | 8.670 | 13.720 | 8.670 | 102.83 | 04-009-1081 | I |
| mC21.38 | Ho4 S4 Te2.68 | Ho4 S2 Te | Ho4 Te2.68 S4,mS22,12 | 12 | 0.488 | 0.488 | 8.668 | 13.657 | 8.668 | 102.72 | 04-008-8960 | B |
| mC20.00 | Mo P4 | Cr P4 | Cr P4,mS20,15 | 15 | 0.522 | 0.477 | 5.820 | 11.139 | 5.313 | 110.64 | 00-026-1273 | I |
| mC20.00 | Mo P4 | Cr P4 | Cr P4,mS20,15 | 15 | 0.522 | 0.477 | 5.820 | 11.139 | 5.313 | 110.64 | 04-006-6086 | P |
| mC20.00 | P4 V | Cr P4 | Cr P4,mS20,15 | 15 | 0.535 | 0.478 | 5.879 | 10.997 | 5.259 | 110.07 | 00-036-1401 | I |
| mC20.00 | P4 V | Cr P4 | Cr P4,mS20,15 | 15 | 0.535 | 0.478 | 5.879 | 10.997 | 5.259 | 110.07 | 04-003-4672 | S |
| mC20.00 | Cr P4 | Cr P4 | Cr P4,mS20,15 | 15 | 0.536 | 0.482 | 5.771 | 10.760 | 5.191 | 110.65 | 00-026-1141 | C |
| mC20.00 | Cr P4 | Cr P4 | Cr P4,mS20,15 | 15 | 0.536 | 0.482 | 5.771 | 10.760 | 5.191 | 110.65 | 00-026-0438 | I |
| mC20.00 | Cr P4 | Cr P4 | Cr P4,mS20,15 | 15 | 0.536 | 0.482 | 5.771 | 10.760 | 5.191 | 110.65 | 04-007-1322 | S |
| mC20.00 | Au Cs Se3 | | Cs Au Se3,mS20,15 | 15 | 0.555 | 0.470 | 7.551 | 13.709 | 6.403 | 112.17 | 04-008-4025 | S |
| mC20.00 | Ge2 Se3 | Ge2 Se3 | Ge2 Se3,mS20,9 | 9 | 0.572 | 0.571 | 6.661 | 11.652 | 6.649 | 108.84 | 00-044-1012 | S |
| mC20.00 | Ge2 Se3 | Ge2 Se3 | Ge2 Se3,mS20,9 | 9 | 0.572 | 0.572 | 6.680 | 11.650 | 6.680 | 108.12 | 01-078-2310 | I |
| mC20.00 | Cu2 Se3 | Cu2 Se3 | Cu2 Se3,mS20,9 | 9 | 0.572 | 0.572 | 6.680 | 11.650 | 6.680 | 108.20 | 04-001-8837 | D |
| mC20.00 | Cu2 Se3 | Cu2 Se3 | Cu2 Se3,mS20,9 | 9 | 0.572 | 0.571 | 6.661 | 11.652 | 6.649 | 108.84 | 04-003-1839 | P |
| mC22.00 | C5 Nb6 | C5 Nb6 | Nb6 C5,mS22,12 | 12 | 0.577 | 0.577 | 5.461 | 9.459 | 5.461 | 109.47 | 00-037-1201 | S |
| mC22.00 | C5 Nb6 | C5 Nb6 | | 12 | 0.577 | 0.577 | 5.461 | 9.459 | 5.461 | 109.47 | 01-072-2380 | I |
| mC22.00 | C5 Nb6 | C5 Nb6 | Nb6 C5,mS22,12 | 12 | 0.577 | 0.577 | 5.461 | 9.459 | 5.461 | 109.47 | 03-065-1169 | I |
| mC22.00 | C5 Nb6 | C5 Nb6 | Nb6 C5,mS22,12 | 12 | 0.577 | 0.577 | 5.447 | 9.435 | 5.447 | 109.47 | 03-065-1180 | I |
| mC22.00 | C5 Nb6 | C5 Nb6 | Nb6 C5,mS22,12 | 12 | 0.577 | 0.577 | 5.460 | 9.457 | 5.460 | 109.47 | 04-005-7856 | I |
| mC22.00 | C5 Nb6 | C5 Nb6 | Nb6 C5,mS22,12 | 12 | 0.577 | 0.577 | 5.447 | 9.435 | 5.447 | 109.47 | 04-007-1466 | I |
| mC22.00 | C5 Nb6 | C5 Nb6 | Nb6 C5,mS22,12 | 12 | 0.577 | 0.577 | 5.460 | 9.457 | 5.460 | 109.47 | 04-007-6990 | S |
| mC20.00 | B Se3 Tl | | Tl B Se3,mS20,9 | 9 | 0.601 | 0.609 | 7.031 | 12.109 | 6.100 | 113.08 | 04-008-8162 | S |
| mC22.00 | Li2 Ni P2 S6 | Li2 Ni P2 S6 | Li2 Ni P2 S6,mS22,12 | 12 | 0.615 | 0.543 | 6.718 | 10.917 | 5.926 | 104.40 | 00-037-1228 | H |
| mC22.00 | Li2 Ni P2 S6 | Li2 Ni P2 S6 | Li2 Ni P2 S6,mS22,12 | 12 | 0.615 | 0.543 | 6.718 | 10.917 | 5.926 | 104.40 | 01-084-0819 | I |
| mC22.00 | Li2 Ni P2 S6 | | Li2 Ni P2 S6,mS22,5 | 5 | 0.615 | 0.543 | 6.718 | 10.917 | 5.926 | 104.40 | 04-010-1073 | B |
| mC20.00 | Cr P Se3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.632 | 0.581 | 6.689 | 10.690 | 6.149 | 107.71 | 00-033-0403 | I |
| mC20.00 | Ag P2 Se6 V | Ag P2 Se6 V | Ag V P2 Se6,mS20,6 | 6 | 0.634 | 0.575 | 6.962 | 11.020 | 6.340 | 106.02 | 00-041-0906 | S |
| mC20.00 | Ag P2 Se6 V | Ag P2 Se6 V | Ag V P2 Se6,mS20,6 | 6 | 0.634 | 0.575 | 6.962 | 11.020 | 6.340 | 106.02 | 04-008-0329 | D |
| mC20.00 | Cd P S3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.638 | 0.578 | 6.887 | 10.793 | 6.218 | 107.58 | 00-033-0243 | I |
| mC20.00 | Cd P S3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.638 | 0.578 | 6.887 | 10.793 | 6.218 | 107.58 | 01-083-0468 | S |
| mC20.00 | Cd P S3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.638 | 0.578 | 6.887 | 10.793 | 6.218 | 107.58 | 04-005-1517 | I |
| mC20.00 | Cd P S3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.639 | 0.578 | 6.920 | 10.670 | 6.170 | 107.10 | 04-001-4865 | P |
| mC20.00 | Ag Cr P2 Se6 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.640 | 0.578 | 6.991 | 10.917 | 6.305 | 107.70 | 00-040-0017 | I |
| mC20.00 | Ag Al P2 Se6 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.640 | 0.578 | 7.028 | 10.888 | 6.348 | 107.20 | 00-040-0018 | I |
| mC20.00 | Ag0.5 Cr0.5 P Se3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.640 | 0.578 | 6.991 | 10.917 | 6.305 | 107.70 | 04-007-7414 | D |
| mC20.00 | Ag0.5 Al0.5 P Se3 | Fe P S3 | Fe P S3,mS20,12 | 12 | 0.640 | 0.578 | 7.028 | 10.989 | 6.348 | 107.20 | 04-007-7415 | P |


