

Organic and Pharmaceutical Subcommittee Meeting Minutes
Wednesday, 16 March 2011
4:00 pm – 5:00 pm
David Rendle, Pro-tem, Fred. Wireko

1. Call to Order and Opening Remarks
D. Rendle started the meeting at 4:00 pm

D. Rendle

2. Appointment of Minutes Secretary
Fangling Needham was appointed as the Minutes Secretary.

3. Roll Call and Attendance
D. Rendle circulated the attendance sheet in the meeting room.

4. Approval of Minutes from March 2010
The minutes were approved.

5. Mission Statement
D. Rendle said that the wording of the mission statement is fine.

The mission of the Organic and Pharmaceutical Subcommittee shall be to increase the value and successful use of the organic section of the PDF by the diffraction community. To that end the subcommittee shall (1) provide technical support for all organic database products, and (2) support efforts demonstrating its capabilities.

Attendees did not have comments about the mission statement.

6. Board of Directors' Liaison Report

J. Miguel Delgado

M. Delgado mentioned that there was no motion received last year. D. Rendle concluded that there will be no report for this item.

7. Update on selection of important compounds from IUCr collection
The task group members are Graciela Delgado, David Rendle, and Frank Rotella.
D. Rendle provided the following slide to show the background information.

D. Rendle

“From an original list of 30,000 compounds (from IUCr), ~3,000 have been selected by the Editor-in-Chief on the basis of potential commercial importance, and hence of value to the PDF.

The Task Group's work is to review the list of 3,000 compounds, and to refine it further, by identifying which of the entries are of greatest importance.

The selected compounds will then have their powder patterns calculated by the Editorial Section”.

So far the task group has processed >800 entries. About 50% of the entries were classified as important. The classification is subjective to some extent.

D. Rendle presented two spreadsheets sent to the task group by S. Kabekkodu. The first spreadsheet contains information such as file name, chemical formula, chemical name, space group, possible subfile type, and important(Y/N?). The other spreadsheet contains literature reference information. To use the reference requires access to the IUCr journal on-line for other information. From the journal information, the task group populated columns in the first spreadsheet to indicate whether the subfile designation is correct, and the compound is considered to be important. Comments were added, if required.

D. Rendle showed three examples – pigment, pharmaceutical, and forensic material.

The task group will continue to process entries on the list, continuing from the initial 800 processed data.

T. Fawcett pointed out that web fungicides will be labeled bioactive and pharmaceutical if it applies to human. Graciela Delgado pointed out that the task group will not enter a subfile designation if no information concerning the use of the compound can be obtained from the WEB or from the Merck Index. D. Rendle mentioned that the paper from the journal does not always give the source of the material. T. Fawcett asked about the success rate of finding information on the web after the journal search. G. Delgado answered that the success rate is low. T. Fawcett stated that only 20% - 25% of the entries in the organic database have subfile designations and the rest have no specified use.

8. PPXRD-10 Report Update

T. Maguire

T. Maguire reported that PPXR-10 will be held from May 16th to 19th in Lyon, France. We did not have a PPXRD symposium this fiscal year because there were two symposiums one in Glasgow, Scotland and Hilton Head Island USA, the prior year. The format of PPXRD-10 includes a one-day workshop – “Understanding Amorphous Materials,” followed by two and a half day technical sessions. The symposium will end on Thursday afternoon with a post-symposium excursion to the European Synchrotron Research Facility.

The instructors for the workshop are Dr. Shawn Yin, Dr. Ann Newman, Dr. Valeri Petkov, and Dr. Loren Schielaer. The workshop topics include:

- An Introduction to Amorphous Materials and Pharmaceutical Applications
- Amorphous Basics
- How to Prepare Amorphous API
- Using PXRD for Amorphous Materials
- Using ss-NMR and Other Techniques for Amorphous Materials
- Using Thermal Techniques for Amorphous Materials
- Optional Panel Discussions

The sessions planned are:

- Patent and Regulatory Issues
- Formulation & Product Development
- Polymorph & Salt Screening
- Complementary Techniques
- Amorphous, Activated and Nanomaterials
- New Frontiers in XRD in Pharmaceutical R&D
- XRPD Structural Techniques
- Crystal Structure Prediction

The deadline for the abstracts has passed, but we are still accepting them. We are happy to accept abstracts in any of the topics. We also will have a poster session held in conjunction with the exhibits. We will accept applications for posters as well as oral presentations.

PPXRD-11 will be held in the United States. We are still searching and the location is to be determined.

9 Future Tasks

General

T. Fawcett stated that there were some additional features that came out of last year's product. HQ Staff has done a very good job on cross-referencing, so that bioactive materials have extended to non-Cambridge Structural Database entries and increased the subfile population. We also cross-referenced drug common names in conjunction with the right chemical formula to increase the pharmaceutical subfile population. The pharmaceutical subfile population has increased 20% in the last year. The population of other subfile categories, such as amino acids, also greatly increased due to the cross-referencing effort. This cross-referencing activity for subfiles is an on-going process.

10. Other Matters

General

D. Rendle stated that T. Fawcett indicated during the Regional Co-chair Meeting that ICDD has money to spare related to Grant-In-Aid Program. During their 5-10 minutes presentation at British Crystallography Association meetings (BCA) every year, Dave Taylor and D. Rendle informed attendees that ICDD will compensate grantees for submitting good quality X-ray

powder diffraction patterns. Despite their efforts, there were no takers. D. Rendle asked T. Fawcett for input concerning the means to encourage people to submit PXRD patterns with compensation.

T. Fawcett stated that there had been a surplus of GiA applicants five years ago. However, the situation has changed for the last two years. We have started to reactivate the activities and advertise the GiA program again. ICDD grants are designed for supplemental purposes. It is difficult to fully subsidize a diffraction operation with the ICDD grants, especially due to the laboratory cost in the United Kingdom. The situation has completely changed in different parts of the world, such as China and Russia, due to the price of the US dollar. It is a good idea to make the offer of GiA at BCA. Many beam lines have user facilities and GIA will support XRD data collected from the beam line too. The ICDD grantees are not required to have a diffractometer.

11. Adjournment