

DIVISION OF PHYSICAL AND BIOPHYSICAL CHEMISTRY

Minutes of the Milano off-year meeting of IUPAC Division I Committee (31 May – 03 June 2018)

31 May 2018, starting at 9:00 a.m.

Participants:

Ron D. Weir (RDW, Division I President (DIP), from Canada)
Timothy J. Wallington (TJW, Division I Vice-President, from the US)
Attila G. Császár (AGC, Division I Secretary, from Hungary)
Jeremy G. Frey (JF, TM, from UK)
Roberto Marquardt (RM, TM, from France)
Pierangelo Metrangolo (PM, TM, from Italy)
Frances Separovic (FS, TM, from Australia)
Hiroko Tokoro (HT, TM, from Japan)
Bert Weckhuysen (BW, TM, from the Netherlands)
Modou Fall (MF, AM, from Senegal)
Theo Kurtén (TK, AM, from Finland)
Zhigang Shuai (ZS, AM, from China)
Vladislav Tomisic (VT, AM, from Croatia)

Apologies:

Angela Wilson (AW, Division I Past-President (DIPP), from the US)

1. Welcome, introductions, apologies for absences (RDW)

2. Finalization of agenda (RDW)

No further discussion.

3. IUPAC Mission (reminder) (RDW)

4. Rules of engagement (Division I) (RDW)

No further discussion apart from elections, see separate agenda item.

5. Minutes of Division meeting (Sao Paulo, July 2017) (RDW)

RM suggested that minutes be distributed by the DS and DP after checking.

At this meeting the Minutes were updated by all simultaneously; PM made the changes on the screen.

Several decisions were mentioned with a follow-up discussion on arising business.

RM to finish layout and approval of minutes was moved toward the end of the meeting.

5.1 Minute 7 item:

RM: highly welcomed projects on thermodynamics.

JF: projects on non-equilibrium thermodynamics are missing.

RM: these should be discussed under item of future projects.

Minute 8, 9 items:

RDW, RM, JF: confirm assignment to ICTNS and CPCDS.

MF, FS: both liaise with CCE (FS will keep contact for the forthcoming meeting of CCE in Australia).

RM: mentioned IUPAP, see also with ZS, JF.

other representatives: RDW write to Fabienne.

Project Management or Tracker:

TJW: discuss with RM format of tracking and present to DC later during the meeting (new item 10.0)

BW: should have a document for internal use so that statements can be traced back.

RW: some changes made to the duties of the DIVP, specifying details of the oversight.

Motion: One task of the DIVP is to maintain oversight of Division projects; the DIVP will define the details of the oversight.

Advisory Board:

RDW: AW said Advisory Board had not been formed.

RM: RDW should now approach people on the list decided in Sao Paulo.

Color Books:

RM: Stuart Chalk input in Sao Paulo re Gold Book.

JF: project is supported by NIST; explains world wide use of XML for books in general;

FAIR (Findable, Accessible, Interpretable, reusable) principle; digital data standard representations; will be presented at CPCDS at meeting in Amsterdam in the end of July, will share document with DC to get feedback from specialists.

BW: JF should share document.

RM, JF: short story about Gold Book; many errors and omissions have been spotted such as in the definition of the hydrogen bond, the halogen bond is missing.

RM: strongly suggested to have a task group within the DC to check Gold Book contents for coherence with Green Book or other recommendations supported by the Division.

Furthermore, the Division should make a MOTION that all Divisions establish similar tasks groups so that the Gold Book revision is carried out coherently throughout IUPAC.

JF: Gold Book project is with CPCDS; request them to ask similar action from all Divisions; Stuart has the priority list of terms for physical chemistry.

RM: the visibility of the Color Books on the IUPAC website needs to be improved by putting the link to the corresponding pages more prominently on the first page of the website.

RDW: MOTION to add to procedural guidelines that each project recommendation and TR has an appropriate summary of its contents in a few sentences that will be used in the Gold Book.