Results - (SubFile/Subclass (Metals ...
File Edit Fields Results Similarity Index Help
Results (355 of 340,653)
Search Preference Set: ICDD Defaults
Pearson
Empirical Formula
Prototype Structure (Alpha Order)
LPF Prototype Structure
SG #
XtlCell a/b
XtlCell c/b
XtlCell a (Å)
XtlCell b (Å)
XtlCell c (Å)
XtlCell β (°)
PDF #
QM
mC22.00 Li2 Ni P2 S8
mC20.00 Ag P2 Se8 V
mC20.00 Ag P2 Se8 V
mC20.00 Cr Cu P2 Se6
mC20.00 Cu P2 Se6 V
mC20.00 Cu P2 Se6 V
mC20.00 Cu P2 Se6 V
mC22.00 In K P2 S7
mC22.00 Cr K P2 S7
mC22.00 K P2 S7 V
mC22.00 P2 Rb S7 V
mC22.00 P2 Rb S7 V
mC22.00 Ce P2 S7 V
mC22.00 Hg2 P2 S7
mC22.00 Hg2 P2 S7
mC20.00 B5 Ca2 Os3
mC20.00 B5 Ca2 Os3
mC20.00 B5 Eu2 Os3
mC20.00 B5 Eu2 Os3
mC20.00 Be H3 Li
mC20.00 Ga2 Se3
mC20.00 Ga2 Se3
mC20.00 Ga2 Se3
mC20.00 Ga2 Se3
mC20.00 B Se3 Tl
mC20.00 Ga1.9 In0.1 S3
mC20.00 Ga2 S3
mC20.00 Al2 Se3
mC20.00 Ga2 S3
mC20.00 Ga2 S3
mC20.00 Ga2 S3
mC20.00 Ga2 S3
mC20.00 Al2 Se3
mC20.00 Ga2 S3
mC20.00 Ga2 S3
mC20.00 Ga2 S3
mC20.00 Ga2 S3
mC20.00 Ga2 S3
Search Description
{Subfile/Subclass (Metals & Alloys)} And {{{Crystal Symmetry (Monoclinic)} And {Lattice Centering (End-Centered)} And Atom Count Between 20 - 22}}
Calculations
Mean:
Median:
ESD:




