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Frontiers in Geochemistry

Goldschmidt 2003

Abstract Deadlines
- 14 April
  (Grant Application or Hardcopy)
- 5 May (Electronic)

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The Geochemical Society

The Geochemical Society is a nonprofit scientific society founded to encourage the application of chemistry to the solution of geological and cosmological problems. Membership is international and diverse in background, encompassing such fields as organic geochemistry, high- and low-temperature geochemistry, petrology, meteoritics, fluid-rock interaction, and isotope geochemistry. The Society produces a Special Publications Series, The Geochemical News (this quarterly newsletter), the Reviews in Mineralogy and Geochemistry Series (jointly with the Mineralogical Society of America), the journal Geochimica et Cosmochimica Acta (jointly with the Meteoritical Society), and co-publishes the electronic journal G3 (jointly with the American Geophysical Union: AGU); grants the V.M. Goldschmidt, F.W. Clarke and Clair C. Patterson Awards, and, jointly with the European Association of Geochemistry (EAG), the Geochemistry Fellows title; sponsors the V.M. Goldschmidt Conference, held in North America in odd years and elsewhere in even years, jointly with the EAG; and co-sponsors the Geological Society of America annual meeting and the AGU spring meeting. The Society honors our first President, F. Earl Ingerson, and our first Goldschmidt Medalist, Paul W. Gast, with the Ingerson and Gast Lectures, held annually at the GSA Meeting and the V.M. Goldschmidt Conference, respectively. The Geochemical Society is affiliated with the American Association for the Advancement of Science and the International Union of Geological Sciences.

Members of the Organic Geochemistry Division are individuals with interests in studies on the origin, nature, geochemical significance, and behavior during diagenesis and catagenesis of naturally occurring organic substances in the Earth, and of extraterrestrial organic matter. GS members may choose to be affiliated with the OGD without any additional dues. The OGD presents the Alfred E. Treibs Award for major achievements in organic geochemistry, and Best Paper awards (student and professional) in organic geochemistry.

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The Geochemical News

April 2003

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Newsletter of the Geochemical Society
From the President:

The 2003 Goldschmidt Conference
“Frontiers in Geochemistry”

As spring approaches, we can begin to put the gray days of winter behind us and turn our thoughts to the major geochemical event of this coming summer, the 13th Annual Goldschmidt Conference to be held at Kurashiki-Sakuyo University in Kurashiki, Japan from 7 to 12 September 2003. In late February, many if not most of you received an e-mail invitation to attend the Conference, which announced the appearance of the second circular at http://www.ics-inc.co.jp/gold2003/. I would like to congratulate the Organizing Committee, chaired by Yukihiro Matsuoka (Geological Survey of Japan), for their excellent (i.e., user friendly) web site. If you have not, as yet, taken the opportunity to peruse the electronic circular, please do so. It is easy to negotiate your way through the various pages and find any information you might wish to know concerning the Conference. In particular, check out the list of symposia, preview the contents and learn about the invited keynote speakers. The Goldschmidt International Program Committee has once again produced an interesting and stimulating program. The special symposia touch on all of the current topics in geochemistry, highlighting the theme of the Conference, “Frontiers in Geochemistry”. It will undoubtedly be a very comprehensive and exciting meeting with something for every geochemical or cosmochemical inclination.

The 13th Annual Goldschmidt Conference is the first to be organized outside of the USA or Europe. It promises to be both a scientific and cultural experience, an opportunity to interact with fellow scientists coming from around the world to review state-of-the-art geochemistry in a unique setting. In addition to the scientific program, you will have the opportunity to enjoy Japanese hospitality through a number of scheduled field trips and social events. And, while you are looking at the web site, browse through the links under Kurashiki to learn more about this well-preserved historical town, as well as other important cultural centers in the region, such as the cities of Okayama, Kyoto and Nara. The web site provides helpful information on accommodations, even making available arrangements for those who wish to stay in a traditional Japanese style inn (ryokan). The travel information section is also very useful providing detailed instructions on how to travel within Japan. Having visited Japan on previous occasions and having experienced first hand the tremendous welcome given to visitors from abroad, I highly recommend that you contemplate combining additional sightseeing with your participation in the 2003 Goldschmidt Conference. And, please mark the following fast approaching deadlines in your calendar: 14 April 2003 for paper submission of abstracts and grant applications, and 5 May 2003 for electronic submission of abstracts.

Congratulations to the 2003 Medalists and Fellows

You may have noticed that each year a call is advertised in the Geochemical News requesting nominations for The Geochemical Society medal awards, as well as for the joint EAG-GS Geochemistry Fellows. This past year was no exception and the evaluation process of the various GS committees began in earnest after the November 15th deadline. Under the guidance of the committee chairs, the nominations are reviewed and the committee members have the difficult task of selecting from among a group of outstanding individuals nominated by their peers. Once a consensus is reached, the nomination of each committee is then reported to the GS Board of Directors who gives the final vote on the selected candidates. And, finally with the approval of the BoD, I have the great pleasure, as President of The Geochemical Society, to inform and congratulate the newly elected Medalists and Fellows.

