

International Centre for Diffraction Data
Organic and Pharmaceutical Subcommittee Meeting Minutes
Wednesday, 25 March 2015
Fred Wireko, Chairman

1. Call to Order Fred Wireko
 - a. Staff liaison - Amy Gindhart
 - b. Welcomed new member on the subcommittee.
2. Appointment of Minutes Secretary - Megan Rost was appointed to record minutes.
3. Roll Call and Attendance on record at headquarters.
4. Approval of 2014 Minutes

Motion moved by: Jeffrey Deschamps
Second by: David Rendle
4-Yes, 0-No, 0-Abstain
5. Review of Mission Statement - No changes
6. Report of Board Liaison Robert Papoular

No Report
7. PPXRD-13 Report Update Terry Maguire
 - a. No PPXRD last year
 - b. PPXRD-13 will be held 18 -21 May 2015, Black Forest, Germany
 - i. Pharmaceutical symposium
 - ii. Workshop for quantitative phase analysis
 - iii. Technical sessions
 - iv. Vendor exhibition
 - v. Poster session
8. Update-Energetic Materials Database Jeffrey Deschamps & David Rendle
 - a. Progress in 2014-2015
 - i. 1623 current entries reviewed (658 unique)
 - ii. All entries categorized as:
 1. Explosive
 2. Explosive, Common
 3. Explosive, Ingredients
 4. Explosive, Exotic
 5. Explosive, Residue
 6. Non-Explosive
 7. Uncategorized

Action Item #1:

- 1) The explosive flag should be removed from non-explosive entries.

- 2) An extra descriptor should be added (common, ingredient, exotic, or residue) to current entries as needed.
- 3) Uncategorized explosive entries need to be studied to complete classification.
- 4) A review of new entries should be completed annually to ensure all entries actually belong to explosive subfile and assigned to a subcategory, ~ 50 per year.

9. Future Tasks

General

- a. Open to discussion is 2D-data structure and fragment search capabilities.
 - i. Concerns:
 1. Implementation steps required are unknown.
 2. How to standardize our current entries?
 3. Financial cost to accomplish; a valid estimate is needed.
 - ii. Suggestions:
 1. Begin adding "smiles" to new entries.
Roy Garvey has already given SMILES for entries he worked on.
 2. Plan project into smaller steps to execute.
- b. Review of organic excipient subfile.
 - i. Suggestion was to bring this up at PPXRD-13 meeting to recruit volunteers.
 - ii. Gregory Stephenson from Eli Lilly

Motion #1:

The Organic & Pharmaceutical Subcommittee recommends to the Technical Committee that ICDD evaluate the ability of 2D chemical structure data and fragment search capability.

Motion moved by: Fred Wireko

Seconded by: Jeffrey Deschamps

9-Yes, 0-No, 0-Abstain

Action Item #2:

Get volunteers for organic excipients entries to be reviewed.

10. Other matters

General

- a. Naming entries and fixing nomenclature
- b. Business analysis
 - i. Pharmaceutical companies
 - ii. Law enforcement- Forensic analysis
 1. Moved over inorganic entries to organic product
 2. Cleaned up explosive subfile
 - iii. Added more commercial material entries with atomic coordinates

11. Adjournment

Motioned moved by: Stacy Gates

Seconded: David Rendle

0-Yes, 0-No, 0-Abstain