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## Executive Committee Meeting Minutes

Division of Computers in Chemistry  
Anaheim, California

*Jeff Evanseck*

March 27<sup>th</sup>, 2004

Convention Center, Room 206B, Convened at 3:00 pm

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### Present

Michelle Francl (Chair, Councilor), Andy Holder (Chair-Elect, Editor, JMGM), Jeff Evanseck (Secretary), Curt Breneman (Treasurer), Peter Jurs (Councilor), Michelle Lamb (Newsletter Editor), Ralph Wheeler (Program Chair), Lisa Balbes (Web Master), Wendy Cornell (Assistant Program Chair), Dominic Ryan (Guest), David Spellmeyer (Editor, Annual Reports), Jennifer Miller (Councilor), Jeffry Madura (Alternate Councilor), Frank Yan (Guest), Alex Tropsha (Alternate Councilor).

### 1. Chair's and Past Chair's Report (Michelle Francl and Peter Grootenhuis)

- Michelle handed out the agenda (see Attachment 1)
- Michelle honored Ralph for his hard work as the Programming Chair with an official ACS plaque and ACS mug. It is clear that Ralph has had a tremendous impact on the COMP Division under his reign as the Program Chair.
- Michelle introduced Frank Yan to the Executive Committee.

### 2. Secretary's Report (Jeff Evanseck)

- Jeff handed out the secretary's report (see Attachment 2).
- The total membership for 2003 is down 3.2% compared to 2002. We are down 87 members. Two age groups have declined dramatically: 25-30 years olds (-53 members) and 35-40 years old (-36 members).
- Jeff then presented the demographic data for the 2003 year.

- The election needs (1) Chair Elect, (2) Secretary, (3) Councilor, and (4) Alternate Councilor. We are on track for the election this year.
- Jeff reported upon the Division Recognition Award, which he submitted. We put forth three activities: (1) Awards and Recognition, (2) Symposia Programming, and (3) Annual Reports of Computational Chemistry.
- Jeff then discussed a “welcome letter” that he crafted (see Attachment 3). There was a number of comments and changes needed to be made. Everyone agreed to examine the letter and send Jeff changes to the document.

### **3. Treasurer’s Report (Curt Breneman)**

- Curt handed out the treasurer’s report (see Attachment 4).
- Curt reported that 2003 has been a good year so far.
- Operating account including the Dewar Symposium is approximately \$23K
- The assets to operating budget ratio is 1.42.
- Funds are slowly growing
- The ACS investment pool grew from ~85K to 100K (a 17% increase) over the year.
- The COMP operating budget is ~\$116K, thus the EZ tax form can no longer be filled out. The 990 form must be now filled out.
- As in NYC, the audit liability is now gone.
- So far this year, we have spent \$7-8K more than we have brought in. However, we will make up for it with the higher dues. The bottom line is that we must watch how much we spend.
- Financially the Division is healthy.
- David S. commented that we will spend a lot of money on the ARCC. So far, he knows that it will be ~\$8 per copy for the 2800 copies printed (~\$36,400).
- Michelle suggested that maybe the retreat be skipped this year.

### **4. Program Chair’s and Vice-Chair’s Report (R. Wheeler and W. Cornell)**

- Ralph handed out the program chair’s report (see attachment 5).
- Ralph W. described the Anaheim meeting. It has eight symposia, four of which are co-sponsored with four other Divisions. He considers the meeting to be strong from a programming viewpoint with 378 talks and posters.
- Wendy C. thanked Ralph for his excellent service.
- She reported that COMP is in good shape for Philadelphia.
- The docking and scoring symposium is big in Philadelphia. CINF had overlap with their programming, thus the docking component was cut back.
- CINF’s programming is strong over the next few meetings.
- For the San Diego Meeting in 2005 there are seven symposia slated
- Wendy said that we need to follow up on the funding from Scott Kahn. Will Acceryls sponsor the ACS Award for Computers in Chemical and Pharmaceutical Research? This requires \$60K up front for five years. The Award winner gets \$3-4K.

