
Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

DRAFT Minutes for E13.15 Subcommittee Working Group DRAFT

10:35 am – 12:12 pm EDT

Friday, August 4, 2005

Virtual Meeting

I. Introductions and Welcome: Gary Kramer, NIST, E13.15 Chair called the meeting to order at 10:35 am EDT. Len Morrissey was introduced as the temporary ASTM/E13.15 liaison. Carolyn Sheahan has left the ASTM to return to school.

II. Review of Agenda and Minutes. The agenda was approved without change.

A motion was made to approve the minutes for the July 7, 2005 meeting as circulated. Second. The motion passed unanimously.

III. Attendees:

Mark Bean, GSK

Tony Davies, Waters

Maren Fiege, Waters

Gary Kramer, NIST

Richard Larsen, JASCO

Peter Linstrom, NIST

Charlie Manfredi, Agilent

Dave Martinsen, ACS

Len Morrissey, ASTM

Mark Mullins, SSI

Anh Dao Nguyen, NIST

Burkhard Schäfer, Univ. Kaiserslautern

IV. Location of Schemas. There was a discussion concerning the need for a permanent location for the AnIML schema files. On the one hand, XML only requires a unique namespace for schemas, not the actual existence of files at the specified locations. However, if one wants to validate AnIML files, then the schema files do need to exist. When AnIML files are moved from one environment to another, significant editing would be required, unless the schema files were available from a standard, unchanging, location. Several possible locations were discussed: xml.org, animl.org, sourceforge, IUPAC, ASTM. The ASTM position on schemas is still evolving; at the current time, files won't be posted until some documentation is available for the standard. In addition, standards files are generally stored in an access-controlled area of the ASTM site. If access control is required to validate AnIML files against the schemas, then the usefulness of AnIML will be severely curtailed.

The requirements for the schema location are

1. 24x7 availability
2. permanent availability (meaning, in practice, that it will likely be available for a long period of time)
3. no access control
4. sample documents should be allowed, in addition to schema files.

Given these requirements, Mark Bean volunteered examine xml.org, and to return with a recommendation as to whether it meets the requirements.

Burkhard Schäfer will investigate the possibility of using a url whose only function is to redirect to the then-current location of the schemas. This would allow the schemas to be moved from one location to another, while the url reference within AnIML documents could remain the same.

V. AnIML Website Redesign. The new website was deployed, and the comments were generally favorable, as an improvement over the previous site. The following changes were requested:

1. The text in the navigation bar is hard to read. Suggestion was made to use bold arial font in a slightly larger point size.
2. The need for a “Project Links:” category, with 4 entries, was not clear. Suggestion was to make all of the links in the navigation bar at the same level.

VI. AnIML Subgroup Membership. Gary Kramer presented his listing of the subgroup membership. A couple of corrections were noted. Following is the updated composition of the AnIML subgroups:

IR & UV/Vis	Richard Larsen (chair) James Duckworth Stuart Chalk
Chromatography	Frank Tontala (chair) Alex Mutin Mohan Cashyap Michael Harzheim
MS & IMS	David Varley (chair) Mark Bean (GSK) Someone from Thermo Someone from Shimadzu
NMR	(no one selected; need to ask for help from Bruker, JEOL, Varian, & perhaps Woody Conover)
Core and Technique Schemas:	Burkhard Schäfer Maren Fiege Someone from Scientific Software to replace Mark Mullins Mohan Cashyap Mark Bean

VII. Formal AnIML Requirements Document. Mark Bean circulated a draft requirements document for the meeting. However, it was requested that discussion be delayed until members have a chance to review the document. Tony Davies will attempt to merge the items from Mark’s list into the diagram he circulated at the last meeting.

VIII. Core Developer’s Meeting. The core group has been unable to meet due to vacations and other scheduling problems. There is some urgency for the group to meet, since Anh Dao is leaving Gary Kramer’s group in three weeks, and the current core schema fails with both the latest version of XMLSpy and Microsoft Visual Studio. The core group agreed to try to meet at 10:30 am EDT on

August 12, 2005, with the goal of correcting the known schema errors. Burkhard Schäfer will review the previous documents and notes from virtual meetings, and prepare a list of known problems and Mark Bean will prepare a list of previously agreed changes. These modifications will be made to the frozen version 1.0 of the schema. Len Morrissey will set up the meeting and send invitations to the Core Group.

IX. AnIML Example. Richard Larsen noted that he had looked at the IR examples, and had some questions which he will be communicating with Anh Dao. He also commented on a problem with the way the IR spectrum was plotted in the example, in a format which no IR spectroscopist actually uses. It was noted that the way in which the viewer displays data is up to the viewer software, not AnIML.

X. PittCon Session on AnIML. Gary Kramer needs to submit today the final plan for a PittCon Session on AnIML. After much discussion, the following talks were decided on:

1. Introduction – Gary Kramer
2. Requirements – Mark Bean
3. Architecture – Burkhard Schäfer
4. Technique Definitions – Maren Fiege
5. Data Model – Peter Linstrom
6. Vendor experience – Alex Mutin
7. Vendor experience – Mark Mullins
8. Regulatory considerations – Tony Davies
9. Path to the standard – Dave Martinsen
10. Concluding remarks – Gary Kramer

XI. Miscellaneous.

1. Several ASTM E13 standards documents are open for balloting. Included are two renewals for ASTM E13.15, and a reorganization of ASTM E13 which has an impact on ASTM E13.15.

XII. Agenda Items for Next Virtual Meeting.

1. Review of AnIML requirements document.

XIII. Action Items:

- Web page redesign: Dave Martinsen will make the suggested changes to the website.
- PittCon Session: Gary Kramer will forward the list of presentations and speakers to the PittCon committee. Each presenter is requested to prepare an abstract for submission upon request of the PittCon committee.
- Requirements document: Tony Davies will update his requirements figure with new items from Mark Bean's document.
- Mark Bean will determine whether or not xml.org will satisfy the requirements for the AnIML schema location.
- Burkhard Schäfer will determine whether a redirecting url will work as a permanent placeholder for the AnIML schema location.
- Core Group will update the core schema.

XIV. Future Meetings:

- Working Group Teleconferences

- If possible, Fridays are preferred days for E13.15 meetings. However, due to availability, the next meeting is scheduled for a Thursday.
- August 25, 2005, 10:30 am – 12:30 pm EDT
- IQPC/ALI (January 30 – February 1, 2006, San Diego) and Lab Automation (January 21-25, 2006, Palm Springs, CA)
 - The dates of IQPC/ALI were changed to avoid collision with Lab Automation. A joint symposium/workshop is planned to accommodate attendees of both conferences.
- EAS, November 13-17, 2005, Somerset, NJ, Doubletree Somerset, Room 211
 - Working Group Meeting, November 13, 2005, 3:00 – 5:00 pm
 - Business Meeting, November 14, 2005, 5:00 – 7:00 pm
- PittCon, March 12-17, 2006, Orlando, FL
 - Business Meeting
 - Symposium/Workshop

XV. Adjournment. Motion to adjourn. Second. Carried unanimously at 12:12 pm EDT.

Submitted by David Martinsen, ACS, ASTM E13.15 Secretary