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INTRODUCTION

Mark S. Gordon

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This special issue of Theoretical Chemistry Accounts marks the 65th birthday of Professor Mark Gordon, celebrated by a meeting on the island of Maui from 15–18, January 2007. Attendees at this meeting, entitled "Practicing Chemistry with Theoretical Tools", included a majority of Mark's current and former students and postdoctoral fellows, and a few close collaborators. Wife Joan, son Michael, and niece Teresa were in attendance, as well. The 80 participants contributed a total of 47 oral presentations and 21 posters. The scientific presentations were interspersed with several more personal tributes to Mark, and an after-dinner roast by Tom Barton on January 18, exactly 65 years to the day after Mark's birth. The papers in this special issue are an outgrowth of the Maui meeting.

Mark was born in New York, NY in 1942, attending high school at the Newburgh Free Academy, where his studies included an emphasis on advanced science and math courses. After obtaining a B.S. from Rensselaer Polytechnic Institute in 1963, he began graduate school at Carnegie Institute of Technology. Carnegie Tech would offer Mark two excellent opportunities: the chance to study with Professor John Pople, newly arrived from England, and the appeal of wedding bells, culminating in his marriage to Joan Novak. After writing the original Z-matrix program "model builder", and completing a thesis titled "Applications of Approximate Molecular Orbital Theory to Organic Molecules", Mark undertook postdoctoral studies with Professor Klaus Ruedenberg at Iowa State University from 1967 to 1970. He then moved to North Dakota State University, rising to full Professor, and serving as Chemistry Department chair from 1981 to 1989. NDSU honored Mark during those years with a Distinguished Professorship award in 1987, and his selection as the University Faculty Lecturer in 1988. In 1992, Mark moved to Iowa State University's Chemistry Department and the US Department of Energy's Ames Laboratory. He was appointed Director of the Applied Mathematical Science program of the DOE lab, overseeing the local parallel computing laboratory in 1997. Mark was also viewed highly at ISU, being named Distinguished Professor in 1998 and Master Teacher in 2005, and becoming the first holder of the Craig Chair in Chemistry in 2006. As might be expected, Mark has earned several important scientific awards, including being named a Fellow of the American Physical Society in 2001, holding a Fulbright Senior Scholarship from 2003 to 2004, receiving the American Chemical Society Midwest Award in 2004, and election to the International Academy of Quantum Molecular Science in 2004. Sabbatical visits made over the years include UC-Irvine (Warren Hehre 1978), Minnesota (Don Truhlar 1985), Institute for Molecular Science (Keiji Morokuma 1991), and the Australian National University (Leo Radom 2003, Mick Collins 2007).

The many students and postdoctoral fellows who have worked with Mark will attest that his research is characterized both by an interest in development of new methods, and then once implemented, demonstration of the methods through solving practical chemistry problems. Such a robust research program inherently produces young scientists grounded in both theory and application, and these generations of scientists are most surely regarded by Mark as his primary achievement. To date, Mark has mentored a total of 48 undergraduate students, of whom 25 are known to have been awarded an advanced degree or are currently enrolled in graduate school. Mark's own graduate students are listed below, in a list that will surely continue to grow,

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Fred Marsh, MS, 1976	Kurt Glaesemann, Ph.D, 1998	Jonathan Bentz, MS, 2006
Patrick Saatzer, Ph.D, 1976	Brett Bode, Ph.D, 1998	Ryan Olson, Ph.D, 2006
James Caldwell, Ph.D, 1981	Dmitri Fedorov, Ph.D 1999	Deborah Zorn
Kim Baldridge, Ph.D, 1988	Vanda Glezakou, Ph.D, 2000	Jonathan Mullin
Jerry Boatz, Ph.D, 1989	Yousung Jung, MS, 2001	Bosiljka Njegic
Theresa Windus, Ph.D, 1993	Mark Freitag, Ph.D, 2001	Daniel Kemp
Kiet Nguyen, Ph.D, 1994	Mike Pak, Ph.D, 2002	Toni Smith
Nikita Matsunaga, Ph.D, 1995	Yuri Alexeev, Ph.D, 2002	Sarom Sok
Jan Jensen, Ph.D, 1995	Heather Netzloff, Ph.D, 2004	Pooja Arora
Jon Rusho, MS, 1996	Ivana Adamovic, Ph.D, 2004	Luke Roskop
Galina Chaban, Ph.D, 1997	Jamie Rintelman, Ph.D, 2004	Andrey Asadchev
Simon Webb, Ph.D, 1997	Christine Aikens, Ph.D, 2005	Sean Nedd
Jim Shoemaker, Ph.D, 1997	Sergej Varganov, Ph.D, 2005	Spencer Pruitt