In my opinion, the 2003 deliberations of the various GS committees have resulted in an outstanding selection of Medalists and Fellows. I am very pleased to announce that Bernard J. Wood, University of Bristol (UK), will be awarded the 2003 V.M. Goldschmidt Medal, the highest honour of the Geochemical Society. Roger E. Summons, Massachusetts Institute of Technology (USA), will receive the 2003 Alfred Elbe Medal for major achievements in organic geochemistry. William F. Fitzgerald, University of Connecticut (USA), will be given the 2003 C.C. Patterson Medal for his innovative breakthroughs in environmental geochemistry. For his outstanding early career contributions, Paul D. Asimow, California Institute of Technology (USA), will be honoured with the 2003 F.W. Clarke Medal. In recognition of his exceptional service to the Society, Hubert L. Barnes, Pennsylvania State University (USA), will receive the 2003 Geochemical Society Distinguished Service Award. Finally, the list of new GS/EAG Fellow for 2003 includes 7 prominent geochemists: Robert C. Aller, SUNY, Stony Brook (USA), Richard W. Carlson, Carnegie Institution of Washington (USA), Marilyn Fogel, Carnegie Institution of Washington (USA), S. Krishnaswami, Physical Research Lab, Navrangpura, Ahmedabad (India), John W. Morse, Texas A & M University (USA), Herbert Palme, Universität zu Köln (Germany) and David Rickard, Cardiff University, Wales (UK). I am sure you will join me in congratulating the 2003 Medalists and Fellows, who will be formally honoured during the Awards Ceremony at the Goldschmidt Conference in Kurashiki, Japan.

I would like to take this opportunity to thank the members of the various award committees who have contributed their time to this important task of nominating fellow geochemists to be honoured by The Geochemical Society. I would particularly like to acknowledge the committee chairs and heartily thank the following persons for their service to the Society: Peggy Delaney (Clarke Committee), Lynn Walter (Geochemistry Fellows Committee), Lee Kump (Goldschmidt Committee), and Erwin Suess (Patterson Committee). It is my impression that the selection process for honouring our fellow geochemists is very fair, open and thorough. The process does, however, require your input. I cannot emphasize strongly enough how important your nominations are. Next to volunteering to participate on a GS Committee, submitting nominations to the committees is also an important way to contribute to The Geochemical Society. Please consider that it is not too early to begin thinking about possible candidates for 2004. Remember it does take time and some effort to gather the material to submit your nominations before the next November 15th deadline.

In my next letter, I will be able to provide you with an up-to-date report on the progress of the 13th Annual Goldschmidt Conference. Until then, I am already making my travel plans for September and will look forward to meeting you in Kurashiki.

With best wishes,

Judith A. McKenzie
GS President
EDITOR’S CORNER...

As we go to press, military forces of the US have initiated an invasion of Iraq. There are no registered members of the Geochemical Society in Iraq, however we have many members in surrounding nations, including Iran, Turkey, Israel and the West Bank. The editors offer best wishes to our colleagues there, and hope they survive the present conflict with minimal disruption of their lives or the lives of their families.

This conflict in the Middle East, no matter the strategic outcome, will ultimately call upon our profession to assess and address the aftermath. In Iraq, the detonation of munitions laden with uranium, the dispersal of war toxins into soils and aquifers, coastal marshlands suffocated in petroleum, and the abiding threat of radionuclide dispersal will demand the attention and the labors of environmental scientists for years to come.

More fundamentally, the global thirst for petroleum - the root cause of this particular conflict - continues to weigh heavily upon our civilization. Though geochemistry has (in part) been traditionally associated with petroleum exploration, a new cadre of geochemists - such as this issue’s featured interviewee Prof. Alexandra Navrotsky - seeks to understand the physical and chemical properties of solids, both geologic and synthetic, that promise revolutionary advances in photovoltaics, advanced ceramics, and superconductors, potentially blazing a path to a post-petrocarbon era. Prof. Navrotsky offers a gleaming example of how our discipline can inform and include a truly monumental range of issues.

Wishing all our members, in the Middle East and elsewhere, good fortune in the coming months,

Johnson R. Haas and Carla Koretsky, Editors

Geochemical Society Business Office News

- Please check the mailing labels on your issues of Geochemical News and Geochimica et Cosmochimica Acta for accuracy. If corrections are necessary, please send them to the GS business office.

- Some GCA subscribers have experienced delivery problems with v.67 issue 3, namely that the shipping bag was not sealed and the contents fell out during shipment. As always, if there are issues of your subscription that have arrived damaged, or not at all, please let me know and I will strive to resolve the matter as painlessly as possible.

- Also, if you are having problems with your personal on-line subscription to GCA, Elsevier has an address you can contact for assistance: loginsupport@elsevier.co.uk

- The Geochemical Society, in collaboration with the Society of Economic Geologists (SEG) and the Institute of Geological and Nuclear Sciences (GNS), is working on a volume to honor the memory of Werner F. Giggenbach. SEG has commenced copyediting of reviewed manuscripts that have been received from the editor, Stuart Simmons, and plans on a late 2003 release date.

