

IUPAC Database Enhancements

Teleconference  
8:30am - 9:00am EST  
December 9, 2015

**Draft Minutes**

\*\*\*\*\*

**IUPAC Attendees:** Colin Humphris, IUPAC Secretary General, Bonnie Lawlor, Chair, IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS)

**De Gruyter Attendees:** Katharina Butsch

The meeting opened at 9:00am EST. The objective of today's teleconference was to follow-up on the discussion held on October 29, 2015 regarding possible enhancements to the IUPAC Standards and Recommendations database for introduction in 2017.

**Status of Phase One**

Katharina Busch said that the contractor who is responsible for the conversion of articles from PDF to XML did not have everything turned over by the end of November as expected. Plans are to have it delivered by the second week of January with a test database available by the end of January. This delay should not have any impact on the database release date.

Katharina said that the sample content that she has reviewed to date is of very high quality and all of the search functions have been tested. In addition to the e-publishing group, the database will get support from the De Gruyter database publishing group. The manager, Hella Behrend, will be the point person and she is a colleague of Spencer McGrath. Hella will be responsible for looking at the regular updates of the file and will handle the freelancer once Katharina leaves De Gruyter later this month. Katharina will provide her email address.

Katharina said that De Gruyter has found her replacement. He is an organic chemist, Dr. Oleg Lebedev, and he will start immediately following the Christmas holidays as Senior Acquisitions Editor, Chemistry. He will have responsibility for the entire chemistry section and will probably be IUPAC's main contact for the database. Katharina's functions regarding the database, however, will be fulfilled by Hella Behrend and probably Karin Sora will make the introductions in the New Year. (*Note:* Bonnie has since heard from Dr. Lebedev who said that we will have the test version of the product for review in the beginning of February and that the 2015 articles will be added to the database in March before the launch).

Katharina said that De Gruyter would like IUPAC to provide a supplementary document to the database that talks about IUPAC, the history and importance of the Standards and Recommendations, IUPAC members - anything that IUPAC wishes (even a membership application form). There is no specific format nor any page requirements. A PDF version is needed by the end of February 2016. Colin suggested that Bonnie seek input from Ron Weir on the standards; e.g. their value, limitations, how they should be used, etc. The PDF will be on the same page as the database along with other supplementary material such as the user manual.

**ACTION:** *Bonnie Lawlor* will draft the supplementary material page for review, comment, and editing by the Secretariat. She will request Ron Weir's input on the value, limits and use of the standards.

### **Enriched Database**

Katharina noted that Colin Humphris and Karin Sora have already connected about a source for the InChI codes, so that is a great first start. Karin will be traveling for the remainder of this year and will probably reach out to Alan McNaught in January when Dr. Lebedev is on board. Katharina then asked about the status of IUPAC's perspective on using a Periodic Table as a search feature for the database.

Bonnie Lawlor said that she did not want to speak for Lynn Soby, but that her personal opinion when she left the October 29<sup>th</sup> discussion was that IUPAC had no problem with having the periodic table as a search feature of the database. Lynn was more concerned with how IUPAC itself will use the periodic table on its own website. Colin agreed that IUPAC has no problem with the periodic table being used as a search portal to the database. But he suggested that the design of the periodic table should perhaps be in alignment with the design on the new IUPAC website since in a way it is a signatory logo for IUPAC. In fact, he believes it would look odd for the periodic table in an IUPAC database not to replicate the design of the periodic table on the new IUPAC website that will be launched early in 2016. Bonnie agreed. Katharina said that the e-publishing group at De Gruyter has not yet worked out the technical implementation of the periodic table, but she will inform them of IUPAC's desire regarding the design.

**ACTION:** *Katharina Butsch* will notify the De Gruyter e-publishing group that the design of the periodic table portal to the database should replicate the design of the periodic table on the new IUPAC website that will be launched early in 2016.

Katharina asked if either Colin or Bonnie needed her to convey anything to Karin. Colin said that he wanted Karin to know that she can work through him at any time regarding the InChI codes. He knows Alan McNaught very well as Alan is both the Secretary for the IUPAC Division VIII subcommittee on InChI and the Secretary of the InChI Trust. Colin also noted that Richard Hartshorn, the new IUPAC Secretary General, is on the InChI Trust Board of Directors. He suggested that Karin might want to consider having De Gruyter become an Associate Member of the Trust and use the codes in other De Gruyter products since InChI is becoming more broadly accepted and utilized.

Katharina thanked both Colin and Bonnie for their cooperation over the past two years and said that she will miss working with them when she leaves De Gruyter this month. They both said that they will miss Katharina on a personal level as well and that it has been a pleasure working with her. Katharina said that she can now tell them where she is going. She will be joining a little start-up as a content editor for a company that is programming a teaching platform for students. The company has two locations - Berlin and Cologne, and that this job change will allow her to return to her home town in the Cologne area and be close again with family and friends.

She said that she has been away from teaching for five years and away from direct involvement with science for two. She found that she was losing her skills and wanted to get back into working creatively with chemistry before she lost everything. Working on the IUPAC database allowed her to do just that and she found that this is what she wants to do moving forward. She said that her leaving De Gruyter is not IUPAC's fault, but that IUPAC was definitely an influence. Colin complimented Katharina on her command of the English language and said that it played a major role in the success



## **(CPCDS) Committee on Publications and Cheminformatics Data Standards**

of the working relationship on the database. Katharina said that she is sad that she will not see the final results of the database, but is confident that from what she has seen to date that all will go well as it is in good hands at De Gruyter.

The meeting closed with goodbyes and best wishes for a Merry Christmas and a Happy New Year.

There being no further discussion, the meeting was adjourned at 9:00am EST.

Respectfully Submitted,

Bonnie Lawlor, Chair  
IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS)  
January 25, 2016

\*\*\*\*\*