

**Minutes of CPCDS Meeting August 9-10, 2015  
Busan, Korea**

**Titular Members:**

Bonnie Lawlor (Chair)  
James Liu (Secretary)  
Jeremy Frey (Absent)  
Kazuhiro Hayashi  
Lene Hviid  
Wolfram Koch (Absent)  
Robert Lancashire  
Bono Lučić (Absent)  
Leah McEwen  
Miloslav Nič (Absent)

**Associate Members:**

Mark Kinnan (Absent)

**Ex Officio:**

Hugh Burrows (*PAC* Scientific Editor)

**IUPAC**

Colin Humphris (IUPAC Secretary-General)  
Fabienne Meyers (IUPAC Associate Director, Secretariat)  
Lynn Soby (IUPAC Executive Director)

**Observers:**

Brynn Hibbert, President, IUPAC Division V  
Ron Weir, Chair, Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS)  
Illie Guzei, Director Crystallography, Univ. Wisconsin  
Yeon Gyu Yu

**De Gruyter:**

Katharina Butsch, Acquisition Editor, Chemistry  
Spencer McGrath, Senior Project Manager

**Schedule:**

**Sunday, August 9, 2015:** 8:00am - 4:20pm

**Sunday, August 10, 2015:** 9:00am - 12:00pm

**Meeting was held at:**

Busan Exhibition and Convention Center (BEXCO)  
55 APEC-ro, Haeundae-gu  
Busan, South Korea  
Room 317

**Agenda:**

**Sunday: August 9, 2015**

**1. Welcome and Introduction of Members and Guests**

Bonnie Lawlor opened the meeting at 9:00am. Before proceeding, introductions were made around the table.

**2. Finalize the Agenda**

The agenda was accepted as submitted.

**3. Minutes from the 2014 Meeting were approved.**

The minutes from the Committee meeting held in Berlin, Germany on July 26-27, 2014 were accepted as submitted at a prior meeting. Robert Lancashire and James Liu both noted that the minutes in the agenda book were not the final, corrected set.

**4. Review of Membership Roster**

The 2015 membership roster was reviewed and it appears on page 18 of the agenda book. Lene Hviid's term dates were corrected to read 2013-2016 as she was an observer in 2012.

**5. CPCDS Role and Responsibilities**

Bonnie Lawlor reported that the changes to section (i) of the Committee's Terms of Reference were approved by the IUPAC Executive Committee in November 2014. These changes are as follows: (changes are bolded).

(i) To advise the President, Executive Committee, other Standing Committees, Divisions, and Commissions on all aspects of the design and implementation **of publications and data-sharing**, including computerized databases of all sorts, and to promote the compatibility of **the** electronic transmission, **storage, and management of digital content through the development of standards for the creation of a consistent and interoperable global framework for human and machine-readable chemical information.**

Bonnie noted that the changes will be put forth to Council this week for approval.

**6. Report from the Secretariat**

IUPAC Executive Director, Lynn Soby, gave an overview of Union activities in the past year. She first gave a brief review of the Secretariat, especially the new office facility at Research Triangle Park, North Carolina. The constraints of the old facility brought many challenges to the Union from both administrative perspective and the technical support and development of the IUPAC website.

Lynn then shared the perspective on the current situation and the future. The IUPAC Secretariat moved into the new 2,500 square feet office space in March 2015, with all electricity included in the rent for the new facility. The most important aspect of the new facility is the IT infrastructure. They have moved from an original storage shed to a state-of-the-art facility. All the servers have backups and all phones are VOIP phones.

