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Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

Minutes for E13.15 Subcommittee Working Group

10:30 am – 12:30 pm EST

February 9, 2007

Virtual Meeting

I. Introductions and Welcome: Gary Kramer, E13.15 Chair called the meeting to order at 10:30 am EST. The ASTM release form for recording the session was displayed on the screen. There being no objections, the meeting was recorded.

II. Attendees:

Mark Bean, GSK
Michael Boruta, ACD
Stuart Chalk, Univ. of N. Florida
Tony Davies, GSK
Maren Fiege, Waters
Patrick Gleichmann, NIST
Joe Koury, ASTM
Gary Kramer, NIST

Robert Lancashire, UWI
Peter Linstrom, NIST
Dave Martinsen, ACS
Alex Mutin, Shimadzu
Dale O'Neill, Agilent
Kordian Placzek, NIST
Burkhard Schaefer, BSSN

III. Next Virtual Meeting: March 16, 2007, 10:30 - 12:30 EST.

- The UV/Vis Technique Group will meet on February 13, 2007 at 10:30 am.
- The Core Group will meet March 20, 2007 at 10:30 am EST. They generally meet every other Tuesday.

IV. Minutes: On the November 3, 2006 minutes, no changes were noted. On the December 8, 2006 minutes, the name of Maren's colleague should be changed to "Rolf Grigat". A motion was made and seconded to approve the November 3 minutes as distributed, and the December 8 minutes as amended. The motion carried.

V. Pittcon Preview: Each of the presenters gave an overview of their presentation for PittCon.

- a. Gary Kramer's introductory talk will include only a brief definition of XML, but will concentrate on the fact that XML is really a mainstream technology. He will also introduce each of the other talks in the rest of the session.

- b. Burkhard Schaefer will cover validation, and will also talk about the basic AnIML structure - the core, techniques, and building blocks. He will be very generic, so as not to cover the material for later talks.
- c. Maren Fiege will talk about UV, and will use Anh Dao's holmium spectrum updated to the current AnIML schema. She will also try to use Robert's viewer to display the spectrum.
- d. Dale O'Neill will talk about long term storage, proliferation of data, storage formats, regulations and SOPs, and the necessity for a neutral format. He will also get into the chromatography technique.
- e. Mark Bean will talk about the hybridized technique, LCMS, building up from separate techniques, and the challenges of multidimensional data.
- f. Robert Lancashire will discuss his viewer, which can now handle JCAMP, CML, and AnIML. He will also discuss Stuart's online converter.
- g. Peter Linstrom will talk about publishing AnIML files using web servers, covering some of the XML tools available. He will also talk about server side parsing, client side parsing, graphs/xslt. He will also talk about how standard tools can be used to build specialized applications. A discussion about the location of schemas will not be included, because that hasn't yet been decided.
- h. Alex Mutin will talk about controlling instruments using XML, and so won't get into the data model very much at all. He will discuss network layouts, different instrument configurations, and advantages of using XML to control multiple instruments. He will also show some Shimadzu instruments that are using XML control, as well as possibilities for the future. A suggestion was made to look at other systems that might for instrument control, and perhaps make mention of those.
- i. Gary Kramer will close with a summary, and also an invitation for technique experts to join the process, particularly in NMR.

VI. Pittcon Details:

- a. The session starts at 1:30. Speakers should arrive early to make sure that their laptops will work.
- b. After Pittcon, please submit presentations to Gary or Peter, and they can be loaded onto the web site.

VII. Other AnIML Meetings at Pittcon:

- a. Business Meeting: 3:00 - 4:00 pm Tuesday
- b. Working Group: 3:30 - 5:30 pm Sunday - as published.
- c. Stuart Chalk workshop on Wednesday. He will put link on the AnIML wiki.

VIII. The AnIML wiki:

- a. Mark Bean demonstrated the AnIML wiki site. The site is restricted to those who have accounts, including a guest account. Documents can be edited, files can be uploaded. Discussions can continue offline. All developers have

accounts, which Mark set up and sent to the developers. Search engines can not index the site, so it is not visible to the world.

- b. Eventually, some parts of the wiki could be made public, and be used as the AnIML web site.

IX. Adjourn: 12:30 pm EST.

Minutes prepared by David Martinsen, ACS
ASTM E13.15 Secretary