- The 2003 Goldschmidt conference will be upon us before too long. Be sure to not only register early, but to take advantage of your conference registration membership discount.

- The 2003 Medalists and Award Recipients have been announced. Congratulations to:

  - Bernard J. Wood 2003 V.M. Goldschmidt Medal
  - Roger E. Summons 2003 Alfred Treibs Medal
  - William F. Fitzgerald 2003 C.C. Patterson Medal
  - Paul D. Asimow 2003 F.W. Clarke Medal
  - Hubert L. Barnes 2003 Geochemical Society Distinguished Service Award


Cheers,

Seth Davis
Geochemical Society Business Manager

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Newsletter of the Geochemical Society
In Memoriam: Harmon Craig (1926-2003)
Scripps Institution of Oceanography, UC San Diego

Professor Harmon Craig, a leader in global investigations of the earth’s chemical properties and a world explorer at Scripps Institution of Oceanography, University of California, San Diego, died Friday, March 14, at Thornton Hospital in La Jolla, Calif., from a heart attack. He was one day shy of his 77th birthday.

During his 47-year career with Scripps Institution of Oceanography, Craig led scientific expeditions to such remote spots on Earth as Tibet, Polynesia, and the Great Rift Valley in East Africa. He searched for elusive gases and rocks in some of Earth’s most inaccessible places, such as 12,000 feet deep in the Pacific Ocean’s Mariana Trough, where he discovered hydrothermal vents; and in the crater of an active underwater volcano off Hawaii.

“Harmon’s curiosity and sense of adventure knew no bounds,” said Dr. Charles Kennel, director of Scripps Institution of Oceanography. “His drive for scientific achievement was unparalleled in my experience. The ocean and earth science world has lost a truly spirited adventurer and one of the greatest geochemists of the 20th century.”

In 1998, Craig was the first geochemist to receive the Balzan Prize, the international honor considered to be the equivalent of the Nobel Prize in the fields of natural sciences, humanities, and social sciences that are not Nobel award categories. Craig was recognized by the Balzan Foundation for his work as “a pioneer in earth sciences who uses the varied tools of isotope geochemistry to solve problems of fundamental scientific importance and immediate relevance in the atmosphere, hydrosphere and solid earth.”

Craig was listed among the top Earth scientists in the world in the recently published “A to Z of Earth Scientists,” part of a notable scientists series published by Facts On File, Inc. His entry begins, “If there were an Indiana Jones of the Earth sciences, it would be Harmon Craig. Not only does he work on some of the most important problems in Earth science, he does it while having the most daring of adventures.”

Harmon Craig was born March 15, 1926, in New York City. He entered the University of Chicago in 1943 and served in the U.S. Navy as an ensign during 1944-46. In 1951, he received his Ph.D. from the University of Chicago in geology/geochemistry and stayed on as a research associate at the University’s Enrico Fermi Institute for Nuclear Studies until 1955. At the University of Chicago, Craig studied the isotopes of carbon in the earth and the element iron in various classes of meteorites under Nobel Laureate Harold C. Urey, who joined the fledgling UC San Diego faculty in 1958.

Craig had joined Scripps Institution of Oceanography in 1955 and, in 1957, he published a paper on the distribution of radioactive carbon-14 in the earth’s atmosphere and oceans and concluded that atmospheric carbon dioxide is replaced once every seven years by exchange with the oceans and that the global oceans circulate vertically at a rate of once every 700 years.

Craig was awarded a Guggenheim Fellowship in 1963. He spent a year in Pisa, Italy, at the Istituto de Geologia Nucleare. In 1970, Craig joined forces with W.S. Broecker of Lamont-Doherty Geological Observatory, Arnold E. Bainbridge of Scripps Institution, and Derek W. Spencer of Woods Hole Oceanographic Institution to initiate and direct a multi-institutional and international oceanographic project called Geochemical Ocean Sections Study (GEOSECS) for a global investigation of chemical and isotopic properties of the world oceans. The results obtained by the GEOSECS program represent the most complete set of ocean chemistry data ever collected and contributed significantly to the advancement of chemical oceanography. Based upon the data obtained during this program, Craig estimated the rate of oxidation of organic carbon in the deep ocean. Another result was the discovery of the scavenging of lead and other trace elements from the deep sea by sinking particulate matter.

Craig also has investigated geothermal and hot springs processes, which are a manifestation of the upward transportation of heat and materials from the earth’s interior. A series of papers published in the mid-1960s by Craig and his associates demonstrated how the isotopes of hydrogen and oxygen can be used to understand the origin of the volcanic gases. In 1969, Craig in collaboration with W.B. Clarke and M.A. Beg of McMaster University, Canada, demonstrated for the first time that the isotope helium-3, which was trapped in the earth’s interior at the time of its formation some 4.5 billion years ago, is being released from mid-ocean volcanoes and sea-floor spreading centers. Release of primordial hydrogen and neon gases has subsequently been added to his list of discoveries.

A major finding by Craig’s group during the GEOSECS Pacific Expedition was the existence of two major primordial helium-3 plumes that mark the cores of westward flowing water at mid-depths (~2,500m) from the East Pacific Rise. The discovery of these two jets revealed for the first time the direction of horizontal flow and the nature of the deep circulation pattern in this major region of the Pacific.