A summary of the past year's activities at the Secretariat is as follows:

- Stabilized the bleeding of the website infrastructure; the new Website development and server setup is in progress.
- Evaluated all staff capabilities and the necessary capacity - is ongoing.
  - √ Identified key staff gap and hired Jay Lucido on July 1, 2015, who will serve as IUPAC's Financial Comptroller.
  - √ Rebuilt the Financial Management system and initiated Cost accounting/GAPP standards rather than continuing with the cash accounting procedure that was used in the past
- Identified space and negotiated new lease for Secretariat. March 13<sup>th</sup> move in date.
- Resolved *Chemistry International (CI)* and De Gruyter print label issues. IUPAC numbers have been stabilized and the focus is on the costs of complimentary vs. paid subscriptions (Lynn stressed the importance of getting to know the people and establish relationship with our partners at De Gruyter. We are working well with each other. Lynn and others visited De Gruyter in their Boston office earlier in the year.)
- Improved *CI* workflow issues and the partnership perspective is also improving.
- Held on-site meetings to enable open, direct communication and problem resolution.
- Clarified Copyright for *Pure and Applied Chemistry (PAC)* and *CI* author - open source documentation. We wanted a more open source approach. We already set this up for *CI*. Sales for *PAC* are going really well. *PAC* revenue is up while the cost of *CI* goes down. *PAC* is now well under control.
- Book and royalty contracts are now centralized in the Secretariat.

#### **7. Website Update and demo (Lynn Soby)**

Lynn Soby then gave a brief demonstration of the new website prototype. It is based on the report provided by the Web Vision Task Force (including data from their survey regarding user needs and desires), as well as on the backend needs, issues and future operational capabilities. The first step is to stop the bleeding of the current website, rebuild iupac.org, and move to a new platform).

She sent out a call for website development proposals and received four responses. She narrowed them down to two and made a final decision to work with TheeDesign, a company local to the IUPAC office. A prototype website was built for gathering user input here in Busan. It balances the needs of both external and internal audiences and builds capabilities and future capacity for Phase II and beyond. The new site will have unlimited capability and capacity. Lynn noted that the website is built on WordPress and that a soft launch is scheduled for January 2016.

On the very top level of the Home page are the following tabs: "Contact," "Forum," "Join," "Login," and "Search." At the next level are: "Who We Are," "Member Organizations," "Events," "Projects," and "News." Lynn noted that on the main carousel section of the home page, there will be five or six things that we may want to feature and a "Take Me There" button will lead to the detail pages of the features (this content will be regularly freshened). The next level of the Home page highlights an inspirational placeholder about IUPAC; e.g. "advance the worldwide role of

chemistry.” This is followed by a member section that includes the various membership programs and then the next section has icons representing the various fields of chemistry. There was a brief discussion of security concerns. The Committee thought that the prototype was very well done and members were encouraged to go to the Secretariat office at BEXCO to “play” with it and post comments/suggestions.

**8. *Pure and Applied Chemistry (PAC).***

Dr. Hugh Burrows gave an extensive update on the journal activities since the last meeting in Berlin. He noted that Joshua Gannon has taken over from Allie Struzik as *Journal Manager of Pure and Applied Chemistry*, and has also taken on editorial functions that were previously handled by Cheryl Wurzbacher. This transition has gone smoothly and they are currently developing a realistic timeline between invitation and publication of manuscripts. The time from a Conference to publication in *PAC* should be around nine months - ideally two months for submission, two months for review, one month for revision and two months for production of the online version. Issues will then be published up to two months afterwards. We should make sure that authors know that manuscripts can be submitted before Conferences, and aim for a deadline of maximum of two months after the meeting. In the past this has been complicated because of a breakdown of communication with IUPAC on Conferences. It has been arranged that both the Scientific Editor of *PAC* and Fabienne Meyers should receive application for IUPAC sponsorship of Conferences and meetings and the approval letter. This will include current email contact details of the Conference Organizer so that publication negotiations can take place smoothly. Because of the above-mentioned staff changes, the proposed introduction of Graphical Abstracts of Conference papers has not yet started. All future invitation letters to submit to *PAC* will indicate the need for a Graphical Abstract, and we will try to make sure that all papers published after January 2016 have Graphical Abstracts in the Table of Contents page.

Hugh also discussed the publication of conference articles in the last volume of *PAC* (2014, 86); provided an overview of the papers published to date in the current volume (2015, 87); and gave an indication of the publication prospects for late 2015/early 2016. An additional publication project involves preparation of special topic issues. The first of these will be in the area of Chemistry and Cultural Heritage, and should be published in early 2016.

