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**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

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

10:37 am – 12:37 pm EST

Wednesday December 21, 2005

Virtual Meeting

- I **Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 10:37 am EST. Peter Linstrom agreed to take minutes for the meeting since the subcommittee secretary was unable to attend the meeting.
- II **Attendees:**
- |   |                         |
|---|-------------------------|
| Mark Bean, GSK                            | Gary Kramer, NIST       |
| Stuart Chalk, University of North Florida | Peter Linstrom, NIST    |
| Maren Fiege, Waters                       | Mark Mullins, SSI       |
| Ronny Jopp, NIST                          | Alexander Roth, NIST    |
| David Joyce, Thermo                       | Burkhard Schaefer, BSSN |
| Joe Koury, ASTM                           |                         |
- III **Schedule for next virtual meeting:** It was agreed to have the next virtual meeting from 10:30 am to 12:30 pm EST on Friday January 13 2006.
- IV **Approval of minutes**
- The minutes for October 14, 2005 virtual meeting were reviewed. Gary Kramer indicated that in section VI, subsection k, “RFC 1129” should be “RFC 2119”. The minutes were approved with requirement with the noted correction be made.
  - The minutes for October 28, 2005 virtual meeting were reviewed. Gary Kramer indicated that in section VIII the names “Alex Ropp and JK” should be “Alex Roth” and “Ronny Jopp”. The minutes were approved with the requirement that this correction be made.
  - The minutes for the November 13, 2005 E13.15 working group meeting at EAS were reviewed. Gary Kramer noted that in section IV, subsection d the term “ISO 111179” should be replaced by “RFC 2119”. The minutes were approved with the requirement that this change be made.
  - The minutes for the November 14, 2005 E13.15 business meeting at EAS were reviewed. Gary Kramer noted that in section IX, second bullet subparagraph iii, the name “Alex Ropp” should be “Alex Roth”. These minutes could not be voted on in this meeting because they are for a business meeting.
  - The minutes for the December 2, 2005 virtual meeting were reviewed. Maren Fiege noted that the name “Joop” in the last sentence of section V should be corrected to “Jopp”. Gary Kramer noted three corrections. He indicated that Burkhard Schaefer’s Affiliation should be corrected in section II; it is now BSSN. He noted that the AnIML workshop at Pitttcon will run from 1:30 pm to 5:15 pm rather than 1:00 pm. To 5:00 pm as noted in the second sentence of section IV. In the third correction, he indicated that the term “would be” in section VI, third sentence, should be changed to “is”. It was also noted that several spelling errors need to be corrected in the first paragraph of section VII; the terms “namespaces” and “namespace” are incorrectly spelled as “name spaces” and “name space”. The minutes were approved with requirement with the corrections noted above be made.
- V **AnIML at scientific meetings**
- The Pittcon meeting from 3/12 to 3/17 2006 in Orlando, Florida was discussed. It was noted that the AnIML workshop will be from 1:30 to 5:15 pm on Thursday March 16, 2006. Stuart Chalk indicated that he would be teaching an XML in Chemistry short course all day on Thursday March 16, but that he would try to re-schedule the course. It was decided that the subcommittee would try to schedule an E13.15 working group meeting at 5:15 pm on Wednesday or Thursday. The E13.15 business meeting will be Monday, March 13 from 5:30 to 7:30 pm.
  - The upcoming Lab Automation conference was briefly discussed. It appears that only 4 or 5 people will be attending this conference. It was not possible to obtain a meeting room at the conference location on the day after

the conference. It was decided to informally arrange a meeting of subcommittee members who would be attending the conference.

- Gary Kramer indicated that he would be giving a talk on AnIML at the upcoming IQPC conference in San Diego.
- Discussion on AnIML talks at the ACS national meeting in Atlanta was postponed until a later meeting. It was noted that it would be more appropriate to discuss this meeting when Dave Martinsen, the XML session chair, was in attendance.

## VI Core working group report

A schema change to allow pages to reference siblings in addition to parents was made. This was done to support some experimental scenarios where the parent page does not properly reflect the relationship between the siblings or does not exist. This change only involved adding one attribute to the AnIML core markup language.

There was extensive discussion of whether references should be value or index based. Currently references are based on an integer index which indicates the data point the reference points to. Use of value based references would allow references to points where no data were collected. There was extensive discussion of this issue including examples of cases where one approach or another would be advantageous. There was discussion of the idea that points with no dependent axis values could be placed in data to provide places for references to link to. No conclusion on this topic was reached.

Peter Linstrom indicated that there could be cases where the parent experiment might not be collecting data, but samples from the experiment might still be collected and analyzed.

Burkhard Schaefer provided the example of the case where one may wish to annotate data after the fact. In this case one may not have data at the point where the annotation should be placed. This might be the case if the purpose of the annotation was to note that a peak was not present in a particular location. If the original data was digitally signed, the signature would be invalidated if extra points were inserted to provide points for annotations to point to.

Gary Kramer suggested that data should be indexed based on the time axis where possible. In cases, where a time axis is not available, other values can be used. The selection of indexing axes will be chosen by the technique definition developers.

Mark Bean indicated that he strongly disagreed with the other core developers on some of the ways data can be stored in the AnIML core schema. He indicated that he did not see the need to link one experiment step to another. As an example he discussed the case of summary GC-PDA data. In this case full traces are kept for only a few frequencies, but full spectra are stored for selected points on the chromatogram. Under the AnIML data model this would result in a large number of spectra with just a few points along with a few spectra with a larger number of points. He indicated that he had been considering developing his own schema to address issues with the AnIML core schema, but now will be working with the current approach to help speed the release of AnIML.

Burkhard Schaefer indicated that the AnIML core is designed to be flexible and that technique definitions should enforce formats for techniques. He noted the modular design of the AnIML core was designed to capture the semantic relationships present in analytical chemistry experiments.

VII **NDRs for AnIML schemas:** Gary Kramer is currently revising the document on naming and design rules for the AnIML core schema. The revised document should be ready for the next AnIML VM.

VIII **Website for AnIML standards:** This agenda item was postponed to a later meeting. Joe Koury had left the meeting by the time it came up and it was concluded that he should be involved in any discussions on this matter.

IX **Technique definition questions from Stuart Chalk:** Stuart Chalk had a couple of questions for the working group:

Stuart asked how he could encode and decode AnIML's base64 data. Peter Linstrom indicated he will send Stuart a base64 encoder and decoder program. Mark Bean indicated that program to do this in C# was available on the Source Forge site. Burkhard Schaefer described how the data could be encoded and decoded in C++ or Java.

Stuart indicated that he has almost completed a flow technique definition and asked how he could present it to the group. It was noted that there is currently no procedure for reviewing technique definitions.

X **Adjournment:** The meeting was adjourned at 12:36 pm EDT.

Minutes taken by Peter Linstrom