| Pearson | Empirical Formula | Prototype Structure (Alpha Order) | LPF Prototype Structure | SG # | XtlCell a/b | XtlCell c/b | XtlCell a (Å) | XtlCell b (Å) | XtlCell c (Å) | XtlCell β (°) | PDF # | QM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| mC22.00 | Ca1.4 Eu2.6 Ge4 In3 | | (Ca0.35 Eu0.65)4 In3 Ge4,mS22,12 | 12 | 3.697 | 1.656 | 16.300 | 4.566 | 7.640 | 98.30 | 04-017-3117 | S |
| mC22.00 | Ca1.6 Eu2.4 Ge4 In3 | | (Ca0.35 Eu0.65)4 In3 Ge4,mS22,12 | 12 | 3.686 | 1.656 | 16.266 | 4.565 | 7.629 | 98.38 | 04-017-3118 | S |
| mC22.00 | Ca1.99 Eu2.01 Ge4 In3 | | (Ca0.35 Eu0.65)4 In3 Ge4,mS22,12 | 12 | 3.669 | 1.656 | 16.188 | 4.548 | 7.626 | 98.40 | 04-017-3121 | S |
| mC22.00 | Ca1.86 Eu2.14 Ge4 In3 | | (Ca0.35 Eu0.65)4 In3 Ge4,mS22,12 | 12 | 3.680 | 1.656 | 16.376 | 4.549 | 7.531 | 98.38 | 04-017-3120 | S |
| mC22.00 | Ca2.27 Eu1.73 Ge4 In3 | | (Ca0.35 Eu0.65)4 In3 Ge4,mS22,12 | 12 | 3.693 | 1.656 | 16.363 | 4.541 | 7.520 | 98.44 | 04-017-3122 | S |
| mC21.90 | Ca2.06 Eu1.33 Ge4 In3 | | (Ca0.35 Eu0.65)4 In3 Ge4,mS22,12 | 12 | 3.622 | 1.651 | 16.357 | 4.516 | 7.499 | 98.56 | 04-017-3123 | S |
| mC22.00 | Ca2.77 Eu1.23 Ge4 In3 | | (Ca0.35 Eu0.65)4 In3 Ge4,mS22,12 | 12 | 3.626 | 1.662 | 16.296 | 4.496 | 7.473 | 98.68 | 04-017-3124 | S |
| mC20.00 | Ag P S3 | Ag P S3 | Ag P S3,mS20,12 | 12 | 1.282 | 0.982 | 8.972 | 6.998 | 6.751 | 90.06 | 00-032-1019 | C |
| mC20.00 | Ag P S3 | Ag P S3 | Ag P S3,mS20,12 | 12 | 1.282 | 0.982 | 8.972 | 6.998 | 6.731 | 90.06 | 04-010-1637 | S |
| mC20.00 | Ag P2 Se6 V | Ag P2 Se6 V | Ag V P2 Se6,mS20,6 | 6 | 0.634 | 0.676 | 6.982 | 11.020 | 6.340 | 106.62 | 00-041-0896 | S |
| mC20.00 | Ag P2 Se6 V | Ag P2 Se6 V | Ag V P2 Se6,mS20,6 | 6 | 0.634 | 0.676 | 6.982 | 11.020 | 6.340 | 106.62 | 04-009-0328 | D |
| mC20.00 | Cu P2 S6 V | Ag P2 Se6 V | Ag V P2 Se6,mS20,6 | 6 | 0.648 | 0.677 | 6.687 | 10.299 | 6.946 | 107.25 | 00-047-1181 | S |
| mC20.00 | Cu P2 S6 V | Ag P2 Se6 V | Ag V P2 Se6,mS20,6 | 6 | 0.649 | 0.677 | 6.687 | 10.299 | 6.946 | 107.25 | 01-078-2472 | S |
| mC20.00 | As1.95 In0.05 Te3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.525 | 2.400 | 14.100 | 4.000 | 9.600 | 97.00 | 04-001-7214 | P |
| mC20.00 | As2 Te3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.556 | 2.449 | 14.400 | 4.050 | 9.920 | 97.00 | 04-001-7213 | P |
| mC20.00 | As2 Te3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.568 | 2.457 | 14.364 | 4.025 | 9.809 | 95.14 | 04-004-5730 | S |
| mC20.00 | As2 Te3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.571 | 2.462 | 14.387 | 4.029 | 9.888 | 95.11 | 01-076-1470 | S |
