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Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

Minutes for E13.15 Subcommittee Working Group

10:38 am – 12:25 pm EST

Wednesday February 10, 2006

Virtual Meeting

- I Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 10:38 am EST.
- II Attendees:**
- | | |
|----------------------|-----------------------|
| Mark Bean, GSK | Mark Mullins, Agilent |
| Michael Boruta, ACD | Dale O'Neill, Agilent |
| Joe Koury, ASTM | Alexander Roth, NIST |
| Gary Kramer, NIST | Karen Wilson, ASTM |
| David Martinsen, ACS | |
- III Approval for Taping the Meeting:** Joe Koury had polled meeting attendees prior to the meeting that taping was a possibility. The question was asked of meeting attendees. No objections were voiced to taping the meeting, so it was taped.
- IV 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 March 3 2006.
- V Approval of minutes:** Two corrections were suggested for the Minutes of the January 13 meeting.
- The AnIML Workshop at Pittcon starts at 1:30, not 1:00 pm on Thursday, March 16.
 - On the 2nd page, “ARSTM” should be ASTM
 - A motion was made and seconded to approve the minutes as amended. The minutes were approved as amended.
- VI AnIML at conferences.**
- At the next virtual meeting, Gary suggested that speakers have a powerpoint of their presentations for PittCon available. That way, we can coordinate our talks to make sure we don't have major overlaps.
 - Gary reported on Lab Automation. Attendance was around 75-100 people. There was a fair amount of interest. Several people came up to ask questions, but Gary had to rush off to another meeting. Bristol-Myers Squibb said they would assign someone to attend the virtual meeting.
 - Also at Lab Automation, there was a long discussion of the Naming and Design Rules.
 - IQPC was a smaller meeting, but still good interest.
 - ACS meeting: 10 papers will be presented on XML, a full-day session. A number of papers from the AnIML committee are included.

VII Core working group report

The core group discussed the complexity of AnIML. Part of the complexity lies in the alternate ways in AnIML files could be laid out. This stems partly from the view of what a technique is, and partly from the way in which AnIML defines samples. If a vial is divided into 2 separate vials, is that 1 sample or 2? What if measurements are made on the contents of the same vial, but 6 months apart? The sample is a function of both time and location. The problem is that there is no industry consensus. Or a chemist makes a mixture, purifies, and sends on the purified sample. What is the sample?

The concern is that if AnIML is too complex, the chances for wide acceptance will be lessened. On the other hand, if AnIML is not complex enough, it won't be able to handle the requirements of the range of analytical instruments. AnIML should describe industry practice, but there is no real consistency across techniques. Perhaps the sample/child

approach leads to complexity, and we should instead take a minimal approach to sample. However, there needs to be some linkage to relate the material in the instrument with a physical reality. This leads to the difficulties in striking a balance.

There was some further discussion regarding the decision to use the technique definition files instead of schema files for techniques. Using non-standard protocols means that standard tools cannot be used. Tools have been posted on the AnIML web site, under the CVS structure (see https://sourceforge.net/cvs/?group_id=76803).

The question was raised about the generic viewer, and how it could handle alternative types of AnIML files. It is possible, for example, to store 2D data with x data on one page, and y data on another. How does the viewer understand extensions? Generic viewers can not understand extensions, only the base level documents. But could a base level document viewer understand alternate formats? JCAMP failed because one couldn't look at MSMS data. We need to be concerned more about encoding, not viewing.

The question was posed for the committee to discuss the following three options at a future meeting: 1) time is of the essence and we should proceed along the path we are on, right or wrong; 2) delay, and try to modify and improve the standard; 3) the standard is right as is, and we should continue. This could be a topic for discussion in the working group meeting in Orlando.

VIII NDRs for AnIML schemas: The Naming and Design Rules were discussed in Palm Springs. The document has been rewritten. One of the changes surrounds the versioning and name space. Three digits will be used to describe the versions and file names: the release number, major version, and minor version, and the distinction between major and minor versions is provided. The document makes use of suggestions from other standards environments, and these are referenced in the document through abbreviations and section numbers. Since the document was sent only a short time before the meeting, we were requested to review the document and make comments.

IX Adjournment: The meeting was adjourned at 12:25 pm EST.

Minutes taken by David Martinsen