

Metals & Alloys Subcommittee Minutes
Wednesday, 14 March 2018
International Centre Headquarters
Conference Room A
11:00 a.m. - 12:00 noon
P. Wallace, Chairman

1. Call to Order P. Wallace
2. Appointment of Minutes Secretary M. Carr
3. Approval of Minutes of March 2017
4. Review of Mission Statement

The Metals and Alloys Subcommittee shall be responsible for (1) assuring that the metals and alloys subfile meets present and future needs of metallurgists and materials scientists, (2) developing and updating the metals and alloys subfile, (3) editing metals and alloys data and products to ensure a high standard of quality, (4) extending the coverage and usefulness of the metals and alloys subfile, and (5) maintaining a web page to communicate with members and other materials scientists.

5. Board of Directors' Liaison Report J. Dann
6. Update on the PDF Phase Diagram Capability J. Blanton

See power point from Justin Blanton (Metals and Alloys Subcommittee 2019.pptx) for further info on implementation of motion from last year's spring meeting. Binary, Ternary, and Quaternary are as far as it goes right now, after that it gets too cumbersome to be useful according to P. Wallace, but A. Payzant says it should move to 5 component or higher order systems for the user. This is very useful in China according to A. Payzant. A. Payzant also says this needs to move from just being a list to including a graphical component. Referring to Phase Diagram as Composition Diagram to not mislead customers.

P. Wallace recommends to Technical committee that headquarters explore 5 component or higher systems in composition diagram capability.

C. Foris seconds.

7, 0, 0

P. Wallace recommends to Technical committee that headquarters explores graphical representation of composition diagram capability for binary and ternaries.

C. Foris seconds.

7, 0, 0

7. M&A Prototype Structure Profiles, a revised motion P. Wallace

See P. Wallace power point (M&A Subcommittee VGs 03-14-18.pptx) for further detail.

P. Wallace recommends to the Technical committee that prototype structure profiles be made available to PDF ® users. See P. Wallace power point (M&A Subcommittee VGs 03-14-18.pptx) for further detail on motion.

A. Roberts seconds.

6, 0, 0

8. The M&A prototype structure tables contain 8,089 entries P. Wallace
(up from 7,930 last year) and are on the M&A web page.

See P. Wallace power point (M&A Subcommittee VGs 03-14-18.pptx) for further detail.

9. M&A Working Group Activities. P. Wallace
 - 9.1 The Pearson Symbol Code Index (PSCI-IV) Review
 - 9.2 Recent PSCI-IV results
 - 9.3 M&A Web Page

- 9.4 M&A Tutorials
10. M&A Editor's report P. Wallace
See P. Wallace power point (M&A Subcommittee VGs 03-14-18.pptx) for further detail.
11. Next M&A Working Group meeting is October 19-22, 2018. P. Wallace
12. New/Old Business: *Thoughts on M&A Data Mining* C. Hubbard
13. Adjournment

Thanks to All M&A Working Group Members

- Jeff Dann
- Cathy Foris
- Cam Hubbard
- Howard Jones
- Terry Kahmer
- Monika Kottenhahn
- Andy Roberts
- Earle Ryba
- Rajendra Sadangi

M&A Subcommittee Agenda – Items 1-5

1. Call to Order.
2. Appointment of Minutes Secretary.
3. Approval of Minutes of March 2017.
4. Review of Mission Statement.

The Metals and Alloys Subcommittee shall be responsible for (1) assuring that the metals and alloys subfile meets present and future needs of metallurgists and materials scientists, (2) developing and updating the metals and alloys subfile, (3) editing metals and alloys data and products to ensure a high standard of quality, (4) extending the coverage and usefulness of the metals and alloys subfile, and (5) maintaining a web page on the ICDD site to communicate with members and other materials scientists.

5. Board of Directors' Liaison Report. (tbd)

6.0 M&A Prototype Structure Table

- The M&A library of prototype structures now has more than 8,082 entries and cross-entries (up from 7,930).
- Each entry has a Wyckoff sequence and other useful information.
- Z-values are being added in the current revision.
- This library is available on the M&A web page.