6. Division Communications (RDW)

6.1 – Website

RM: he takes responsibility for this biennium.

JF, PM, RM: no new website, just update.

PM: news window?

TW: no news window.

JF: should increase visibility but can be dangerous.

BW: Why dangerous?

JF, PM: sharing documents on website not efficient.

RM: Current website is not showing all projects. The GB 2007 project was not found using the search engine.

6.2 GoTo Meetings

PM: green chemistry example, suggested time: GMT 12:00, every 3rd month, 1st week, choose actual date by a Doodle poll. Supported by all.

RDW: will contact Fabienne at Secretariat.

6.3 Twitter

ALL: no use of a separate DI Twitter account, but could use the IUPAC central Twitter account to send tweets.

BW: young generation looks at these short pieces of information.

RM: Tweet GB link might be more efficient than to put it on the web, or in the lecture notes, ask IUPAC central who is collecting contents to tweets.

RDW: contents should go through DIP before reaching out to Central.

7. NAO Cuba (RDW)

RDW: Cuba has not paid its dues (1000 USD); thus, the current TM from Cuba (Prof. Luis Alberto Montero Cabrera) cannot continue to serve.

JF: There are two questions: (1) personal membership was introduced, separates person from country; ask the Secretariat if we can go down that route, and (2): is Prof. Montero Cabrera a personal member himself?

TJW: perhaps bring in South Africa.

FS: choose a personal membership only if we lack the expertise otherwise. All agreed.

RM: he will follow up on this issue.

8. ISMSC 2019 (PM)

PM: introduces 14th ISMSC in Lecce, endorsement received from IUPAC. Details: conference series started by Jean-Marie Lehn; 2016 chemistry Nobel prize winners (Feringa and Stoddart) will be present in Lecce, limited number of talks, 500-600 expected participants. It is up to the President to support the suggestion or not. IUPAC support is max. 4000 USD/conference. Requirements: conference held in a scientifically emerging region (SER) or defines new directions in chemistry (FSC) (funding can go either to lecturers or to young scientists). Ask DIP to endorse the proposal, money comes from Central.

RM: For a FSC, it is important to know who is the "IUPAC lecturer". The Project Committee will ask that the IUPAC lecturer promote IUPAC achievements.

RDW: In principle willing to support the application, new aspect for physical chemistry must be stressed in the application and the role of IUPAC in the congress should be clarified.

PM: need to know what is expected from the “IUPAC lecturer”, who can be chosen, *etc.*, RM should clarify this with central.

RDW: Prior to end of meeting, RDW contacted Doug Templeton (Project Committee) and obtained the information. Division I will support initiative.

9. IUPAC 100 GA, Paris (RDW)

9.1 Short stories project

RDW: up to 24 short stories project (one per month), reach non-scientists and the general public, there are 3 stories already (one of the stories: space launches).

RM: together with Zoltán Mester from Div V, we want to include a video interview with an IUPAC personality engaged with the new SI; the deadline is March 2019.

RDW: Asked TJW about atmospheric chemistry story.

TJW: Can try, story published in CI and get videos if possible, good interview, will discuss with subcommittee how feasible this is.

TJW: in the past provided some short write-ups to Fabienne.

RDW: story about InChI.

FS: How about how to unboil an egg (Australian Academy of Science got 9.9 million views)?

JF: Is the difference between the roles of IUPAC100, GA and Congress clear?

RDW: No direct control over Congress, can contribute to GA, should have suggestions for IUPAC100.

RDW: showcase IUPAC as part of IUPAC100.

RDW: increase public support for IUPAC.

RM: 20 May 2019 SI will launch the new units.

9.2 WCLM

RDW: Bureau decided that the target in 2019 will be NAOs (putting official representatives at the same table). Bring NAOs to the meeting, with briefing what IUPAC does. Division I should find appropriate persons willing to participate during the GA.

PM: Are we going to target the presidents or someone else? Not clear.

RDW: An example: an NAO administrator was convinced about the true value of IUPAC (volunteers are working for IUPAC, money supports students, *etc.*).

