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**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

**Minutes for E13.15 Subcommittee Working Group**

5:22 - 7:30 pm EST

Wednesday March 15, 2006

Pittcon, 2006, Orlando, FL

Convention Center West 230C

- I Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 5:22 pm EST.
- II Attendees:**
- |                                |                          |
|--------------------------------|--------------------------|
| Mark Bean, GSK                 | David Martinsen, ACS     |
| Stuart Chalk, U. North Florida | Mark Mullins, Agilent    |
| Maren Fiege, Waters            | Alex Mutin, Shimadzu     |
| Gary Kramer, NIST              | Chip Patterson, Shimadzu |
| Richard Larsen, JASCO          | Burkhard Schäfer, BSSN   |
| Peter Linstrom, NIST           |                          |
- III Schedule for next virtual meeting:** The next working group meeting will be held on March 31, 2006 as a virtual meeting.
- IV Approval of minutes:** The minutes for the March 3 meeting were not yet available. No action taken.
- V Ballot Reminder.** There is an E13.15 ballot item on LIMS. April 11 is the deadline for voting. Please be sure to vote.
- VI Technique Definition Teams.** A suggestion was made that each technique task group should be chaired by an active member of the E13.15 Working Group. The chair should contact Joe Koury at ASTM to set up virtual meetings to get the task groups started. There was some discussion regarding whether all of the groups should be activated, whether we should concentrate on a subset, and whether we should work on the simplest or the hardest first. The current technique committee make-up was displayed. The status of the technique committees was discussed:
- **IR and UV/Vis.** Richard Larsen will continue as chair of the task group. He has the material from Anh Dao. Stuart Chalk will also continue to work with the committee and has a greater understanding of the format from his work on the JCAMP converter - see below. Burkhard Schäfer will also participate. ThermoElectron is moving to XML (GAML) for a number of their products, including UV/IR, OMNIC, and Atlas. It was noted that the GAML site is back on line. It is unclear whether they plan to use AnIML. Possible new members include David Joyce from Thermo. The most common procedures should be covered, not the less common ones. From the Lab Automation meeting, it became clear that there needs to be a way to focus on a single peak and look at data over time. The group set a target date of May 21 to deliver a draft technique definition by May 1.
  - **Chromatography.** Frank Tontala is the current chair, but is not able to work on the committee any more. Mark Mullins may take Frank's place. Chromatography was fairly complete, but the core has changed since Maren wrote the technique definition, so it needs to at least be re-examined in the light of those changes. Burkhard received comments as a result of a talk at Agilent in Germany, and these were passed along to Mark Mullins. Frank Tontala will be kept on the list, but the chair will transfer to Mark Mullins. Michael Harzheim will be removed, since he is no longer at Waters.
  - **Mass Spectrometry.** A question was raised as to why IMS is included as one of our primary techniques. The reason is that it was part of the original specification because it has a JCAMP definition. It was noted that there is a draft technique for MS on the AnIML web site. David Barley is currently listed as chair. Mark Bean will take over as chair as the active committee member. Gary Kramer received a specification on MZXML from Northwestern, which

he passed to Mark Bean. Peter Linstrom requested a copy as well, and suggested that Steve Stein also review the format. This specification is starting to appear in proteomics work. Stuart mentioned that one of his students is now part of Rick Yost's group. He will check to see if that student would be interested in joining this group.

- **NMR.** It was suggested that this be left for the second set of techniques, since we don't have any expertise in the committee. However, Gary Kramer volunteered to contact NMR companies, because E13.15 was given the NMR standard as a result of an E13 vote last year. It needs to be updated, but should not hold up AnIML. Michel Boruta, ACD, was suggested as a possible NMR person, or perhaps someone at Bruker.

A suggestion was made that the committee chairs share with each other information on progress of their groups. Gary Kramer offered to include a section at each virtual meeting on a status from the committees.

**VII JCAMP-AnIML Converter.** Stuart Chalk described the JCAMP-AnIML converter. Whenever someone submits a file, an email is sent back to him. Robert Lancashire has tried it, and provided some helpful feedback. There was some discussion what action to take when AnIML has a required element which is not in the JCAMP file. The suggestion was made that such cases should be forwarded to the core group. While there is no requirement that AnIML be backwards compatible with JCAMP, it is worth considering whether such elements should be required in AnIML. Another case is elements in JCAMP which have no counterpart in AnIML. Similarly, there may be uncertainty over how JCAMP parameters can be mapped to parameter enumerations in AnIML. Another issue is how to represent the JCAMP conversion as part of the audit trail. Currently, the JCAMP header is stored as a comment in the AnIML file. Maren noted that when she was testing, she triggered an attack condition after submitting 5-6 files from the same IP address. Stuart will address that problem.

**VIII Generic Viewers.** Robert Lancashire sent a note describing a new JCAMP viewer on SourceForge at [jspecview.sf.net](http://jspecview.sf.net). It includes examples and documentation. Stuart commented that it works well, and noted that Lancashire intends to include AnIML support at some point.

A discussion of generic viewers followed, particularly the problem of dealing with multi-dimensional data in a generic fashion. Even technique-specific viewers have problems with data of this complexity. Various approaches were discussed, such as using clues in the AnIML file, and then displaying 2-d or 3-d slices of the data. It was noted that the job of the committee is not to develop such a viewer, but only to expose the data in such a way that a viewer could be written. A generic viewer wouldn't make sense of every technique.

**IX A View of Samples.** Gary Kramer made a presentation discussing different concepts of sample in different techniques. A PowerPoint file is available on the web site. A simple concept of sample can not be extended to all analytical problems. A sample may be very simple - the material in a test tube. But it could also be quite complex - a particular well in a 96-well plate, or in a set of stacked plates, or in a particular location, but at different points in time. Image spectroscopy is becoming important, and there is a need to handle complete images as well as spots. The presentation fostered considerable discussion. While no conclusions were reached, some of the areas discussed were sample inheritance, where one experiment step inherits sample from a previous step; processes which perform some action on the sample to create a derivative sample, or on the data, such as subtraction of background; and annotation, in order to label data points with a label. The core group will consider these concepts in future meetings.

**X Outreach.** The committee has done a good job with publications and presentations in the past year. In the business meeting (March 13), there was discussion about a number of possible ways to publicize AnIML. There are other XML initiatives in ASTM, such as E27: Colorimeters. An article for Standardization News (ASTM's publication) would be a useful way to help make other committees aware of our work. Other venues could be *Analytical Chemistry* or *Spectroscopy*. A caution was given - not to overdo the publicity aspect until AnIML is really ready, but to try to attract others to the process so we don't need to modify the standard later. Other possibilities include presentations at EAS (abstracts due by April 15) and FACSS (abstracts due by April 28).

**XI Adjournment:** The meeting was adjourned at 7:30 pm EST, with coordination of rides/walks for the AnIML dinner.

Minutes taken by David Martinsen