- The following suggestions were made:
  - “Signal Processing” UCLA or IRVINE suggested by Ralph W. PHYS may want to cosponsor a quantum dynamics symposium.
  - “Protein Modeling for Drug Discovery” Wendy has a few people in mind. Not involving docking.
  - “Memorial for John Pople” Joint with PHYS. They have a complex procedure.
  - “Disease Targets” Joint with MEDI on ion channels
- The national ACS meeting is in Washington DC Fall 2005
- Dewar Symposium in Atlanta 2006.
- COMP programming is split; big at the beginning and big at the end.
- Curt B. would like 20 abstracts to get 6 or 7 invited talks for the Emerging Technologies Symposia.
- Wendy stated that the Division of Laboratory Automation is dissolving. There are 300 members. Do we adopt them? The fit may be better with ANAL.

## **5. Councilor’s Report (Michelle Franci, Peter Jurs and Jennifer Miller)**

- Peter J. announced that the new editor of JCICS is Bill Jorgensen. This is good for the journal and good for COMP.
- Bill described two big changes, where the journal will split into two.
  - JCICS (1/05) name changed to “Chemical Information and Modeling”. The articles will be of the same flavor as the previous JCICS articles.
  - The new journal’s name is “Chemical Theory and Computation”. It should attract the theory and computational articles that are published in JACS.
- AICHE gave all of its publications to Wiley. They need infrastructure.
- Jenn reported on the Public Relations and Communication meeting. A three year plan was described.
  - Goal of evaluating scientific progress
  - Expanding chemistry
  - Make the world better
- The committee has mostly local section representation. The committee is looking for better interaction with Divisions.
- Ralph W. has tried to publicize before, but has had problems in the past.
- One comment is that it is difficult to translate the science into layman terms.
- Andy H. stated that the PR training conference was interesting and informative.
- Michelle and Ralph both have had no feedback when contacting PR.
- David S. Stated that we need to do a better job in making our science understandable.

## **6. Annual Reports in Computational Chemistry (David Spellmeyer)**

- David S. handed out the proposed Elsevier agreement (see Attachment 6)
- David S. stated that we have selected Elsevier. Other options were too expensive. The next closest was \$19/copy higher than the one accepted.

- We have agreed to purchase 2800 copies
- We can sell the back cover. IBM has been approached at \$25K
- The ACS lawyers have checked the contract and do not find anything of concern.
- Ralph W. asked about the renew date. "In-print" needs to be defined.
- The cost is \$8/copy which is the same as with MEDI.
- David will make changes and resend to the committee. Please send comments back to him.

## **7. JMGM Report and Related Issues (Andy Holder)**

- Andy H. handed out the JMGM report (see Attachment 7)
- In 2003, 48 papers were received and 29 were accepted for publication.
- To date in 2004, 27 papers have been received and eight have been forwarded for publication.
- Elsevier Science and JMGM are sponsoring a symposium at the Anaheim meeting at \$3K. The symposium is "Computational Approaches to problems in Environmental Chemistry" organized by Doug Tobias.
- Elsevier and ACS-CAS and ACS Publications have agreed to provide linking between their services for scientists. Thus, Science Direct, MDL databases and ChemWeb will be able to link directly to ACS journals.
- Andy H. has agreed to continue for three more years as the US Editor.

## **8. Web Site (Lisa Bables)**

- Lisa handed out a website summary (see Attachment 8).
- Lisa reported that during 2004, the site is averaging 136 visits per day, 219 page views per day and 7 minutes/visit.
- These statistics are up from 2003. Just over half of the visitors are from the US.
- 34% enter from google and 17% enter the URL.
- An entire 350+page report (per year) is available upon request.
- The Division of Inorganic Chemistry is the only Division approved for electronic elections. Rubber is considering it. The number of votes doubled when electronic voting was the only format available.
- Lisa estimates from preliminary research that the cost to switch to electronic voting is \$7-10K.

## **9. Elections (Andy and Peter)**

- Nominations for the 2005 posts have been determined.
  - Chair-Elect lined up.
  - Three people for Councilor
  - Two individuals for Secretary

## **10. Other**

- To save money, the Newsletter and Abstracts will be posted on the website only.

- Michelle will draft the postcards to be sent to the membership to describe the change. The postcards should be sent out in the June or July time frame.
- Another idea is to modify the election ballot. Indicate e-mail on the ballot.
- Michelle presented the Newsletter (see Attachment 9).