

Organic and Pharmaceutical Subcommittee
March, 13 2013
ICDD Headquarters
F. Wireko, Chairman

1. Call to Order and Opening Remarks

Fred Wireko called the meeting to order.

2. Appointment of Minutes Secretary

Bridget Gavaghan appointed minute's secretary.

3. Roll Call and Attendance

4. Approval of Minutes from March 2012

Motion: Timothy Fawcett

Second: David Rendle

March 2012 meeting minutes approved.

5. Review of Mission Statement

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.

6. Board of Directors' Liaison Report (M. Delgado)

M. Delgado reviewed a special project to examine the top 200 pharmaceuticals by sales. The project has been a collaborative effort between Argonne National Laboratory, Jim Kaduk, and ICDD (S. Pagola). S. Pagola identified 63 pharmaceuticals that had no entry in the product. Thirty-two of the 63 were purchased. Data has been collected at Argonne and sent to Jim Kaduk to review. So far, data collected for eight pharmaceuticals and structures have been solved for three.

7. Update—Energetic Materials Database (J. Deschamps)

J. Deschamps has been comparing contents of Naval Research Laboratory (NRL) in-house database with the PDF to identify entries to be added to the PDF. NRL has 1186 entries for energetic materials. The explosives subfile in the PDF has 925 entries. J. Deschamps detailed the process of finding entries and showed examples of new, existing, and overlap entries. He also shared issues he encountered. There are entries in the PDF that are categorized as EXP that are not energetic materials. There are entries in the PDF that are energetic materials but are not in EXP subfile. And there are energetic materials that are not in the PDF at all. J. Deschamps proposed creating a new subcategory or to better define criteria for the explosives subfile. J. Deschamps presented a classification scheme that had already come up with 35 new entries and 2 new phases. It was proposed that a new task group be formed to classify energetic materials. J. Deschamps was made chairman and David Rendle joined the new task group. The subcommittee also welcomed suggestions for other people to join the new task group.

8. PPXRD-12 Report Update Headquarters (T. Maguire)

T. Maguire presented a report. PPXRD will run from 20-24 May 2013 at the Institute of Physics, Chinese Academy of Sciences, Beijing, China. There will be a two-day workshop on Fundamentals and Applications of XRD presented in Chinese. This workshop will be followed by 2.5 days of technical presentations from experts.

9. Future Tasks

T. Fawcett addressed potential new subfiles that are currently being populated that should be brought up at next year's meeting. He called these the 'anti-s and -icides'. This refers to compounds that are herbicides and fungicides or exhibit antibacterial, antiviral, or any kind of anti-biological activity. Currently, these compounds are being put in the Bioactive (BIA) subfile.

10. Other Matters

No other matters discussed.

11. Adjournment