# Dos Arroyos
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# memorandum


*To:* Distribution
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*Filename:* M&A Minutes 03-10.doc
*Date:* March 25, 2010


**Subject: Metals & Alloys (M&A) subcommittee minutes for March 17, 2010**

*Business Items*

The meeting was called to order at 11 am. The agenda is Attachment 1, and the attendance list has been sent to ICDD Headquarters for archiving. Cathy Foris and Jeff Dann took meeting notes, and Pete Wallace wrote the minutes. The M&A subcommittee minutes of March 2009 were approved as written.

*Upcoming M&A Working Group Meetings*

1. **2010 Fall Meeting:** Will be held the four days before the regular sessions of the DXC (July 31 – August 3), 2010.
2. **2011 Spring Meeting**: Will be held during the four days before the ICDD annual meeting as time and competing meetings permit. To gain an additional day, we may begin this meeting on the Friday before the annual meeting. A final decision on this will be made later.
3. **2011 Fall Meeting**: Tentatively, we will meet on October 23-26, 2011.

*Board of Director's Liaison Report*

Ray Goehner noted that the M&A subcommittee passed no motions last year, and hence he has nothing to report.

*M&A Web Page*

All that remains for the M&A web page to be open is the addition of several small documents referenced in M&A Working Group notes. These will be supplied to ICDD Headquarters soon.

*M&A Electronic Editors' Book*

The M&A subcommittee is working with Suri Kabekkodu at ICDD Headquarters to produce various electronic tables aimed at helping the M&A volunteers in their editing. Suri has completed initial versions of these tables and needs M&A volunteers to review and comment on them.

*Actions:*

1. Suri Kabekkodu will supply copies of the (a) Pearson Symbol code index (PSCI) anorthic (aPn) table [Ref. Section 3.0], (b) both monoclinic PSCI tables, mPn and mCn [Ref. Section 3.0], and (c) the Prototype Structure PSCI [Ref. Section 4.2] to Pete Wallace for distribution to the M&A Working Group. [The references shown in square brackets refer to sections of the *Electronic Metals, Alloys, and Related Phases (M&A) Editor's Book.*]
2. Pete Wallace and M&A volunteers will review these tables both before and during the M&A Working Group meeting before the 2010 DXC.

*Status of the Pearson Symbol Code Index (PSCI-III) Editorial Review*

Introduction:

This review uses Pearson symbol code index tables created in 2005, after a very large increase in the population of the M&A subfile occurred. This review is the first review where M&A volunteers are working directly on electronic files and submitting their recommendations in electronic form, first to the M&A subcommittee chairman for a quality check and then to ICDD Headquarters for approval and implementation. The ICDD is adding about 7,000 to 10,000 entries to the M&A subfile each year. So, we have our work cut out for us. Fortunately, we believe that the work we have done (and will do) establishes a basis for automatically assigning prototype structures based on established *prototype structure profiles*. ICDD Headquarters is working on this possibility now. A caveat: Computer-assigned prototype structures still will need a review until we have confidence that the assignment is done correctly.

The task requires the review of about 101,000 M&A entries focusing on the addition of prototype structures and correction of (generally minor) database errors. Microsoft Excel files in PSCI format are used for the review. We use a two step review process: (1) An M&A volunteer does the first, or primary, review. (2) Then the chairman performs the quality assurance review. M&A volunteers include Harlan Clark, Jeff Dann, Catharine Foris, Andy Roberts, Earle Ryba, and Pete Wallace (chair).

Status:

We are approximately 80% done with the PSCI-III review. See Attachment 2 for the details. To date, about 95% (or more) of the M&A entries have assigned prototype structures, and many small errors have been corrected. When we complete this review cycle, we will have established a baseline for subsequent reviews that should make the future assignment of prototype structures easier whether the assignment is done manually or automatically with manual oversight. Attachment 3 shows the effect of the PSCI review on the last 6,400+ entries of the hexagonal (primitive) file. For this file, we have assigned prototype structures to over 94% of the entries.

During the subsequent discussion, Suri noted that ICSD is now adding prototypes to the data they send us. Some of these prototypes are not in the PDF. On another subject, Mike Bennett noted that zeolites are classified based on topography and not on prototype structures and the space groups.

*Review of Current M&A Patterns*

This review involves from 100 to 200 experimental patterns a year. Most of these patterns are from grant-in-aid recipients. We are current in these reviews.

*Report on the October 2009 and March 2010 M&A Working Group Meetings*

The recent M&A Working Group meetings continued the work on the PSCI-III review with the results shown in Attachments 2 and 3.

*New/Old Business*

Three motions were brought to this subcommittee.

