

Minutes for Micro and Meso Subcommittee
Scott Speakman, Chairperson
Wednesday, March 12, 2008

1. CALL TO ORDER

Meeting was called to order by Scott Speakman.

2. APPOINTMENT OF MINUTES SECRETARY

Michael Carr

3. DISCUSSION OF MEMBER INTEREST

This is a brand new subcommittee, created as a by product of the Minerals Subcommittee because the Zeolite Task Group was being assigned more and more compounds that were out of the context of zeolite study. These materials did not fit into the scope of any other subcommittee, so it was determined that a new subcommittee needed to be formed. The group is trying to figure out exactly what type of materials will be studied as part of this group and why.

Projected materials for subcommittee study:

- Zeolite and sieve materials
- Oxalates
- Micro and mesoporous materials
- Clathrates
- Prussian blues
- Pillared clays
- Metal-organic frameworks
- Others including quantum dots, modulated structures, and nanomaterials

4. DISCUSSION OF MISSION STATEMENT

- MOTION #1 Scott Speakman moved, motion seconded by Sue Quick.

The Micro and Meso Subcommittee recommends the following mission statement:

The Micro and Meso Subcommittee will identify systems in which 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.

Vote: 16-0 in favor of the motion.

Group agreed to use this as the current mission statement, but acknowledged that it may be subject to change at a later date.

5. CONSIDERATIONS OF ZEOLITE TASK GROUP

Questions were raised about whether or not quantum dots will be part of this subcommittee. Discussion was back and forth, but the general consensus of the group was that they don't know, at this point, because the subcommittee is so new. Discussions will have to continue regarding how quantum dots will be covered.

Chairpersons comment: this group was initially formed to address zeolites and other micro and mesoporous materials (MMM). The ongoing discussion is to what extent do we want, or are we able, to include other

material groups where micro- or mesostructural components are important; this includes quantum dots, ordered mesoporous materials, and modulated structures. A mission statement was adapted that gave us the flexibility to expand into these other areas as we see fit.

6. REPORT OF ZEOLITE TASK GROUP

The task group met in June 2007 and reviewed 295 patterns and met again in January 2008 to review 167 patterns. Along with the review of patterns, several other tasks were performed by the task group. The task group requested that Headquarters review the IZA web site annually for new structure type codes for input to the database. This task was put on hold due to prioritizations of work assignments.

- MOTION #2 Sue Quick moved the motion, motion seconded by Scott Speakman.

The Zeolite & Molecular Sieve Task Group requests \$5000 to allow the members to meet twice in 2008-2009 fiscal year. During these meetings they plan to

- Continue review for primary vs. alternate
- Review of unnamed zeolites
- ID of non-flagged zeolites in currently published databases
- Evaluate automated procedures to assign zeolite structure type code
- Continue evaluation of new patterns

Vote: 12-0-4 in favor of the motion, Mike Bennett and Sue Quick abstained by name.

7. Al Rohrman is a new member of the subcommittee.
8. Scott Speakman asked the members to brainstorm a better name for the subcommittee. The group was asked to contact Scott Speakman if they are interested in joining the new subcommittee.
9. Adjournment
Please see [Scott Speakman's presentation](#) for details of the adjournment.
The attendance sheet is on file at headquarters.

Micro and Meso Subcommittee

Scott Speakman

12 March 2008

Agenda

- Call to Order
- Appt of Minutes Secretary
- BoD Liaison Report
- A Brief History
- Discussion of Member Interest
- Discussion of Mission Statement
- Report of Zeolite Task Group
- New Business

A Brief History

- Created on the recommendation of the Minerals Subcommittee in March 2007
- To support work of Zeolite & Molecular Sieve Task Group
- To address phases other than zeolites and molecular sieves that are micro- or mesoporous
 - these are currently not flagged in a manner for discrete retrieval in PDF
 - The MMM supergroup may address materials containing pores and channels with the smallest dimension of $>4 \text{ \AA}$

Micro and Mesoporous Materials

- Zeolite and Molecular Sieves
- Oxalates
- Mesoporous Materials
- Clathrates
- Prussian blues
- pillared clays
- metal-organic frameworks
- other

Other materials to consider

- quantum dots
- nanostructured/mesostructured

Discussion of Member Interest

- Are there any doubts or concerns about the establishment Micro and Meso Subcommittee
- Any concerns about pitfalls in the creation of such a subcommittee

Mission Statement

- A very rough draft of a mission statement
- The Micro and Meso Subcommittee will identify systems in which ordered non-atomic/super-atomic/poly-atomic 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.