He noted that a challenge for *PAC* is that some authors are reluctant to submit to the journal due to its impact factor and the number of citations and commented that annual Impact Factors may drop, but the five-year average shows a fairly consistent Impact Factor and may be more appropriate to use.

**Comparative data sets for *PAC*: 2011 - 2014**

	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>
Impact Factor	2.789	3.386	3.112	2.492
Total Cites	12,669	13,333	13,894	14,265
Immediacy Index	0.928	0.382	0.514	0.439
5-Year Impact Factor	2.987	3.115	3.080	3.202
Eigenfactor	0.01425	0.01327	0.01270	0.01168

Article Influence      0.9126      0.936      0.906      0.921

**Citations (as of 4/8/2015)**

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>
<b>Total</b>					
Number of articles	183	153	187	160	162
Number of times cited	2639	2238	1000	751	186
Citations/article	14.42	14.63	5.35	4.69	1.15
<b>Conference papers</b>					
Number of articles	174	133	176	143	149
Number of times cited	2339	996	939	379	108
Citations/article	13.44	7.49	5.34	2.65	0.72

Bonnie Lawlor shared the comments and frustrations from *PAC* authors about errors being introduced during the proofing. Fabienne Meyers pointed out that measures are being taken to address the errors and that they are exceptions rather than the norm. Colin Humphries commented on the *PAC* Editorial Advisory Board. He believes that it is critical now to reinvigorate the Board and to work with the IUPAC Divisions to incorporate their content in *PAC*. There will be a *PAC* Advisory Board meeting on Monday evening here in Busan.

**9. *Chemistry International (CI)***

Fabienne Meyers reported on the major changes in the past year. She worked with Chris and now with Josh Gannon – the transition has not been a smooth one and the results of the replacement of Cheryl have been less than optimal. Fabienne pointed out that she now has to do more complete work for *CI* and that Josh realizes that he does not have the experience of news magazine publishing. His experience is with traditional scholarly publishing. The content of *CI* has suffered in the last two issues. There was much less information and details than in prior issues. Fabienne would like to be able to spend more time to work on the magazine. She noted that the September issue will be late, but that the November issue is under control.

**10. *Chemistry International Strategy***

Bonnie shared the survey results of the *CI* strategy discussion. A series of questions were addressed with the following results:

- a) Who is the primary audience for *CI* today?
  - ✓ IUPAC members (comment: some committee members never heard of *CI* until they become involved with IUPAC)
  - ✓
- b) What is the primary role of *CI* today?
  - ✓ Internal organ for IUPAC members
  - ✓ External articles for non-members (comment: the balance content for IUPAC members and non-members is well-done)

- c) What primary role should *C/* play for IUPAC as we move forward?
- ✓ Promotion of IUPAC's value to science in conjunction with the IUPAC website
  - ✓
- d) What content is needed to allow *C/* to fulfill the role it should play?
- ✓ Broader support of conferences (before and after)
- e) In what formats should *C/* be distributed – print, digital or both? If “both”, should they be published at the same frequency? Should the print be distributed less frequently and if so, should the content be the same as in the digital version; e.g., should it only contain content that has a longer shelf life – full articles; summary of annual events, etc.? – serve as more of an archive for reference? Will *C/* be an integral part of the IUPAC website?
- ✓ Digital should be the main focus
  - ✓ During a transition period, print should remain as a secondary focus with less-frequent publication cycle and article-only content (content with a longer shelf life) – has value in reading rooms.
  - ✓ Some comments point to a new format that should be developed for *C/* on the web; there should be more use of visual graphics/photos/videos; the creation of blogs should be considered as a tool for engaging interaction with members and non-members)

Bonnie summarized the two action items from the discussion to date:

- ✓ Survey young IUPAC members to get their opinion
- ✓ Repeat survey at Busan Meeting to reach a broader audience.