**Motion 1:** The Metals and Alloys Subcommittee recommends to the Technical Committee that for M&A phases Greek-letter formula modifiers (e.g., alpha-Al2O3, beta-Pu, alpha-Ti, etc.) as well as other commonly-used formula modifiers (e.g., 6H, 12R, etc.) (a) be added to the database and (b) be searchable. For the other commonly-used formula modifiers, M&A volunteers would create the needed list beginning with SiC, SiO2, and other similar phases and expand it as appropriate.

*Supporting information* from a 2/24/10 e-mail from Pete Wallace to Ray Goehner:

In response to your question about alumina polymorphs, I tried the following searches using the "All Names" search:

- Searched for "alpha": Got 37 answers, none of which was alumina.
- Searched for "alpha alumina": Got no answers.
- Searched for "beta": Got 5 answers, none of which was alumina. All were ternary or higher oxides that contained aluminum.
- Searched for "beta alumina": Got 5 answers, none of which was alumina. All were ternary or higher oxides that contained aluminum.
- Searched for "gamma": Got 7 answers including one alumina (01-074-4629, SG 141, PSC = tI26.66).
- Searched for "gamma alumina": Got one answer which was an alumina phase (01-074-4629, SG 141, PSC = tI26.66).

Then just for fun I searched for:

- "alpha plutonium" and got no answers.
- "beta plutonium" and got no answers.
- "gamma plutonium" and got no answers.

I suspect we both knew what the results of these searches would be even though each of these phases exists in the PDF. A lot of labeling work needs to be done for both metals and non-metals.

Motion 1 was moved by Pete Wallace, seconded by Andy Roberts, and passed 11-0-0.

**Motion 2:** The Metals and Alloys Subcommittee recommends to the Technical Committee that the Crystal Data cell axial ratios are made available in PDF4+ through *Preferences*.

Motion 2 was moved by Pete Wallace, seconded by Jeff Dann, and passed 10-0-0.

**Motion 3:** The Metals & Alloy Subcommittee moves that the Technical Committee either:

1 Allow the Prototype Structure field to have multiple entries so that former prototype designations and Strukturbericht symbols can be added, *or*

2 Create a field called Other Prototype Structures that allow multiple entries.

*Supporting information*

Example 1

| | |
|---|---|
| Chemical Name | Aluminum Barium |
| Prototype Structure | Ba Al4 |
| LPF Prototype Structure | Al4 Ba,tI10,139 |
| Other Prototype Structures | Cr2 Si2 Th  Al2 Ce Ga2  $D1_3$ |

Example 2

| | |
|---|---|
| Chemical Name | Rhenium Oxide |
| Prototype Structure | O3 Re |
| LFP Prototype Structure | Re O3,cP4,221 |
| Other Prototype Structure | Cu3 N  $D0_9$ |

Motion 3 was moved by Jeff Dann, seconded by Pete Wallace, and passed 12-1-0.

After the motions, Jim Kaduk said that a new ICDD 3-year strategic plan is coming and asked M&A members to think about (1) new ways to add value to the PDF and (2) what useful physical properties can be calculated and/or added to enhance the value of the PDF.

As one suggestion, Pete Wallace said that customers could be given an automated tool to identify possible prototype structures for a new material.

> *Action:* M&A members should think about (1) new ways to add value to the PDF and (2) what useful physical properties can be calculated and/or added to enhance the value of the PDF and give their input to Jim.

*Adjournment*

The meeting was adjourned at about 12:00 pm.

**Attachment 1: The M&A Agenda for March 17, 2010**

1 Call to Order
2 Appointment of Secretary
3 Approval of Minutes
4 Board of Directors Liaison Report (Ray Goehner)
5 M&A Web Page (Pete Wallace)
6 M&A Electronic Tables for Editors / Prototype Structure Profiles (Pete Wallace and Suri Kabekkodu)
7 Status of the Pearson Symbol Code Index (PSCI-III) Editorial Review
8 Review of Current M&A Patterns
9 Report on the October 2009 and March 2010 M&A Working Group Meetings
10 M&A Working Group will meet at the 2010 DXC
11 New/Old Business
12 Adjournment

Reference: M&A Agenda 03-09.doc

**Attachment 2: Status of the Metals and Alloys (M&A) Pearson Symbol Code Index (PSCI) Review, Third Pass (PSCI-III)** **Page 1**