Other recent work by Craig and his colleagues include the discovery of submarine hydrothermal vents found on the Galapagos spreading center, as well as discoveries of similar vents on the East Pacific Rise, on Loihi submarine volcano in the Hawaiian chain, and in the Mariana Back-arc Basin, using the Alvin submersible, and the emission of abioticogenic methane from the earth’s interior in submarine volcanic regions. In other work on Continued on Page 22
AAAS Annual Meeting
Denver, February 13th – 18th

Once again the AAAS failed to disappoint! Two dominant themes emerged at the meeting: Water Resources and Global Climate Change. All sessions were well attended by scientists, policy-makers, media and the general public. Interdisciplinary symposia of particular interest to our community included:

- Does All Water Flow Up Hill Towards Money in the West? (Organized by R. Hannigan)
- Microbes Beneath the Earth’s Surface (Co-organized by M. Fisk and L. Criscenti)
- Nonpoint Source Water Pollution: Science and Public Policy
- Removing Damns, Restoring Rivers
- Implications of Climate Change for Soil and Water Conservation
- Comparative Assessment: Carbon Sequestration as a Greenhouse Gas Mitigation Strategy
- Understanding and Managing the Global Carbon Cycle
- Climate Change Mitigation Strategy: Technical Challenges for Geologic Carbon Sequestration
- Disruptions of Ancient Land Ecosystems: Lessons from the Fossil Record

The ideas for potential symposia for the annual meeting arise through discussions at the various section meetings that are attended by the AAAS section council members and affiliate representatives. Most symposia run for between 1.5 and 6-hours. The Geochemical Society is affiliated with two AAAS sections: Chemistry and Geology/Geography. Geology/Geography sponsored or co-sponsored 38 symposia. Chemistry sponsored or co-sponsored 17 symposia. In addition to symposia, the sections also sponsor topical lectures. This year topical lectures of interest to the Geochemical Society included the George Sarton Award Lecture in History and Philosophy of Science presented by Stephen Pyne of Arizona State University and lectures by Kirk Dirkson of the Denver Museum on “Tropical Rainforests: Dinosaurs, and Drinking Water” and Warren Washington of NCAR on “Predicting the Climate of the 21st Century”. A topical lecture by Charles Great of the USGS was highly anticipated but due to outside circumstances, Charlie was unable to attend the AAAS this year. We hope he will be able to make it in 2004!

At the AAAS affiliates meeting, several speakers discussed emerging policy changes and their potential impact on how science is done within the university community. Ron Atlas, president of the American Society of Microbiology, discussed “Scientific Openness and National Security Needs in the New Age of Bioterrorism”. While most of the GS membership will be unaffected by them, several of the new policies may be of interest including the U.S.A. Patriot Act which places restrictions on selected chemical agents and the Biopreparedness Act which requires registration of possession of bioagents including certain agri-chemicals. Access to these chemicals has to be cleared through the Department of Justice. U.S. Department of Agriculture policies related to this act took effect on 02/11/03. Full compliance of research labs to the U.S.A. Patriot and Biopreparedness Acts is required by 11/12/03. One point stressed by Atlas is that the days of graduate students going into the lab on a Saturday night to complete an experiment alone and unsupervised are OVER. Another point raised by Atlas is that the dissemination of scientific information including the publication of results may be restricted in order to comply with these Acts. Atlas and others are seeking to protect the traditional openness of the scientific endeavor while still upholding new policy requirements. The American Society of Microbiology wants to maintain scientific censorship as a societal responsibility, and is relying on the journal editors to balance the need to document scientific methods with the need to eliminate potentially “dangerous” information from articles. The consensus is that this responsibility should be that of the scientific community, not of the government.

Al Teich, Director of Science and Policy Programs at the AAAS, provided an update on foreign student and exchange visitor policies. As of 2/15/03, all Universities must be in compliance with the Student and Exchange Visitors Visa Information System (SEVIS). SEVIS is designed to track students and visitors from their admission to a university, through updates in their status including changes in address, name, disciplinary action, GPA, to their, graduation and/or termination. VISA officers, and perhaps Universities, are liable if a student turns out to be a terrorist. A small percentage of foreign students in the U.S. will be screened by the Interagency Panel on Advanced Science Security (IPASS). IPASS will focus on students from specific countries who are studying potentially dangerous fields. The panel will include members from the Homeland Security Office, the National Science Foundation and other science agencies. The student screening process is still in development and can be enacted by Executive Order.

Carol Manahan introduced the new National Postdoctoral Association (NPA). The NPA is associated with AAAS through Science NextWave (the weekly online publication that covers scientific training, career development, and the science job market). The NPA is currently funded through a $450K grant from the Alfred P. Sloane Foundation. The association hopes to become self-sustaining, to provide a unique voice for postdoctoral researchers, build consensus regarding “best-practice” policies for postdocs, improve the lives of postdoctoral fellows, and make science more attractive to young people. Details about this new organization can be found on-line at http://www.nationalpostdoc.org.

