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**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

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

10:30 am – 12:30 pm EDT

September 15, 2006

Virtual Meeting

- I. Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 10:30 am EDT. The ASTM release form for recording the session was displayed on the screen. There being no objections, the meeting was recorded. Gary noted that Patrick Gleichmann and Kordian Placzek were joining NIST as guest researchers.
- II. Attendees:**
- |                                   |   |
|-----------------------------------|---|
| Mark Bean, GSK                    | Alex Mutin, Shimadzu                        |
| Stuart Chalk, Univ. of N. Florida | Matt Olcese, ASTM                           |
| Patrick Gleichmann, NIST          | Dale O'Neill, Agilent                       |
| Joe Koury, ASTM                   | Kordian Placzek, NIST                       |
| Gary Kramer, NIST                 | James Powers, Wyeth                         |
| Richard Larsen, JASCO             | Alexander Roth, Fachhochschule<br>Wiesbaden |
| Dave Martinsen, ACS               |   |
- III. Next Meeting:** October 13, 2006, 10:30 - 12:30 EDT.
- IV. Minutes:** Because the minutes of previous meetings were distributed late, the approval will be deferred until next time.
- V. PittCon:**
- Abstracts have been submitted. Mark Bean hasn't heard back from PittCon. Gary suggested that he contact [hackley@pittcon.org](mailto:hackley@pittcon.org) and make sure they got it. This year, AnIML has a better time slot than last year, Monday afternoon, February 26.
  - Dale questioned what we plan to do. Gary noted that each technique talk was scheduled for 20 minutes. Dale will be talking about chromatography, and will concentrate on how the technique is laid out, how it fits into AnIML, and also will touch on TNF.
- VI. Other meetings:**

- a. Lab Automation: Gary has received no word from Burkhard Schäfer on whether he was able to submit a talk. Abstracts were due on 11 September. Two posters on AnIML have been submitted by Patrick and Kordian. They will present on the validator. Dominik's validator doesn't work any more because of the changes to the core schema. In addition, they will build in the validation for the NDRs. We need more than a single validator. There will need to be one for AnIML documents themselves, and one for the technique definitions. Ultimately, we won't be the only ones writing these. People will also write extensions. We need to make sure these are being done in the proper ways.

It was noted that another reason the validator doesn't work is that no one could get it working on their own environment. Not only does the validator need to work, but the environment also needs to be documented. The same libraries need to be available on the installation machine as were on the development machine. Dale O'Neill suggested testing the installation by starting with a clean OS. Agilent sometimes uses a virtual machine, with nothing installed. Installing in such an environment, and getting it to work there, gives confidence that the install documentation is complete.

**VII. Style and format of the ASTM specification:** Matt Olcese, an ASTM editor, joined the meeting to answer questions about the format of the AnIML specification. This section of the meeting took the form of a Q&A. In the dialog below, MO refers to Matt Olcese, JK to Joe Koury.

Q: We will have a lot of references that exist in electronic form. These could include websites, comments, rules for XML, rules for using the Web. How should these be handled?

MO: At one time, ASTM was not keen on websites. But this has changed. The current practice is that the title of the document should be included within the body of the ASTM specification, as "see 'title of document'", with the title hotlinked to section 2. In the reference document, a footnote would contain the title and the url, such as "'document title' accessible from url".

Q: Many times people reference web sites, giving a date last viewed. Does ASTM want us to do that?

MO: No, the date is not required. The editors will make sure the links still work.

Q: Section 2 has a footnote which says: <http://...> Where do we put the title?

MO: The title appears in section 2, like "2.2.2 Other standards", so people can see what they are going to read. This is the "AnIML Core Schema Documentation".

Q: With respect to references, if you look at this document, there are other related AnIML standards documents referenced. These will not exist at the time the first document is submitted for ballot. How should we handle this?

MO: ASTM is open to suggestions. This is a type of forward linking. If a document doesn't yet exist, and doesn't have an ASTM number, it shouldn't be referenced.

Q: We could leave these references out initially, and when the new document is complete, make a revision to the main document to add the references. In this case, only the revisions need to be balloted. Would this be a valid approach?

MO: Yes.

Q: This is a question about terminology. RFC2119 is a one page document from W3C which defines the meaning of must, must not, should, and may, and recommends a particular format. In ALL CAPS, it means the RFC2119 definition. Since most people reading the definitions will be computer scientists, and familiar with the W3C definitions, can we use those in all caps? If material is in all caps, will the editors try to change it?

MO: ASTM has its own mandatory meanings, and the ASTM style is not very lenient on caps. However, if the convention is stated in the terminology section, the editors should allow it. It is not against the ASTM style per se.

Q: What is the recommendation on paragraph numbering? Should single subparagraphs be given a number?

MO: All paragraphs are numbered, even if only a single subparagraph.

Q: How should software code be included in the documents?

MO: In standards, computer code may be done as a figure, or as an interior table, to distinguish it from other text. The interior table is defined in the SGML code for the document. It's not covered in the style document, because it's only in the markup language. It normally will be labeled, but labels could be suppressed.

