International Centre for Diffraction Data
Organic and Pharmaceutical Subcommittee Meeting Minutes
Thursday, 11 March 2021; 1:00 pm – 2:00 pm
Fred Wireko, Chairman

1. **Call to Order** **F. Wireko**
   Attendance tracked through Zoom.

2. **Appointment of Minutes Secretary**
   Megan Rost was appointed to record minutes.

3. **Approval of Minutes from March 2019**
   Minutes approved by unanimous consent.

4. **Review of Mission Statement – no changes**
   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.

5. **Board of Directors Liaison Report** **J. Kaduk**
   There were no motions to the Board from previous year. Headquarters' report on various Organic database activities part of the meeting presentations.

6. **Activities Update** **S. Gates-Rector**
   a. 2021 PDF-4/Organics
      i. 2019 tasks -enable use of SMILES notation (2D structure search), authors/grantees have option to submit SMILES notation, editors can view and edit 2D structure with in-house software; DataQuaker.
      ii. 2021 PDF-4/Organics now has 2D structure search capability
          526,513 entries- SMILES notation converted
          6,675 entries – SMILES notation supplied by database department

   b. CCDC Collaboration re-established in 2020
      i. Targeted entries from priority subgroups
         (BIA, PHR, EXC, FOR, EXP, PIG, POL, CAT, MOF)
      ii. 6,000 new entries per year
      iii. 60,000 catch up entries over 2020-2023
      iv. Now able to publish atomic coordinates in PDF entry
      v. Working with CSD for refinement of data delivery

   c. PDF-4/Organics Production
      i. Release 2021
         - ICDD-05- 3,002 processing/2,584 published
         - CSD-02- 8,354 processing/5,478published
      ii. Release 2022

- ICDD-05- 1,330 processing
- CSD-02- ~46,000 processing

d. Density issues. Calculated electron density vs. structural electron density that differ over 15% are excluded from the database. Many of the CSD entries have this error.
   i. "SQUEEZED' solvents, chemical formula and published atomic coordinates have discrepancy, disordered structure where atom occupancies are not given, and hydrogen atomic positions are not given.
   ii. Headquarters request advice and a task group to address this issue. Suggestions on how to address these entries:
      - Add entries with warning as partial powder entry with low quality marks
      - Only add entries that the DB is missing completely

e. Pharmaceuticals Project — A. Gindhart
   i. Set 70 – 15 patterns
   ii. Set 71 – 22 patterns
      - Issues with ordering new samples due to COVID-19

f. PPXRD-17 Report Update — T. Maguire
   i. 2020 Meeting cancelled due to COVID-19
   ii. EPDIC17 - Pharma satellite for June 2022

7. Future Tasks

ACTION ITEM:

a. Headquarters requests a task group to address electron density issues from CSD database entries.
   Suggestions for task group are S. Kabekkodu, S. Gates-Rector, M. Rost, F. Wireko, T. Fawcett, J. Kaduk, G. Stephenson

b. Suggest some meetings continue virtually due to COVID, when possible.

8. Organic and Pharmaceutical chair

G. Stephenson will take over as the Organic and Pharmaceutical Subcommittee Chair.

9. Other Matters

Nothing to report

10. Adjournment

Motion moved by S. Gates-Rector
Second by T. Blanton
Meeting adjourned.