7.0 M&A Prototype Structure Profiles

M&A prototype structure profiles are based on the Crystal Data cell and contain observed ranges for the:

- Pearson Symbol Code,
- Lattice parameters, cell angles, and axial ratios,
- Atomic volumes,
- Calculated densities, and
- If possible, elements that are found in specific atomic positions of the structure.
- Examples follow.

7.1 Metrics of the HfGa₂tI₂₄,141 Structure

There are **28 PDF entries** including duplicates.

Variable	Low Value	High Value
Pearson Symbol Code	tI24	tI24
a(0)	3.929 (Ga ₂ Ti)	4.726 (Bi ₂ Eu)
c(0)	23.898 (Al ₂ Ti)	34.221 (Bi ₂ Eu)
Axial Ratio [c/a]	6.027 (Al ₂ Ti)	7.241 (Bi ₂ Eu)
Atomic Volume	375.63 (Al ₂ Ti)	764.33 (Bi ₂ Eu)
Calculated Density	2.289 (Al ₂ Mg)	13.09 (Pb ₂ Pu)

7.1 *Chemistry* of the HfGa₂,tI₂₄,141 Structure

The Wyckoff Sequence = e3.

Sites	Atoms
2 of the 3 e-sites [approximately (0, 0.25, 0.125) (0, 0.25, 0.789)]	Al, Ga, In, Bi, Sn, Pb
The remaining e-site [approximately (0, 0.25, 0.30)]	Mg, Ti, Zr, Hf, Eu, Pr, Pu

7.2 Metrics of the CoSn,hP6,191 Structure

There are **65 PDF entries** including duplicates.

Variable	Low Value	High Value
Pearson Symbol Code	hP6	hP6
a(0)	4.536 (InNi)	5.678 (PbRh)
c(0)	3.852 (CoGe0.67Sn0.33)	5.100 (In0.5NiSn0.5)
Axial Ratio [c/a]	0.745 (CoGe0.67Sn0.33)	0.978 (InNi)
Atomic Volume	77.40 (InNi)	126.21 (PtTl)
Calculated Density	6.971 (FeGe)	15.767 (PtTl)

7.2 Chemistry of the CoSn, hP6, 191 Structure

The Wyckoff Sequence = *fda*.

Site	Atoms
f-site [0.5, 0, 0]	Fe, Co, Rh, Ni, Pt, Tl
d-site [0.33, 0.67, 0.5]	Sn, Ge, Pb, In, Sb, Tl, Pt
a-site [0, 0, 0]	Sn, Ge, Pb, In, Sb, Tl, Pt

7.3 Metrics of the Cr₃S₄,mS₁₄,12 Structure

There are **229 PDF entries** including duplicates.

	Low Value	High Value
Pearson Symbol Code	mC12 (Cr _{0.5} Se ₄ V _{1.5})	mC14.16 (Ni _{3.08} Sn ₄)
a(0)	10.185 (S ₄ V ₃)	12.89 (Te ₄ V _{2.72})
b(0)	3.000 (CrPr ₂ S ₄)	4.061 (Ni _{3.08} Sn ₄)
c(0)	5.224 (Ni _{3.08} Sn ₄)	7.090 (Te ₄ Ti _{2.96})
Beta (degrees)	90.00 (Cr ₃ S _{2.46} Te _{1.05})	101.48 (S ₄ V ₃)

7.3 Metrics of the Cr₃S₄,mS₁₄,12 Structure

There are **229 PDF entries** including duplicates.

	Low Value	High Value
Axial Ratio [a/b]	2.765 (Rh _{2.3} Te ₄)	3.709 (P ₄ Re ₃)
Axial Ratio [c/b]	1.624 (Cr ₃ Se ₄)	2.006 (P ₄ Re ₃)
Atomic Volume	186.47 (S ₄ V ₃)	355.56 (Te ₄ Ti _{2.96})
Calculated Density	3.716 (Cr ₃ S _{2.46} Te _{1.05})	11.205 (P ₄ Re ₃)

7.3 Chemistry of the Cr₃S₄, mS₁₄, 12 Structure

Cr₃ S₄ has a *Wyckoff Sequence* = $i3a$.

