



**Address** 100 Barr Harbor Drive  
PO Box C700  
W. Conshohocken, PA  
19428-2959 | USA

**Phone** 610.832.9500  
**Fax** 610.832.9555  
**e-mail** [service@astm.org](mailto:service@astm.org)  
**Web** [www.astm.org](http://www.astm.org)

---

**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

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

10:37 am – 12:15 pm EST  
Wednesday January 13, 2006  
Virtual Meeting

- I Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 10:37 am EST.
- II Attendees:**
- |                     |                         |
|---------------------|-------------------------|
| Michael Boruta, ACD | Peter Linstrom, NIST    |
| Tony Davies, Waters | David Martinsen, ACS    |
| Maren Fiege, Waters | Mark Mullins, Agilent   |
| Ronny Jopp, NIST    | Alex Mutin, Shimadzu    |
| Joe Koury, ASTM     | Dale O'Neill, Agilent   |
| Gary Kramer, NIST   | Alexander Roth, NIST    |
| Joe Koury, ASTM     | Burkhard Schaefer, BSSN |
- 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 February 10 2006.
- IV Approval of minutes**
- The minutes of the December 21 meeting were approved as distributed.
- V AnIML at scientific meetings**
- The Pittcon meeting from 3/12 to 3/17 2006 in Orlando, Florida was discussed.
    - Business Meeting: Monday 3/13, 5:30 – 7:30 pm
    - Working Group Meeting: Wednesday 3/15, 5:15 – 7:30 pm, followed by dinner
    - AnIML Workshop: Thursday, 3/16, 1:30-5 pm
  - Lab Automation: Informal Working Group meeting scheduled for 1/26. No room information yet. The topic will be naming and design rules. Ronny Jopp, Alex Roth, Burkhard Schaefer, and Gary Kramer are expected.
  - IQPC: End of January. Only Gary Kramer and Tony Davies are expected.
  - ACS: 3/28: All day session on XML in Chemistry. Several working group members are presenting.
- VI Website for AnIML Standard:** Joe Koury had a number of questions regarding the AnIML requirements for the ASTM web site, in order to better understand the needs of the XML world. The following summarizes the requirements:
- Available 24x7.
  - Fixed urls for the xml files, since they will be referenced automatically by application software. If the location changes, many applications will not be able to run.
  - No password protection. Anybody, and any application, must be able to read the XML files without the need for a password.
  - The XML files are intended to be machine-readable, and machine-processable. They are not human-readable files, like Word documents.
- VII Core working group report**
- The core group had two meetings since the last task group. One issue they would like to discuss with the entire group has to do with the use of modules within AnIML. The module concept was introduced to allow a file to be “included” into several different technique definitions. For example, sample attributes could be used in multiple techniques without the need to maintain the same coding in several files. This can be accommodated now with the W3C “XInclude” recommendation. Use of the include in this way would make it easier for developers to work with AnIML, since they

wouldn't need to code for a proprietary include scheme. We settled on modules earlier in the AnIML process, with the intention of providing a tool for technique definition authors to use to handle modules. However, while modules do make things easier for technique writers, they put a burden on software developers. This is not an end-user issue, since end users will not be writing technique definitions. In summary: modules make things easy for technique developers, more difficult for software developers.

The proposal from the core group is for technique developers to use the XInclude specification when writing the techniques, but to perform the inclusion when releasing the files for use, and for balloting. The intention is that any technique definition released to the public will have all the inclusions already applied. In either case, the data files in AnIML format would be unaffected.

There was some concern over the procedures required when one modules, or XInclude files, is updated. Whenever something in one of the XInclude files changes, all existing technique definitions would need to be updated, and distributed. However, this would need to be done anyway, whether using XInclude files or modules. We could make each XInclude file a ballotable item, and just rebalot the definition. However, we would still need to modify each technique definition to point to the new XInclude files.

There was also a concern over the ultimate usability of the AnIML specification. The core group is confident that the XInclude syntax is easier to use than the modules. Therefore we should migrate to the use of XInclude, since this will make AnIML easier to use in the long run. Technique writers could use the XInclude files, and we could distribute the merged files. The technique document could be awkward, a problem for those implementing the standard. Writing documentation could also be a problem. In the end, we need enough information, stored in a recognizable way, so vendors can use it in their instruments. The specification should be simple enough to handle simple techniques, like UV, but must also be rich enough to handle complex hyphenated techniques. We decided on technique files, using modules, to provide this flexibility, but because it is not a standard protocol, IBM, Microsoft, and Oracle are not writing applications to support our protocol. Schematron is one possible method for data validation. Another possibility is to write a validator application. Two validator prototypes have been written at NIST. Such an environment is still somewhat complex; some software companies may find problems with the validation software, and may need to make fixes themselves.

The core group will continue to explore the issue of modules vs. XInclude files, taking into account the discussion of the full working group.

VIII **NDRs for AnIML schemas:** Gary Kramer is currently revising the document on naming and design rules for the AnIML core schema. The revised document is not ready yet. The goal is for the next working group meeting.

IX **Miscellaneous related efforts:**

- **UnitsML:** The OASIS technical committee for UnitsML is moving forward. If anyone is interested, please let Gary Kramer know. The first meeting is to be in April.
- **IUPAC Chemometrics Group:** Meeting in Dublin on January 20.
- **ASTM Medical XML Documentation:** Tony Davies noted that a medical committee at ASTM has posted documents for balloting, and pointed out that we already have more material than they do. We might be able to have three documents read for ballot in September.

X **Adjournment:** The meeting was adjourned at 12:15 pm EST.

Minutes taken by David Martinsen