Point of Discussion 1

- What is the scope of this subcommittee?

Point of Discussion 2

- What can this subcommittee contribute to the ICDD and the PDF?
 - enhancing the datamining capabilities
 - new physical properties
 - description of pores

Point of Discussion 3

- Is there a more descriptive name for this group?

Report of the Zeolite Task Group

**Zeolite & Molecular Sieve
Task Group
Report
March 2008**

Zeolite Task Group Report

- Review patterns to be published
 - Confirm that they are Zeolite and Molecular Sieve Materials?
 - Assign zeolite structure type code (3 letters)
 - Assign a “zeolite” name
- Respond to problems identified by ICDD editorial staff.

Current Publication

- 1429 flagged Zeolite and Molecular Sieve patterns in experimental (00)
- 1257 flagged Zeolite and Molecular Sieve patterns in ICSD (01)
- 445 flagged Zeolite and Molecular Sieve patterns in LPF (04)

June 2007

- 295 patterns reviewed
- New zeolite and molecular sieve phases in experimental PDF (Lisa)
- Referred 15 patterns to Mesoporous group(?)
- Referred approximately 40 patterns to mineral task group for name
- Removed zeolite flag from approximately 20 patterns (mostly in LPF)
- Printout of recommended changes was given to Lisa.

January 2008

- 167 Patterns reviewed
- Experimental zeolite and molecular sieve phases to be published (Lisa)
 - 27 were reviewed and 3 were rejected
- Reviewed 43 patterns in experimental data base and added zeolite name
- Reviewed 92 patterns in 6 STC for primary vs. alternate designation. Cross references between primary and alternate were recommended.

Current Rules Primary vs. Alternate

- Designation of primary vs. alternate phases – Add both a calculated and experimental pattern when available.
- Add both a hydrated and dehydrated pattern when available.
- New primary representative for $>3\%$ change in volume (still not fully tested) independent of chemistry
- When same reference is in 01 and 04 sets, designate 04 as primary because structural parameters are available

Review for Primary vs. Alternate

- Beginning with smaller populated STC to establish rules, then apply to larger populated STC.
 - FAU STC (includes faujasites, zeolites X and Y) - Currently has approximately 300 patterns.
 - LTA STC - currently has approximately 350 patterns

March 2008

- Identified 5 patterns of FAU STC that should not be flagged as zeolites. (Will ask Lisa to remove name, zeolite STC, and zeolite name.)
- Identified 55 patterns that have not been flagged as zeolites at this time. HQ will receive a report of these materials plus STC and zeolite name.

Motion 1

- The Zeolite & Molecular Sieve Task Group requests \$5000 to allow the members to meet twice in 2008-2009 fiscal year. During these meetings we plan to
 - Continue review for primary vs. alternate
 - Review of unnamed zeolites
 - ID of non-flagged zeolites in currently published databases
 - Evaluate automated procedures to assign zeolite structure type code
 - Continue evaluation of new patterns

New Members

- Anyone interested in joining this task group should contact Mike Bennett, Cyrus Crowder, Sue Quick, or HQ.

Questions

Other Micro- and Meso- Porous Materials

- Currently in the Database there are patterns, other than zeolites and molecular sieves, that are micro- or meso- porous. These patterns are not flagged in a manner that allows easy retrieval/identification.

Possible Supergroup

- Micro- and Meso-porous materials (MMM) – materials containing pores and channels (> 4 angstroms)
 - Zeolites & Molecular Sieves (already a task group)
 - Oxalates (possibly Natalie or Thierre from France)
 - Mesoporous materials
 - Clathrates
 - Prussian Blues
 - Pillared Clays
 - Metal Organic Frameworks (MOF)
 - quantum dots

Motion

- The Zeolite Task Group recommends that ICDD should create a Micro- and Meso-porous Materials supergroup. Preliminary definition for this supergroup is materials containing pores and channels with smallest dimension of > 4 angstroms. Zeolite and Molecular Sieve Materials would be one member of this supergroup.

Motion passed 8-0-0

Questions ?????

New Business

- prototype structures for zeolites
- tracking humidity information