In addition to symposia and topical speaker proposals, an underlying theme at both the Geology/Geography and Chemistry section meetings was AAAS membership and Fellow nominations. AAAS has adopted a new mission, “advance science and innovation throughout the world for the benefit of all people”, as part of its broader initiative to increase membership. A concern within AAAS is that as more libraries purchase site licenses for Science magazine and Science on-line, fewer individuals will become members of AAAS. AAAS is considering several strategies to improve AAAS recognition like linking the AAAS logo to Science magazine and to improve future membership, possibly by offering AAAS membership without a Science magazine subscription in the hopes of attracting more student and young professional members. AAAS membership declined by 3.24% between 2001 and 2002 and was accompanied by a loss in advertising.

Fellow nominations are requested by each section. AAAS Fellows are individuals who have made significant contributions to the advancement of science. Many deserving scientists remain to be nominated for this prestigious award. Fellow nominations may be made by the Steering Groups of the Association’s 24 sections, or any three Fellows who are current AAAS members, so long as two of the three sponsors are not affiliated with the nominee’s institution, or the Chief Executive Officer. Details on nomination can be found on-line at http://php.aaas.org/about/aaas_fellows/index.php. The nomination contact for the Geology and Geography section is Carol Ann Hodges (cahodges@att.net). The nomination contact for the Chemistry section is Jeff Aube (jaube@ku.edu).

The theme for the 2004 AAAS meeting in Seattle, WA February 12th – 17th is “Science At The Leading Edge”. Proposals for symposia are due to the AAAS by March 17th 2003. Rumor has it that proposals on gas hydrates and on environmental geochemistry and public health are in the works. Both Robyn and Louise have successfully sponsored symposia at the 2003 AAAS annual meeting and would be delighted to help you plan for a strong GS presence in Washington, D.C. in 2005. Robyn and Louise would like to thank our speakers: Roger Bales, Susan Brantley, David Brookshire, Rick Colwell, Martin Fisk, Steve Gloss, Ravi Kukkadapu, Tullis Onstott, and Everett Shock for making our symposia successful. If you have any suggestions about what AAAS can do for the GS please contact either one of us.

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Newsletter of the Geochemical Society
Adventures in Geochemical Molecular Modeling

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Introduction

Somewhere between the ideas that we can calculate everything we need to know about chemical systems and that everything coming out of a computer is nonsense, lies the truth about molecular modeling. In essence, we might be able to calculate everything if we could solve the Schrödinger equation for macroscopic systems. However, numerous approximations to the full Schrödinger equation are generally made in even the most sophisticated quantum mechanical calculations.

Furthermore, the size of most simulated systems involves dozens to perhaps thousands of atoms and therefore does not approach the molar-sized scale of materials, to say nothing of a geochemical system of macroscopic aqueous solution and minerals. Limitations, such as these, should not discourage the use of molecular modeling techniques in geochemistry. Judicious choice of model systems and techniques allows a great deal of useful information to be extracted from a “computer experiment.” In this article, we outline a variety of techniques that can be employed to address different types of geochemical problems.

A need to explain experimental results motivated the earliest molecular modeling by scientists from the earth science community (Gibbs et al., 1972; Tossell et al., 1972; Woodcock et al., 1976). That motivation remains just as compelling today as it was 30 years ago. Tossell et al. (1972), Tossell (1973), and Collins et al. (1972) focused on the molecular orbital interpretation of X-ray emission and photoelectron spectroscopy of minerals. Though G. V. Gibbs shared an interest in X-ray emission spectroscopy (White and Gibbs, 1967), his more immediate motivation was a desire to explain mineral structure: bond lengths and angles (Brown et al. 1969; Brown and Gibbs, 1969; Gibbs et al., 1972).

An unmistakable trend in recent years finds mineralogists and chemists augmenting traditional phenomenological observations with atomic-scale measurements using physical methods, including spectroscopy plus magnetic and X-ray scattering methods. This shift in experimental approach creates an increasing demand by laboratory experimentalists for...
atomic-scale simulations. The link between atomic-scale processes, the point of departure for molecular modeling, and macroscopic observables remains tenuous, a result of the inherent heterogeneity and complexity of earth materials. The connection between molecular modeling and observables is more direct when both are on the same time and length scale.

Molecular Modeling Methods

A number of molecular modeling techniques have been developed, each with advantages and disadvantages. Practical computational limits generally force trade-offs when selecting a method to study a given chemical system. One can either choose highly accurate quantum mechanical methods that detail the position of every nucleus and the electron density within a system but limit the number of atoms explicitly included, or a molecular mechanics approach can be adopted where up to millions of atoms may be simulated but atomic interactions are approximated by simple equations. As computational hardware and software become more powerful, the gap between these two end-members diminishes. Quantum mechanical calculations will handle larger numbers of atoms and molecular mechanics simulations will have increasingly accurate interatomic potentials. The two approaches have been linked recently by the development of embedded simulations (Dapprich et al., 1999) in which simple interactions such as bond stretching are handled analytically but more subtle interactions are funneled into subroutines for quantum mechanical calculations. Figure 1 summarizes the various choices the theoretical geochemist has in pursuing accurate molecular simulation.

