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**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

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

10:35 am – 12:37 pm EST

Friday December 2, 2005

Virtual Meeting

I. **Introductions and Welcome:** Gary Kramer, NIST, E13.15 Chair called the meeting to order at 10:35 am EST. He asked Peter Linstrom to take minutes for the meeting, since the subcommittee secretary was unable to attend the meeting.

II. **Attendees:**

Michael Boruta, ACD  
Mark Bean, GSK  
Tony Davies, Waters  
Maren Fiege, Waters  
Ronny Jopp, NIST  
Joe Koury, ASTM

Gary Kramer, NIST  
Peter Linstrom, NIST  
Alex Mutin, Shimadzu  
Alexander Roth, NIST  
Burkhard Schaefer, Univ. Kaiserlautern

III. **Schedule for the next virtual meeting:** It concluded that the next virtual meeting would be held on Wednesday December 21, 2005 from 10:30 am – 12:30 pm EST.

IV. **Presentations at scientific meetings:** The schedule is out for the Pittcon meeting. The AnIML workshop will be a Thursday March 16, 2006 from 1:00 to 5:00 pm. The subcommittee will schedule a working group meeting at 5:30 to 7:30 on Thursday March 16. The subcommittee will arrange a business meeting at 5:00 to 6:30 pm on Monday March 13.

There will be no AnIML working group meeting at IQPC in San Diego because too few people from the group will be attending.

The subcommittee will seek to schedule an AnIML working group meeting on January 26, 2005, (the day after the Lab Automation conference ends). The meeting will tentatively be held at the Lab Automation conference site in Palm Springs. Gary Kramer will check with ALA to see if he can secure a room for this meeting.

Several abstracts have been submitted for some AnIML related talks at the XML session at the ACS national meeting in March. The following abstracts have been submitted:

- Maren Fiege – general discussion of AnIML
- NIST (Ronny Jopp and Alexander Roth) – two talks UnitsML and NDRs for AnIML
- Tony Davies – IUPAC/XML in chemistry (will cover much more than AnIML)

V. **Core schema team report:** The implementation of Naming and Design Rules (NDRs) for AnIML was discussed. The core schema team would like to address other issues (validation problems with

the schema, work with hyphenated experiments). There was concern that dealing with NDRs now would delay current work on the schemas.

Mark Bean suggested that it might be useful if a person with additional XML experience could join the core schema working group. Burkhard Schaefer noted that the addition of Alexander Roth and Ronny Joop could help in this regard.

**VI. Requirements document discussion:** Changes discussed in previous meetings have been added to the document by Tony Davies. At EAS it was decided that this document probably should not be balloted. It was concluded that this document would be important in the development of AnIML. There was some discussion over whether or not to ballot this document. Tony Davies will locate the other ASTM group that balloted a similar requirements document. Gary Kramer indicated that these sorts of documents are generally not balloted.

There was some discussion about the requirement of SI Units. Mark Bean was concerned about having the ability to convert units to non-SI units. He will add a requirement relevant to this issue to the requirements document.

Burkhard Schaefer had two corrections for the document. In reference 1.4.15 on page 2, the web site URL is incorrect; it should be <http://animl.sf.net>. On page 3, section 2.3.5, the text indicates that the core can be extended; this wording should be clarified to indicate that technique definitions are extended. Agreement was reached on the need for significant re-wording of this section, although the exact wording was not developed. Mark Bean will make these corrections to the document.

**VII. Skepticism over progress with AnIML:** There was some discussion of the concerns of customers that the AnIML is not making progress. Tony Davies discussed some of these concerns. There is skepticism in industry that E13.15 will not be able to deliver the product that will be needed by industry. Mark Bean suggested that there may be a need for additional resources for AnIML development. Mark Bean also suggested that the complexity of AnIML may be a problem. Maren Fiege suggested that this is not the case. There was extensive discussion of the complexity of AnIML. Tony Davies indicated concerns about companies claiming they already support AnIML.

**VIII. Naming and design rules:** There was a discussion of the name spaces for the AnIML schemas. Burkhard Schaefer noted that name spaces in the XML schema context are used for documents with multiple schemas. AnIML uses this for digital signatures and scalable vector graphics (SVG). Burkhard Schaefer noted that it is unlikely that the AnIML schema will be used with other schemas; so schema name space issues are less important for AnIML than other markup languages. There was discussion of the various meanings of the term “name space” in context of the AnIML schema and documents.

The AnIML versioning system was discussed; the current versioning system supports major and minor version types. The idea of providing two versions of the schema; one with comments, and one without was also discussed. It was decided that this would not be an issue for AnIML since the savings from using a schema with the documentation stripped out would be minimal. There was some discussion of the language to be used for schema documents. It was decided that schema documents would be in U.S. English but a specific dictionary was not chosen.

The need for a standardized set of acronyms was discussed. Mark Bean noted that ASMS defines a standard set of acronyms. Tony Davies indicated that it would be wise to use existing standards

where possible. There was discussion on the use of the slash (/) or the hyphen (-) for hyphenated experiment. Gary Kramer indicated that IUPAC documents would be examined for rules in this area.

It was decided to use upper camel case for element tags and data types. Lower camel case will be used for attributes.

It was suggested in the proposed naming and design rules that AniML avoid the xsd:anytype datatype. AnIML uses this to allow inclusion of information such as chemical structures in XML (CML). There was some discussion on the merits of such flexibility versus more strict control of document content. Gary Kramer suggested that the schema be examined for instances of xsd:anytype.

It was noted that the language in the report on NDRs needs to be cleaned up to improve readability.

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

Minutes taken by Peter Linstrom