

COMP Exec. Committee Meeting
August 27, 2005
Washington DC

Present: Curt Breneman, David Spellmeyer, Andy Good, Jennifer Miller, Wendy Cornell, Jeff Madura, Kerwin Dobbs, Ralph Wheeler, Orlando Acevedo, Jeff Evanseck, Lisa Balbes, Hanneke Jansen, Andy Holder, Christopher Whitehead, Michelle Francl, Peter Jurs, Peter Gund

Agenda is handed out (Appendix I).

1. "The List of Topics We No Longer Discuss" was read as a reminder (Appendix II).

2a. Minutes from the San Diego meeting were approved with one change: the CHED symposium will probably be scheduled for Fall 06 or Winter 07, not Dec '05-Jan '06 as mentioned in point 18. This change is made and minutes will be forwarded to Lisa for inclusion on our website.

The committee discusses whether the demographics overviews are useful. Current version on our website is from 2003. Hanneke will look into how much work it is to compose those overviews. The decision is to not spend a lot of time on it.

During review of the latest update on membership it is noted that there are resignations as well as immediate resignations and future cancellations. A question for the ACS is what the differences are.

The committee decides that we should send a postcard or letter to those who resign. Ask them to contact the past chair to find out why they resigned and remind them of all the good things COMP has to offer (Andy and Kate will work on this). Hanneke will prepare the relevant address lists from the rosters and forward to Kate. David mentions he made a new letterhead, using the new logo. He will forward that to Andy & Kate.

2b. Ballots for the elections are due by October 1st. They're coming in at a good rate. The Secretary will keep ballots for one year.

3a. Treasurer's report (Appendix III): the division is in good shape, although there is a little decline. Reasons for the decline have to do with our increased membership outreach. We're still in the black and on-track. Note on the report: the amount due from CCG for the ARCC back cover is \$10,000, not \$25,000

3b & 3d. Registration fee reimbursement happens at the early registration rate. There will be one reimbursement per half-day symposium. Curt needs complete and timely information from symposium organizers to process reimbursement requests.

3c. The observed decrease in allocations appears to be due to the fact that we were undercounting attendance. We will pay close attention to this in the future. The most recent allocation payment was around 14K, which is good.

4. The “General Travel Support Policy for the Division” (Appendix IV) is reviewed. The ACS cap for councilors is currently \$874. Requests for reimbursement should be forwarded to the treasurer within 2 weeks after the end of the meeting. The Division will only cover the remainder of travel expenses for councilors who are from academia or who are independents. Andy to rewrite the document with these notes added, Lisa to post on the website.

5. Councilor’s reports

Michelle: DAC met this morning. A new vision for 2008 is being developed, which will change reimbursements for programming and will change programming. This will also be discussed at the long range planning meeting / divisional summit (Jeff E. will attend).

Peter J: The publications committee met yesterday and dealt with routine business mainly. New name and direction for JCIM and JCTC are going well.

Jennifer: Public Relations Committee has strong focus on local sections, not so much on divisions. They’re meeting later this week, so no news to report.

David: Chemical Abstracts Service committee met last night. There is ongoing debate between ACS and NIH around the Molecular Libraries Initiative and in particular PubChem. There is a request to have all questions and comments go through ACS, not CAS. The open meeting for the CAS committee, scheduled for Monday afternoon, is a place where society members can discuss this since relevant ACS representatives will be present.

CAS is also working on clarification on what can be done with downloaded records. Historically, an additional fee was necessary for downloading more than a set number of records. New policy is going to include very specific language that you cannot download records and then analyze with 3rd party tools or share with others.

6. The JMGM report is reviewed (Appendix V). The journal is strong.

7. The Annual Report Report is reviewed (Appendix VI). The division is considered to be in generally good health. All divisions got the advice to incorporate. This is an issue the committee has discussed in the past and does not consider to be beneficial. The item is moved to the list of topics we no longer discuss.

8a. Programming in DC has 9 symposia beyond the general oral sessions. There are 4 symposia lined up for Atlanta and 2 for San Francisco and Chicago.

Note: Wendy will stay on as Program Chair for the next 2 meetings, then Jeff M. will cycle in as Program Chair.

8b. Novartis has provided sponsorship for food at the DC poster session. Wendy will follow up with them for support for the 2006 Spring Meeting. A suggestion is made that we could ask for a 1-year commitment of this sponsorship, so we don't have to ask twice a year. There has been concern that many non-COMP members are coming to eat the food. A note is made that if membership of divisions were on the badges, there would be a way to monitor that.

