PDF Editorial Staff Subcommittee Minutes
Wednesday, 17 March 2010
ICDD Headquarters
Chairman - Suri Kabekkodu

Call to Order

Appointment of Minutes Secretary
Lisa Lanno

Motion 1:
The minutes from the March 2009 PDF Editorial Staff meeting were approved.
Kabekkodu, Wallace
8 Yes, 0 No, 0 Abstain
Motion passed.

Board report (Scott Misture)
The Board approved the motion to define the "R" quality mark as: "The "R" quality mark is used for patterns where it is clear that the d-values are directly the result of whole powder pattern fitting methods such as the Rietveld or decomposition methods. The entry should meet all the requirements of star quality mark."

Editorial Progress Report
Annual routine tasks, such as subfile and quality mark assignments, duplicate reviews, reviewing raw data, cross references, etc. were performed as normal. This year we had some targeted materials, i.e., polymers and amorphous materials that were included in the database.

S. Kabekkodu reported on the details of Release 2010 and the editorial work that went into it. There are a total of 59,510 new entries being published. S. Kabekkodu's report begins on page 3.

A. Roberts helped with a mineral editorial flag clean up. A new flag (NAT – naturally occurring mineral) was created and the non-ambient flag for minerals, because it exists elsewhere, was removed.

Metals and Alloys structure types – about 30,000 were updated by the Metals and Alloys Task Group. Beginning this year, we are reviewing ANX formulas from ICSD. J. Dann worked on this project and reviewed close to 17,000 ANX formulas.

Pattern distribution was also shown. Close to 60,000 entries were removed during the duplicate review.

Summary of Sunday's Editors' Meeting

- Seven new subfiles have been added to the PDF-4/Organics 2010: Alkaloids (ALK); Amino Acids, Peptides & Complexes (APC); Carbohydrate (CAR); Nucleosides & Nucleotides (NUC); Porphyrins, Corrins & Complexes (PCC); Steroids (STE)
- A guide, to assist abstractors and editors, to help standardize physical property comments is being established. Work on this guide is on-going in an attempt to make the list more complete.
- A brief background and introduction of modulated structures was given the importance of them and the work that is being done at ICDD.
- Headquarters is beginning to include non-crystalline materials in the PDF. The first target material is an amorphous cellulose pattern.
- The DataQUACkER program is in use and continues to be modified and tweaked.

Motion 2:
The PDF Editorial Staff Subcommittee recommends to the Technical Committee that headquarters use two (2) new Quality marks for non-crystalline materials. The proposed quality marks are: good (G) and minimal acceptable (M), and defined as:

1. Good (G) patterns should have chemical analysis, characterization of local structure (either by pair distribution function or spectroscopy) & good signal/noise
2. Minimal acceptable (M) patterns should have good signal/noise & chemical analysis

Kabekkodu, Wallace
14 Yes, 0 No, 1 Abstain
Motion passed.

Motion 3:
The PDF Editorial Staff Subcommittee recommends to the Technical Committee to approve a round robin for amorphous and poorly crystalline materials.

Kabekkodu, Rotella
11 Yes, 0 No, 1 Abstain
Motion passed.

Physical Properties (see Joel's presentation beginning on page 13 for further details)
J. Reid gave a status report on the work being done at Headquarters on physical properties. We have been thinking about what additional types of properties that are in the literature that we would like to capture and how we would like to standardize and express them. We would like to give users key quantities that will help them avoid going back to the original literature. We started by looking at our subfiles and specific related quantities that are widely available within our subfiles and prepared a guide. We would like to get some feedback and suggestions to help us expand the guide.

General Discussion
There was no general discussion or new business.

Adjournment
Motion to adjourn meeting.
Kabekkodu, Wallace
6 Yes, 0 No, 0 Abstain
Motion passed.