

PDF Editorial Staff Subcommittee
Wednesday, 21 March 2012
ICDD Headquarters
Chairman - Suri Kabekkodu

Call to Order

Appointment of Minutes Secretary

Lisa Lanno

Minutes Approved

The minutes from the March 2011 PDF Editorial Staff meeting were approved.

J. Dann moved.

S. Kabekkodu seconded.

8 approved

0 opposed

0 abstained

Board report (Jim Kaduk)

No motions from last year.

D. Sagnella sent L. Bernstein proposed modifiers. L. Bernstein reviewed and sent back to headquarters for Release 2013.

Non-ambient conditions motion was to capture additional non-ambient information not just having a flag but what the conditions are (example: electric or magnetic field) and there are ~1000 entries under review and will be in Release 2013.

S. Quick working on non-ambient conditions and has abstracted them. It is under review and will be in Release 2013.

Future plans - D. Sagnella is working on new program for a look-up table.

Non-ambient Subcommittee would like to work on multiple patterns per entry being implemented especially digitized patterns.

A. Roberts found missing non-ambient flag while searching ICSD. S. Kabekkodu will look at examples and investigate problem.

Editorial Progress in PDF Release 2012

Polymers for the past 2 years are target materials to be included in database and many are being contributed by T. Blanton. Many polymers are being abstracted and being captured from the Dow Polymer Book.

New entries for atomic coordinates are increasing in the experimental database mainly from the Grant-in-Aid Program and from literature articles.

The number of ICSD atomic coordinates is lower because of ICDD's contract with LPF. We cannot put all the atomic coordinates in our database.

LPF entries have a good percentage of atomic coordinates.

Raw data is visually checked and if not correct does not get used for the new release and gets put on hold until corrected.

The major reason for not publishing atomic coordinates is that the experimental and calculated do not match, the formula versus the structure density difference is $\geq 3\%$ and once corrected they get published the following year.

More ICSD patterns are being replaced by LPF because of duplication.

Subfile population has increased with the polymers and pharmaceuticals this year which also can be viewed on ICDD's website.

General discussion

For the modulated structures all tools are now in place to incorporate into our database. ICDD needs editors to work on this project and are asked to contact S. Kabekkodu. The first priority on the list is targeting minerals for modulated structures.

Another targeted area is polymers which in an ongoing process.

Other developments: Contributions for writes has had a significant increase in the past year because we can process the raw data in-house.

J. Dann questioned the policy on Tradenames – in product it is as an also called but flagged in database as 'T' for Tradename.

Primary and alternate – we don't use cluster analysis for primary and alternate.

Zeolites done on basis of cluster analysis and this process works for zeolites and S. Kabekkodu will not overwrite the Zeolite Task Group decision on primary and alternate patterns.

ICDD receives structure types from multiple sources (LPF, ICSD, Metals & Alloys and literature).

They are all flagged according to the source, experimental, LPF, Metals & Alloys, literature and ICSD. A mapping table needs to be implemented and is still in the works. Volunteers are needed to work in these areas and should contact S. Kabekkodu.

All grantees are expected to submit data through DataQUACKER. D. Sagnella is now working on a format for the corrections from the editors to be done directly on the P1 forms which can be submitted electronically.

Adjournment

Motion to adjourn meeting

S. Kabekkodu