

Minutes of Non-Ambient Diffraction Subcommittee:

March 21, 2012

- Call to order – Andrew Payzant
- Minutes from 2011 Spring Meeting approved.

Board of Directors Liaison Report: Jim Kaduk

- Past motions: Abstracted 1400 entries to date for experimental conditions stating in-situ. Changes in the 2013 release, speed increase, separate numeric fields, which will include the non-ambient fields. This will make it easier to search for these. Possible to tag multiple datasets in individual PDF entries. ICDD (i.e., Suri) is looking for data sets to test. To date no consideration of changing past entries for consistency; however, it was agreed this needs to be done to make all entries uniform.

Discussion and New Business

- Reviewed past and upcoming non-ambient workshops and meetings: noted one N/A session at upcoming ACA 2012 meeting, several sessions at EPDIC.
- New discussion:
 - Discussion of inclusion of lattice thermal expansion coefficients in the PDF-4 comments field whenever available. It was noted that there was some opportunity for development of web-based tutorials to instruct users how to do search-match on data collected under non-ambient conditions.
 - Standards for non-ambient calibration: Knowing the correct temperature of sample is very challenging; consequently, it would be useful to have some recommended standards. When such standards are utilized in data collection, it would be helpful to add this standard information in the PDF-4 entries. In PDF-4, suggest adding comments regarding how the data were obtained and/or what is the level of accuracy (of the non-ambient condition). If added as a comment, is it searchable? When possible attach a graph or graph + equation. Discussion of use of known melting point materials as temperature standards.
 - Subcommittee members requested to consider recommending potential standard materials as external and/or internal standards. Discussions will continue in next meeting (Spring 2013).
 - Estimated error on the temperature/pressure included in PDF-4?
- No Motions to go to Board this year
- Task Group: Agreed that a “best practices” document for non-ambient measurement would be of considerable value. Andrew Payzant will e-mail subcommittee members for input and once consensus is reached will submit to ICDD.
- Motion to adjourn.