FS: Pulled up a Report on the Benefits of Australian membership to the International Council for Science (ICS) which shows the benefits with quantitative measures.

9.3 Special symposia

RM: these appear on the webpage of IUPAC100, there are three symposia proposed (called 8.1, 8.2, and 8.3 on the website).

RM: Zoltán Mester attempting to attract people to talk about the new SI.

JF: It would be inappropriate to have a discussion on the new units.

01 June 2018, starting at 8:30 a.m.

10. Project list for Division I

10.1 Completed 2016-17

RW: nothing to be done now.

10.2 Projects in progress

| | | | |
|----------------|--|----------------|-------------|
| 2015-038-1-100 | Evaluated data for atmospheric chemistry | Tim Wallington | 01 Dec 2015 |
|----------------|--|----------------|-------------|

RDW: Fabienne asked for an update on 2015-038-1-100.

TJW: 2015-038-1-100 is really finished, will send a one-page report to Fabienne.

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|----------------|--------------------------------|------------------|-------------|
| 2015-002-2-100 | Diffusion in nanoporous solids | Rustim Valiullin | 01 Aug 2015 |
|----------------|--------------------------------|------------------|-------------|

RDW: 2015-002-2-100 should be finished by August 31, 2018 according to Fabienne.

RM: currently has no knowledge about this project, should follow up.

RM: do not take decisions where we do not have enough information, make decisions at the next GoTo meeting.

Decision: FS will monitor this project.

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|----------------|---|---------------|-------------|
| 2014-028-2-100 | Chemical kinetics of gas-phase elementary reactions at high temperature | Tamás Turányi | 15 Mar 2015 |
|----------------|---|---------------|-------------|

RM: Jürgen Stohner was the monitor of this project up until the Sao Paulo meeting.

Decision: AGC will monitor this project in future, will write a mail to the TG leader, follow up, make decision at next GoTo meeting, need to see a preliminary Technical Report.

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|----------------|--|----------------|-------------|
| 2014-021-1-100 | Green Book 4 th revised printing of 3rd edition | Jürgen Stohner | 01 Nov 2014 |
|----------------|--|----------------|-------------|

JF: summary of changes since the last printing, no issue about this project, more or less ready to send it to the printer.

RM: asks for support as this is an important project, JF and RM have been working on this for a long time, long ongoing project

RM: provides an update on activities of Commission I.1 to inform new members of Division I

Decision: project on track, RW will monitor this project

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|----------------|--|---|-------------|
| 2012-044-1-100 | Basic terminology of crystal engineering | Pierangelo Metrangolo Giuseppe Resnati | 01 Feb 2013 |
|----------------|--|---|-------------|

PM: large project, involved a large number of people, identified 22 terms, 10 brand new definitions, 6-7 are on the way, Kristin used to monitor this project, connection with Division II (some definitions come from this division).

RW: suggest to submit an interim Technical Report by November 2018, indicate a one-year no-cost extension.

Decision: BW will monitor this project, submit an interim Technical Report by November 2018, indicate a one-year no-cost extension.

RDW: no special request from Fabienne about the other projects.

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|----------------|--|----------------|-------------|
| 2016-031-2-100 | Notations and conventions in molecular spectroscopy: Rotation-vibration spectroscopy | Robin McDowell | 22 Feb 2017 |
|----------------|--|----------------|-------------|

Decision: RM will monitor this project.

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| 2016-038-1-100 | Translation Green Book (Portuguese) | Romeu Rocha-Filho | 01 Mar 2017 |
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RM: project has finished successfully.

RM: there are several translations of the Green Book, some are not yet online (e.g., the Italian one). The French version is not available online, have to buy it from de Boeck (see the website <https://www.deboecksuperieur.com/ouvrage/9782804172077-grandeurs-unites-et-symboles-de-la-chimie-physique>).

Decision: inform Fabienne that the project has finished. Contact project leader to send a final report to Fabienne.

