

PDF Editorial Staff Subcommittee Minutes
Wednesday, 16 March 2016
ICDD Headquarters
Chairman-Suri Kabekkodu

Call to Order

The meeting was called to order at 9:00 a.m.

Approval of Minutes

The minutes from the March 2015 PDF Editorial Staff Subcommittee meeting were approved.

Approval: All Abstained: 0

Review of Mission Statement

The PDF Editorial Staff shall be responsible for evaluating and recommending improvements in the editorial and bibliographic procedures of the ICDD.

Board of Directors' Liaison Report (Scott Mixture)

No motions were brought before the Board from the committee last year. A majority of the Board's discussions revolve around the capabilities of the database and enhancements. The Board is looking forward to seeing and discussing new ideas and recommendations that the committee has to offer.

Editorial Progress in PDF Release 2016

Chairman and Editor-in-Chief, Suri Kabekkodu, gave a presentation and the following items were discussed:

- New EXP data
- New LPF data
- New ICSD entries
- Modulated Structures
- Abstracted Atomic Coordinates
- Editorial and Duplicate review
- Assigning Calculated pattern QM
- Raw Data
- Target Materials (Polymer, Top 200 Pharmaceuticals)
- Cross Referencing
- Subfile population

New Entries

Database	Diffraction Patterns	Atomic Coordinates
Experimental	1,669	1,444
ICSD	10,798	5,659
LPF	10,397	10,397
Modulated	149	149
TOTALS	23,013	17,649

Processed vs. Published

Database	Processed	Published
LPF	10,500	10,397
ICSD	11,621	10,798
Atomic Coordinates (exp)	1,832	1,444
Raw Data	1,524	1,219

Pharmaceutical and Polymers Update:

- Twenty-nine Pharmaceutical
- Twelve Polymers

Editorial Updates:

- Metals & Alloys: Reviewed the task group work and approved updating 17,047 structure types.
- Added 10,313 ANX formula and corrected 97.
- Phase designation review of Alumina by comparing with Alcoa.
- Continuation of adding In-Situ experiment description in comments and classifying dehydrated zeolites.

Mineral Classifications:

- Review of the mineral classification for inconsistencies (family, super group, group, subgroup).
- Identified and fixed more than 1,000 entries.
- 9,190 entries have been assigned with mineral group.
- 16,622 class/subclass added.

New Chemical Class:

- Bioactive (BIA)
- Narcotic (NAR)
- Psychotropic (PSY)

New Features:

- Modifications: New table with phase designations. Some of these are with other comments under comment type PM (Polymorphism)
- Two new comment types:
 - CM- Chemically related
 - PT- Phase transition
- New quality mark for experimental star patterns collected with internal standard
- New table mapping mineral structural formula

Database Status:

- All the patterns were classified into Primary/Alternate using Composition, QM and Temperature/Pressure of data collection.

Update on Organic Database:

- 5,988 new organic atomic coordinates.
- 5,022 atomic coordinates abstracted and added to previously published patterns.
- 8,018 ICSD atomic coordinates newly added this year
- In total 19,028 new atomic coordinates will be added in PDF-4/Organics 2016

New “Bioactive” Subclasses: Narcotics and Psychotropic

Senior Scientific Editor, Stacy Rector-Gates, gave a presentation and the following items were discussed:

Project Goal: Generate a ‘Narcotics’ subset/subfile/subclass for PDF products:

- Acquire guideline for known narcotics through the “Yellow & Green” list of the International Narcotics Control Board’s Drugs under International Control
- Review the current database entries to locate possible matches to the list (s)
- Determine coverage percentages

New Subclasses:

Narcotics (NAR): Defined as listed by the International Control Board **Yellow List**. All polymorphic or chemically modified forms of the narcotic should be included in the subclass.

Psychotropic (PSY): Defined as listed by the International Control Board **Green List**. All polymorphic or chemically modified forms of the psychotropic should be included in the subclass.

Subclass content for Newest Releases are as follows:

Narcotics: PDF-4+, 147 entries, PDF-4/Org, 245 entries.

Psychotropic: PDF-4+, 189 entries, PDF-4/Org 300 entries

Methods to obtain missing controlled substances will include member contributions, references and Grant-in-Aid. The possibility of a special project linked to Grant-in Aid was also mentioned and the committee was asked for any suggestions or recommendations.

General Business

James Kaduk suggested to the committee to always be thinking of more efficient ways of processing data that any ideas or suggestions can always be discussed.

New Business

Suri Kabekkodu posed the question of whether it was needed to distinguish between “R” quality mark and “star” quality mark. He suggested to merge them due to the fact that the only thing that distinguishes them is the way the data is processed. Peter Wallace discussed whether the user will lose anything and does it help the user? Suri confirmed that the user does not lose anything. Justin Blanton explained that last year the quality marks were color coded and “R” and “star” quality were both given a green code to distinguish them as top quality. Amy Gindhart stated that we will still be able to flag/comment during the processing that it’s Rietveld. The key factor agreed upon by all in this discussion was that essentially nothing would be removed or lost by merging the quality marks to star.

PDF Editorial Staff Motion: Proposal for Merge of Quality Mark

The PDF Editorial Staff recommends to the Technical Committee that the Star (*) and Rietveld (R) quality marks are merged into Star (*) quality mark.

Suri Kabekkodu moved the motion, Peter Wallace seconded the motion.

In Favor: 11 Yes, Opposed: 0 Abstained: 0 Motion was passed

Other Discussions

Graciela DelGado brought into discussion the wording of how to request the data for patterns. Some are cautious about providing data and that they are worried and concerned exactly where the data is going to be, and also what do they receive from submitting the data. Suri addressed her question and explained that if it is new data they can submit through the Powder Diffraction Journal as a Data report. If it is published, it will have a PDF number. More than ten submissions they receive a plaque, otherwise they will be given a certificate.

Adjournment: The meeting was adjourned at 9:55 a.m