Collin Humphries raised the importance of a business model for *C/*. Bonnie questioned whether or not we need to work with a print partner and if we need additional staff in order to add new content to *C/*. Collin noted that we need to decide what to do before the end of the first quarter of 2016

Bonnie and Leah wondered if it is feasible to have CPCDS committee members as volunteers to help create the content for *C/*. Lene Hviid supported the exploratory effort, but cautioned the downside of having committee members to be involved in such daily activities. Colin mentioned again the idea of Editorial Advisory Board. The committee was in general agreement.

Bonnie emphasized that CPCDS will have to address the following questions if *C/* is published in two formats:

- Publication frequency of each format.
- Content of each format.
- Will the new IUPAC website support *C/* production?
- What will the 2017 production schedule look like and when does it need to begin?
- What business model(s) should be implemented for *C/* distribution?
- Can IUPAC create/market/distribute *C/* as we have now defined it without a publishing partner?



- What production support is needed? Do we add staff/volunteers responsible for supplying regular reports from Divisions, NAO's, etc.?
- Does *CI* need an active Editorial Board?
- In what time-frame do we need to bring De Gruyter into the discussion?

The goal is to have an agreed-upon game plan by the end of this year for 2017 as the business plan needs to be finalized in the first quarter of 2016. The meeting convened for lunch at noon.

#### 11. Meeting with De Gruyter

The meeting reconvened around 1:00pm and the committee was joined by De Gruyter staff: Katharina Butsch, Acquisition Editor, Chemistry, and Spencer McGrath, Senior Project Manager. Spencer reported on the status of *CI* and *PAC*.

##### *Chemistry International Report*

##### Online member access to *CI*

In 2016, *CI* will be accessed through a firewall. IUPAC members will have access via an authentication link from iupac.org. Additionally, those who receive *CI* through the American Chemical Society (ACS) or a National Adhering Organization (NAO) will need to have a similar authentication link. De Gruyter needs to know how IUPAC will handle this. Spencer went through the P&L for the *CI* account and noted that *CI* is now freely-available due to lack of user authentication. Starting in January 2016, De Gruyter will put it behind a firewall and IUPAC will provide user authentication.

**ACTION:** **IUPAC** must provide member authentication as of January 2016 for access to *CI*.

**ACTION:** **IUPAC** must provide user authentication for those who receive *CI* through the American Chemical Society (ACS) or a National Adhering Organization (NAO).

Communications to members and subscribers/Increased Awareness of *CI* Online De Gruyter is recommending that in December 2015, an email is sent to all members who receive *CI* in print format with information regarding the online version. They also recommend that IUPAC (and NAO's) approve that for months in which issues are published, e-TOC alerts will be sent to all members and subscribers in advance of their receipt of the printed issue; and for months in which issues are not published, email blasts will be sent with highlights from past issues, forthcoming content, highlights from past or current *PAC* issues, events calendar, conference reports, etc. Either IUPAC or De Gruyter can do the actual e-mailings. De Gruyter will draft the content.

**ACTION:** **IUPAC** needs to approve the above suggestions, especially with regard to the emails.

##### Content acquisition and development initiatives

There needs to be better cross-promotion between *CI* and *PAC*. Conference reports in *CI* and *PAC* issues must be connected. Other initiatives may include *CI* thematic issues, cover contests, student member perspectives.

### Proposal

Transition *CI* to a seasonal print publication. It makes sense both financially and contents wise (online first). It is \$11,000 per issue for the print version (printing and distribution). So there would be a saving of \$22,000 by going seasonal.

**ACTION:** *IUPAC* needs to respond regarding the proposal to create a “seasonal” *CI* (four issues rather than six)

### 2016 Target Subscription sales

The 2016 sales objective for *CI* is 40 online-only institutional subscribers and 20 print & online institutional subscribers. The \$20 subscription fee will be retained. They will target institutions receiving complimentary print *CI* and *PAC* subscribers (the latter used to get *CI* free). Individual subscription fees for non-members will be \$49/year. The numbers are based upon the 2014/15 member files.

### Advertising sales

Solvay purchased the back cover of *CI* issues 1-3 to advertise the Solvay Prize. De Gruyter is developing an advertising sales strategy as follows:

- Compile membership demographic data.
- Create editorial calendar for forthcoming content (need to be at least one issue ahead).
- Create rate card and share current print distribution numbers along with NAO distribution.