An equally vital contribution to Mark's research programs comes from his postdoctoral fellows, who are listed below,

Kazuo Takatsuka, 1979–1981	Wei Chen, 1994–1995	Hiroyuki Tamura, 2003
Satoshi Yabushita, 1982–1984	Takako Kudo, 1995	Tim Dudley, 2003–2004
Mike Schmidt, 1982–1985	Jan Jensen, 1995–1996	Jie Song, 2003–2004
Shogo Sakai, 1985–1986	Graham Fletcher, 1998–2000	Hui Li, 2004–2006
Shiro Koseki, 1987–1989	Rob Bell, 1998–1999	Ian Pimienta, 2004-
Marshall Carroll, 1990–1991	Grant Merrill, 1998–1999	Takeshi Nagata, 2005-
Tom Cundari, 1991	Cheol Ho Choi, 1999–2001	Lyuda Slipchenko, 2005-
Kyungsun Kim, 1991	Pradipta Bandyopadhyay, 2000–2001	Yingbin Ge, 2005-
Paul Day, 1991–1993	Akihiko Yoshikawa, 2001–2002	Soohaeng Yoo, 2006-
Shujun Su, 1992–1993	Yoshinobu Akinaga, 2002–2003	Hirotoshi Mori, 2006-
Tetsuya Taketsugu, 1994	Baudilio Tejerina, 2002–2005	

The organizers are particularly pleased that 16 of Mark's former students, 7 of his current students, and 21 of his postdoctorals were able to attend the meeting, along with a few of Mark's various senior visitors to Ames: Keiko Takano, Haruyuki Nakano, Joe Ivanic, and Bob Damrauer. Some of the organizers personally witnessed a quote famous enough to have been officially archived in the list of happy thoughts at the end of some computational chemistry data outputs,

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1309 FORMAT(1X,'MY GROUP MEETINGS AREN"T VERY STRUCTURED.'/
   $ 5X,'- PROF. M. S. GORDON, OCT. 5, 1984')
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and, with bad weather in the 48 states delaying travel, a missing box of programs, and various other fine meshes, the meeting in Maui proved no exception to the rule.

To date, Mark has published over 450 papers, and a current listing of these can be found on a web site [1]. These papers document a career devoted to both theoretical and computational chemistry. Nearly all of the developed methodology from Mark's group, and a growing list of collaborating groups, is captured in the GAMESS program [2,3], which is made freely available to the chemical community [4]. A simple way to measure the success of this is to count the download requests for GAMESS: over 9,200 in calendar year 2006. One could also point to the "lines of code" statistic: the growth of GAMESS from 65,000 lines in 1982 to 820,000 today. However, a more meaningful tribute would be to list some of the high points in Mark's scientific career, along with a sampling of his papers. It is with great pride that not only Mark, but his many colleagues, continue to develop and foster the growth of the GAMESS software program, in support of both research and education.

The early years of Mark's career were focused on the comparison of silicon chemistry with that of carbon, establishing that these two elements, albeit in the same group, are more often different than similar. This included discovery [5] of the near isoergicity of silylenes (H_3Si–SiH) with double bonds ($H_2Si{=}SiH_2$), and studies of strained rings [6], silylene insertions [7], pyrolysis [8], π bonding [9], aromaticity [10], hypervalency [11], thermochemistry [12], the clean Si(100) surface's electronic structure [13], chemistry on that surface [14–16], and polyhedral oligomeric silsesquioxanes [17]. Several reviews of Mark's research on silicon chemistry

are available [18–21]. A number of these topics were pursued in other 4e$^-$ atoms: germanium and tin [22], and eventually titanium [23,24], which opened up the subject of catalysis through Ti's hydrosilation [25] and bis-silylation [26] reactions. Investigations involving titanium led to other transition metal systems [27], including more recent interest in gold catalysis [28]. One might find it more difficult to pick out a central "theme" in Mark's recent work, as his interests have expanded to nearly every aspect of chemistry. However, one recurring topic involves research into high energy molecules, such as prismanes [29], N_2O_2 [30], Si_8R_8 [31], N_3F [32], N_5F [33], $C_{36}H_{16}$ [34], or ionic liquids [35–37], as potential propellants.