Molecular Orbital and Density Functional Theories

Ab initio molecular orbital theory is a method used to model the electron density in an atom or molecule with respect to the average electron density. The term “ab initio” signifies that there are no adjustable or empirically-derived parameters used in calculating the molecular energy. Ab initio calculations are preferable because there is less chance for the results to be biased by the researcher or in error due to inadequacies of the interatomic potential. In practice, a number of approximations are made within the molecular orbital calculations that have a direct bearing on the reliability of the results obtained. For example, the Hartree-Fock approximation allows a large saving of computer time and memory, but it neglects the effect of electron correlation on the calculated energy of the system. Methods such as Møller-Plesset second-order perturbation theory (MP2; Møller and Plesset, 1934) and density functional theory (DFT; Kohn and Sham, 1965) can be used to account for electron correlation, but the added computational demands can make including these corrections prohibitive for moderate-size molecules. DFT is much faster than MP2 and is increasingly used in conjunction with molecular orbital calculations. Semi-empirical quantum methods provide a computationally faster but less theoretically robust alternative method (Pople and Beveridge, 1970).

Molecular Mechanics

Some molecular modeling simulations avoid calculation of electron densities altogether. Instead, each atom is given a set of parameters that fit into analytical equations used to describe atomic interactions such as Coulombic, van der Waals, bond stretching, etc. The equations and parameters governing these interactions are termed a force field. Neglecting to solve for the electron density of the system saves vast amounts of computer time, so many more atoms—up to millions in some recent cases—may be treated with molecular mechanics. The main problem in utilizing this approach is determining that the force field accurately represents the atomic interactions.

Once an appropriate interatomic potential has been set up to describe the interactions of all the atoms in a system, several
possible methods exist for modeling the system. In order of increasing complexity these are static energy calculations, energy minimizations, lattice dynamics, Monte Carlo calculations, and molecular dynamics simulations. As the name implies, static energy calculations simply take an input configuration, subject the system to the force field equations, and derive an energy for the given state. For example, static energy calculations can be used with molecular orbital theory or molecular mechanics where configurations have been predetermined or obtained by refinement of experimental data.

Monte Carlo calculations are useful for investigating complex systems where several potentially stable structures may exist and where sampling many initial configurations often leads to the equilibrium structures. Molecular dynamics simulations take atomic movement one step further. Time is explicitly included in the calculation and all the atoms move in concert according to classical mechanics equations based on the potential energy surface and the kinetic energies of the atoms for a given temperature. Molecular dynamics is the method of choice for studying dynamical properties of systems, such as diffusion or other time-dependent processes.

Several books on molecular modeling techniques are available (Cygan and Kubicki, 2001; Hehre et al., 1986; Frenkel and Smit, 1996; Young, 2001) and may help in choosing the appropriate method for an application. Commercial software is available for most of the above types of simulations through companies such as Accelrys, Inc. (San Diego, California), Gaussian, Inc. (Carnegie, Pennsylvania), Hypercube Inc. (Waterloo, Ontario), and Tripos Inc. (St. Louis, Missouri). Additionally, clearinghouses such as the Quantum Chemistry Program Exchange (Indiana University) and CCP5 (Daresbury, United Kingdom) make programs and subroutines available at nominal cost.

Mineralogy and Interfacial Processes

Molecular simulations of mineral structures have been performed since the 1980’s using molecular mechanics (e.g., Catlow et al., 1982) and later in the 1990’s with periodic quantum methods (e.g., Brodholt et al., 1996). However, only recently have geochemists attempted to simulate the complex chemistry associated with mineral surfaces and mineral-fluid interfaces (e.g., Greathouse et al., 2002). The development of an accurate interfacial model would greatly benefit our understanding of adsorption, dissolution, growth, and reactions that occur at or near the mineral surface, and that control many environmental processes. Clay minerals, in particular, present a noteworthy challenge due to their complex crystallography and composition, and nano-sized grains—all contributing factors to our inability to fully characterize these common soil phases. Cygan and coworkers have recently developed an adsorption model of the kaolinite-solution interface based on the large-scale molecular dynamics simulation of cesium sorption. Figure 2 presents the periodic simulation cell used to evaluate the partitioning of Cs and Cl ions from an aqueous solution to either the siloxane or hydroxyl basal sheets of the kaolinite, and the equilibrium atomic density profile. The simulation results indicate that ion pairing may contribute to adsorption of Cs to the hydroxyl sheet and not just solely to the negatively-charged siloxane surface. Recent synchrotron-based measurements of real systems exhibit evidence of this form of metal-anion complexes on the mineral surface.

Isotope Geochemistry

A few studies have used molecular modeling techniques in isotopic geochemistry. Casey et al. (1990) performed one of the
first studies of H$_2$O-silica dissolution that combined experimental data and ab initio results relevant to isotopic effects. Driesner et al. (2000) performed ab initio calculations to model H and O isotope fractionation by hydrated ions. Schauble et al. (2001) used molecular mechanics methods to estimate Fe-isotope fractionation factors. Because isotope exchange fractionation depends on the zero-point vibrational energies of reactants and products, this type of study is also helpful in estimating fractionation values when they are difficult to obtain experimentally.

