

Micro and Meso Subcommittee Meeting Minutes
Wednesday, 14 March 2018
International Centre Headquarters
Conference Room D
11:00 a.m. – 12:00 noon
Cyrus Crowder, Chairman

1. Call to Order Cyrus Crowder
2. Appointment of Minutes Secretary Melissa Mitchell
3. Approval of Minutes of the 2017 March Meetings

Motion: S. Mixture moved to approve the 2017 Micro and Meso Subcommittee Meeting Minutes.
Seconded by S. Quick
Motion passed. 15 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 material, 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

Leoni stated that Vladislav Blatov is working on a Topology project with ICDD. Blatov will be here at ICDD training staff on the use of his program TOPOS_PRO.

6. Automated Framework Topology Tom Blanton
(Response to Motion/AI)

Suri put together a group of phases for Topology and TOPOS studies. Blatov will be here in May to assist with his TOPOS project/tool. JBlanton will be setting up an additional tab in the database. The additional information will only work with the data that has structural information and will identify if the structure is 2D or 3D. Looking to get about 1600 additional entries from the project into the 2019 PDF-4+ database.

7. Report from Zeolite Task Group Susan Quick

Quick stated the Zeolite Task Group met in October to continue the review of Zeolites in the database that have not be assigned structure type codes. Kaduk worked on cluster analysis to get primary patterns for those codes that have more than 10 patterns to facilitate search/match for zeolite patterns in the database. Over the last week (Friday, 3/9/18-Sunday, 3/11/18), the group continued their review and overall added about 200 structure type codes to phases that did not have them in the past. Also, they found new zeolite information and identified phases that were not previously filed as zeolites. In addition, the group found representatives for previous structural type codes that are assigned by the International Zeolite Association. Currently there are about 300 structure type codes and we are missing representatives for about 25. Currently we have good coverage with 275 out of 300 represented in the database. The Zeolite task group is continuing to work and do what headquarters needs assistance with first, then move on to doing more research.

8. Proposed keywords TBD
Discuss keywords to add to PDF
 - a. Definitions

b. Criteria for ICDD to add keyword to a reference

Since searching for Metal Organic Frameworks (MOFs) is not optimized in the database, we would want to look into getting keywords in the database to make searching easier. Crowder did a search for MOF in the PDF database; there were only 27 hits on the search, and in reality, only 7 were actual MOFs. Crowder has done extensive searching and a spreadsheet of information for reference has been made – there has been much discussion within the group.

Question comes up: Do we need a small group to work on a definition change for MOF in the ICDD database? (Gates-Rector) There are currently 265 labeled as a MOF Subclass in database.

Peterson will be attending a MOF conference in December in Australia and will talk to her contacts for help and assistance with the database. She will then bring back what she learns to ICDD.

Decisions on keywords and MOF definitions are delayed for a year until the Topology/TOPOS Project is implemented and the MOF Conference results are available.

9. New Business

Mesoporous Task Group

No one would chair, therefore no task group was put together. Could be 100 sitting unnamed in the database. We will revisit after the topology project with Blatov is implemented.

10. Adjournment