Micro and Meso Subcommittee Meeting Minutes
Wednesday, 13 March 2019
International Centre Headquarters
Conference Room D
2:00 p.m. – 3:00 p.m.
Cyrus Crowder, Chairman

1. Call to Order — Cyrus Crowder

2. Appointment of Minutes Secretary — Melissa Mitchell

3. Approval of Minutes of the 2018 March Meetings

   **Motion:** C. Crowder moved to approve the 2018 Micro and Meso Subcommittee Meeting Minutes. Seconded by S. Quick
   **Motion passed. 8 Yes, 0 No, 0 Abstain**

4. Review of Mission Statement

   The Micro and Meso Subcommittee will identify systems in which ordered pores, channels, and/or cages on the nano, meso, or microscale are important in the diffraction and the performance of the material; and will identify how the ICDD and PDF can serve the scientific community by providing reference and resource materials, by creating or adapting a formalized description of these materials, and contributing to techniques by which these materials can be characterized.

5. Board of Directors' Liaison Report — Matteo Leoni

   Nothing to Report at this time.

6. Automated Framework Topology — Suri Kabekkodu

   No time remaining to cover this topic. Will need to refer to S. Kabekkodu to elaborate on results of the Topology & Topos Studies project from V. Blatov's visit in May.

7. Report from Zeolite Task Group — Susan Quick

   No time remaining to cover this topic. However, Susan Quick's report that was to be presented is included here:

   **Zeolite and Molecular Sieve Task Group Report March 13, 2019**

   **October 2018 Meeting**
   - 4 task group members attended.
   - Reviewed ~1900 entries
   - Assigned IZA structure type codes
   - Assigned primary vs. alternate designations using cluster analysis
   - Reviewed new IZA structure type designations and searched for representative entries in PDF.
   - Identified PDF entries that were not flagged as zeolites and consequently had no structure type code.

   **March 2019 Meeting**
   - 3 task group members attended.
   - Reviewed ~ 400 entries
   - Assigned IZA structure type codes
   - Assigned primary vs. alternate designations using cluster analysis
   - Reviewed entries with zeolite flag, but without STC designation.

**2020 Release of PDF4**

- Contains ~5600 entries for zeolites and molecular sieves.
- Missing 36 of the 245 IZA structure types.
- About 10 of these 36 have PDF entries that were identified during March and October meeting.

**Future Work**

- Continue the current work
- Contact IZA structure commission about phases that "appear" to be zeolites, but do not have STC designations at this time.

8. Proposed keywords TBD

Discuss keywords to add to PDF

a. Definitions
b. Criteria for ICDD to add keyword to a reference

V. Peterson gave a report on the 6th International Conference Metal Organic Frameworks & Open Framework Compounds that she attended in New Zealand. Plenary speakers were Omar Yaghi & Richard Robson. V. Peterson spoke with several people, all refer back to the IUPAC paper ("Terminology of Metal-Organic Frameworks and Coordination Polymers (IUPAC Recommendations 2013)", Batten, et.al.,Pure Appl. Chem., Vol. 85, No. 8, pp. 1715–1724, 2013), and they recommend that they do not go outside of that detail to identify MOFs and hold to that standard. Terminology recommendations are as follows: IUPAC proposed a hierarchy of terminology from the most general to general terms starting with Coordination Polymers, then Coordination Networks is a subset of that, then MOFs are a further subset of that. There was much discussion with differing opinions being presented. At the end of the discussion the following motion was passed for presentation to the Technical Committee.

**Motion:** **The Micro and Meso Subcommittee recommends to the Board of Directors that ICDD follow the guidelines specified in the paper by Batten, et al. for giving the IUPAC names for MOF's, and if not available, use the name prescribed by the author and/or the chemical name.**

C. Crowder moved to approve the motion.
Seconded by V. Peterson
**Motion passed. 9 Yes, 0 No, 1 Abstain**

9. New Business

Mesoporous Task Group – No time remaining to cover this topic.