

Micro and Meso Subcommittee Meeting Minutes
Wednesday, 16 March 2016
S. Quick, pro-tem, Chairman

1. Call to Order S. Quick
2. Appointment of Minutes Secretary – Michael Carr
3. Approval of Minutes of the 2015 March Meetings

Motion #1: The Micro and Meso Subcommittee recommends to the Technical Committee that the 2015 minutes be approved.
M. Leoni moved. C. Crowder seconded. 8 in favor, 0 oppose, 0 abstain

4. Review of Mission Statement

The Micro and Meso Subcommittee will identify systems in which ordered features 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 M. Leoni
6. Automated Framework Topography T. Blanton/S. Kabekkodu
(Response to Motion/AI)

S. Kabekkodu gave a brief report on programs explored to assess pore size and other micro/meso characteristics. S. Kabekkodu commented on the three programs below and summarized them as being impractical and too time consuming for headquarters to attempt to implement into the database due to difficult output analysis. A script cannot be used to automate the process because probing radius needs to be changed on a case by case basis.

- a. ToposPro – pore size, pore volume calculation, Voronoi-Dirichlet polyhedral
- b. PLATON – Pore volume calculation, Solv module (crystal structure solvents)
- c. MOFormics (from Princeton) – Web based, more than day per structure. Many jobs failed.

7. Report from Zeolite Task Group (ZTG) S. Quick

ZTG met in October and March to assess zeolite names, zeolite structure type codes, respond to staff problems, confirm molecular sieve or zeolite, revise/update already existing patterns, primary/alt. flags, and cluster analysis (J. Kaduk).

8. Proposed keywords S. Speakman
Discuss keywords to add to PDF
 - a. Definitions
 - b. Criteria for ICDD to add keyword to a reference

9. New Business

Mesoporous Task Group

Discussion of creating a task group to assess porous framework materials. Not all porous materials are Metal Organic Frameworks. Need to determine what is a MOF and what is not. Vanessa Peterson expressed interest, but needed time to determine how much time she can commit to the effort and what volunteers may be available to join the group. There also needs to be more coverage on conditions of measurement (ambient/non-ambient) for zeolites.

10. Adjournment