

Organic and Pharmaceutical Subcommittee Meeting Minutes
Wednesday, 25 March 2009
International Centre Headquarters
Conference Room A
4:00 p.m. - 5:00 p.m.
F. Wireko, Chairman

1. **Call to Order and Opening Remarks (F. Wireko)**

F. Wireko gave welcoming remarks.

2. **Appointment of Minutes Secretary**

F. Needham was appointed as the Minutes Secretary.

3. **Roll Call and Attendance**

Attendance sheets were passed around for signatures.

4. **Approval of Minutes from March 2008**

The minutes from March 2008 were approved.

5. **Review Mission Statement**

F. Wireko emphasized that one of the important goals of this subcommittee is to increase the value of the ICDD organic database, to support and to demonstrate its capability. And therefore, we should discuss how to improve this process.

Organic classification for subfiles

S. Kabekkodu suggested expanding subfiles. T. Fawcett noted that the current subfiles are effective and there are over 300,000 patterns that can be further classified with amino acid, peptide, and protein subfile options. F. Wireko noted that he found CSD classifications very useful himself. He differentiated the Organometallic and other Organic compounds for searching. D. Rendle remembered that years ago, CSD had more than thirty different groups, such as alkaloids and some basic definitions. ICDD could use either the CSD or its own classification system. T. Fawcett mentioned that the PDF has a more elegant periodic table search than that of the CSD in response to F. Wireko's elemental search question. The following motion was adopted by the subcommittee to be recommended to the Technical Committee.

Motion:

The Organic & Pharmaceutical Subcommittee recommends to the Technical Committee that the compound classification traditionally used in the Cambridge structure database be adapted along with current and any reasonable functional classifications as subfiles for the Organic PDF to aid in database search.

Nine votes were in favor of adopting CSD classification. There were no opposing votes, and none abstaining.

6. **Board of Directors' Liaison Report (S. Mixture)**

S. Mixture reported that there were no motions last year. He urged this subcommittee to send motions of comments and thoughts, not necessarily monetary in nature, to the Board. F. Wireko requested more elaboration on Web PDF-4⁺. T. Fawcett indicated that a few people had purchased Web PDF-4⁺. ICDD has sped up its web access by purchasing high-speed lines. We also get information about web product usage to gather data. Questions to ICDD on the web include inquiries as to how to use Jade or HighScore Plus. Since dongles need new code and a special version, we are waiting to see the sales volume demand before moving the organic product to the web. Users of the Web PDF-4⁺ product can work from home and other sites. C. Crowder noted that the Web PDF-4⁺ is exactly the same as PC PDF-4.

7. Update on Disordered (S. Kabekkodu/Headquarters)

We have discussed this for 5 or 6 years. Last year, we looked at commercially important pharmaceutical compounds. Densities were compared to find missing atoms. CSD does not store site occupancies.

D. Rendle: Some information is in the comments.

S. Kabekkodu: Someone has to read the comments.

T. Fawcett: It is time consuming to read comments.

D. Rendle: There is information in Mercury too.

S. Kabekkodu: Mercury does not take the disorder into consideration. ICDD asked CCDC to correct the disordered entries' problem.

T. Fawcett: We gave them a list of commercially important compounds for correction. CCDC is looking into the important list. CCDC have 60% raw data in electronic format. They agreed to send us files in CIF format, but we have not received them yet.

S. Kabekkodu reported that this year we received 30,000 compounds with atomic coordinates from IUCr. Most of them are organic compounds. D. Rendle is working on 2,000 of them. S. Kabekkodu is requesting about three volunteers who are interested in looking at them. D. Rendle needs to get access to online journals for his editorial purpose. It takes about five minutes per compound for the editorial process. To speed up the process, G. Delgado and F. Rotella volunteered to join D. Rendle on editing the atomic coordinates of organic compounds upon F. Wireko's and D. Rendle's solicitation. D. Rendle will be the task group leader.

8. PPXRD-8 Report Update Headquarters (T. Maguire)

The PPXRD-8 will be held from May 4th to May 7th 2009, in Glasgow Scotland, which is different from the traditional February meeting in the past. This year's organizing committee members were introduced, and is headed by a new chairperson, C. Crowder. The format of PPXRD-8 will be started with a one-day optional workshop - "Characterization of Pharmaceutical Solids." The workshop instructors will be Detlef Beckers, Cyrus Crowder, Tim Fawcett, Geert Vanhoyland, and Raj Suyanarayanan (chairperson). There are 14 people registered for the workshop. The workshop will be followed by two and one half days of technical sessions. The topics are XRPD Structural Techniques, Crystal Structure Prediction, Formulation Product Development, Drug Delivery, Polymorph & Salt Screening, Amorphous Activated and Nanomaterials, complementary Techniques, New Frontiers in XRPD Pharmaceuticals, Patent Regulatory Issues, and Round Robin Results from last year. Currently, there are 52 people from 13 countries registered for the symposium. Among them are six students. There will be 10 table top exhibits from nine companies. There is no sponsorship up to now. We will accept any sponsorship if anyone is interested. So far, there will be about 26 to 30 talks and 11 posters. We are still accepting registrations if anyone is interested in attending the PPXRD-8 symposium. T. Fawcett commented that we are pleased about the healthy number of registrants despite the world economy. The professional survey company hired by ICDD reported that polymorphs, salt screening, and patent research were most frequently utilized by the users. DDView+ and SIeve+ come with the database without additional charge. ICDD is committed to educate customers how to data mine the database. ICDD has a tutorial web site for education purposes and any additional examples submitted will be welcome. PPXRD past abstracts are available on the ICDD web site.

9. Future Tasks General

This subcommittee would like help to put out a better product. Disorder structure problems were tackled two years ago. Today, we found the solution. ICDD asked CCDC to provide us correct data.

10. Other Matters General

At this subcommittee meeting, there are many guests who are not subcommittee members. F. Wireko will obtain guests' e-mail addresses from F. Needham and request whether they would like to be an Organic and Pharmaceutical Subcommittee members.

11. Adjournment

The meeting was adjourned at 5:00 PM.