8c. Financial consequences of co-listing/co-sponsoring: the issue is a complicated one and rules will change again in a year. There may be a dependence on attendance, how many sessions, etc. Michelle, Jeff M. & Wendy to check on this.

8d. Doug Tobias organized the Elsevier sponsored symposium at the Spring 2004 meeting, "Computational Approaches to Problems in Environmental Chemistry". Elsevier will sponsor a symposium again in 2006, which will also result in a special issue in JMGM. Andy & Wendy to discuss and select a symposium off-line.

8e. Kenny Merz will organize the MJS Dewar symposium in San Francisco, Fall 2006.

9. The P2C2 meeting used to be Program Chairs only. ACS now added a Divisional Summit/Long Range Planning track. Jeff M will attend the programming sessions, Jeff E will attend the Divisional Summit/LRP sessions. The division will cover additional reasonable business expenses if they need to stay longer in order to attend additional sessions.

10. All material for the website that Lisa received has been posted. She will post the San Diego minutes there as soon as she receives them from Hanneke (who will make the correction mentioned under 2).

We cannot (yet) put a password protected area up on our website, nor a news-feed (because of ACS rules). Several committee members note that an RSS news-feed is particularly useful if there is not a lot of news and it comes irregularly, which describes COMP news pretty well. Michelle offers to mock up some RSS feed for the next meeting, so we can try it and think about it a bit more. Lisa will work with her on this.

11. ARCC report

Volume 1

- Mailing cost so far was 9K USD.
- On the roster download from 082705 there were 51 members listed with a bad address. They were excluded from the mailing. Additionally, there were some books that were undeliverable, and returned to Jeff E. David, Jeff E., and Hanneke to come up with ways to deal with "bad address" members. One specific action item is to send email to bad address members in the roster (none have email flag

set to “No”) to ask them to correct their address at ACS for ARCC volume 2 mailing and to send corrected address to Jeff E. who will mail them volume 1. Since the numbers are not large, these additional mailing costs will be manageable.

- The Division has not been paid yet by CCG for the back cover advertisement, because we did not send them a bill or notice. This will be corrected.
- Several members of the committee reported receiving positive feedback from COMP members, and all present agreed that it is a wonderful new benefit for all members.

Volume 2: There is a delay in publication timeframe for Volume 2. After publication and mailing of Volume 1 it was apparent that we needed to push publication 6 weeks out in order to get the relevant mailing list from ACS (official year-end list). There is now an additional 6 weeks delay because there were not enough quality submissions that were received on time. Current publication date for Volume 2 is June 2006.

ARCC process discussion: David would like to appoint an assistant editor who will be groomed to be the next editor. He suggests we discuss this at the next planning retreat. Another discussion item at that time should be new and/or additional section editors. The goal is to have 6 recurring sections, and then have some sections that are there sometimes but not always. We should also discuss section selection at the planning retreat.

12. The extra copies we have for ARCC Volume 1 have been part of email discussions between executive committee members (excerpts in Appendix VII). We have many extra copies (at least 300) that we cannot sell or give away other than to our membership because of contract limitations. One proposal is to investigate an option where Elsevier buys back a portion of these books for re-selling to MGMS members. Our implicit goal with this proposal is to recruit MGMS members to COMP. Andy H. and David will discuss this with Elsevier. Note that Elsevier is currently selling ARCC Volume 1 at \$140 (Amazon). The committee does want to retain some books for recruiting purposes and for CCG awardees. Hanneke will look into lists of new/rejoined members and lists of resigned members to help decide use of ARCC Volume 1 in retention activities.

13. Andy reports for Phil on activities around regional meetings and local section activities. We have so far received several (5) requests for financial support of regional meetings. Phil established the following guidelines:

- The program has to be related to computational chemistry
- The requestor has to write a summary on what they need the money for, and how they will spend it
- Phil will then bring the proposal to the executive committee

Only 1 of the 5 requestors has responded so far.

The committee suggests that Phil should request COMP advertising in order to be eligible for COMP support. This could be a table with materials from the COMP division (Newsletter, brochure).

14. Michelle reports on the CHEMED online conference. This will most likely happen in the Fall of 2006. She requests suggestions for contributors, esp. from industry and notes that she will remind committee members of this request next Spring.

15. There is no Divisional Service Award Committee yet, so we will not hand out this award for 2005. Andy will appoint a committee for the 2006 Divisional Service Award.

16. Many thanks are expressed to Curt for getting the CCG Excellence Award program set up and started. Andy Good is welcomed as the new CCG Excellence Award coordinator. Current practices, concerns and questions are discussed.

