

**Program meeting  
March 12, 2005  
San Diego, CA**

Present: David Spellmeyer, Wendy Cornell, Jeff Madura, Jeff Evanseck, Orlando Acevedo, Kate Lindholm, Andy Holder, Hanneke Jansen, Lisa Balbes, Curt Breneman, Ralph Wheeler, Jennifer Miller

Agenda is handed out: see Appendix I

1. Jeff Madura is appointed as assistant program chair.

2. Program statistics are reviewed using the graph presented in Appendix II.

3a. Wendy discusses the COMP schedule for the San Diego meeting. The 2 biggest symposia are the Pople Memorial symposium and the Mike Klein birthday symposium. The ACS award symposium (Peter Willett receiving the award) is a full day symposium on Tuesday. In the past, this award symposium was often half a day.

3b. There are 9 half day general oral sessions. Wendy needs more chairs for these oral sessions. It is noted that finding chairs has been a struggle. A suggestion is made to use reimbursement of registration fees as an incentive for people to chair a general oral session. This suggestion should be added to a later discussion on COMPs registration fee reimbursement guidelines.

3c. Wendy goes over related symposia in other divisions for San Diego: see Appendix III. In addition to the symposia listed, there is also a session in FUEL that is COMP related.

4. COMP symposia scheduled for future meetings are listed in Appendix IV. COMP is the primary sponsors on all those listed in the appendix.

The Fall '05 schedule for Washington DC is a very full program, with currently 9 specific symposia scheduled. All but 2 of these have co-sponsors and COMP needs clarification on the impact of that on the ACS allocation.

The Exec. Committee is reminded of an opportunity we get every other year to request Elsevier/JMGM sponsoring and a special journal issue on a selected symposium. Our next opportunity for this is in 2006.

5a. ACS provides a website where speakers that qualify for registration fee reimbursement can register, with the bill going directly to the treasurer of the sponsoring division. COMP has not really used this service and Curt notes that it will eliminate our flexibility to approve the use of funds for alternative reimbursements. Again, the Exec. Committee needs a more general discussion on registration fee reimbursement guidelines.

On a related note, Curt mentions that we have maybe 4-5 foreign speakers in San Diego that are requesting their reimbursement in cash. The Exec. Committee prefers to not do

cash transactions. If there is really no viable alternative for specific recipients, we will reimburse in cash and make sure the recipient signs a cash receipt.

The Exec. Committee also discusses current sponsorship related to programming:

Accelrys: ACS award

Novartis: poster session (Wendy will approach them to also sponsor that in Washington)

PRF & IBM (through PHYS): Pople symposium

Bayer, Merck, Leadscope: CINF cosponsored symposia

Merck: general oral session “drug discovery” (refreshments)

Some money is left after San Diego from the Merck donation and Wendy suggests we look into using that for DC general oral drug discovery session refreshments.

5b. The subject of registration of special non-chemist guests is discussed with respect to Pople relatives that are attending his memorial symposium. The Exec. Committee feels that in cases like this, the guests should not have to pay a registration fee. ACS has been unresponsive when Wendy approached them on this subject.

5c. Wendy goes over the list of repeat symposium organizers: people who organize the same symposium (or very similar ones) on a regular schedule. The Exec. Committee suggests that as long as the symposia feature new speakers every time, and are well-attended and lively, this should not be a problem. The Program Chair and Assistant Program Chair should keep an eye on the speaker lists in such cases and also possibly suggest the addition of a new co-organizer.

5d. Ideas for bolstering the General Oral sessions include getting sponsoring for refreshments (like the Merck donation) and allowing for 25 minute talks.

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**COMP Exec. Committee meeting**  
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Present: David Spellmeyer, Wendy Cornell, Jeff Madura, Jeff Evanseck, Orlando Acevedo, Kate Lindholm, Andy Holder, Hanneke Jansen, Lisa Balbes, Curt Breneman, Ralph Wheeler, Jennifer Miller, Michelle Francl, Peter Jurs, Phil Bowen

Agenda is handed out: see Appendix V

1a. Fall 2004 meeting minutes are approved unanimously.