| mC20.00 | As2 Te3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.578 | 2.468 | 14.356 | 4.012 | 9.903 | 94.97 | 00-083-0178 | I |
| mC20.00 | As2 Te3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.579 | 2.465 | 14.359 | 4.006 | 9.873 | 95.00 | 00-015-0407 | B |
| mC20.00 | As2 Te3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.579 | 2.465 | 14.339 | 4.006 | 9.873 | 95.00 | 04-005-5729 | P |
| mC20.00 | As2 Te3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.579 | 2.466 | 14.338 | 4.006 | 9.873 | 95.00 | 04-008-0175 | D |
| mC20.00 | As2 Se3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.564 | 2.486 | 13.370 | 3.750 | 9.310 | 95.00 | 04-003-2838 | P |
| mC20.00 | As2 Se3 | As2 Te3 | As2 Te3,mS20,12 | 12 | 3.564 | 2.504 | 13.370 | 3.750 | 9.340 | 95.00 | 04-006-8091 | P |
| mC20.00 | As1.95 In0.05 Se0.06 Te2.94 | | As2 Te3,mS20,12 | 12 | 3.591 | 2.459 | 14.420 | 4.016 | 9.875 | 95.00 | 04-005-5730 | P |
| mC20.00 | Au2 P3 | Au2 P3 | Au2 P3,mS20,12 | 12 | 0.406 | 0.324 | 5.865 | 14.435 | 4.671 | 106.40 | 00-023-1087 | I |
| mC20.00 | Au2 P3 | Au2 P3 | Au2 P3,mS20,12 | 12 | 0.406 | 0.324 | 5.863 | 14.438 | 4.674 | 106.39 | 04-007-1320 | S |
| mC20.00 | Ba2 Bi Nd O6 | | Ba2 Nd Bi O6,mS20,12 | 12 | 1.413 | 1.007 | 8.669 | 6.137 | 6.178 | 90.20 | 04-009-3157 | I |
| mC20.00 | Ca2 Fe N2 | | Ca2 Fe N2,mS20,12 | 12 | 1.903 | 1.380 | 9.437 | 4.960 | 6.844 | 97.31 | 04-009-9308 | B |
| mC20.00 | Ca2 Ir2 Si | | Ca2 Ir2 Si,mS20,15 | 15 | 1.658 | 1.254 | 9.657 | 5.825 | 7.302 | 100.21 | 04-010-8561 | S |
| mC20.00 | In Pt2 Sr2 | | Ca2 Ir2 Si,mS20,15 | 15 | 1.714 | 1.386 | 10.268 | 5.990 | 8.303 | 103.17 | 04-014-9303 | S |
| mC20.00 | Al La2 Ni1.79 Ru0.21 | | Ca2 Ir2 Si,mS20,15 | 15 | 1.721 | 1.397 | 9.701 | 5.634 | 7.940 | 104.34 | 04-017-3144 | S |
| mC20.00 | Al La2 Ni1.24 Ru0.76 | | Ca2 Ir2 Si,mS20,15 | 15 | 1.726 | 1.398 | 9.800 | 5.735 | 7.846 | 104.28 | 04-017-3146 | S |
| mC20.00 | In Pd2 Sr2 | | Ca2 Ir2 Si,mS20,15 | 15 | 1.738 | 1.378 | 10.467 | 6.035 | 8.308 | 105.88 | 04-014-9302 | S |
| mC20.00 | Ca2 In Pt2 | | Ca2 Ir2 Si,mS20,15 | 15 | 1.765 | 1.429 | 10.043 | 5.689 | 8.131 | 104.25 | 04-014-9336 | S |
| mC20.00 | Ca2 In Pd2 | | Ca2 Ir2 Si,mS20,15 | 15 | 1.773 | 1.416 | 10.176 | 5.741 | 8.127 | 104.54 | 04-014-9335 | S |
| mC20.00 | Al Gd2 Ge2 | | Ca2 Ir2 Si,mS20,15 | 15 | 1.781 | 1.367 | 10.126 | 5.684 | 7.768 | 104.73 | 04-012-4296 | S |
| mC20.00 | B5 Ca2 Os3 | B5 Ca2 Os3 | Ca2 Os3 B5,mS20,6 | 6 | 2.167 | 1.866 | 8.686 | 4.068 | 7.889 | 103.78 | 04-009-0036 | I |
| mC20.00 | B5 Ca2 Os3 | B5 Ca2 Os3 | Ca2 Os3 B5,mS20,6 | 6 | 2.211 | 1.988 | 8.871 | 4.013 | 7.971 | 105.80 | 04-009-0083 | I |