The number of downloads is not enough for ad sales online and they will need to track online usage. The tools are in place to track clicks, views, etc. They are in pilot now and will be rolled out at the end of this year.

### Usage

Spencer then went through the online usage between 2014 and 2015. Through the first half of 2015, the usage in general has gone up. There were close to a maximum of 400 downloads per issue. In 2014, *CI* was downloaded 1,867 times. Through June of 2015, issues have been downloaded a total of 1,437 times. In 2015, the non-AMP member copies have increased nearly 50%, while AMP and ACS member copies have remained consistent. The majority of downloads (95%) are to the most recent issue.

They are formalizing a *CI* reuse policy with a Creative Commons license. *IUPAC* will retain copyright and authors will still assign copyright to *IUPAC*. It will be a simple and clear reuse and sharing policy for authors and readers through CCBY-NC-ND licenses.

Spencer also noted that we are behind financial plan because the subscription agent (SWETS) filed for bankruptcy. A new agent is attempting to recoup the subscriptions. Moving Cheryl's position in-house to De Gruyter saved money (reduced pre-press costs).



*Pure and Applied Chemistry* Report

PAC conference papers

Spencer noted that there are better ties between *PAC* and *CI*. The Graphic abstracts for conference papers will be made a mandatory field in the Scholar One manuscript submission workflow in order to increase author participation. The transition to a De Gruyter-managed editorial office is complete and they are supporting the acquisition of *PAC* conference papers and symposium-based issues.

**ACTION:** *De Gruyter* will make the Graphic abstracts for conference papers a mandatory field in the Scholar One manuscript submission workflow in order to increase author participation.

PAC Reports and Recommendations (typesetting and article proofing)

Spencer agreed that there are needs to improve the workflow for article proofing. Errors are introduced when *serif* font in the author submitted manuscripts are changed to the *sans serif* fonts, which are the De Gruyter house style fonts. We need to get a better understanding of the formatting changes that result from this process and there need to be better guidelines for authors to improve author proof corrections (for an author to say that a superscript “isn’t high enough” does not provide adequate feedback to the proofing editor). The introduction of errors during proofing was a major discussion topic and all agreed that there are several factors - typesetting and font styles, lack of proofing tools, poor communication across the stakeholders, etc. De Gruyter is addressing the issues. Spencer asked that Bonnie suggest that Ron Weir stop by the De Gruyter booth (#21) so that he can go over the errors with him. (*Note: Ron and Spencer did meet and an interim solution was agreed upon*).

**ACTION:** *De Gruyter* will develop a workflow process/guidelines that will eliminate the introduction of errors during the PAC proofing process.

Usage

*PAC* article downloads have increased in 2015 as compared to 2014. The monthly average has increased to 1,951, up from a monthly average of 1,225.

Open Action Items

The CitedBy functionality (formerly entitled Forward Linking) was implemented in the June 25, 2015 platform release (see example at: <http://www.degruyter.com/view/j/pac.2014.86.issue-3/pac-2013/pac-2013-1023.xml>). CrossMark is being reviewed, but there are no current plans to implement it on De Gruyter Online.

Researchers who have registered with ORCID provide their ID upon manuscript submission and the ID is included in the published paper both online and in print. The Altmetrics pilot produced very little results and with no metrics to display online De Gruyter has no plans for its future implementation. However, this decision will be revisited in the future.

IUPAC Standards Online Report

Katharina provided a status report on the IUPAC Standards Online database. The database will be launched in 2016 and its content will be up to 2015. The database will not include information from the current publication year. The initial product will

cover content from more than one thousand articles (over 22,000 print pages) from 1960 through December 31, 2015. The database will have the following features:

- Advanced search functionalities.
- Topical structure for browsing.
- Enriched list of keywords.
- Enriched linking.
- Granular content.
- Thesaurus

Katharina presented sneak previews of *IUPAC Standards Online*, particularly the following features: Building Ontologies, like keywords, title, full text, captions, etc.; Browsing through the first level navigation tree (there are 19 subject categories, 172 sub-categories and 12 independent search functions); Sorting criteria, via relevancy, publication year, document type, alphabetic (Title), and author; Filtering (there are six filters that can be used to refine a search – year, author IUPAC Division, article type, collaborative partner, provisional recommendation).