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|----------------|---|----------------|-------------|
| 2013-048-1-100 | A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities | Jürgen Stohner | 01 Dec 2013 |
|----------------|---|----------------|-------------|

RM: project is finished successfully. Report published in PAC.

Decision: notify Fabienne about closing the project off with the following text: "The project is formally closed with a successful completion and a publication in *Pure Appl. Chem.*"

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|----------------|--|------------------------|-------------|
| 2012-051-1-100 | International standard for viscosity at temperatures up to 473 K and pressures below 200 MPa | Josefa Fernandez Perez | 15 May 2013 |
|----------------|--|------------------------|-------------|

RM: should be considered to be completed. Technical Report is with ICTNS. The document should have gone through Division I: contact ICTNS. The DC thanks Josefa for completing the project.

Decision: Once ICTNS approves the Technical Report, the project can be considered completed.

RW: Email to Jürgen Stohner.

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| 2011-037-2-100 | Recommended Reference Materials for Phase Equilibrium Studies | Ala Bazyleva | 01 Jan 2012 |
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RM: project terminated at the 2016 off-year meeting, should not have appeared on the list.

Decision: this information should be sent to Fabienne and remove the project.

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| 2010-048-3-100 | Common values of nuclear electric quadrupole coupling terms for appropriate nuclei in functionalized hydrocarbons | Stephen Cooke | 01 May 2011 |
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RM: project terminated at the 2016 off-year meeting, should not have appeared on the list.

Decision: this information should be sent to Fabienne and remove the project.

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| 2007-055-1-100 | Ultrafast intense laser chemistry | Kaoru Yamanouchi | 01 Jan 2008 |
|----------------|-----------------------------------|------------------|-------------|

JF: important project, should keep it, perhaps a new proposal is appropriate.

Kaoru Yamanouchi: agreed in an email to submit a manuscript before the end of 2018.

Decision: RDW will monitor the project.

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| 2007-032-1-100 | Green Book - Abridged Version | Roberto Marquardt | 27 Nov 2007 |
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RM: still need some more work to be done, text is basically finished. Jürgen Stohner finished the indexing. Needs review.

Decision: HT will monitor the project.

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| 2016-001-2-300 | Categorizing Chalcogen, Pnictogen, and Tetrel Bonds, and Other Interactions Involving Groups 14-16 Elements | Pierangelo Metrangolo Giuseppe Resnati | 01 Jul 2016 |
|----------------|---|---|-------------|

PM: kick-off meeting will take place in a couple of days. Project on track.

Decision: submit interim report (by the end of this year). TK will monitor the project.

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| 2016-032-2-020 | IUPAC's role in developing interdisciplinary/ collaborative work in the Chemistry community and beyond - the focus for the 2017 WCLM | Hemda Garelick Christopher Ober | 24 Jan 2017 |
|----------------|--|------------------------------------|-------------|

RW: WCLM discussed on May 31.

Decision: ZS monitors the project on behalf of Division I.

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|----------------|--|-----------------|-------------|
| 2006-050-3-100 | Wet surface vibrational spectroscopy experiments | James McQuillan | 14 Mar 2007 |
|----------------|--|-----------------|-------------|

RM: AW has been monitoring the project. The TG Chair is approached during the meeting via email. His reply is that the TG is still waiting for some data, because they had to avoid pure perchloric acid because of safety issues; they want to submit the J Chem Ed article which will be the main part of the project completed.

Decision: A no-cost extension is granted, but the article has to appear before the next meeting if the project is not to be considered terminated.

10.3 Green Book translation into Portuguese

RM: accomplished (see above).

10.4 Project proposal: Green Book 5th ed.

JF: described the status of the project, 1 September 2018 is a sensible start date, but 1 January 2019 is better starting date to first finish 4th-edition issues.

Decision: update how to spend the money, change starting date to January 1, 2019; JF should amend the proposal.

10.5 Project proposal on Proton affinity...

RDW: critical reviews.

Decision: allow the authors to amend their proposal and resubmit.