Theoretical studies of isotopic exchange have used ab initio calculations to describe the pathway between reactants and products in a step-by-step manner and to find the transition state and activation energy barrier to isotope exchange (Felipe et al., 2003). Although isotopic exchange equilibria have been measured, limited experimental data exist on the rates of isotopic exchange for many important geochemical species. Hence, these modeling studies are used to provide estimates of the rate data and can be tested against the known isotope exchange equilibrium constants. Figure 3 represents such a reaction pathway as the potential energy changes during O-isotopic exchange in aqueous H$_4$SiO$_4$. The results predict that oxygen exchange between dissolved silicic acid and water should occur on the order of tens of seconds. Consequently, oxygen isotopes in silica precipitated from solution should reflect the isotopic composition of the solution rather than the original source material.

**Organic Geochemistry**

As in isotope geochemistry, the number of papers employing molecular modeling techniques in organic geochemistry is disproportionately small. This is surprising given that much of the development of molecular modeling techniques has focused on organic chemistry. Many of the force fields have been parameterized for organic compounds. In addition, the emphasis on detailed reaction mechanisms found in many organic chemistry textbooks suggests that molecular modeling would be useful for addressing problems in organic geochemistry. The reason for this discrepancy may be that much of naturally occurring organic matter (e.g., humic and fulvic acids, black carbon, etc.) is poorly characterized on a molecular scale. This makes the step of creating a fundamental molecular model difficult.

Despite this difficulty, some recent studies have made excellent use of molecular modeling methods. For example, Cody and Ságghi-Szabó (1999) predicted changes in the $^{13}$C NMR chemical shielding in lignin based on ab initio calculations designed to constrain the calculated values as a function of torsion angle. Peters (2000) used molecular mechanics to predict the elution behavior of epimers in order to help interpret chromatographic results on petroleum samples. Kubicki and coworkers have been modeling soot and its interactions with polycyclic aromatic hydrocarbons (PAHs). In this case, MD simulations of hexane soot material have resulted in a structure that is similar to what is known about soot particles. However, the same force field that produced a reasonable soot structure predicts incorrect values for PAH-soot partitioning. Ab initio calculations at the MP2 level of theory were required in order to obtain partitioning energies that would correlate (Figure 4) with observed equilibrium constants (Bucheli and Gustafsson, 2000). This illustrates the point that the correct prediction of one property of a system by molecular modeling does not guarantee the correct prediction of all properties. Verification of modeling results by as many pieces of experimental data as possible is critical in producing a robust methodology.
Biogeochemistry

Biogeochemistry has become a hot area of research and some workers are beginning to bring molecular modeling techniques to bear on these problems. Molecular simulations have been common in biochemistry, especially drug development, for some time. However, the complication of dealing with biological molecules and inorganic geometries is a daunting challenge. For example, a great deal of work has been carried out on polysaccharides, a major component of bacterial surfaces, but only a few studies address the chemistry of these biomolecules under geochemical conditions. Notably, the simulation of bacterial membranes by Straatsma and coworkers (e.g., Shroll and Straatsma, 2002) has been advancing this field. Another good example of biogeochemical molecular modeling is provided by Sahai and Tossell (2002) in their calculations relating to the stabilities of biogenic silica species. Also, studies that model geochemical reactions relevant to microbial processes in the environment are beginning to be published (e.g., Duff et al., 2002).

One area where biology and geology meet is in the cycling of silicon. This process and related germanium complexation with natural organic material can then affect the Ge/Si ratio in river waters that eventually reach the ocean. NMR spectroscopic studies have suggested that Si may form complexes with certain organic molecules in aqueous solution, and XAFS studies have shown that other types of organic molecules preferentially bind to Ge rather than form Si complexes. However, the interpretation of NMR spectra of Si-organic solutions has been controversial. Kubicki and Heaney (2003) demonstrated Si-organic complexation could be responsible for the observed NMR peaks and that other aquatic species did not fit the analytical data. This role for molecular modeling—testing proposed structural models based on spectral interpretations—is an excellent one that allows experiment and theory to complement one another. Such an approach is catching on with spectroscopists in geochemistry as they attempt to decipher the often ambiguous data collected on complex and often disordered geologic materials.

Future Directions in Geochemical Molecular Modeling

The phenomenal growth in computing power is allowing researchers to rapidly increase the realism and accuracy of their molecular simulations. In addition, more emphasis is being placed on reaction kinetics and understanding fundamental mechanisms in geochemistry. Just about everywhere one looks for equilibrium situations, the effects of kinetics and disequilibrium can be seen. Process-oriented geochemistry is evolving to examine mechanisms to explain reactions. Understanding initial and final states is not enough; the path between the two should also be understood.

