



Executive Committee Meeting Minutes

Division of Computers in Chemistry
Orlando, Florida

April 7, 2002
Convened at 3:30

Present

Bill Jorgensen (Chair), Peter Grootenhuis (Chair-Elect), David Spellmeyer (Past-Chair), Curt Breneman (Treasurer), Jeff Evanseck (Secretary), Peter Gund (Councilor), Peter Jurs (Councilor), Michelle Francl (Councilor), Hanneke Jansen (Alternate Councilor), Michelle Lamb (Newsletter Editor), Ralph Wheeler (Program Chair), Lisa Balbes (Web Master), Wendy Cornell (Assistant Program Chair), Jennifer Miller (Guest), Dominic Ryan (Guest), Andy Holder (Editor, JGM)

Chair's and Past Chair's Report

- Bill Jorgensen had the committee members introduce themselves.

Secretary's Report

- Andy Holder met with Jeff Evanseck to transfer COMP documents and records.

Treasurer's Report

- From the final 2001 report submitted to the ACS, Curt Breneman reported that the COMP division is in good financial shape.
- The asset to expense ratio is 2.03, which is slightly lower than last year's number.
- The division's activities are up 17% as compared to last year, which explains the slightly lower asset to expense ratio.
- COMP has the same assets as last year (\$167,584), which is good considering the current economic trend.

- The Division's taxes were filed on time and correctly this year.
- COMP has a reserve of funding, in case something goes wrong.
- The Chemical Computing Group (CCG) will make the student travel grant money available once a year. It was not clear, but multiple payments seemed to be problematic.
- ACS Stop/Gap funding helps our financial situation (\$ 6,500).
- Michelle Francl briefed the committee about ACS Stop/Gap funding. An imbalance between divisional and local section funding has caused serious financial problems for a few divisions. The ACS has recognized this problem and has made the Stop/Gap funding available until its by laws can be changed to redirect more funding to Divisions.
- The annual strategic meeting is new and an additional cost for COMP.
- Curt Breneman agreed to run for treasurer for 2003.

Councilor's Report

- Michelle Francl went into more detail concerning ACS Stop/Gap funding. The Divisions will receive more money. In addition, membership and programming will receive more financial assistance. The bylaws are being changed to correct the current situation.
- Encourage COMP members to scan their badges at the exposition center, since COMP gets credit when its members get their badges scanned at any of the booths.
- Peter Jurs will check if ACS books will go electronic.
- Peter Gund was reappointed as councilor. He reported from the Science and Technology Subcommittee.

Program Chair's and Vice-Chair's Report

- Ralph Wheeler thanked Wendy Cornell for preparing the preliminary and final Orlando schedules on very short notice.
- The number of symposia and presentations increased significantly in 2001, as compared with 2000. There was a 78% increase in presentations, 100% increase in sessions, and 58% increase in symposia.
- The programming for Orlando (2002) was strong compared to Chicago (2001). Orlando has 316 presentations and 13 symposia.
- Boston programming looks light (currently 261 presentations), probably due to the early closing date. Most committee members found the early closing date unacceptable, and wanted the councilors to take this message back to the ACS. For this time only, Ralph Wheeler was willing to accept late abstracts.
- Only 2 abstracts have been received for the "Chemistry of Computers" symposium. It is questionable if the symposium will be held. One problem is that it may be competing against "Computational Nanotechnology" in New Orleans (2003).
- Ralph described how the schedule is built and how he is trying to achieve more balanced programming.
- Ralph said that other divisions needed to be reached. In this way broader topics could be established that result in symposia with larger attractions. Andy Holder suggested dual talks between experiment and theory. The committee agreed that this was a good idea, and should be followed up.

- Andy Holder brought up the issue of Dimitris Agrafiotis (Guest Editor) and Elsevier having an annual combinatory chemistry symposium. The committee thought it was an excellent idea, but had serious reservations of having a single program chair. The issues of exclusive sponsorship and required papers were discussed.
- Ralph Wheeler requested topics or organizers for future symposia. Jennifer Miller agreed to organize a conference for New York (Fall 2003). Wendy Cornell indicated she would organize a conference on computational materials in Anaheim (Spring 2004). Jeff Evanseck volunteered to organize a conference on the developments and progress in DNA/RNA computational studies for New York (Fall 2003).
- Ralph Wheeler's term expires in New Orleans (Spring 2003). He has not decided if he would be willing to continue as the Program Chair.

JMGM Report

- Rod Hubbard has resigned as MGMS Editor in the UK, John Essex has been named as the new European Editor.
- Andy Holder became the USA Editor May 2001. Since this time, 37 papers have been received for publication.
- JMGM should return to a normal publication schedule, since the remaining backlogs have been published this year.
- Two special issues are in progress for 2002.
- JMGM is getting ready to put electronic submissions online and would like to have a link to this page from the COMP web page describing JMGM. The committee agreed.
- Elsevier would like to offer all COMP members electronic subscription to JMGM, for the discounted cost of \$10 each. Previously, David Spellmeyer and Andy Holder were asked to consider how this could be accomplished. The amount needed is ca. \$27,000 given our current membership.
- Advertisement on the back page of a journal is meaningless in electronic format. It was suggested that an electronic banner for advertising would be a more appropriate format.
- Bill Jorgensen and David Spellmeyer suggested that this idea be expanded to other journals on behalf of the COMP membership. Andy agreed to continue the discussions with Elsevier (JMGM), Bill would approach Wiley (JCC), and David would contact the ACS (JCICS).

Other Business

(a) Elections (David Spellmeyer)

- Potential candidates for 2002 COMP elections were discussed. It was decided that Curt Breneman would run for treasurer. A few names were mentioned for the other positions, but nothing definite was decided. The four positions needed are Chair-Elect, Treasurer, Councilor, and Alternate Councilor.

(b) COMP Electronic Elections (Jeff Evanseck)

- National plans on going to electronic elections within the next 3-5 years.

- The Organic Division has held successful electronic elections over the last 3 years.
- Electronic elections will requires us to change our bylaws.
- David Spellmeyer said that we should move quickly, since it takes a number of years to change the bylaws.
- The bylaw change is a topic of the long-range planning meeting at Yale this year.

(c) Web Site (Lisa Balbes)

- Lisa Balbes reported that she volunteered to participate in the Gated Web Community Project, but has had no response since November 2001.
- The COMP home page was the 18th most visited divisional page. There were a total of 3643 visits, which represents 0.33% of all traffic.
- From the new web counter, the COMP site had 310 visitors since March 7th.
- Lisa had our site removed from the East Bay Technology's database of multimedia-content and multimedia related websites.

(d) Newsletter Editor (Michelle Lamb)

- Michelle requested that all material be sent before April 26, 2002 for the August newsletter.

(e) 2003 Dues (Curt Breneman)

- After some discussion, it was decided that the dues will remain the same. ACS members dues are \$10, students \$5, and nonmembers \$15.

(f) Summer Retreat (Bill Jorgensen)

- The 2002 annual strategic meeting (July 19-20) in New Haven was briefly described. A number of activities are planned.