1b. Action item and decision list from the Kansas City planning meeting is reviewed. The following decisions from that meeting are recorded here:

- i) Program Chair, Chair, Secretary & Treasurer can make decisions on sponsorship for COMP related symposia at regional meetings for an amount up to \$500 per symposium. If more than 2 such symposia per year are recommended for sponsorship, the matter is referred back to the Exec. Committee.

ii) COMP will co-sponsor an online symposium with the Division of Chemical Education (especially Committee on Computers in Chemical Education, CCCE) on "WHAT DO CHEMISTS AND CHEMISTRY STUDENTS NEED TO KNOW ABOUT COMPUTERS AND COMPUTING?". Presumably, the conference will be held in the Fall or Winter of 2006 or in 2007. Michelle Francl will serve on the organizing committee and COMP will publicize this event.

iii) COMP will sponsor the Bill Jorgenson symposium on April 29-30 with \$500.

iv) COMP will sponsor CADD Gordon Conference (summer 2005) with \$500.

From the action item list, the mailing list for ARCC labels is discussed. This list has now been created and was delivered by ACS on 3/10/2005. Following is a description of the make-up of the list: members of the ACS COMP Division as of yearend 2004 plus new or rejoining members in 2005 who were not in the 2004 yearend list. Hanneke had requested new or rejoining members as of the run date in 2005; however, ACS membership staff did not want to mix an official membership list for yearend 2004 with an unofficial membership list in 2005, so they provided the official 2005 members as of monthend February. Because of the delay in getting the official year-end membership list from ACS, we will send out ARCC volume 1 by April 1<sup>st</sup>.

The Exec. Committee reiterates that we need the official yearend membership list for sending ARCC. For the first volume, we allowed members with payment status "unpaid delinquent" on the mailing list. We requested a duplicate list from ACS with all members on the ARCC mailing list and their payment status. We can use this list for sending "unpaid delinquent" members a separate post-card to point out that if they value this member benefit, they should pay their dues for 2004 and 2005.

1c. The list of "not-to-be discussed" items is read.

The Exec. Committee agrees to add "we will not discuss journal access to members".

2a. Candidates for the upcoming election are proposed as listed on the agenda:

Chair-Elect: Lisa Balbes & Ralph Wheeler

Councilor: Jennifer Miller & Kerwin Dobbs

After the meeting, the Exec. Committee realized that one additional candidate for councilor is needed according to our Bylaws. Charles Reynolds was proposed and accepted as an additional candidate to run for councilor.

2b. Andy has an appointment this week with the chairman of ACS's C&B (Constitutions and Bylaws) to discuss the process & language for bylaw changes that will allow for electronic voting as well as electronic distribution of Newsletter and meeting abstracts. The upcoming election will have to be done by mail ballot, but the Exec. Committee will work to get the Bylaws changed before the next election.

3a. Curt distributes Appendix VI, describing the general state of our financial affairs, which is judged to be good.

3b. The decrease in divisional allocation is discussed. The Exec. Committee will get a full break-down of all the monies because the decrease is significant. We suspect that ACS did not get all the Fall 2004 attendance sheets, so Michelle will check that they had

the right input and get that information to Curt & Wendy. This issue will be revisited at the Fall meeting. Wendy has reminded every organizer for San Diego to do the attendance sheets.

3c. The question of “Formula and effect of co-sponsorship on national meeting revenue” is referred to the Fall 2005 meeting. The Exec. Committee needs updated information from ACS. We are also told that the formula will change once again. A related item to be addressed at the Fall meeting is the question of co-sponsorship vs co-listing of symposia.

3d. Dues for retired, emeritus, and student members are discussed. A motion is made to have students pay half of the full price, i.e. \$7.50/year. The motion carries. The Exec. Committee decides to keep dues for retired and emeritus members at \$15/year. Overseas members pay an extra charge for postage. The Exec. Committee decides to increase that charge from \$3/year to \$8/year in order to cover mailing ARCC.