Q: Another difference with this document is that it will have schema, with a multiply indented formatting style showing the hierarchy of the elements. Is there a way we can put this in, without reformatting?

MO: If is presented as a figure, it will be scanned into document as is.

Q: Some of the figures will graphically show how the schema is laid out. These will come from XMLSpy. We need to see if there are any copyright issues from XMLSpy.

MO: We haven't run into this before. I will need to bring up with my manager. ASTM would clearly state in a footnote where the images come from. Also, ASTM would indicate that ASTM does not authorize this software, and would like to name an alternative application as well.

Q: Would ASTM have a problem if XMLSpy output has a copyright notice?

MO: ASTM would also add a trademark footnote to Altova. Note that figures should be black-and-white, preferably, since they scan better.

Q: There is a comment in the style manual saying please don't use Microsoft Word outlining. Is there a problem with using Word?

MO: Word outlining is different than the standard ASTM practice. ASTM would rather you use the ASTM template. But if our document looks ok, then it shouldn't be a problem.

Q: In one sense, the whole idea of a standards document for AnIML is somewhat questionable. The XML schema is, in essence, the documentation of the standard - the official standard. We are now documenting the document, repeating it in English form. It doesn't really help anyone. Would there be any value for this committee to suggest how ASTM should handle XML standards? Would ASTM be open to suggestions?

JK: There is an xml schema now - E31.25. I will check and send the document name to everyone. The schema is available as an annex.

MO: An annex is mandatory, but an appendix is not. For E13.15, the schema would be an annex.

Comment: XML will be in ASTM's future. We should step back and help ASTM to define the way these standards should be handled. The way XML standards work require that they be downloadable and machine-readable. There is a difference from the normal ASTM standards.

Note from JK: As requested, I will send ASTM style guide to Dale O'Neill. If anybody else wants one, contact Joe Koury.

**VIII. Core Developers Meeting:** The core group dealt with a question from Dale O'Neill: Should we have a header at the top of the document indicating who created the AnIML file, the software, etc., or should this be in the audit trail. If these fields were present at the beginning of the file, you wouldn't need to read the entire file to find out what they were. However, this raises the question of what to put in the header if an application reads an AnIML file, processes the data, and writes out a new AnIML file. Who is now the creator? The original

creator, or the new application? Would we just be creating another audit trail at the front of the file? Agilent is ahead of the group in creating files, so we should listen to their input. The core group will continue to discuss this issue.

The group is catching up on bugs, and making additions. The last major issue is how to deal with chromatograms and spectra. There are three proposals, from Mark Bean, Burkhard Schäfer, and Alex Roth. Mark Bean would like to get people in Sciex, Waters, Micromass involved in decision, since they have a lot of experience. Meetings are occurring often, and the group is working together well. Alex Roth has stayed active, even after finishing his time at NIST. That has been terrific.

- IX. UV/Vis Technique Group:** One meeting was canceled. The group is still working in the general part, dealing with samples. There has not too much progress. The UV/Vis base technique was written by Alex Roth and Ronny Jopp. Version 1.2 was generated from the tool Burkhard Schäfer wrote, and from information in the technique document itself. Burkhard also sent around a marked up version of the document, with comments from the group meetings. The tool was written to help technique experts, who were not XML experts, to write technique documents.
- X. Validators:** There was some discussion on validators, and where they would be used. We need to know that people are creating the technique definition documents in valid format, to help us weed out non-standard definitions, such as those which have become a problem in JCAMP. A validator should help to ensure that these problems don't creep into AnIML. There could be documents which validate against the schema. However, because AnIML is not sufficiently constrained in an XML sense, the validators can be used to check on the additional constraints, including the presence of required elements. Validators will be the subject of a future meeting.

Some of the features the validators will check for include: a) that the NDRs are followed; b) check the contents of certain elements, e.g., "yellow" is not allowed as a boiling point, an entire XML file is not allowed as a string variable.

NIST will update the earlier validator, to get it into working order again. As to who maintains the validators in the long run, this is not yet decided. Should it be under the purview of this committee? If so, then a standards document on the validator needs to be developed as well.

- XI. Generic Viewers:** One more item from the Core Group discussion related to the generic viewer requirement. The need to support a generic viewer brings with it some constraints on the way data is stored. In support of a generic viewer, there was an assumption that one would click on a point in a chromatogram, for instance, and view a spectrum. But in practice, most people would click on a chromatographic peak, not a point. This immediately becomes more specialized.

The presentation of data is separate from the structure. If we can give hints to the display, that is good. A suggestion was made that the group look at the three different models, and evaluate each on the basis of storing data. Then analyze what each would need to support a generic viewer. Then evaluate those results.

**XII. Other business:**

- a. Joe Koury noted that the schema referred to earlier is E31.25, E2369. It is in Volume 14.01.

**XIII. Adjourn:** 12:35 pm EDT.

Minutes prepared by David Martinsen, ACS  
ASTM E13.15 Secretary