More than five thousand keywords have been added and more than three hundred articles have been transformed into short database entries. There is enriched metadata, deep indexing, enriched linking, granular content, thesaurus-enabled data mining, etc.

Katharina reviewed the project schedule. The next step is to build the thesaurus and deploy a test version on the De Gruyter platform. (See <http://www.degruyter.com/view/db/iupac>).

Katharina summarized CPCDS' decisions on the database and then reviewed the current state of the "living" structure of the subject categories. The following additional points were discussed:

- Errata: it was suggested to have an indicator to the errata on the first page. Katharina will go back to ePress to explore options.
- Plans for updates/further enrichment: Bonnie Lawlor mentioned that we already have a list of possible enhancements for future implementation depending upon the success of the database. CPCDS will review the list next year.
- Fabienne Meyers suggested that De Gruyter write a report on the database to publish in *CI*.
- Thesaurus: Leah McEwen asked how it will be built. De Gruyter will have a freelancer to provide the synonyms. This should be completed by November.
- A test version of the database will be loaded on the De Gruyter platform in December 2015.

**ACTION:** **Katharina Butsch** will explore what options are available for the display of errata (ideally on the first page);

**ACTION:** **Bonnie Lawlor** and **Katharina Butsch** will discuss how best to "proof" the database in light of the errors that have been noted when converting manuscripts for *PAC*.

## 12. ***Chemistry International (CI)* - Continuation of the Strategy discussion**

Bonnie pointed out that the topics were well-covered in the morning session under Agenda Item 10. Robert Lancashire added that *CI* should cover material of interest to non-members.

Lene Hviid pointed out that all readers still prefer the print version. Leah McEwen, as a member of the *Chemical and Engineering News (C&EN)* editorial board, shared that the magazine met challenges similar to those facing *CI*.

The meeting was adjourned at 4:20pm to be reconvened at 9:00am the following morning.

**Monday: August 10, 2015**

## 13. **Subcommittee Reports**

### Subcommittee on Electronic Data Standards

Robert stated that it has not reached the stage to put in a project. The team tried to generate a single JCAMP-DX file to include infrared and NMR data. At this time, it is still a work in progress. But definitely there are potentials. This same conversation had happened several times. They will be applying for a project by end of the year. But need manufacturers' buy in to produce an instrument to gather the data.

### Gold Book Committee

A Content Management System (CMS) is being developed (an IUPAC Project) in order to easily update the Gold Book Content. The Gold Book is not in the scope of Phase I of the new website, but it is part of the conversation. There is a meeting here in Busan to discuss how to move forward for the new website and how to include the Gold Book. Bonnie will send an update after the meeting. (Note: the first step is to edit the Gold Book content that has been made into a database. This will be done before the end of this year if not sooner).

### InChI Project

Leah McEwen gave some background on the project concept that has been submitted for review (see p. 33 of the Agenda Book). Recent highly damaging events in chemical laboratories and classrooms have led to increasing focus on chemical information management in laboratory organizations. The diverse teaching and research environment in the academic sector particularly is raising awareness of the complexity of chemical safety information resources and formats available. A key concern in this regard is that documentation of chemicals with current identifiers is a persistent challenge for tracking and managing chemicals across the chemical enterprise, from process planning to manufacture to waste disposal and emergency response. The objective of this project is to establish requirements and guidelines for the generation of a unique identifier for all forms of a chemical (liquid, gas, solid, powder, etc.). Currently, many chemical identifiers exist, but very few reflect these bulk properties of substances, which may commonly exist in many forms and mixtures. Furthermore, most existing identifiers present cross-referencing challenges

between systems designed around different initial applications and editorial principles.

The intended outcome of this project is global adoption of the InChI notation in chemical inventories and information systems across commercial, industrial, government, academic and educational sectors to facilitate accurate documentation, handling and exchange of chemical information in support of safer management and use of chemicals.

