

Minerals Subcommittee
March 21, 2007
3:00 – 4:00 pm
A. Roberts and S. Quick, Acting Co-Chairs

1. Call to Order: The Minerals Subcommittee was called to order by A. Roberts and S. Quick.
2. Appointment of Minutes Secretary: J. Dann was appointed as secretary.
3. Approval of Minutes of the 2006 March Meetings: Minutes from the March 2006 meeting were approved.
4. Board of Directors' Liaison Report: E. Antipov reviewed responses to motions from March 2006 subcommittee meeting.
 - a. R. Goehner moved that a sum of up to \$1,500 be allocated for a Zeolite Task Group meeting in June 2006 to cover travel expenses. The meeting will be coincident with the XRD-1 clinic. (Travel R&D fund)

Response: These funds have been added to the TC R&D funds in the 2006-2007 Budget. The meeting was held and conducted.

- b. R. Goehner moved that a sum of up to \$3000 be allocated to finance travel for P. Bayliss to attend the March meeting 2007.

Note: As suggested in prior correspondence, the Minerals Task Group expects to receive a list of proposed changes to the Experimental Mineral Database by January 1, 2007. This is to ensure that the Minerals Task Group has adequate time to review the suggested changes.

Response: These funds have been added to the TC R&D Funds in the 2006-2007 Budget. However, notification to P. Bayliss was not timely and P. Bayliss did not have the proposed changes available by January 1.

Publication – The list of proposed changes was not submitted to HQ by January 1, 2007. T. Kahmer sent correspondence to P. Bayliss asking if he would like to submit the changes in time to come to the Task Group meeting in June 2007, or if he would prefer to come to the March 2008 meeting.

- c. R. Goehner moved that useful books are added to the ICDD library. The books include data to be considered in the database.
 - i. Dana's New Mineralogy: The System of Mineralogy of James Dwight Dana and Edward Salisbury Dana (\$325).
 - ii. Handbook of Mineralogy; full set of 6 books (silicates have volumes) by Anthony, Bideaux, Bladh, Nichols (\$600).
 - iii. Strunz Mineralogical Tables (9th Edition) by Strunz and Nickel (\$158).

- iv. An Introduction to the Rock-Forming Minerals (2nd Edition) by W. A. Deer, R. A. Howie, J. Zussman (\$90, paperback; 170, hard cover).

Headquarters will purchase the books (motion not necessary).

Response: Books were purchased by the Publication Department and are in the ICDD library.

5. Report from Minerals Task Group: A. Roberts reported that L. Bernstein, A. McDonald, A. Sabino and he met June 20-21, 2006 to review 57 patterns. The Task Group also met on Sept. 13, 2006 to review an additional 50 patterns. The ICSD and LPF editorial work was also discussed.
6. Report from Zeolite Task Group: S. Quick reported that the Zeolite and Molecular Sieve Task met twice last year. The accomplishments were shown via PowerPoint and are summarized below.

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.

In 2006 Release

- 1363 flagged Zeolite and Molecular Sieve patterns in experimental (00)
- 829 flagged Zeolite and Molecular Sieve patterns in ICSD (01)
- 17 flagged Zeolite and Molecular Sieve patterns in LPF (04)

June 2006 Meeting

- 247 patterns reviewed
- New zeolite and molecular sieve phases in experimental PDF (L. Lanno)
- Review of names in calculated patterns (F. McClune)
- ID of phases not designated as zeolite and molecular sieve material (S. Kabekkodu’s program)
- Assigning 3 letter code (F. McClune/L. Lanno)
- Printout of recommended changes was given to L. Lanno.

November 2006 Meeting

- 78 Patterns reviewed
- Experimental zeolite and molecular sieve phases to be published (L. Lanno)
 - 18 were reviewed and eight were accepted
- Designation of primary vs. alternate phases – reviewed patterns of a few of zeolite structure type code with low population of patterns (<20). Cross references between primary and alternate were recommended. Developing and revising criteria.
 - Include both a calculated and experimental pattern when available

- Include both a hydrated and dehydrated phase when available
- New primary representative for >3% change in volume (still not fully tested) independent of chemistry
- Noted that flag indicating a shoulder for a peak was missing from new display format. Problem was reported to F. McClune.
- List of recommended changes were given to L. Lanno.
- Gave HQ a list of new zeolite structure type code designations and structures for these materials so the patterns could be calculated by HQ.

The task group had three motions:

A. The Zeolite Task Group (C. Crowder, M. Bennett, S. Quick) requests \$4000 to allow the three members to meet twice in 2007. 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

Moved by S. Quick and seconded by P. Wallace.

Motion passed 8-0-3 with abstentions by the task group members.

B. The Zeolite Task Group recommends that a comment (notification) be automatically added to Zeolite and Molecular Sieve patterns that have been designated as primary. This comment should indicate that alternate patterns may potentially exist with different chemical composition and that a match with a primary phases does not infer chemical composition. This comment is to supplement the cross-reference.

After discussion, the motion was tabled.

C. The Zeolite Task Group recommends that ICDD investigate the addition of a new flag indicating atypical atmosphere surrounding the sample produces a pattern that is distinct from the pattern that would be obtained under typical conditions.

Moved by S. Quick and seconded by C. Crowder.

Motion passed 9-0-1.

7. What defines a "Mineral Related" Phase?: T. Fawcett reported that a Mineral Related Subfile has been created to include materials such as minerals/gems/non-ambient mineral phases, synthetic minerals, etc. These materials may not be considered minerals by the usual criteria, but are still useful.
8. Mesoporous and Microporous Supergroup: M. Bennett reported that the database currently contains patterns from phases other than zeolites and molecular sieves that are micro- or meso-porous. Currently, these phases are not flagged in a manner that would allow easy retrieval. These phases are often referred to the Zeolite Task Group, but do not fit criteria for the Zeolite and Molecular Sieve subfile. Therefore, it is recommended that a supergroup be

created. This supergroup could be called Micro and Meso- porous Materials (MMM) and would be populated with phases that contain pores and/or channels >4angstroms. Subgroups could be:

- a. Zeolites & Molecular Sieves (already a task group)
- b. Oxalates (possibly N. Audebrand or T. Bataille)
- c. Mesoporous materials
- d. Clathrates
- e. Prussian Blues
- f. Pillared Clays
- g. Others

Therefore the following motion was proposed:

D. The Zeolite Task Group recommends that ICDD 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.

Moved by M. Bennett and seconded by P. Wallace.

Motion passed 8-0-0.

9. New Business: None at this time.

10. Adjournment: The meeting was adjourned a 4:10 pm.