

Synchrotron Subcommittee Minutes
16 March 2011
ICDD Headquarters
M. Suchomel, Chairman

Call to Order

M. Suchomel called the meeting to order.

Appointment of Minutes Secretary

A. Gindhart appointed as minute's secretary.

Approval of Minutes from March 2010 Meeting

March 2010 meeting minutes approved.

Motions: M. Suchomel

Second: S. Misture

4 For

0 Opposed

0 Abstained

Board of Directors' Liaison Report (J. Faber)

Synchrotron Subcommittee Motions

- 26 BoD 310-19A(1)i Misture moved to encourage Grant-in-Aid recipients to utilize increasingly available mail-in synchrotron powder diffraction resources to compliment in-house lab based measurements, especially for complicated patterns or patterns prone to preferred orientation and related effects.

Note: Subcommittee will help to write the letter.

Response: Publication Department – The following sentence was added to the Grant-in-Aid acceptance letters: “The Grant-in-Aid Committee encourages the recipients to use increasingly available mail-in synchrotron powder diffraction resources to compliment in-house lab-based measurements, especially for complicated patterns or patterns prone to preferred orientation and related effects.”

- 27 BoD 310-19A(1)i Misture moved that DataQUACKER be modified to support web based powder diffraction submissions, with corresponding communications to the data submitter to ensure that the data has been transmitted properly.

Response: Publication Department – Initial meeting with the Science Department took place for the program design. However, since that meeting, D. Sagnella's priority has been modifying the DataQUACKER program to abstract modulated structures in timing with the commercial release of the modulated structure subfile. Work is continuing on the web submission.

Response to First motion- Publication Department added a line into the Grant-in-Aid acceptance letter encouraging the Grantees to use the mail-in synchrotron powder diffraction resources.

Response to Second motion- Publication Department's initial meeting with the science Department took place for the program design. However, since that meeting D. Sagnella's priority has been modifying DQ program to abstract modulated structures in timing with the commercial release of the modulated structures subfile. Work is continuing.

General Discussion

It was discussed that the subcommittee should provide a detailed list of the currently available mail-in powder diffraction programs available to the user. The subcommittee asked that ICDD headquarters make this information available to all of its Grantees. This could be done via the website, emails, etc.

Online Submission Discussion

It was discussed to make the submission program restricted to 1 compound per CIF. The user can submit as many CIF's as they choose. D. Sagnella mentioned that more than one compound would make the CIF import too complex discouraging the submitter.

D. Sagnella will continue to work on a "Slim" version of DataQUACKER keeping it simple and sticking with the most important items needed for the database (Formula, Cell parameters, etc.).

R. Papoular mentioned about trying to have data submitted to the ICDD concurrently as users submit to different Journals. S. Kabekkodu replied that the ICDD has been unsuccessful in the past at having journals agree, but he mentioned it is highly encouraged by the ICDD. Currently, the information is written for once the article has been published and retrieved by the bibliographers.

R. Papoular also wanted to know how many entries a user should submit to the ICDD when they do several temperature or pressure experiments. S. Kabbekodu's response was to submit all the entries that the user would like to submit and then, at the Editorial level, the ICDD will choose a select number of those entries to continue through processing.

Expanding the Subcommittee Scope

M. Suchomel suggested expanding the scope of the subcommittee to include Neutron Diffraction. A new name and Mission Statement was presented to the subcommittee.

The new subcommittee name introduced was:
"Synchrotron & Neutron Scattering Methods."

The Mission Statement was as follows:

"The Synchrotron & Neutron Scattering Methods Subcommittee of the International Centre for Diffraction Data (ICDD) will connect the ICDD's Technical Committee with the international synchrotron and neutron scattering community. It will educate ICDD members about advances within the community, and help identify new opportunities to enhance ICDD databases. The subcommittee will provide recommendations to address unique aspects associated with these experimental methods, and will assist the technical staff of the ICDD to integrate information obtained at synchrotron and neutron scattering facilities into the ICDD databases."

Synchrotron Subcommittee Motions

Motion 1

The synchrotron subcommittee recommends to the Technical Committee that additional information about mail-in powder diffraction resources as provided by this subcommittee, be made available to grant-in-aid recipients, and that there is continued encouragement to use the resources for complex patterns.

Motions: M. Suchomel

Second: S. Misture

4 For

0 Opposed

0 Abstained

Motion 2

The synchrotron subcommittee recommends to the Technical Committee that DataQUACKER be modified to support web based powder diffraction submissions, with corresponding communications to the data submitter to ensure that the data has been transmitted properly.

Motions: M. Suchomel

Seconds: J. Faber

5 For

0 Opposed

0 Abstained

Motion 3

The Synchrotron Subcommittee recommends to the Technical Committee that the name and mission of the subcommittee be modified to include both Synchrotron and Neutron scattering methods. As such; the new subcommittee name would be:

"Synchrotron & Neutron Scattering Methods"

The new mission statement will be:

"The Synchrotron & Neutron Scattering Methods Subcommittee of the International Centre for Diffraction Data (ICDD) will connect the ICDD's Technical Committee with the international synchrotron and neutron scattering community. It will educate ICDD members about advances within the community, and help identify new opportunities to enhance ICDD databases. The subcommittee will provide recommendations to address unique aspects associated with these experimental methods, and will assist the technical staff of the ICDD to integrate information obtained at synchrotron and neutron scattering facilities into the ICDD databases."

Motions: M. Suchomel

Second: V. Peterson

5 For

0 Opposed

0 Abstained

Adjournment