



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

(SCDS) Subcommittee on Cheminformatics Data Standards

IUPAC

Committee on Publications and Cheminformatics Data Standards (CPCDS)
SubCommittee on Cheminformatics Data Standards (SCDS)

March 6, 2017, 9am - 10am US-EST

(Web conference)

Minutes

SCDS Members Present: Greg Banik, Ian Bruno, Stuart Chalk, Chris Fellows, Robert Lancashire, Bonnie Lawlor, Leah McEwen, Dave Martinsen, Claudio dos Santos, Andrey Yerin

1. *Welcome new members, from the Polymer Division Subcommittee on Terminology*
 - a. **Chris Fellows**, Royal Australian Chemical Institute
 - b. **Claudio dos Santos**, Federal University of Ouro Preto, Brazil

2. *Acceptance of Minutes of February 9, 2017*

Approved

3. *São Paulo General Assembly GA*
 - a. Planning to attend: Claudio, Chris, Ron, Dave, Leah, Ian, Stuart, Andrey, Jeremy
 - b. Dave will look into web conference for remote attendees to SCDS

4. *Cheminformatics Color Book*
 - a. Proposal soon to be submitted to CPCDS
 - b. Most task group members should be able to attend the proposed open meeting in São Paulo
 - c. Emerging need to address 'machine-readable' data published with articles as part of funding requirements
 - d. Semantic interpretation increasingly important, but metadata management is concern
 - e. Who are working on Cheminformatics Data Standards
 - a. CPCDS working on a list
 - b. SCDS start listing known standards in Google Doc (in SCDS GDrive)

ACTION: SCDS members brainstorm existing chemical digital data standards

5. *JCAMP-DX status and future continued* (<http://old.iupac.org/jcamp/>)
 - a. Started in 1980s, latest version 1999, available on most spectroscopy instruments, still widely used among vendors in spectroscopy disciplines.



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JCAMP-DX 6.0 development was put on hold in 2002 for AnIML, need to move forward now

- i. See 2013 article by Tony and Robert:
<http://www.spectroscopyeurope.com/articles/tony-davies-column/3760-updating-iupac-spectroscopy-recommendations-and-data-standards>
 - ii. Tony Davies considering a project proposal for the next generation of JCAMP-DX
 - iii. Coordinate with AnIML and other analytical data reporting efforts (e.g. Allotrope)
 - b. Suggestions for input and feedback for updating JCAMP-DX
 - i. Target stakeholders: instrument vendors, spectra reference sources, pharma, instrument facilities, chemistry research depts
 - ii. Survey of chemistry community, can we put this thorough IUPAC member channels?
 - iii. Consider a workshop of key stakeholders to consider the type of needs for an open file format standar: Pittcon (annually in March), other analytical conferences in US, EU, Asia
 - iv. Discuss with Div V at IUPAC GA
 - c. Issues with JCAMP-DX
 - i. Writing files can be problematic, easy to be incomplete
 - ii. Useful for archiving and exchange - between software, and between machines
 - iii. Concern about converting so many files from current JCAMP-DX into any new format, could take long time, the volume of data is large in numbers and file sizes
 - d. Robert, Leah and Dave looked at the existing files on the jcamp-dx.org to migrate to new iupac.org. This material may become part of the new Cheminformatics Color Book.
 - e. Brief AnIML update - Stuart
 - i. <https://animl.org/>
 - ii. Status: specification frozen two years ago to work on documentation; may be formally out end of 2017
6. *Gold Book Update*, Stuart Chalk
- a. Forming static visual pages for new site
 - b. Will post as soon as approved
 - c. Looking into the CrossRef account for Gold Book, not associated with DG registration of PAC or CI, mgmt of DOI and can help us understand use



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ACTION: Stuart and Leah will look at the CrossRef data for the GoldBook DOIs

Respectfully submitted,

Leah McEwen, Co-Chair, Subcommittee on Cheminformatics Data Standards

May 9, 2017