10.6 Gold Book update

RM: suggested to check the Gold Book entries by a subcommittee (2-3 persons) formed within the Division and ask other divisions to do the same (see above). All divisions should be involved in this project. Our division should send a request to the Bureau about this.

JF: showed mail from Stuart Chalk and new web site related to the Gold Book.

JF: suggested to form a project which other divisions can join but start it in our division with a small budget.

Decision: JF should be project chair and submit a proposal. FS, RDW, RM and TJW join the project. Keep the update on the agenda of all future meetings of the division, part of the duty of the division members is to find problems in the Gold Book. Our division should send a request to the Bureau about this.

11. Elections, 2019-20 biennium

RDW: after presenting the appropriate Division I Operating Procedures, suggested to choose Nominating Committee (NC) and Chair (NCC) and overview of openings for different positions.

RM: NC needs two members from outside and two from inside (fifth is the chair).

RM: based on the data available, PM, RM and BW need to step back as TMs, and AW has to step back as PP.

RDW: TJW is happy to become the president in the next biennium, which means that the VP position will become open.

RDW: after asking everyone individually, everyone unanimously agreed that RM should be the chair of the NC, a role he accepted.

RDW: AMs present could become TMs.

RDW+RM: HT and FS were asked to serve on the NC, they agreed.

RDW: choose outside experts, suggested by Kristin Bartik.

RM: look for a member from North/South America in thermodynamics and/or spectroscopy, suggested Frank van Veggen (Canada) or Juris Meija (Canada).

RM: looking for further candidates from Africa or elsewhere

RM: will ask Enid to send the eligibility list.

12. State of the IUPAC union

RDW: treasurer's position, not discussed in detail.

RDW: Less money coming in compared to annual expenses; thus, IUPAC needs to raise money. Most of the money comes from subscription. Bureau has plans to get countries (*e.g.*, Cuba) back.

RDW: Questions: (1) How should the divisions be structured? (2) Can private funding be raised?
(3) Some providers are not willing to support administration. (4) How to capitalize on the brand name. (5) Work on the NAOs.

RM: (1) Work to increase efficiency and relevance. (2) Add more scientific content to the meetings (*e.g.*, discussion of Gold Book).

BW: (1) Great organization of the meeting is important. (2) Have a shorter meeting (arriving Wednesday evening, leave Friday evening).

FS: Perhaps tack the Division I meeting onto a scientific meeting which would make the meeting more attractive to those flying from a long distance.

JF: (1) Leave the job of attracting NAOs to the Treasurer. (2) Make the meeting more cost-effective. (3) Solicit projects with set preferences. (4) Perhaps move off-year meeting to a country needing to be convinced about the role of IUPAC.

PM: (1) We have always had problems with projects. (2) How to increase attractiveness of Division so that people will submit proposals?

BW: Restructuring and rejuvenation of the division structure of IUPAC: decrease the number of divisions to 4-5 and give new names (*e.g.*, materials chemistry, methods of chemistry). Make division structure more attractive to society and industry at the same time.

All: Interdivisional committee on green chemistry and sustainable development should be folded into another division, most likely Environmental Chemistry.

All: Division VIII merged into CPCDS.

Decision: (1) Division meeting should not be longer than two days (four half days). (2) GoTo meetings would help to improve efficiency. (3) Have a scientific part to the meeting.

13. Other business

13.1 Evaluation Committee Questionnaire:

- 1.) Yes.
- 2.) Perfectly.
- 3.) Rejuvenate divisions and contribute to the future vision of IUPAC.
- 4.) We are working on the succession plan.
- 5.) Yes and yes.
- 6.) Yes. We work hard on selection.
- 7.) All except one (PP), three AMs out of 5 present. Zero NRs present.
- 8.) PC underpins all aspects of the divisions.

Projects:

- 1.) Majority yes, remainder: TGCs contacted.
- 2.) Yes.
- 3.) Yes.
- 4.) Done, via Excel spreadsheet keeping track of progress of all projects.
- 5.) Yes.
- 6.) Problem with the proliferation of small projects.