Last update: March 25, 2010 Filename: M&A PSCI-III Review Status 03-25-10.xls

| Volunteer | Crystal System | Pearson Symbol Codes | Entries | Status | Completion Date | Date Quality Review Complete | Date Submitted to ICDD | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| Andy Roberts | Anorthic | aP … | 682 | Complete. | 07/16/07 | 07/16/07 | 10/27/07 | |
| | | | | | | | | |
| Pete Wallace | Monoclinic | mC… + mP… | 6599 | Complete. | Ca. 7/1/06 | 07/13/06 | 7/13/06 | |
| | | | | | | | | |
| Harlan Clark | Orthorhombic | oC… + oP … | 3,557 | Part 1 - Complete. | 08/11/08 | 08/26/09 | 08/26/09 | |
| | | | 3,594 | Part 2 - Complete. | 12/14/08 | 09/14/09 | 09/14/09 | |
| | | | 3,501 | Part 3 - Complete. | 07/28/09 | 09/30/09 | 09/30/09 | |
| | | | 3,321 | Part 4 - Complete. | 03/04/10 | | | Needs QA |
| | | | | | | | | |
| Andy Roberts | | oF… | 620 | Complete. | 07/26/06 | 09/26/06 | 09/26/06 | |
| | | | | | | | | |
| Andy Roberts | | oI… | 1,852 | Complete. | 07/26/06 | 09/26/06 | 09/26/06 | |
| | | | | | | | | |
| Andy Roberts | Tetragonal | tI… | 10,806 | Complete. | 03/10/08 | 08/05/09 | 08/05/09 | |
| | | | | | | | | |
| Harlan Clark | Tetragonal | tP… | 3000 | Part 1 - Complete. | 07/21/07 | 05/11/09 | 05/11/09 | |
| | | | 3929 | Part 2 - Complete. | 03/12/08 | 07/15/09 | 07/15/09 | |
| | | | | | | | | |
| Andy Roberts | Hexagonal | hP… | 20,591 | To be done in 6 parts of about 3,500 entries each. | n/a | n/a | n/a | 12,046 done |
| [first 14170 entries] | | | 3,530 | Part 1 - Complete | 03/15/09 | 10/08/09 | 10/08/09 | |
| | | | 3,530 | Part 2 - Complete | 03/15/09 | 10/17/09 | 10/17/09 | |
| | | | 3,530 | Part 3 - In process | | | | |
| | | | 3,580 | Part 4 - In process | | | | |
| Pete Wallace | Hexagonal | hP… | 3,480 | Part 5 - Complete | 03/07/10 | | | Needs QA |
| [last 6421 entries] | | | 2,941 | Part 6 - Complete | 03/07/10 | | | Needs QA |

| Attachment 2: Status of the Metals and Alloys (M&A) Pearson Symbol Code Index (PSCI) Review, Third Pass (PSCI-III). | | | | | | | Page 2 | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| **Volunteer** | **Crystal System** | **Pearson Symbol Codes** | **Entries** | **Status** | **Completion Date** | **Date Quality Review Complete** | **Date Submitted to ICDD** | |
| | | | | | | | | |
| Jeff Dann | Hexagonal | hR… | 5,613 | To be done in 2 parts of about 2,800 entries each. | n/a | n/a | n/a | 1,960 done |
| | | | | Part 1 | | | | |
| | | | | Part 2 | | | | |
| | | | | | | | | |
| | Cubic | cF… | 20,355 | To be done in 6 parts of about 3,500 entries each. | n/a | n/a | n/a | |
| Pete Wallace | | | 3,500 | Part 1 - Complete | 11/05/09 | | | Needs QA |
| Earle Ryba | | | 3,500 | Part 2 | | | | 1,221 done |
| Not assigned | | | 3,500 | Part 3 | | | | |
| Pete Wallace | | | 9164-9253 | A portion of Part 3 | 10/24/09 | | | |
| Not assigned | | | 3,500 | Part 4 | | | | |
| Not assigned | | | 3,500 | Part 5 | | | | |
| Cathy Foris | | | 2,855 | Part 6 | | | | 1,677 |
| Cathy Foris [trial] | last 1000 | | | | | | | 1000 done |
| Earle Ryba [trial] | 3800-3900 | | | | 11/05/09 | | | 100 done |
| Earle Ryba [trial] | 3901-4800 | | | | 11/05/09 | | | 900 done |
| | | | | | | | | |
| Jeff Dann | | cI… | 4,369 | Complete. | 07/21/08 | 08/13/09 | 08/13/09 | |
| | | | | | | | | |
| Pete Wallace | | cP… | 8,383 | Complete. | 12/17/08 | 12/17/08 | 12/17/08 | |
| | | | | | | | | |
| Pete Wallace | All Systems | Incomplete Pearson Symbols | (photocomps) | Have not been requested yet. | | | | |
| | | Total | 100,766 | [Includes unpublished patterns.] | | | | |

**Attachment 3: A comparison of the last 6,421 hPn entries before and after PSCI-III review. These entries cover the PSC range from hP13 to hP2090.**

| | Before Review | | After Review | |
|---|---|---|---|---|
| | **No.** | **%** | **No.** | **%** |
| **Total entries from hP13 to hP2090** | 6,421 | - | 6,421 | - |
| **Those having no space group** | 212 | 3.3 | 194 | 3 |
| **Those having no ICDD prototype structure** | 4,589 | 71.5 | 289 | 4.5 |
| **Those having no LPF prototype structure** | 3010 | 46.9 | 346 | 5.4 |

File: PSCI Snapshot 03-24-10.xls