

PDF Editorial Staff Subcommittee Meeting Minutes
Wednesday, 15 March 2017
International Centre Headquarters
Conference Room A
9:00 a.m. – 10:00 a.m.
S. Kabekkodu, Chairman

Call to Order

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

Appointment of Minutes Secretary

Lisa Lanno

Approval of Minutes from March 2016

The minutes from the March 2016 PDF Editorial Staff Subcommittee were approved.

Jeff Dann moved, second by Pete Wallace

Approved 6

Opposed 0

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 (Jeff Dann reported for Scott Misture)

There was a motion brought to the Board last year and approved that the Star (*) and Rietveld (R) quality marks are merged into Star (*) quality mark. This is implemented with Release 2018.

Editorial Progress in PDF Release 2018

S. Kabekkodu gave a presentation and the following items were discussed:

- New EXP data
- New LPF data
- New ICSD entries
- Modulated Structures
- Abstracted Atomic coordinates (both EXP and PDF-4/Organics)
- Editorial and Duplicate review
- Assigning Calculated pattern QM
- Raw Data
- Target Materials (Polymer, Top 200 Pharmaceuticals)
- Cross Referencing
- Subfile population
- Organic nomenclature
- Physical properties (new feature in PDF-4+)

New Entries

Database	Diffraction Patterns	Atomic Coordinates
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Experimental	1,547	647
ICSD	5,514	11,234
LPF	10,374	10,374
Modulated	78	78
TOTAL	17,513	22,333

Processed vs. Published

Database	Diffraction Patterns	Atomic Coordinates
LPF	10,500	10,374
ICSD	5,742	5,514
Atomic Coordinates (exp)	1,022	647
Raw Data	~1,500	1,077

Pharmaceuticals and Polymers

- Pharmaceuticals → 25
- Polymers → 14

Subfile Population

A library database has been built to provide an automated system which compares patterns, chemistry, structure and names to matches in database with classifications to those with no classification, if there is a match it is assigned a subfile classification, if no match is found it proceeds through an editorial review.

Structure Type Updates

Metals & Alloys: reviewed the task group work and approved updated 16,804 structure types.
Added 10,420 ANX formula and corrected 61.

Mineral Classifications

Review of the mineral classification for inconsistencies (family, super group, group, subgroup).
1311 entries have been assigned with mineral group.
Identified 15,087 mineral entries with no classification corresponding to 3,338 distinct mineral names.
Assigning mineral structural formula.

Cross Referencing

Cross referencing to patterns with atomic coordinates to patterns which do not have atomic coordinates is a good feature in our product experimental to LPF.

Constant Wavelength Neutron Diffraction Database

Since first released in 2014 enabling search/match using CW neutron diffraction pattern, more than 275,000 entries are in Release 2018.

Organic Chemical Classification

Several papers get published with no proper chemical name. Roy Garvey is involved with the task of assigning IUPAC chemical name, Structural formula, alternate and trade name (if available), organic functional group, 2D molecular diagram.

Organic Production

PDF-4/Organics Release 2017	PDF-4/Organics Release 2018
Processed: 15,845	Processed: 15,297
Published: 12,241	Published (<i>in progress</i>) currently ~9,500

Electron Diffraction

Main purpose of this project is to calculate structure factors using electron form factors for those entries we cannot publish atomic coordinates in PDF-4+ because of our contractual agreements. 5,698 new electron diffraction patterns were calculated for better representation of electron diffraction intensities in our product.

New Features

Phase Designation in previous releases (Prior to 2016) of the database, were stored in the comment section which made it difficult to recognize the phase immediately. A special table was created this year “Phase Designation” as one of the preferences which is easily identified during data retrieval and search/match. Release 2018 contains 36,847 entries with phase descriptor(s).

Neutron Time of Flight Database created with John Faber was a big factor in the development of this project which contains ~14,000 entries belonging to common phase and some applied material subfiles from LPF, using ORNL POWGEN instrument parameters, detector bank that has most intense peak, ~280,000 TOF patterns, new grant targeted TOF in-situ experimental patterns. Demo version of PDF-4+ has 96,500 TOF patterns and estimated time to complete by March 31, 2017.

Metal & Alloy Specialty Table - reviewed and created table to display standard empirical formula, Z, space group and Wyckoff sequence per M&A Subcommittee motion with ~29,500 entries for Release 2018.

Phase descriptor and classification of important cement phases was worked on with Cyrus Crowder.

International Mineralogical Association assigned number to mineral species (IMA number, Year-XXX) was worked on with Megan Rost.

New Chemical Subclass under Bioactive

- Depressants (DEP) → 216
- Stimulants (STM) → 63
- Pesticides & Antimicrobials (PES) → 397

New Chemical Class for clay minerals are being populated with Stephen Hillier chairing the task group which was proposed prior to this meeting.

General Discussion

Pete Wallace thanked the PDF Editorial Staff for starting on previous year’s motion.

John Faber suggested any help would be beneficial for the TOF project.

Adjournment