

Organic and Pharmaceutical Subcommittee Meeting Minutes
Wednesday, 21 March 2012
4:00 pm – 5:00 pm
Fred Wireko, Chairman

1. Call to Order and Opening Remarks
F. Wireko started the meeting at 4:00 pm.
2. Appointment of Minutes Secretary
F. Needham was appointed as the minutes' secretary.
3. Roll Call and Attendance
F. Wireko circulated the attendance signing sheet.
4. Approval of Minutes from March 2011
Acceptance of last year's minutes was moved by Davor Balzar and was approved.
5. Mission Statement -- Reminder

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 stated that the ICDD Mission Statement shown here is to remind the old members and to introduce it to new members and guests. He also asked whether the Mission Statement should be changed and concluded that there was no need to change it.

6. Board of Directors' Liaison Report
J. Miguel Delgado stated that there were no motions and there is no message from the board last year. F. Wireko commented that no motions does not mean there is no activity.
7. Update on Commercially Important Organic Structures - Structures-PDF-4 Task Group
F. Wireko stated that the task group, D. Rendle, F. Rotella, and G. Delgado had worked on this project for three years.

D. Rendle's report:

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 Department.

The task group used the information in the CIF file and on-line journal to review and edit the subfile assignment. The task group also determined whether a substance is of commercial importance (1,600 out of 2,977 entries were flagged by the task group as important.)

D. Rendle thanked F. Rotella and G. Delgado for their efforts.

T. Fawcett made a major announcement concerning the termination of ICDD/CCDC (Cambridge Crystallographic Data Centre) contract last month. For future entries, ICDD will extract its own single crystal structure information from published literature for PDF-4+. To this end, additional resources (A. Gindhart and M. Rost) have been directed to the task for targeted pharmaceuticals and commercially important compounds. Full single crystal structure information, including atomic coordinates, for ICDD extracted compounds will be available in the PDF-4 product line. T. Fawcett responded to F. Wireko's

question about the previous CCDC data; i.e. the organic patterns obtained from ICDD during the contract years will remain in the database.

8. PPXRD-11 Report Update

T. Maguire reported the upcoming PPXRD-11 activities: PPXRD-11 will be held from 15th-18th May 2012 at Sanibel Harbour Marriott Resort & Spa at Fort Myers, Florida, U.S.A. The program consists of a one-day workshop on, "Understanding Amorphous Pharmaceutical Materials," and two and one-half days of technical sessions: Regulatory, Formulation/Product Development, Polymorph/Salt Screening, Complementary Techniques, Amorphous/Activated/Nanomaterials, New Frontiers in XRD in Pharmaceutical R & D, XRPD Structural Techniques, and Crystal Structure Prediction.

T. Maguire urged the subcommittee attendees to obtain and/or help distributing brochures.

C. Crowder stated that the organizing committee members are currently reviewing the abstracts; the program is posted on the web.

T. Fawcett attested that the hotel is very good; the average water temperature is around 76 degrees. He urged people to bring their families to visit the nature preserve (2/3 of the island), to talk science in the relaxing environment.

9. Future Tasks

General

J. Deschamps mentioned that he has published 317 energetic materials with polymorphs in his proprietary database. The first step is to identify the entries missing in the ICDD database. F. Wireko stated that no motion is needed for helping him right now since the database is open only to J. Deschamps. So this will be a one-person task group.

T. Fawcett mentioned that our first priority would be targeting the commercial excipients that are mostly inorganic, pharmaceutical, energetic, explosive, metal-organic framework, and pigment. The second priority would be anything else with commercial importance. We will require help from this subcommittee one year from now. Another effort we are conducting now is to correct and identify all pharmaceutical and bioactive materials in the database. S. Kabekkodu responded that the non-commercial ones in the database can be flagged as bioactive materials. T. Fawcett responded to F. Wireko that the 700 explosive materials from J. Deschamps' database will be called "explosive materials."

F. Wireko gave the attendees a heads up about the 2012 International Conference on the Chemistry of the Organic Solid State (ICCOSS) in the United Kingdom. The time and program are not determined yet. T. Fawcett feels that it is good to know in advance to put a place holder for scheduling and funding purposes. T. Fawcett and G. Delgado discussed the possibility of organizing an educational workshop at the ICCOSS meeting with D. Rendle's help.

10. Adjournment

T. Blanton moved, T. Fawcett second and the meeting was adjourned.