

International Centre for Diffraction Data
POLYMERS Subcommittee Meeting Minutes
Wednesday, 16 March 2016
L. Liu, Chairman

1. Call to Order and Opening Remarks L. Liu
2. Appointment of Minutes Secretary
J. Quagliarello was appointed to record minutes.
3. Roll Call and Attendance
See attendance sheet.
4. Review of Mission Statement
Read through by L. Liu and no changes were suggested.
5. Approval of the 2015 Minutes
Minutes were accepted as written.
6. Report of Board Liaison J. Anzelmo
No report to give.
7. Status of Polymer Activity and Discussion

T. Blanton commented about the polymer tutorial, saying it doesn't get into specifics about using the database. T. Blanton presented a PowerPoint presentation starting with a slide mentioning how a Polymer Workshop was planned for October 2015, but was not held due to low number of people signing up to attend. The preferred attendance was at least 10 people. It has not been scheduled for 2016, but they will revisit the idea in the future.

For 2016 release, 46 new entries classified as Polymer will be added to the PDF-4 databases. Meanwhile, we are continuously looking into the database for more Polymers. T. Blanton mentioned how coordination of polymers are not considered polymers, but only compounds with carbon or silicon backbones. In addition, twelve new entries will be added as part of the ICDD polymer project—seven amorphous, five semi-crystalline, and four with unit cell indexing.

T. Blanton displayed a chart with each of the 12 new polymers by PDFID, name, chemical formula, and common name. T. Blanton mentioned that Nylon 11 had an issue with indexing because there were not enough peaks in the powder data.

T. Blanton mentioned we are looking for polymer samples targeted as pharmaceutical-related, specifically the raw data patterns. He mentioned that J. Dann published a paper on Chitosan with figures, but no raw data. J. Dann mentioned that all 1D patterns in the paper came from 2D images. T. Blanton replied that 2D data would be great.

L. Liu commented that he can send data for the PEG polymer. He also stated that crystalline polymers are very important to have. He said for crystalline polymers, we want to have as many peaks as possible, which requires samples to be well crystallized.

T. Blanton agreed with L. Liu. T. Blanton said we have to consider what we're going to see in real polymers. Sometimes it is not possible to get purely crystalline.

J. Anzelmo mentioned something regarding an action item from a previous board meeting about polymers—he said it needs to be clarified. T. Blanton said it was about a tutorial. J. Anzelmo said he already completed the Report of Board Liaison.

L. Liu began a presentation by going through slides with examples of powder patterns for different polymers with 2D patterns. T. Blanton said we need the TPI polymer pattern from L. Liu. L. Liu then began his presentation on the “Importance of Studying Amorphous Polymers.” T. Blanton said we need to collect the patterns, physical properties, raw data, etc., and that it is important to make the step size larger than the crystalline sample.

L. Liu commented again that well-crystallized polymers for data collection are very important.

Someone asked if we have an orientation distribution function in the database for ODF analysis. T. Blanton replied that we do not at the moment because we are not working with 2D patterns directly yet. The technical discussion regarding orientation distribution continues.

8. Adjournment

Meeting adjourned at 2:00 PM.