In recent years, Mark's group has made considerable efforts towards development of a molecular solvation model, called the Effective Fragment Potential [38–40]. The EFP model treats the solvent as a discrete, molecular species, and thus captures the intricate interactions of the solute, including the first solvation shells. The EFP model is intended to capture the details of each kind of interaction, and now includes multipolar electrostatics, dipole polarizability, Pauli repulsion, charge transfer, and dispersion—each modeled by a non-empirical formula based on more exact physics. The ab initio part of Mark's soul is revealed by his insistence that the EFP model retain a firm theoretical basis and numerical accuracy, term by separate term. There are now 40+ papers covering the development and application of the EFP model. Particularly interesting applications and extensions of the EFP theory include a demonstration that MP2-based EFP parameters suffice to describe the structure of liquid water [41], and studies of how many waters are needed to make the dipole of one H_2O reach the bulk limit [42], drive glycine from its neutral to its zwitterionic form [43], or dissociate NaCl to ions [44]. The extensibility of the EFP model means it is not just a model for aqueous solution, as its parameters can now be obtained from ab initio computation on any monomer, as is shown by recent EFP simulations of benzene [45], and styrene [46] clusters, and ionic liquids [47].

Another predominant theme in Mark's career has been the development, with Mike Schmidt, of the MCSCF method [48], due to its native ability to incorporate effects such as bond breaking, electronic excitation, and spin–orbit coupling [49]. Each of these topics has to do with unpairing of electrons, with immediate implications for chemical applications such as: elucidation of methane's inversion [50], proton transfers in excited states [51], treatment of species such as Ti_8C_{12} metcars [52] which are intrinsically not single reference, explanation of observed vibrational structure in spin–orbit coupled levels of diatomics [53], and any number of chemical reactions such as the ring opening mechanism of silacyclobutane [54]. Of course, methodological improvements to the MCSCF program in GAMESS enabled these chemical applications, including a new orbital converger [55], adoption of determinant CI codes from the group of Professor Ruedenberg, scalable MCSCF analytic Hessians [56], and connection of GAMESS' MCSCF code to the surface growing program of Mick Collins [57].

One cannot practice theoretical chemistry without confronting the computers that do the arithmetic. Mark's interest in the parallelization of quantum chemistry began in 1992, with replicated memory parallelization of SCF [2], and now has extended to a full suite of distributed memory closed and open shell MP2 programs [58–60], and very recently, a SMP-optimized program for CCSD(T) [61]. The necessary computer science support for parallelization (the Distributed Data Interface [62–64] included with GAMESS) brought Mark into direct contact with Computer Science as it bears on computational science, particularly as in relation to parallel computing. This led Mark into taking on the position of Director for the Scalable Computing Laboratory in 1997. An extra benefit from the SCL connection to those who use GAMESS is continued development by Brett Bode for the MacMolPlt visualization program [65] for GAMESS.

As the pool of former group members increases, the number of their collaborations and interactions with Mark continues to grow. Only one such project will be mentioned here, due to space limitations. This is the Fragment Molecular Orbital (FMO) method [66], the coding of which has been done by Dmitri Fedorov, a 1999 Ph.D. student. FMO, as developed in the lab of Fedorov and Kazuo Kitaura, divides large molecules into many pieces, and then exploits the native parallelism of the various quantum chemistry methods in GAMESS within subgroups of processors—with different subgroups taking different tasks from the list of many smaller computations required by FMO. The FMO method could serve as a paradigm for Mark's approach to science: judicious approximations made where possible to rigorous methods, with careful control of numerical accuracy, programmed to run on existing computer technology, and directly aimed at chemistry problem of impressive complexity [67]. This method has the potential of bringing ab initio methods as a full partner in the suite of tools necessary to better understand very large materials and biological systems, for the first time.

The organizers [Kim Baldridge (Zurich), Jerry Boatz (Edwards AFB), Theresa Windus (Ames), Tom Holme (Milwaukee), Tom Cundari (Denton), and Mike Schmidt (Ames)] are grateful to the Air Force Office of Scientific Research for financial support of the meeting costs, to Heidi Weber for web design and photography, and to all the participants for a very lively and enjoyable time. Mahalo!

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