Bonnie commented that it is interesting that there is an approved IUPAC Project to develop QR codes for InChI. She suggested the possibility of combining the two projects together.

Lene Hviid pointed out that industries have their own identifier number. If there are academic interests, it should be a good project. Safety should also be an issue to be addressed in universities. It was noted that the CAS registry number was not designed for this purpose.

#### **14. Project Status Reports**

##### IUPAC Color Book Data Management Project

Brynn Hibbert and members of the IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) joined the meeting. Brynn gave a status report on the project. There has been a lack of a clear process for the production and updating of the color books. The identified problem is that the xml is hand written. Nothing has been done to update the Gold Book for a long time, yet it is used as an authoritative resource. Hence the database/color book project. The current status is as follows:

- All text information has been extracted and put into a database.
- A front end CMS system will be implemented to query the database.
- This will be the new Gold Book.
- An audit trail will be added.
- A Word template for the Orange Book has been created.

Brynn shared screenshots of the xml file and the database web page and noted that future work will include:

- Development of a strategy to incorporate Color Book information into the new IUPAC website instead of building a standalone website.
- Use of project funds to help support implementation of the Gold Book on the new website.
- For the next revision, an electronic version will be produced.
- Two processes are required: one for new entries and a second for those entries that have been approved, but are not yet in the system

Bonnie and Ron Weir, Chair of ICTNS, reconfirmed that the two committees work closely together.

**ACTION:** *Bonnie Lawlor* will ensure that a teleconference is held with Lynn Soby to discuss the Gold Book on the new website (Lynn has already had a conversation with Mark Kinnan who heads the project).

**ACTION:** *Bonnie Lawlor* will keep CPCDS informed of progress on the gold Book.

Ron Weir raised two questions. He knows that there is a new contract with the Royal Society of Chemistry (RSC). The Green Book will be updated and he wondered if it will be under the new contract. Bonnie said that she was not involved with the contract and that Lynn Soby can answer that question. Ron then raised the issue of the proof reading errors in PAC and he is concerned about possible litigation since the standards and recommendations are used for legal issues. He asked how we will deal with mistakes due to differences resulting from these errors. Bonnie gave an update from the discussion with De Gruyter and encouraged Ron to visit with Spencer McGrath at the De Gruyter booth.

## 15. Other Reports

### InChI

Bonnie Lawlor noted that Steve Heller has provided a written report which gives a good summary of InChI (see p. 121 of the Agenda Book). There has continued to be good progress in a number of areas, but the progress on membership has been slow. The fact that Steve and others on the InChI development team received the CSA Trust Mike Lynch award in 2014 and Steve will be presented with the Patterson-Crane Award this fall highlights IUPAC's efforts for this initiative.

### CODATA

Robert Lancashire stated that he missed the CODATA General Assembly last year and that communication has been scarce. He observed that the CODATA project approval process needs to be improved. Robert's term as the IUPAC representative to CODATA will end this year and a replacement should be considered.

Bonnie asked if Robert believes that it is important for IUPAC to have the relationship with CODATA. Robert said that it is more a nice to have, rather than a necessity. She asked what IUPAC gets out of the relationship. Robert said that CODATA looks at isotopes, thermodynamic constants, and so on, and more recently big data. So there are complementary needs and interests. It is really a matter of figuring out who is better to look out for these things. He said that as far as he knows IUPAC has had a relationship with CODATA for at least the past ten years.

**ACTION:** *Bonnie Lawlor* will remind Colin Humphries about replacing Robert Lancashire as the IUPAC representative to CODATA.

## 16. Discussion of Future Data/Cheminformatics Initiatives

### IUPAC Digital Proposal

Jeremy Frey put forth the "Digital IUPAC" proposal for IUPAC to take the lead to build a framework for sharing digital data (see p. 40 of the Agenda Book). Jeremy and Colin Humphries were approved to develop a Project proposal. Staffing changes in

the past several years had made it difficult to do so. However, with the staff changes completed, it is now time to move the proposal forward.