Andy notes that the Spring 2005 postcard was not sent to overseas members because of the risk of non-delivery and because the timing was too close to the San Diego meeting already.

Curt will forward these decisions to ACS on the required form. On that form, we also need to answer the following:

Q: Who qualifies for student rate ?

A: Person in a Degree-seeking program

Q: Who qualifies for emeritus status ?

A: Anybody qualifying for ACS emeritus status

4a. Michelle reports on DAC: the focus is on multi-disciplinary efforts and DAC is looking for strategic changes to benefit such efforts. This will probably effect COMP programming efforts: make it easier to program multi-disciplinary topics, add sponsoring/refreshments, etc.

4b. Peter J. reports on the Publications Division: Reminder that JCICS changed name to JCIM (Journal of Chemical Information and Modeling) and the new journal JCTC (Journal of Chemical Theory and Computation) has been launched. The objective of the Publications Division is to monitor every ACS journal on a regular basis, do surveys, etc. Two magazines were recently discontinued: Today’s chemist at work & Modern Drug Discovery. C&EN tries to capture instrumentation advertizing that went to those journals before.

4c. Jennifer has no news to report on the Public Relations Committee.

4d. David reports on the Committee on Chem Abstract Service. A major topic of their latest meeting was the scope of PubChem which is an NIH sponsored repository of compounds w/ biological data. CAS does not have the data-link. Since ACS gets 2/3 of its income from Chem Abstracts, there is a serious concerns that PubChem will negatively impact CAS and thereby ACS. A note is made that since data in PubChem is not tied to publication, there are entries w/o CAS numbers in PubChem.

The Exec. Committee discusses concerns on both sides of the argument: CAS response rate is poor, there is a relatively high charge for small institutions, and CAS has a

monopoly. On the other side are concerns about the government controlling access to scientific data, which they may not understand; there is also the notion that keeping a chemical registry is a scientific activity and should be kept by a professional organization. Two main questions are formulated:

1. Should government control access to scientific data and compete with ACS's main source of income.
2. How should the needs of Pharma & Ag be met with respect to open and free access of data.

David will take some of the comments made and incorporate them in his response to CAS.

5. The JMGM report is handed out, see appendix VII, and discussed with the following two additional notes:

1. On-line submission makes it easier to send papers that are "not good enough", which results in a higher rejection rate.
2. The decline in ACS COMP subscriptions may indicate that no one wants the paper journal.

6a. COMP has 6 symposia scheduled in San Diego, 9 in DC, and 4 so far for Atlanta. Note: ACS award falls in COMP because we brought in the Accelrys sponsorship. If there is no corporate sponsorship, the awardee gets to choose which division to present in.

6b. The Exec. Committee needs more clarification on co-listing vs co-sponsorship. We need to be pro-active and maintain our network of connections with other program chairs to ensure quality and COMP-relevant programming. The suggestion is made to have someone attend P2C2.

6c. Wendy will approach Novartis for sponsorship of the Fall 2005 poster session

7. See 12.

8. There are no stats available from ACS regarding our website. Lisa investigated online polling options with the initial goal of checking the effectiveness of our postcard mailings. Her recommendation is to use survey-monkey. Michelle has used survey-monkey and supports it. It will allow us to put up our logo on the survey site and there are no advertisements. For \$20/month we can have unlimited questions and responses (the free survey-monkey version is limited with respect to number of questions & responses). The question is raised if we want to poll additional topics on COMP member's satisfaction & needs. The Exec. Committee agrees we should expand the online poll and it is decided that the Chair will appoint an ad-hoc committee to develop such a survey. This ad-hoc committee shall discuss the matter by email and propose polling questions to the Exec. Committee for discussion at the DC meeting. Tentative start of the on-line poll would be September 2005.

