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**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

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

5:12 pm – 6:17 pm EDT

November 14, 2005

Eastern Analytical Symposium

Room 211, Doubletree Somerset, Somerset, NJ

**I. Introductions and Welcome:** Gary Kramer, NIST, E13.15 Chair called the meeting to order at 5:12 pm EDT.

**II. Review of Agenda and Minutes.** The agenda was approved without change.

The minutes of the March business meeting at Pittcon were displayed. A motion was made to approve the minutes as circulated. 2<sup>nd</sup>. The minutes were approved unanimously.

**III. Attendees:**

Maren Fiege, Waters

Herbert Hoover

Gary Kramer, NIST

Tim Brooke for Joe Koury, ASTM

Richard Larsen, JASCO

Dave Martinsen, ACS

Alex Mutin, Shimadzu

Jerome Workman, ThermoElectron

**IV. Work Items:** The subcommittee has two work items that are up for review. The first of these, E 1578-93 (1999) "Standard Guide for Laboratory Information Management Systems (LIMS)," is currently being updated under the direction of Jim Powers. Since it is related to the first one, the second one, E 2066-00 (2000) "Standard Guide for Validation of Laboratory Information Management Systems," will be started once the first one has been completed.

**V. Standards Reviewed:** Three standards were balloted that have an impact on E13.15.

- i. E 2077-00 (2000) "Standard Specification for Analytical Data Interchange Protocol for Mass Spectrometric Data" was approved with 54 yes votes and 42 abstentions, or 100%.
- ii. E 2078-00 (2000) "Standard Guide for Analytical Data Interchange Protocol for Mass Spectrometric Data" was also approved with the same totals: 54 yes, 42 abstentions, 100%.
- iii. Reorganization and transfer of E13.07 into E13.15 (E386-90 (1995) "Data Presentation Relating to High-Resolution Nuclear Magnetic Resonance (NMR) Spectroscopy." (Approved with comments from Davies, Martinsen, and Kramer)

**VI. LIMS Guide.** As noted above, Jim Powers is leading the effort to update (actually, to re-write) the LIMS standard. The LIMS standard was originally approved in 1993, and needed much work. Gary Kramer presented a PowerPoint from Jim, describing the approach taken and the status to date. A total of 42 people have been involved in the update effort, divided into several teams. The updated standard is currently in the hands of the ASTM editor, and it is estimated that the standard will be ready for

subcommittee balloting in December, 2005. If it passes, it should be ready for a full E13 ballot in midyear 2006.

**VII. AnIML Status.** Gary Kramer gave a PowerPoint presentation on the status of AnIML. The working group and the CORE developer group have met 11 and 10 times respectively since PittCon. Several presentations and publications have been generated by committee members, and several additional presentations are scheduled, including the Lab Automation and IQPC Conferences in January, and a ½ day workshop at Pittcon. An XML in Chemistry session is also scheduled for the ACS meeting in Atlanta, March 26-31, 2006. Dave Martinsen will send a call for papers to the group to highlight that session as well.

Accomplishments include:

- Redesign of the AnIML web site on Sourceforge.net
- Draft of an AnIML requirements document, based on the conclusions of the organizing meeting at Shimadzu in September, 2002.
- Formation of the CORE
- Draft UV/Vis and IR Technique Definition Documents
- Generic viewer tool
- Draft of a Naming and Design Recommendations (NDR) Document

There are a number of outstanding issues:

- Handling of hyphenated techniques
- Sample concept and information
- Units
- Name spaces – global vs local
- Versioning
- NDR

#### **VIII. Coming Meetings:**

- The next business meeting will be at PittCon in March, 2006. The day will be announced later.
- A working group meeting will also be arranged in conjunction with PittCon.
- After some discussion on the merits of EAS vs. FACSS, a motion was made and seconded to hold the 2<sup>nd</sup> business meeting of 2006 at EAS. The motion carried unanimously.
- Virtual meetings for the working group and the CORE developers group will be scheduled between now and PittCon.

#### **IX. Other Business:**

- In order for the technique definitions to be created appropriately, we need greater participation from the technique experts, both those on other ASTM committees as well as non-ASTM members, to collaborate on the technique definitions. The suggestion was made that it might be time to go to the other E13 subcommittees to let them know their assistance is required.
- While the subgroup members were listed on the screen, some updates were suggested:
  - i. Michael Harzheim is the appropriate Waters representative on Chromatography. He should also be included in the CORE group.
  - ii. Mark Mullins should be listed as the SSI representative on the CORE

- iii. Ronny Jopp and Alex Ropp should be added to the CORE team. They are new guest researchers in Gary Kramer's group at NIST.
- It was noted that the Andi standards, as they have now been approved, should now be ok until they are retired after the completion of AnIML. However, since he has been answering requests about the standards, he would like to be able to send the appropriate documentation to individuals who request assistance.
- Randy Julian has dropped his ASTM membership. Therefore a new vice-chairman is needed. Jerome Workman, Herbert Hoover, and Tim Brooke/ASTM noted that Gary Kramer could appoint a new vice-chair at any time, without the need for a ballot.
- Alex Mutin's name was not printed on the ASTM attendance sheet. Tim/ASTM, will check to see whether Alex is assigned to E13.15.

**X. Adjournment.** Motion to adjourn. Second. Carried unanimously at 6:17 pm EDT.

Submitted by David Martinsen, ACS, ASTM E13.15 Secretary