

## **Minerals Subcommittee Meeting Minutes 13 March 2013**

1. Call to Order – The Minerals Subcommittee Meeting was called to order at 2:02 p.m. on Wednesday, 16 March 2013 by Chair J. Kaduk.
2. Appointment of Minutes Secretary – S. Quick was appointed secretary.
3. Approval of March 2012 Minutes – J. Faber moved that the minutes be accepted and P. Wallace seconded. Motion carried.
4. Board of Directors' Liaison Report – S. Misture reported that the 2012 motion to allocate funds for Mineral Task group was approved.
5. Report from Mineral Task Group and Other Info – A. Roberts reported that the Minerals task group considered 56 new patterns in July of mineral phases. A. Roberts is continuing to the calculated mineral entries (from ICSD and LPF).
6. New Business –
  - a. Task Group Support.

**Motion 1: The Minerals Subcommittee recommends to the Technical Committee that up to \$5000 be allocated to cover expenses for the Minerals Task Group to meet at least once in FY 2013/2014.**

Moved by M. Leoni and seconded by A. Roberts

Motion passed 13-0-2 with L. Bernstein and A. Roberts abstaining by name.

- b. What do mineralogists want?

L. Bernstein reported that some of the new information presented in the software is not considered useful for mineralogists and may discourage them from using the database. The mineral subfile originally had a narrow vision on containing naturally occurring minerals. With the addition of entries from LPF and ICSD and additional information, the data base may have become too cluttered for mineralogists. J. Kaduk asked if a tutorial would help the mineralogical community. M. Leoni asked about feedback from customers. P. Wallace asked how the PDF4+ could be made easier to use. L. Bernstein commented that mineralogists do not use the database for other properties. T. Fawcett stated that there were two questions:

What do mineralogists want?

What do people who work with minerals want?

Mineralogists need to communicate their needs/problems to ICDD so problems can be fixed and/or tutorials can be developed.

- c. Mineral Group Classification for calculated patterns.

J. Kaduk reported that a search on amphiboles retrieved only 64 patterns that were in the experimental patterns (00), but not the calculated patterns from ICSD (01) or LPF (04).

A. Roberts stated that he was working on adding designations to the calculated patterns.

**Motion 2: That all mineral patterns be assigned a Mineral Classification, where appropriate.**

Moved by J. Kaduk and seconded by P. Wallace  
Motion passed 15-0-0.

d. Space Group Number Ranges –sub/supergroups

J. Kaduk reported the ICDD was considering adding the utility of searching on a range of space group numbers. The feasibility and usefulness of using a collection of space group numbers that represented subgroups and supergroups was discussed and resulted in the motion given below. M. Leoni asked if PDF-4+ had the functionality. T. Fawcett replied that it did not, but the addition would not be hard to implement.

**Motion 3: That, as part of searches on multiple space group numbers, searches on maximal sub-groups and minimal super-groups be pre-defined.**

Moved by J. Kaduk and seconded by J. Faber  
Motion passed 13-0-0.

e. NBS\*Lattice functionality in PDF-4+

J. Kaduk stated the ability to sub/supercell searches was a very useful utility in NBS\*Lattice and could be added to PDF4+. C. Hubbard asked about the results for determining high symmetry than that reported. S. Kabekkodu responded that the code for identifying missing symmetry was already in place. The discussion resulted in the following two motions (4 and 5).

**Motion 4: That, in addition to reduced cell searches, the ability to carry out systematic searches on sub-and super-cells (with output of derivative cell calculations) be incorporated into PDF-4+.**

Moved by J. Kaduk and seconded by L. Bucio.  
Motion passed 15-0-1.

**Motion 5: That the reduced cell matrix analysis output (“metric symmetry exceeds crystal symmetry,” etc.) be provided in PDF-4+.**

Moved by M. Leoni and seconded by P. Wallace  
Motion passed 13-0-0.

f. Minerals Group List

J. Kaduk reported that P. Bayliss had sent a message with his concerns that the Mineral Group List contains errors and is not up to date. It was recommended that the corrections and additions should be forwarded to A. McDonald.

g. Cation Site Labels

J. Kaduk reported that a message from P. Bayliss also contained concerns about the cation site labels in the Minerals Group List. A. Roberts commented that he had been part of the group that initially assigned the labels, but does not actually use the

assignments. Again, it was recommended that corrections and additions be forwarded to A. McDonald.

h. Other

T. Fawcett reported that the consummation and production of minerals remains very high and should remain a fertile business for the next 10 years.

7. The meeting was adjourned at 3:00 p.m.