The program so far was run with a letter of understanding, not a contract. Some changes have been made and agreed on mutually but those changes were not put in writing. For example, originally there were 5 awards/meeting, which was later changed to 10 awards/meeting. The understanding was that we were operating under a 3-year term.

A new proposal has recently been received from CCG. This includes going back to fewer awardees, with the money going directly to the students, not through COMP. The new proposal has no term mentioned. There is also a change in coverage, in particular the fact that awardees are limited to those residing in the Americas.

Curt points out that it's better for us if the money passes through COMP. That way, it shows on our annual report as a program service, which effects our allocation and the perception of our activities by ACS. The committee agrees that we should point out to CCG that we would really prefer to have the money flow through COMP. We also want to agree on a term, with a 1-year notice on changes. Lisa mentions that she is not getting information and press releases from CCG for the COMP website. Andy H., David, Andy G., and Jeff E to discuss these items further with CCG.

17. Flashmob II is reported on by Michelle. The event will occur on Sept 15th, at Brywn Mawr College. A local section/division award was granted by the ACS for this happening. There is good funding for the event. Michelle notes that she will buy a set of cables for this type of event. COMP will be the formal owner of these, and Michelle will store them. She requests a box of ARCC Volume 1 books (put out with a note "If you join COMP, you will get this") as well as advertising material (newsletter, brochure). Michelle would also appreciate feedback on defining a "bigger problem" as a Flashmob test case.

18. The committee discusses a letter received from Bill Jorgenson regarding COMP relationships with ACS journals (Appendix VIII). Bill mentions that a reduction in subscription rate for COMP members is unlikely. There is no mention of editorial influence as a result of any special relationship between COMP and JCIM/JCTC in Bill's letter.

The committee is happy with the current relationship with JMGM and realizes that promotion/advertising as mentioned in Bill's letter is good for COMP membership as

well. The committee decides to continue working on getting COMP links set up on the home pages of the 3 journals we feel related with (JMGM, JCIM, JCTC). Lisa will also look into how/where to put up links to all 3 journals on the COMP web page. Andy will follow up with Bill & JMGM on these matters.

19. The committee is very upset that the ACS award for “computers in chemical and pharmaceutical research” is being presented in MEDI. Our understanding from Michael Shea was that since COMP brought in the corporate sponsorship from Accelrys, the award would be automatically presented in a COMP symposium.

It is noted that the Accelrys money goes directly to ACS, and does not go through COMP. The proposal is for Andy H. to talk to ACS on the following requirement and suggestion: The committee wants to require that the award winner presents in a COMP symposium and wants to strongly suggest that publication resulting from that address be published in JCTC or JCIM. The program chair and Bill Jorgenson should follow up on that suggestion.

Following this discussion, the question is raised whether is it time to renew negotiations for a new term of the award and/or to start talking about an endowment. The committee needs to find out how much ACS requires for an endowment. Andy will bring this up with ACS as well. The committee agrees to first contact Accelrys through Peter G. (check on endowment or another 3-year term). A possible new sponsor could be Novartis.

20. COMP sponsorship of the Brazilian Symposium on Theoretical Chemistry is discussed. This includes a \$500 travel award for a US-based person to attend the meeting and give a talk. Candidates need to send their resume and an abstract by Sept 15th to Andy H. who will review applications with an ad hoc award committee. This sponsorship should be highlighted in our annual report as a “Global activity”.

21. The member survey committee reports and hands out a draft as well as a survey that was conducted in 1992 (Appendices IX and X, respectively). Demographics questions were included in the draft to find out what part of the membership responds.

Some comments from the discussion: Split out satisfaction between national programming and other member benefits. Ask about primary focus of current perception (like question 13 of old survey) and desired focus (like question 14 of old survey). Do this for both programming and ARCC. Add room for “anything else you’d like to tell us”. Have a test group do the survey to find out how long it takes to allow a statement up-front on time-demand.

Andy H. proposes to survey the membership annually, and then adjust the survey & frequency as we learn more.

Jeff M will submit a new draft including the comments made by the committee.

22. Other business

22a. Executive Committee planning retreat to happen late Jan/early Feb 2006, probably in Pittsburgh.

22b. COMP is one of the finalists for ChemLuminary awards for ARCC and Flashmob. Andy/Michelle will attend the awards event on Tuesday night. Michelle made a poster to be put up at this event, covering ARCC and Flashmob. If we win, the committee agrees that Michelle keeps the trophy.

22c. Thanks to Andy for his care as Chair, welcome to Jeff E. as incoming Chair.

Adjourned at 7.19