

## **Organic and Pharmaceutical Subcommittee Meeting**

Wednesday, 21 March 2007

Conference Room D

1:00 p.m. – 2:00 p.m.

F. Wireko, Chairman

### **1. Call to Order and Opening Remarks**

Fred Wireko emphasized the power of the subcommittee and encouraged the attendees to take advantage of it.

### **2. Appointment of Minutes Secretary**

Fangling Needham was appointed as the Minutes Secretary.

### **3. Roll Call and Attendance**

The Attendee list was circulated for signatures.

### **4. Approval of Minutes from March 2006**

The March 2006 meeting Minutes were posted on the Web and were approved.

### **5. Board of Directors' Liaison Report**

T. Blanton reported that last year's motion about supporting the International Conference on the Chemistry of the Organic Solid State (ICCOSS) in Venezuela in July 2007 was approved and asked for details. T. Fawcett and H. McDonnell responded that while the mechanics (exhibits...) will be worked out, there was no foreseeable problem. F. Wireko stated that M. Delgado will give a report about it later at this meeting.

T. Blanton mentioned that it was brought to his attention that SiO<sub>2</sub> has many forms and not all SiO<sub>2</sub> are excipients or pharmaceuticals. He promised M. Bennett that we will discuss the issue at this meeting.

T. Fawcett stated that ICDD had talked to United States Pharmacopeia (USP) about identifying polymorphic forms in their publication. None of the excipient publication (US and British) sources specifies forms. Due to lack of the authoritative source, we decided to put all excipients and their polymorphs in the subfile. ICDD's purpose is to solve problems for the customers. We would rather have all excipients and their polymorphs in the subfile than not having the subfile at all. Customers cannot solve their problems if there is no subfile at all. However, we will remove any compounds from the subfile if any individual has valid scientific logic to show that those compounds can not be used as excipients.

M. Davidovich mentioned that one form of calcium silicate is a suitable excipient for one drug but not for another. At Bristol Myers Squibb (BMS), different forms were tried for different drugs.

F. Wireko: It is better to have polymorphs in the subfile than not to have the subfile at all.

C. Floris was concerned about the ICDD image. She asked whether ICDD has a disclaimer about this.

The answer is that ICDD did state in the help file that the pharmaceutical/excipient subfiles contain their polymorphs.

T. Blanton will tell M. Bennett that the subcommittee discussed this issue and decided to keep available polymorphs in the subfiles until a scientific justification can be given otherwise.

#### 6. **Update on Disordered Structures-PDF4**

F. Wireko pointed out that part of the subcommittee's mission is to improve the database. This leads to the problems of missing Cambridge Structural Database (CSD) patterns in the ICDD database due to the problem of disorder. S. Kabekkodu gave a presentation about the problem: Disorder is when the electron density error is outside the tolerable limit of 15%. There are about 27,000 disordered entries and this subcommittee can select the important ones to be included into the ICDD database. T. Fawcett reported that Frank Allen of Cambridge Crystallographic Database Centre (CCDC) will re-examine the disordered bioactivity entries supplied by ICDD. T. Fawcett also mentioned that CCDC should have entries with CIF format at least for the last three years. F. Wireko would like to know how many of the disordered entries are duplicates. S. Kabekkodu answered that they are all from different literature references. A list of materials - bioactivity, Merck, sugar, small molecular weight amino acids, and common excipients will be considered. The action plan is for S. Kabekkodu to break down the disordered structures into material classes such as the above so that a task group can be set up to tackle them in order of priority.

#### 7. **PPXRD-6 Report Update**

T. Fawcett reported that PPXRD-6 in Barcelona had nine vendors, 52 attendees. Many attendees are also ICDD database customers. The symposium with the Rietveld quantitative analysis was a success. PPXRD-7 will be Orlando, Florida. PPXRD-8 will be in Asia or Europe with Asia as a priority. Many PPXRD-4 attendees' companies are the same as those of the PPXRD-6 attendees. It indicates that the European community is interested in the PPXRD symposium. Therefore, PPXRD serves its purpose in Europe. ICDD employed a private company to survey the customers' specific interest in the ICDD databases.

#### 8. **Update on (ICCOSS)-- International Conference on the Chemistry of the Organic Solid State**

M. Delgado reported that there is web site set up for the 18th conference. F. Wireko visited the web site and commented that it was very good. The first two days will have courses and two days of talks following. The conference expects 250 attendees. F. Wireko encourages attendees from this committee to attend ICCOSS. ICDD will participate in the conference and provide funding support per last year's subcommittee recommendation.

#### 9. **Adjournment**