

PDF Editorial Staff Subcommittee Minutes
Wednesday, 25 March 2015
ICDD Headquarters
Chairman – Suri Kabekkodu

Call to Order

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

Appointment of Minutes Secretary

S. Wolkov

Approval of Minutes

The minutes from the March 2014 PDF Editorial Staff Subcommittee meeting were approved.

Approved: 8; 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 Report (Scott Misture)

There was a motion brought to the Board last year. M. Leoni moved that headquarters update instrumentation tables to accommodate current instrument parameters.

Editorial Progress in PDF Release 2015

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
- 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	1,533	668
ICSD	2,363	33
LPF	10,373	10,373
TOTAL	14,269	11,074

Processed vs. Published

Database	Processed	Published
LPF	10,500	10,373
ICSD	2,961	2,363
Atomic Coordinates (Exp)	809	668
Raw Data	~1,000	935

ICSD Update

- 25,768 entries were updated using ICSD Release 2014/1
- All of these entries were processed by keeping the ICDD's editorial work on minerals, zeolites, etc.

Editorial Updates

- The Metals & Alloys Task Group provided 48,105 structure types. Reviewed the task group work, and approved updating 48,037 structure types.
- Inserted 13,397 ANX formula and corrected 114
- Continuation of adding *In-Situ* experiment description in comments
- Classifying dehydrated Zeolites

Mineral Classifications

- Mineral classification has been extended beyond experimental set
- 15,619 entries have been assigned with Mineral group
- Example: Release 2014 has 48 entries under Halite group; now the population is 868

New Features

- All experimental entries with indexed, blank and low precision quality marks now have a comment describing the reason to lower the quality
- In neutron diffraction calculation, an author reporting that a structure with deuterium (instead of hydrogen) will be calculated using the proper scattering length

Possibility of a New Quality Mark

This would be an off-shoot from the Star quality mark. An active discussion was held.

Motion: Proposal for New Quality Mark
S. Kabekkodu moved. S. Misture seconded.
In favor: 2; Opposed: 11; Abstained: 2

Motion did not pass.

General Discussion

J. Kaduk discussed and asked the group for comments on what is an experimental pattern.

Adjournment