

Organic and Pharmaceutical Subcommittee Meeting Minutes
Wednesday, 17 March 2010
Chairman: Fred Wireko

1. Call to Order and Opening Remarks

F. Wireko started the meeting at 4:10 pm.

2. Appointment of Minutes Secretary

Fangling Needham was appointed as the Minutes Secretary.

3. Roll Call and Attendance

Fred Wireko circulated the attendance sheet in the meeting room.

4. Approval of Minutes from March 2009

The minutes were approved.

5. Review of the Mission Statement

F. Wireko reintroduced the Mission Statement for the benefit of newcomers:

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.

F. Wireko did not see the need to change this Mission Statement and informed attendees that the ICDD Mission Statement is on the web.

6. Board of Directors' Liaison Report

S. Mixture reported that last year this subcommittee asked headquarters to generate a series of subfiles including amino acids. The subfiles were published. There was a poster about these subfiles at the poster session on 16 March 2010. Cross-linking is still being implemented and the project is on-going.

T. Fawcett mentioned that the staff did a wonderful job on the subfile task. A lot of subfile assignments were tied in with the Cambridge Structural Database (CSD) subfile scheme. An extra effort was to assign the experimental entries to the subfiles by cross-linking with the CSD definition. The task has not yet been finished; one of the reasons is that polymorphs of organic compounds are more difficult than those of inorganic ones for the assignment. The staff exceeded their goals for this particular project.

S. Kabekkodu mentioned that cross-linking required indexed patterns. The effort from this subcommittee is appreciated.

T. Fawcett mentioned that the molecular diagrams were looked at in some cases. About 200 NIST standards, including LaB6, useful for users involved in calibration, were assigned.

7. Update on Disordered Entries

S. Kabekkodu reported that a list of disordered entries was made. T. Fawcett talked to Frank Allen of the Cambridge Crystallographic Data Centre (CCDC) and is waiting for his response. We have a list of IUCR

CIF files for the task group to identify the important/commercially-important ones. D. Rendle has started working on it and the template is done. They will be cycled back to the Grant-in-Aid Committee.

T. Fawcett mentioned that CCDC would get back to him concerning the disordered list and they will discuss this matter face-to-face in three weeks when Tim and the CCDC representative get together at a conference. The task of the IUCR CIF files focuses on high volume, important pharmaceutical materials.

8. PPXRD-9 & 10 Report Update

T. Maguire reported that the ICDD hosted two pharmaceutical symposia – May 2009 and February 2010. The one in Glasgow (May 2009) was very successful whereas the Hilton Head meeting (February 2010) was not so successful due to the state of the US economy. Tim pointed out that Dr. H. Toraya was added to the Organizing Committee. There was a one-day workshop on “*Characterization of Pharmaceutical Solids*,” at Glasgow followed by a two and one half-day symposium. In Glasgow, there were 26 countries, 58 attendees including 8 students and 21 who attended symposia only. At Hilton Head Island, there was also a one-day workshop on “*Understanding Pharmaceutical Amorphous Materials*,” followed by a two and one half-day symposium. There were 31 attendees from 7 countries, 22 participated in the workshop. Seven companies participated and eight exhibits were featured for both symposia.

T. Fawcett noted that we are currently investigating potential PPXRD-11 site in Asia for 2012. The last European PPXRD-8 was very successful. PPXRD-10 will be held in May in Europe.

C. Crowder announced that PPXRD presentations will be made public on the web after one year. The attendees will have password protected access to this web site during that year.

G. Delgado mentioned that the “*International conference on the chemistry of the organic solid state*” (ICCOSS XX) will be held 26-30 June 2011 at the Indian Institute of Science in Bangalore, India. The registration fee will be USD \$400 including meals and accommodations. G. Delgado was asked to inform the Bangalore planners to go to the ICDD website where they could put in an official funding request on-line. ICDD supported the **ICCOSS** XVIII meeting in Venezuela in 2008 where the ICDD database was showcased.

F. Wireko noted that the next scheduled meeting will be held in Italy in 2014 and wondered about the possibility of combining ICCOSS with PPXRD.

T. Fawcett replied that this is a big maybe. We are planning a symposium in the same general area around that time. The low registration fee competes with ICDD sponsored symposia. Education for diffraction is a good idea.

F. Wireko stated that we will mention this request via the board liaison, S. Misure, to the board as a suggestion instead of a motion.

F. Rotella – moved.

T. Fawcett – second.

9. Future Tasks

F. Wireko: Any suggestion to make the DB a better product?

T. Fawcett: Discussion with B. Toby and J. Kaduk to use APS beam line. There are 700 out of 2,800 pharmaceutical entries not in the ICDD database. They will tackle this list.

B. Toby: Co-crystallized materials would be of interest. He mentioned possible cooperation with other beam line users to get high quality data.

T. Fawcett: Only 10% of patent polymorphic patterns passed ICDD editorial process.

C. Crowder: Poor pattern is better than no pattern.

B. Toby: There is value for the database to have entries without x-ray patterns.

T. Fawcett: Our goal is to solve the unknown for the customers.

C. Forris: We put in minimum number of peaks required in patents.

T. Fawcett: It is a worthy debate about putting bad patterns in the database. We do not have to settle the debate today. Ultimately, the database should do what is best for the customers.

F. Wireko: A patent wants to make its definition as broad as possible to expand the coverage. As a user himself, he thinks that it is better to have data in the database. He would like this subcommittee to come up with an opinion.

T. Fawcett: We will continue to get people's input on this subject. The opinion about whether to add the bad patent data to the database at PPXRD-9 was about a 50/50 split.

T. Blanton: During tomorrow's Annual Meeting, we will discuss how good the organic database is. We will award Dr. R. Garvey for his significant impact on it through his involvement since the early days. S. Kabekkodu stated that R. Garvey gave him 33,000 compound names to review.

10. Other Matters

There are no motions and one suggestion.

T. Fawcett stated that a lot of vendors are interested in the organic database because congress is putting a national health care bill forward. India and China currently have a national health care bill under consideration. The legislative issue globally argues well for ICDD as there will be increased use of the database to validate generic compounds.

The subcommittee had one suggestion and no formal motions this year.

11. Adjournment

The meeting was adjourned at 4:55PM