Other activities:

- 1.) In 2019: 14th International Symposium on Macrocyclic and Supramolecular Chemistry.
- 2.) None beyond the projects.

AC will submit the completed questionnaire to the Secretariat.

13.2 Scientific talks

13.3 Criteria on continuation criteria

All: Regular communication with TGC. Regular reports and updates. Evidence of progress.

13.4 Conflicts of interest matter

At the start of the meeting, remind participants.

Presentations about individual Division member's research

- 1.) Tim Wallington
- 2.) Zhigang Shuai
- 3.) Hiroko Tokoro
- 4.) Theo Kurtén

02 June 2018, starting at 9:00 a.m.

Presentations about individual division member's research

- 1.) Vladislav Tomisic
- 2.) Attila Császár
- 3.) Roberto Marquardt
- 4.) Jeremy Frey
- 5.) Modou Fall
- 6.) Frances Separovic
- 7.) Pierangelo Metrangolo
- 8.) Ron Weir

Unanimous agreement by Division members for future meetings, including the GoTo Meetings:

- (a) invite highest representatives (presidents) of NAOs
- (b) lectures should be part of the off-year meetings, should be given at the beginning of the meetings, perhaps half of the Division members should make presentations, invite public (including local students, colleagues and NAO representatives) to this event.

RDW: two day time limit wanted by most members for the off-year meeting.

RM: The Division needs new projects. Each of us has the potential to propose new projects, and part of our job is to convince colleagues to propose Task Groups (critical assessment and evaluation of data, new standards, *etc.*). This should be on the agenda of the next two GoTo meetings.

TJW: led a discussion about the biennial budget of the Division.

RDW led a review of action items agreed upon during the last two days:

- (1) Agreed on Division representation on different divisions, committees and associations. In detail: Advisory boards: COSI (one representative): TW agreed (he will contact chair of COSI). Atomic weights: at the moment there is no need. CPCDS: JF; IUPAP: RM; ICTNS: RM; CCE: FS.
- (2) Any potential Tweets should go through RDW (DIP).
- (3) Replacement of Louis Montero: RM will contact Brazilians before the next GoTo meeting.
- (4) Lecce conference support is suggested by DIP.
- (5) Projects. Notations and conventions in spectroscopy (McDowell), RM will monitor. Green Book translation finished. Atmospheric chemistry - finished (TW). Chemical kinetics: AGC will monitor. Green Book 4th revised edition: RDW will monitor. Critical review -completed. Viscosity standard: RDW will monitor. Recomm. phase equil.: finished. Nuclear quadruple: finished. Ultrafast lasers: Kaoru Yaamnouchi responded, Technical Report due in October 2018. Categorizing ... (PM): TK will monitor (contact Giuseppe Resnati). Surface vibration (Jim McQuillan): AW will monitor.
- (6) TJW to contact Fabienne to close terminated projects.

- (7) HT agreed to be monitor of the abridged version of the Green Book.
- (8) RM is responsible for the website.
- (9) WCLM. TJW and FS offered help with ideas.
- (10) Special symposium: everything is settled, nothing to do.
- (11) GoTo meetings: 12:00 GTM, mid-September, via Doodle. Secretariat to set it up.
- (12) Incorporating new material in 5th edition of the Green Book: biophysics. JF will review what is needed.
- (13) PA project: AGC will follow up.
- (14) Stuart Chalk (CPCDS). Chair. JF will prepare the project. RM, FS and RDW will be consulted.
- (15) Elections. Decisions about Nominating Committee. Suggestions given, Chair will decide.
- (16) BW and PM: Each needs to decide on future with Division I.
- (17) State of IUPAC: no motions. Decide about motions at the next GoTo meeting.
- (18) Secretary to organize the next GoTo meeting (following instructions from Fabienne).

JR: Announcing the FAIR Chemical Data Workshop.

TJW: Task Group about Critical Evaluation of Data. All divisions are involved.

The meeting adjourned at 1:00 p.m.