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Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

DRAFT Minutes for E13.15 Subcommittee Working Group DRAFT

10:35 am – 11:50 am EDT

Wednesday April 21, 2006

Virtual Meeting

- I Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 10:35 am EST. A poll was taken, and with no objections, the meeting was recorded.
- II Attendees:**
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|-----------------------------|------------------------|
| Michael Boruta, ACD | Gary Kramer, NIST |
| David Farrusseng, CNRS | David Martinsen, ACS |
| Maren Fiege, Waters | Dale O'Neill, Agilent |
| David Joyce, ThermoElectron | Alexander Roth, NIST |
| Ronny Jopp, NIST | Burkhard Schäfer, BSSN |
| Joe Koury, ASTM | |
- III Schedule for next virtual meeting:** The next virtual working group meeting will be held on May 26, 2006, 10:30 am - 12:30 pm EDT.
- IV Approval of minutes:**
- A motion was made, and seconded, to approve the minutes of the March 3, 2006 virtual meeting as sent. The motion was carried.
 - For the March 15, 2006 minutes, it was requested that the statement that ThermoElectron was moving to XML be changed to indicate that they were moving to GAML for UV/IR, OMNIC, and Atlas. A motion was made, and seconded, to approve the minutes as amended. The motion carried.
 - It was noted that on March 31, the recording of the virtual meeting was unsuccessful. The secretary had to leave at 11 am, and was relying on the recording to prepare the minutes. If anyone has notes on the March 31 meeting, please send them to David Martinsen (d_martinsen@acs.org).
 - It was noted that the minutes of the Business Meeting at PittCon 2006 are due to Joe Koury at ASTM by May 1.
- V AnIML PR.**
- Files of PittCon 2006 presentations have been sent to Burkhard Schäfer. He will put them in a PittCon 2006 folder, and make them available on the AnIML web site.
 - Gary Kramer submitted a symposium proposal for PittCon 2007, with 4 speakers. If accepted, the intention is to add more speakers and change it to a regular session.
 - Anand Mudambi and Joe Solsky invited E13.15 to participate in the National Environmental Monitoring Conference, the week of August 28 in Arlington, VA. They are particularly interested in vendor presentations, would like 2-4 speakers. Dale O'Neill will check on whether he, or someone else from Agilent, could participate.
 - Gary Kramer received an invitation for a speaker on AnIML at a Laboratory Informatics Conference, similar to IQPC, being held in Philadelphia, August 1-2. Dave Joyce will check to see if ThermoElectron will be there. Mark Bean is another possibility, since he is from the Philadelphia.
 - Richard Wilhelm of ASTM will write an article on AnIML for the ASTM publication if we answer questions. Burkhard Schäfer and Gary Kramer agreed to a conference call. Joe Koury will work on setting it up for May 2.
 - A Life Science Automation Conference is being held in Rostock, Germany, September 14-15, 2006. Burkhard Schäfer and Maren Fiege are potential speakers. The conference is sponsored by CELISCA.
- VI Technique Expert Groups.** Mark Mullins has left Agilent, and so will no longer be involved with E13.15. Dale O'Neill indicated that he is willing to join the Chromatography technique group in Mark's place.

VII TOPCOMBI. David Farresung made a presentation on the TOPCOMBI effort, <http://www.topcombi.org>. A copy of his slides is posted to the AnIML web site. The effort is a European consortium of 22 partners. The goal is to use high throughput methodologies and combinatorial techniques to reduce costs and speed development to market for chemical processes. This requires normalization and standardization as data from different sources is consumed and propagated through a workflow, from raw data to information to knowledge. The first case study brought data from a Shimadzu SPR16 and an HP GC. The TOPCOMBI approach showed a time gain of a factor of 10 compared to manually extracting and converting data. Interoperability is enabled by using XML. CNRS plans to promote AnIML in Europe through TopCombi. In April 2007, a conference will be held in Bari, Italy. There will be a session on software and databases, and if desired, AnIML can have 2 presentations.

David Farresung and François Gilardoni would like to participate in the AnIML effort with Materials Sciences (David) and Web Services (François). They are ready to use our prototypes and drivers as soon as available.

Some discussion followed David's presentation. Currently, data transport is accomplished using standalone software. Data are gathered into tables of databases. Data can be stored in a database or in files, reloaded and queried. The workflow itself can also be saved, and shared with others.

VIII Core Group: The core group had nothing to report, since they hadn't met since PittCon. It was noted, however, that there had been much activity on the AnIML developer list. This has been driven by Robert Lancashire, resulting from work on the JCAMP to AnIML converter. Questions were discussed on how to incorporate parameters, and whether parameters should be included in a technique definition, or in the core.

The technique groups are meeting to go over the definitions. Richard Larsen, Stuart Chalk, and Burkhard Schäfer have communicated via email, and have been making progress on UV. Then they will switch to IR. A request was made that they include Alex Roth, since he is developing the NDRs.

IX Naming and Design Rules: A question was raised regarding the status of the NDRs. Some thought they were complete. Others weren't so sure. Parts of the NDR have been implemented, but not all. The ones which are left are the more complex to implement, such as making types global. Most of the smaller things are done.

A motion was made and seconded to adopt the NDRs for the AnIML core and technique schemas, version 1.2.3 as implemented just after the February meeting in Palm Springs. After some discussion, a vote was taken and the motion passed unanimously.

Alex Roth described the status of the NDRs for technique definitions. Rules about content are not needed for the technique document. Where applicable, a recommendation was made to use ASTM definitions where they exist, followed by IUPAC. Beyond that, IEEE should be consulted for IT terms. For each definition, an annotation should be included to denote the source of the term. Joe Koury will send a copy of E13 definitions to everyone at the meeting, plus Mark Bean.

X UnitsML: Ronny Jopp is working on an NDR for UnitsML. He will present it at the next meeting. The OASIS technical committee has not been set up yet. Once it is, Gary Kramer will send a note to everyone on the mailing list, in case people want to be involved.

XI Recording: A question came up regarding distribution of the recording of the virtual meeting. If we make it generally available, people might be encouraged to skip attending the session, knowing they could listen to it later. This would make the virtual meetings less effective. The consensus was that we would not announce availability, but if someone asked for it before ASTM deleted it, he or she could get access to the file. Note that recording of sessions can not be decided in advance. Participants must agree at the start of the meeting.

XII Adjournment: The meeting was adjourned at 11:50 am EDT.

Minutes taken by David Martinsen