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**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

**DRAFT Minutes for E13.15 Subcommittee Business Meeting DRAFT**

5:40 pm – 6:45 pm EST  
Monday March 13, 2006  
Pittcon, 2006, Orlando, FL  
Convention Center West 230C

- I Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 5:40 pm EST.
- II Attendees:**
- |                       |                        |
|-----------------------|------------------------|
| Maren Fiege, Waters   | Mark Mullins, Agilent  |
| Joe Koury, ASTM       | Alex Mutin, Shimadzu   |
| Gary Kramer, NIST     | Jim Powers, Wyeth      |
| Richard Larsen, JASCO | Burkhard Schäfer, BSSN |
| David Martinsen, ACS  |                        |
- III Schedule for next business meeting:** The next business meeting will be held at EAS, Somerset, NJ in November, 2006.
- IV Membership Termination:** Gary Kramer noted that four E13.15 members are in danger of being dropped due to missing ballots: Mark Bean, Bob McDonald, Jim Powers, and Frank Tontala. Jim Powers noted that spam filters might prevent ballot notices from being delivered to members, meaning that some may not even know a ballot is pending.
- V Approval of Minutes:** One change was noted for the minutes from the November business meeting. Howard Mark was present for a portion of the meeting, and should be added to the list of attendees. A motion was made and seconded to approve the minutes as amended. The minutes were approved as amended.
- VI E13.15 Ballots**
- **E1578-93:** The LIMS Guide was completely rewritten and is now 78 pages long. It was posted on the ASTM web site on March 10, and voting is open until April 11. This is a subcommittee ballot only, since it was so extensively rewritten. A procedural question was raised regarding whether negative ballots could be resolved in a virtual meeting. Joe Koury replied that they could. June 15 is the target date for the committee/society ballot.
  - **E2066-00:** LIMS Specifications - needs to be updated. Jim Powers agreed to participate. However, he wants to see how the ballot on E1578-93 proceeds before making a larger commitment.
  - **E386-90:** This standard was re-balloted in 2004. It is outdated and needs work. Gary Kramer will try to get participation from the big three. It is not up for re-approval until 2009, but it needs attention sooner.
- VII LIMS Guide:** Jim Powers reported on the update to the LIMS Guide. Over 40 people signed up to participate in the revision, and 10-15 of those were really active. The existing standard was reviewed leading to a decision to completely rewrite it. It was originally authored in 1993, and the re-ballot in 1999 saw little change. The group met electronically twice per month, with one face-to-face meeting. Five subteams met outside of the main meetings to move work along. Some highlights:
- A unique numbering scheme was used throughout to label the sections, and these were referenced in a LIMS checklist at the end.
  - The standard covers the entire LIMS life cycle:
    - Integration, implementation, patching/upgrading, and decommissioning
    - Estimated level of effort, skill sets, project management, common pitfalls, and cost estimates
    - A use matrix by industry
    - LIMS infrastructure

- The benefits of LIMS
- Security of LIMS systems
- An RFP checklist

All E13.15 committee members were asked to take a look at the standard, make comments, and vote.

**VIII AnIML Progress Report:** Gary Kramer presented a PowerPoint discussing the progress on the AnIML standard. Since the last PittCon, 17 virtual meetings have been held, including 6 since EAS. The core group, those who are tasked with developing and finalizing the core schema, have had roughly the same number of meetings.

A requirements document has been written, formalizing the notes from the initial formation meeting at Shimadzu in September, 2002. Initially it was assumed that this would be a balloted document. However, the thinking now is that this document would be for use by the committee. Special thanks to Mark Bean and Tony Davies for their work on this document.

Naming and Design Rules, version 1.2.3, is done, and is now up on the Web site. The NDR forces us to be specific about what we say. The rules can be checked by computer. In this way, interoperability is enhanced. Another aspect of the NDRs is that they will help validate the content within the tagged elements. NIST tools are also under development, to use in conjunction with the Navy NDRs. If our NDRs are done correctly, these tools can be used as well. There has been some concern expressed in the virtual meetings about the extension approach. The NDR approach may help address that concern. There are three NDR documents, one for the schemas, one for technique definitions, and one for instance documents. These won't take the place of standards guides, but will be incorporated into those documents.

AnIML Issues:

- Participation by other ASTM E13 subcommittees has not been very successful. We will address this issue on Wednesday, in the working group meeting.
- AnIML technical issues: Gary Kramer presented a powerpoint covering hyphenated techniques and sample definition
- UnitsML - some concern was expressed about UnitsML, partly due to the concept of layers. In addition, UnitsML has not yet applied any NDRs. It was noted that we are not tied to UnitsML. We already have a UnitsML component. It wouldn't be difficult to switchover to UnitsML, but if UnitsML is not ready for AnIML 1.0, we can look at it later. There are some advantages to UnitsML. If it becomes a universal standard, each markup language would not need to create their own. It would increase interoperability. The plan for UnitsML is to go to OASIS or ISO. Note that UnitsML will also include a units database to do conversions.

Future Meetings:

- Working Group meeting on March 15, 5:15 pm, same room
- XML Session at the ACS meeting in Atlanta
- EAS, Fall, 2006
- A motion was made, and seconded, to hold a E13.15 Business Meeting at Pittcon, 2007, in Chicago. The motion carried unanimously.

## IX Other Business.

- John Hammond noted that there are other ASTM activities involving markup languages, for example, colorimetry. We and other ASTM groups could benefit from knowing about each other's work. A suggestion was made to write up an article for ASTM. Burkhard offered to adapt his JALA article. Gary noted that the colorimetry group is looking at how to output data, and perhaps could use AnIML. Joe Koury will have an editor contact Gary about an article.
- Gary also noted that he had received a letter from the proteomics community on MZXML, a markup language for MS. It might be possible to collaborate with this group as well.
- Other ideas were discussed for publicizing AnIML, in venues such as *Spectroscopy*, *C&E News*, and *Photonics*. Some short columns describing AnIML could help to attract people outside of ASTM. Jim Powers did this for the LIMS committee.
- An article about the restructuring of ASTM E13 could also be helpful. Describing the changes in structure would highlight all of E13, in addition to the AnIML group.

**X Adjournment:** The meeting was adjourned at 6:45 pm.

Minutes taken by David Martinsen