

PDF Editorial Staff Subcommittee
Wednesday, 13 March 2013
ICDD Headquarters
Chairman - Suri Kabekkodu

Call to Order

Appointment of Minutes Secretary

Lisa Lanno

Minutes Approved

The minutes from the March 2012 PDF Editorial Staff meeting were approved.

Board report (Scott Misture)

No motions from last year.

Editorial Progress in PDF Release 2013

- New Experimental, LPF, ICSD, modulated structures (O. Gourdon)
- Abstracting atomic coordinates
- Editorial and duplicate review continuing
- Raw data from our grant program (impurities, etc. are being reviewed)
- Target materials are polymers which are being worked on by T. Blanton and S. Gates
- Subfile population continuing by subfile specialist as well as assigning through queries
- Added additional cross references this year

New Entries

Database	Diffraction Patterns	Atomic Coordinates
Experimental	1513	1255
ICSD	13200	265
LPF	10376	10376

Atomic coordinates are being caught up with a backlog

Processed vs published

Database	Processed	Published
LPF	10500	10376
ICSD	17104	13200
Atomic Coordinates (Exp)	1797	1255
Raw Data	~1300	1178

Atomic Coordinates in the experimental database increased from backlog 1797 vs. 1255 last year

DBStatus - all patterns were classified into Primary/Alternate using Composition, quality mark and Temperature/Pressure of data collection

- Removed 84,754 ICSD duplicates
- Removed 6996 NIST duplicates

Subfile population increase in zeolites, minerals and pharmaceuticals because of cross referencing. Thermoelectric increased from 260 last year to 941 this year because of work from Winnie Wong-Ng.

New - 3 cross references introduced using the criteria below:

- Cross referencing related phases
- Cross referencing
- Temperature series data

New project on organic entries into database. A. Gindhart is the lead working along with interns.

- New novel organic single crystal
- Pharmaceuticals, papers with CIFs, Acta Crystallogr., Sec. E, other papers on key terms, writes project written for in past and have not received responses
- Response and pulled organic papers to process in-house
- Bioactivity flagged 222, pharmaceuticals flagged 76 which is a good population of subfiles.

Historical project

- CIFs, able to extract (A2E), full (less than 20 atoms), project slowed since more has to be done manually
- ~6400 to be calculated for 2014 product
- Total papers tracked ~26,000
- Patterns on hold are due to publication errors, human error, missing atoms
- Issues ~8000 most common not published

Tradenname project

- S. Gates is the lead and E. Foster (intern assisting) if we can add Tradenames looked at 1,700 so far, 530 out of 1,704 and no Tradenames at this time
- Tradename 1423 pharmaceutical
- Inorganic are disregarded since our contract does not allow us to calculate – if good amount of subfiles we ask permission from Pierre Villars

General discussion

New projects – modulated structures (Olivier Gourdon), neutron diffraction data (John Faber)

Adjournment