Jeremy suggested several ideas, including the following:

- Identify what is the core of information that IUPAC controls both in terms of standards and data.
- Identify who is interested in this information and why.
- How much of this information needs to be converted to digital form.
- Identify what new chemical standards are needed.

#### Chemistry Data Interest Group

Leah McEwen represented the Research Data Alliance (RDA) Interest Group to seek collaboration with IUPAC to create a joint RDA/IUPAC interest group (see p. 42 in the Agenda book). Leah mentioned several trajectories have now come together. People already on RDA have started to have the conversation about data. It's an opportunity for IUPAC, ACS and other organizations to address related issues and to see if a relationship can be built between IUPAC and RDA. A Working group can be a good first step.

Leah shared the objectives identified by the interest group and mentioned that the group will start by framing issues specific to chemistry data. More than twenty people have signed on the proposal from the interest group, including IUPAC members, to facilitate the group for communication and collaboration.

Lene Hviid pointed out the group is North America and Europe heavy and suggested to consider including people from central Europe and Asia.

**ACTION:** *Bonnie Lawlor* will pursue the possible collaboration with the Research Data Alliance.

## 17. Industry Trends

The committee briefly discussed a July 2015 report on the Role of Metrics in Research Assessment (<http://www.hefce.ac.uk/pubs/rereports/Year/2015/metricride/Title,104463,en.html>); The Top 10 Tech Trends (STM) published in March 2015 (see: [http://www.stm-assoc.org/2015\\_02\\_20\\_STM\\_Report\\_2015.pdf](http://www.stm-assoc.org/2015_02_20_STM_Report_2015.pdf)); and the ISO Data Exchange Protocol for Interoperability and Preservation that is currently in discussion (see: <http://standardsproposals.bsigroup.com/Home/Proposal/3992>).

## 18. Old/New Business

Bonnie Lawlor asked if the committee thought it would be of value to renew membership in the International Council for Scientific and Technical Information (ICSTI) Membership. The fee is 840€. The consensus is to continue the membership if IUPAC can afford it. It was noted that the RDA relationship may make ICSTI less necessary since it is not totally focused on data curation and management.



**19. Next Meeting**

It was suggested that the next in-person meeting be held in July 2016 at the New Secretariat office.

**ACTION:** **Bonnie Lawlor** will poll committee members to get a date for the next CPCDS in-person meeting.

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**ACTION ITEMS:**

**ACTION:** **IUPAC** must provide member authentication as of January 2016 for access to *CI*.

**ACTION:** **IUPAC** must provide user authentication for those who receive *CI* through the American Chemical Society (ACS) or a National Adhering Organization -NAO.

**ACTION:** **IUPAC** needs to approve De Gruyter suggestions for improved communication with *CI* subscribers, especially with regard to the emails.

**ACTION:** **IUPAC** needs to respond regarding the proposal to create a “seasonal” *CI* (four issues rather than six)

**ACTION:** **Katharina Butsch** will explore what options are available for the display of errata (ideally on the first page);

**ACTION:** **Bonnie Lawlor** and **Katharina Butsch** will discuss how best to “proof” the database in light of the errors that have been noted when converting manuscripts for *PAC*.

**ACTION:** **Bonnie Lawlor** will ensure that a teleconference is held with Lynn Soby to discuss the Gold Book on the new website (Lynn has already had a conversation with Mark Kinnan who heads the project)

**ACTION:** **Bonnie Lawlor** will pursue the possible collaboration with the Research Data Alliance.

**ACTION:** **Bonnie Lawlor** will poll committee members to get a date for the next CPCDS in-person meeting

**ACTION:** **De Gruyter** will make the Graphic abstracts for conference papers a mandatory field in the Scholar One manuscript submission workflow in order to increase author participation.

**ACTION:** **Bonnie Lawlor** will remind Colin Humphries about replacing Robert Lancashire as the IUPAC representative to CODATA.



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- ACTION:** *De Gruyter* will develop a workflow process/guidelines that will eliminate the introduction of errors during the PAC proofing process.
- ACTION:** *Bonnie Lawlor* will keep CPCDS informed of progress on the Gold Book.