



Address 100 Barr Harbor Drive
PO Box C700
W. Conshohocken, PA
19428-2959 | USA

Phone 610.832.9500
Fax 610.832.9555
e-mail service@astm.org
Web www.astm.org

Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

DRAFT Minutes for E13.15 Subcommittee Business Meeting DRAFT

4:00 PM – 5:00 PM EST
Tuesday, February 27, 2007
Pittcon 2007, Chicago, IL
McCormick Place, N129

- I Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 3:05 PM CST.
- II Attendees**
- | | |
|-------------------------|----------------------|
| Joe Koury, ASTM | Alex Mutin, Shimadzu |
| Gary Kramer, NIST | |
| Robert Lancashire, UWI | |
| Richard Larsen, JASCO | |
| David Martinsen, ACS | |
| Burkhard Schaefer, BSSN | |
- III Schedule for next business meeting:** Because of the few people available for the previous business meeting at EAS, the decision was made to skip EAS this year. Instead, a scheduling of a virtual meeting will be examined. A suggestion was made to explore meeting at the IUPAC General Assembly and Congress, August 4-12, 2007 in Torino, Italy. Because IUPAC is involved in the AnIML development, and because several Europeans have been traveling to the US for meetings, this might work well. Gary Kramer will check into the possibilities, and AnIML members will be asked to check their own potential for travel. Even if held in Italy, the capability for virtual participation will also be enabled as well.
- IV Approval of Minutes:** A motion was made and seconded to approve the minutes of the last E13.15 business meeting at EAS in Somerset, November 13, 2006, with typos corrected. (Change “finalized” to “finalize”; “short write up of”; “a E13.15” to “an E13.15”)
- V E13.15 Standards Review**
- **E2066-00 (2000):** Standard Guide for the Validation of Laboratory Information Management Systems. Balloting closed on February 23, 2007. The ballot was approved. As noted before, this standard guide is in need of revision, and someone needs to be found to lead the effort for the next cycle.
 - **E386-90 (2004):** Data Presentation Relating to High-Resolution Nuclear Magnetic Resonance (NMR) Spectroscopy. This effort also requires someone to lead the effort.
- VI AnIML Progress Report:** Gary Kramer presented a brief discussion on the progress on the AnIML standard. The AnIML working group has been holding “virtual meetings” (VMs) once per month. In addition, the Core Group has also held monthly meetings, and has been working to handle time dependent data in a way that will work across different techniques. For example, in an experiment with multiple detectors, the different detectors do not get the same sample at the same time.

The UV/Vis working Group has held meetings every two or three weeks recently trying to finalize the UV/Vis Technique Document.

Alex Mutin reported on his interest in exploring a standard XML definition for instrument control. He presented a talk on this at the workshop on Monday. Such a standard could be a very good complement to the AnIML standard for representing data. The suggestion was made for Alex to see what interest there is among other vendors.

Other AnIML documents, meeting minutes, presentations, etc. can be found on the AnIML SourceForge website (www.animl.org or animl.sourceforge.net).

VII Other Business: A proposal was made to consider adopting the JCAMP data dictionaries, and map those directly to AnIML technique definitions as a way of speeding up the AnIML development. This strategy would allow more rapid development of a standard which could handle legacy data, but not the full complement of information currently envisioned within AnIML. This could be advantageous for legacy NMR data, where we don't have a technique expert. It was pointed out that the problem is not only with the data dictionaries, leading to element or attribute names, but also with the layout of the technique.

There is some precedent for this type of approach. In the library/publishing world, the OpenURL standard adopted the existing SFX standard as version 0.1 of the NISO OpenURL standard. Some time after that, OpenURL 1.0 was finally adopted.

No decision was made on whether to proceed with this suggestion, but it will be discussed at future meetings.

VIII Future Meetings:

- AnIML Working Group VM on March 16, 2007 at 10:30 AM EDT (Note the US has switched to daylight savings time.
- Potential E13.15 Business Meeting in conjunction with IUPAC, Torino, Italy, August 4-12, 2007.
- A motion was made, and seconded, to hold an E13.15 Business Meeting at PittCon, New Orleans, March 2-7, 2008. The motion carried unanimously. Discussion of a workshop will be included in the agenda of the March 16 Working Group meeting, since submission of workshops is very soon.

IX Adjournment: The meeting was adjourned at 4:00 PM.

Minutes taken by David Martinsen, ACS