Site	Atoms
i-sites [x, 0, z]	<ul style="list-style-type: none">• S, Se, Te (in two of the sites)• Metals [Co, Cr, Fe, Mn, Ni, V, Re, Rh, Pr, Bi, Sn, Pb, or Tl singly or in pairs in the third site]
a-site [0, 0, 0]	<ul style="list-style-type: none">• Metals [Co, Cr, Fe, Mn, Ni, V, Re, Rh, Pr, Bi, Sn, Pb, or Tl singly or in pairs]

7.4 A Recommendation

We believe that *Prototype Structure Profiles* are

- A useful analysis tool,
- Easily generated,
- Easily toggled from the profile to the list of examples and back, and
- Would be helpful in marketing our product.

Thus, we make the following motion (revised from the 2017 meeting):

M&A Subcommittee Motion 1

- M&A Subcommittee moves to the Technical Committee that *Prototype Structure Profiles* be made available to PDF users.

Supplemental Information

- M&A *Prototype Structure Profiles* are (a) a useful analytical tool, (b) easily generated, (c) easily toggled from the profile to the list of examples and back, and (d) would be helpful in marketing our product.
- These profiles are based on the Crystal Data cell and contain the value of Z, as well as observed ranges for the:
 - Pearson Symbol Code,
 - Lattice parameters, cell angles, and axial ratios,
 - Atomic volumes, and
 - Calculated densities.

Important Note

- This motion *does not* require *site-specific chemical information for Crystal Data cells* to be a part of these profiles. However, should this data become available, it should be added to these profiles.

8.0 M&A Editor's Report

Several projects are in process:

- Secondary review of the latest M&A patterns.
- A review of the *M&A Prototype Structure File* including the addition of the Z-value for each entry.
- A review of the *M&A Common Names Index* is done periodically to ensure that:
 - (a) Each cited entry has the required M&A common name on it,
 - (b) Each cited entry is the best available entry, and
 - (c) Each prototype structure is in the LPF format.

Both the *M&A Prototype Structure File* and the *M&A Common Names Index* are available on the M&A web page.

9.0 M&A Working Group Activities

- We met in October 2017 and March 2018, and each meeting covered four days.
- Primary tasks:
 - a. Continuing the Pearson Symbol Code Index (PSCI) Review,
 - b. Updating the M&A web page, and
 - c. Developing and updating M&A tutorials.

10.0 The PSCI-IV Review

- The PSCI review of 141,423 M&A entries is about 93.7% complete.
- In this review, entries are
 1. Sorted by (a) Pearson Symbol Code, (b) SG No., and (c) axial ratio(s),
 2. Evaluated individually, and
 3. Given (a) prototype structures, (b) Wyckoff sequences, (c) *standard empirical formulae*, and (d) *standard Z's* whenever possible.

10.0 Recent PSCI-IV results

hP6 to hP10 entries before and after PSCI-IV review.

	<i>Before Review</i>		<i>After Review</i>	
	No.	%	No.	%
Total entries	6024	100%	6024	100%
No space group number	22	0.4%	0	0.0%
No M&A prototype structure	1225	20.3%	45	0.7%
No LPF prototype structure	1817	30.2%	28	0.5%
No Wyckoff sequence	1795	29.8%	40	0.7%

11.0 M&A Web Page

- M&A web page is available on the ICDD website.
- This web page is used to keep M&A Subcommittee members up-to-date, and each member has been notified about it.
- A 2018 review/update will be complete soon.
- Many thanks to Terry Kahmer and Monika Kottenhahn for making this happen.

12.0 M&A Tutorials

- The M&A Subcommittee has created eight tutorials based on the M&A subfile.
- All are available on the M&A web page.
- Many thanks to Terry Kahmer for making this happen.

Final M&A Agenda Items

13. The next M&A Working Group meeting is October 19-22, 2018.

14. New/Old Business.

- Cam Hubbard

15. Adjournment.