# Example mC16 to mC20
## *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?

# Example mC16 to mC20
## *Search Results, continued*

Compare your results with the following discussion.

# Example mC16 to mC20
## *Search Results, continued*

- These sorts show (among other things) that:
  - More than 300 entries fit the search criteria,
  - Many prototype structures are present (the best way to examine these may be to sort on *SG#*, since that makes the evaluation easier),
  - Both the *Pearson* and *XtlCell a/b* sorts separate most of these types,
  - The *LPF Prototype Structure* sort lists the prototype structures within the search criteria, and
  - It may be possible 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 mC16 to mC20
## *Search Results, continued*

If the analyst has an unknown monoclinic metallic phase with a PSC in the search range and the cell, a/b, and c/b are known, there are several approaches that can help in choosing a possible structure.

Some are listed on the next few slides.

# Example mC16 to mC20
## *Search Results, continued*

Comparing 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.

# Example mC16 to mC20
## *Search Results, continued*

Looking 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?

# Example mC16 to mC20
## *Search Results, continued*

Calculating hypothetical powder patterns for the unknown material using the known chemistry and the atom positions for each prototype structure in turn. The resultant patterns could then be compared to the unknown material's experimental pattern.

Again, the analyst is encouraged to study the various sort results, since they have many uses.

# 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

ISO 9001:2008 QUALITY ASSURED COMPANY CERT.NR. 11409.1
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