9. Mailing labels for ARCC were delayed in order to get the right mailing list (see point 1b). Andy will get the 1<sup>st</sup> copy of ARCC on Tuesday from Elsevier. David will design postcard to send to “Unpaid Delinquent” members to encourage them to sign up again (see point 1b). He will circulate this postcard to Andy and Hanneke.

10. Initial new logo designs are handed out (Appendix VIII). We have paid for these initial designs and Andy recommends we chose 1 or 2 for further refinement. From the discussion the following points remained: Use typography from logo #4 with our old molecule, incl 1010101's in molecule but don't add it in COMP letters, and replace “American Chemical Society” with “Division of Computers in Chemistry” (off to the side). Andy will follow up with the designer.

11. The Spring '05 postcard went out 3/3/05. Since we're increasing the postage fee for overseas members, we should include them in the next postcard mailings.

12. The Fall '05 postcard will go out with more time to spare before the start of the meeting. Kate & Andy will take care of the design, Hanneke will request mailing labels. The election will be by paper ballot. Hanneke to collect bio-sketches from the candidates, compose the ballot package, arrange for ballot mailing, and count the votes.

13a. Warm welcome to Phil Bowen as New Regional Meetings/Local Section Activities Coordinator.

13b. Warm welcome to Michelle Franci as Educational Programs Coordinator.

13c. Warm welcome to Jeff Madura as Assistant Program Chair.

14. David and Jennifer have no further information on the opportunity to get involved in a local section event in San Francisco. They will pass all existing information and contact (Lee Latimer, Santa Clara local section) on to Phil.

15. Lisa hands out the proposal from the Divisional Service Award Committee (an ad-hoc committee appointed earlier this year), see Appendix IX. The following addition to the proposal is made: “DSA committee to be appointed annually by the chair”. Andy recommends that the DSA committee will have only one Exec. Committee member and have most of its members come from the outside. The one Exec. Committee member will have a duty to inform the other DSA members on the accomplishments of the nominees. The proposal is accepted with the above mentioned additions and the note that we would like to give our first award at the 2005 Fall meeting.

16. Andy will approach Gerry Maggiora with a request to become the CCG award coordinator.

17. Michelle reports that organisation and advertisement for Flashmob II event in DC is on-going. She has a stack of flyers that she will distribute. The event should be able to accommodate Mac, PC, and wireless. T-shirts will again be available. There is discussion of trying to get sponsorship from a textbook publisher. Michelle mentions that Bob Topper has been using Flashmob in the classroom in collaboration with Pat. This could maybe be used as the example at the DC meeting.

18. The CHED online syposium (“What should chemists know about computing”) will hopefully be run Dec06 or Jan07. Michelle asks for contributions from industry and recommendations of such by the Exec. Committee.

19. Michelle did not yet get info from ACS on what it means to associate with an ACS journal.

The question before the Exec. Committee is: “Should the division associate with a journal and if yes, then which journal” ? The discussion is timely because we need to decide before Nov 2005 if we want to continue with our association with JMGM for another 2 years.

Some general comments:

1. Editorial influence is considered important for association. This means we want to ensure the editor is open to submission from COMP members and is aligned with COMP goals / programming. Note that ACS journals are not going to give us editorial influence. We could get some extra advertizing (logo on website).
2. There is no one journal that covers all our membership. We could associate with more than 1 journal, but are we then diluting the effort (& increasing our time/energy) ? The question is raised whether Elsevier would accept an expanded scope for JMGM ? There is an understanding that very theoretical papers submitted to JMGM get recommended for “theochem” and that if “theochem” gets a “molecular modeling” paper, they recommend it for submission to JMGM.
3. There is a potential for negative branding.

A suggestion is made, and accepted, to invite Bill Jorgenson to the next Exec. Committee meeting to discuss pro’s and con’s of potential association with his 2 ACS journals. Andy will extend the invitation.

As JMGM editor, Andy notes his appreciation regarding the special issues on high impact symposia and the cooperation with the division. He also notes that the division gets more out of the association than the journal does.

Adjourned at 7.10 pm