

International Centre for Diffraction Data
Polymers Subcommittee Minutes
Wednesday, 21 March 2011
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
4. Approval of the 2011 Minutes
L. Liu moved. T. Blanton seconded.

5. Report of Board Liaison Tom Blanton

6. Status of Polymer Activity Lizhu Liu
T. Blanton presented XRD pattern of beeswax (white) and indicated that when this was presented to the editorial staff S. Kabekkodu, he requested chemical composition information. After collecting GCMS, NMR, and other elemental analyses, T. Blanton presents the question of what defines the chemical composition of the material. Discussion was carried out and T. Fawcett and T. Blanton provided literature references to support the findings about beeswax. The group attempted to come to a resolution as to how the materials should be added to the database. T. Fawcett suggested adding these compounds to the database as composite mixtures and S. Kabekkodu indicated that in the past the compounds have been added where the elements were listed and more detailed information could be found in the comments section. Overall outcome was that the group feels it is useful to put compounds such as beeswax into the database; however there are limitations that must be determined. Current suggestion is to obtain an average molecular weight from MS and generate a formula based on that. The major rule decided upon for the inclusion of mixed materials in the database was that each material must be a commercial product with common uses.

Presentation made by L. Liu with a focus on what two-dimensional diffraction information could be useful for polymers in our database. The team decided that two-dimensional images showing different orientation would be good if added to the corresponding polymers in the database. L. Liu also presented the typical crystal structures, oriented 2D patterns of polyethylene and polypropylene as well as polyolefin copolymers. Different polyolefin copolymers can have very different crystal structures, depending on composition and thermal history. Therefore, thermal history is also important information in some cases. GIWAXD was also covered in the discussion and it can be a very good technique for study of both crystal and amorphous orientation of polymer films. In some cases, profile fitting of data obtained from 2D WAXD can be difficult due to the broadening effect. Data with higher resolution from 1D instrument is needed for profile fitting. Discussion also covered how to cross-link or cross-reference polymer patterns of similar structures. More discussion will be carried out in future meetings.

7. Future Focus
Expand more quickly with our polymer data base with 2D information. Presentation was made by L. Liu about what 2D data is needed in the database. T. Fawcett indicated that the 2D data should be submitted as an image file.
8. Adjournment