

International Centre for Diffraction Data
POLYMERS Subcommittee
Wednesday, 13 March 2013
L. Liu, Chairman

1. Call to Order and Opening Remarks Lizhu Liu
2. Appointment of Minutes Secretary
S. Gates 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 2012 Minutes
Minutes were accepted as written.
6. Report of Board Liaison Tom Blanton
No report to give.
7. Status of Polymer Activity Lizhu Liu
T. Fawcett reviewed the polymer patterns published in PDF-4 2012 release as well as the patterns to be published in the upcoming release. He also took some time to acknowledge T. Blanton for his analyses and supplying of polymer raw data to ICDD. He also mentioned the cellulose article that is to be published from ICDD (along with other collaborative members). T. Fawcett discussed pair distribution function data used to distinguish nano crystalline from amorphous materials (courtesy of V. Petkov). He also discussed our recent collaborations with Prof. Ueda and Prof. Wada on the cellulose triacetates. Finally, T. Fawcett explained the new quality mark system that has been established at ICDD to accommodate non-crystalline and/or amorphous compounds (“G” and “M”).

Discussion ensued about techniques used to determine if a material is or is not amorphous; including methods like SSNMR, radial distribution functions, thermal analysis (DSC), microscopy, etc. Members expressed their concerns about whether supporting data was being included in the PDF and T. Fawcett expressed some was being included, but that they should also keep in mind that the full digital pattern of these materials is also being published which should eliminate some of users concerns about these issues.

L. Liu expressed a concern about having different experimental conditions published in the PDF than what the user is using, but T. Fawcett expressed that ICDD’s goal is to at least provide a starting point (common Bragg-Bretano geometry) for analysis/comparison purposes. It is up to the user to manipulate the data from that point.

T. Fawcett announced our newest polymer grantee, I. Bushmarinov, and discussed some of the work he has provided this year.

8. Future Focus

The definition for the “POL” subfile was discussed as clarification is needed for the editorial group to properly identify these compounds. An in depth discussion was carried out and several suggestions were made by T. Fawcett, F. Wireko, T. Blanton, L. Liu, S. Gates, C. Crowder, and S. Leng. The current definition for the “POL” subfile: “A substance composed of very large molecules, which consist of recurring long-chain structural units.” This definition is not clear and thus several grantees are classifying many large inorganic coordination compounds as polymers. Clarification as to how these compounds would be classified was discussed.

In the allotted time a definition could not be determined and so T. Blanton suggested that L. Liu, S. Gates, C. Crowder, S. Leng, and himself meet to specify a definition. Below were the suggestions for POL criteria mentioned thus far:

- i. Use of the phrase “repeating unit” – L. Liu
- ii. Use of the term “covalent” bonds/linkages – C. Crowder
- iii. Use of the term “large molecular weight” – S. Leng (defined on IUPAC **macromolecular** website : old.iupac.org/reports/1996/6812jenkins/molecules.html#1.3)
- iv. Using “POL” to represent “Polymeric Materials” and then providing sub-classes of Organic vs. Inorganic – F. Wireko
- v. Specifying that these are materials with a “ T_g – glass transition temperature”. – L. Liu

L. Liu briefly revisited his request to get 2D images/data included in the PDF. He noted that he has completed all work for this project (which he presented last year) and will soon be submitting it to ICDD. He will also continue to work on 2D data.

T. Fawcett made mention of the success of the current polymer tutorial and indicated that more tutorials in this area are needed. L. Liu indicated that he is working on a new one and will submit it when completed.

Lastly, it was briefly mentioned that we acquired a new member, S. Leng (3M – focus: polymers), and that in the future we hope to also include compounds that cover amorphous analogues based on orientation.

9. Adjournment