Molecular modeling techniques will ultimately become accepted if they can be integrated into coursework at the undergraduate and graduate levels. The beautiful three-dimensional graphics now possible on a desktop personal computer lend themselves to producing visual aids in mineralogy and crystallography. Concepts in geochemical kinetics can also be illustrated clearly by the use of molecular modeling graphics. However, we must always be cautious not to let deceptively accurate graphics make us believe the simulation results are always accurate. Beyond simple graphics, modeling can be used to examine nucleation, adsorption, dissolution, and relationships between structure and thermodynamic stability. Once geochemists begin to see molecular modeling techniques as a tool with weaknesses and strengths—like any other tool in the array of methods for studying geochemical problems—then molecular simulations can be truly integrated into geochemical research rather than being reserved for specialists.
Thirteenth Annual V. M. Goldschmidt Conference
September 7 - September 12, 2003
Kurashiki-Sakuyo University
Kurashiki, Japan

Sponsors
The Geochemical Society of Japan
The Geochemical Society
The European Association for Geochemistry
The Mineralogical Society of America

Website: http://www.ics-inc.co.jp/gold2003/
Invitation to Goldschmidt 2003

On behalf of the Organizing Committee, I am pleased to invite you to the Thirteenth Annual V. M. Goldschmidt Conference to be held from Sunday, September 7th to Friday, September 12th at the Kurashiki-Sakuyo University, Kurashiki, Japan. The Goldschmidt Conference is now the premier annual meeting for geochemistry and cosmochemistry. The abstracts of papers presented at the conference are published in a supplemental issue of Geochimica et Cosmochimica Acta (GCA). Whereas the field of geochemistry is growing wider, it is splitting geochemists into smaller subdisciplines. As a comprehensive meeting, the Goldschmidt Conference is the place to integrate different disciplines where geochemists from all over the world come together to see nature from both subdisciplinary and Interdisciplinary points of view. You are encouraged to participate in sessions that you may not have an opportunity otherwise. We hope Goldschmidt 2003 will create new frontiers in geochemistry and cosmochemistry. The details of the conference and registration procedures will be found in the Second Circular on the conference website (www.ics-inc.co.jp/gold2003/).

We are hosting 55 Special Symposia with the help of the International Program Committee, chaired by Dr. Jun-ichi Matsuda. In addition to these Special Symposia, we prepared nine General Symposia, which cover all the fields of geochemistry and cosmochemistry.

We have arranged reduced registration fees for the members of sponsoring societies. The low registration rates are also applicable to those who join the societies through the Second Circular website. Abstract submission will be handled by the

Facing Page: Old Town of Kurashiki
The city of Kurashiki was a regional trading center in the Seto Inland Sea region in western Japan, during the Edo period of 17th to 19th centuries. The history is well preserved in the Old Town area, where canals and narrow streets are lined with traditional two-story wooden buildings and white plastered walls. Old merchant’s residences are open to public. Museums of paintings, potteries, and Japanese folk crafts are also worth visiting. Most conference hotels are clustered adjacent to the Old Town area (Bikan-chiku) of Kurashiki.

Above: Aso Volcano (photo by Motomaro Shirao)
This picture shows an aerial view of Aso Volcano, which is located in the middle of Kyushu, southwestern Japan, and consists of several central cones and a large caldera, 25 km north to south and 18 km east to west in diameters. The caldera was formed by repeated eruptions with large-scale pyroclastic flows (Aso-1 to Aso-4) in middle to late Pleistocene (ca. 0.3 to 0.09 Ma). The central cones, formed in last 90 thousand years, show a variety of basalt, andesite to rhyolite in composition. Naka-dake (1506 m above sea level), one of the central cones, is still very active as seen in the lower right of this picture, and continually monitored for preventing volcanic hazards. Post-Conference Field Trip PC-1 “Active volcanoes and the Japan’s largest spa in the rift zone in Kyushu” will visit this area.

Facing Page: Old Town of Kurashiki
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Cambridge Publications, UK, with the same format used at the Davos meeting (Goldschmidt 2002). You may reach the page of Abstract Submission via the Second Circular. We provide grants for students and young researchers presenting as the first authors. Those who wish to apply for these grants should submit their abstracts and Grant Application Forms by April 14, 2003, approximately three weeks earlier than the deadline for regular abstract submission.

We have set the abstract submission fee higher than that of the preceding meetings. This has been done to try to prevent the conference bearing the cost of publishing abstracts from authors who may submit but not attend the meeting. To compensate for this expenditure, however, the registration fees have been reduced. As a result, you may find that the total cost for submitting abstract and attending the conference is lower than the preceding meetings.

The city of Kurashiki is located approximately 200 km west of Osaka, easily accessible by Bullet Train (Shinkansen) from major cities of Tokyo, Kyoto, Osaka, Hiroshima or Fukuoka. Thanks to its proximity to the coast and well-developed canal systems, Kurashiki was a regional trading center in the Seto Inland Sea region in Western Japan, during the Edo period of 17th to 19th centuries. The history is well preserved in the Old Town area (Bikan-chiku), where you can enjoy strolling along a canal lined with willow trees and traditional two-story wooden buildings. Small shops and museums are also worth visiting.

The conference venue, Kurashiki-Sakuyo University, is located adjacent to Japan Rail Shin-Kurashiki Station, which is served by both Shinkansen and local commuter trains. Most conference hotels are clustered adjacent to the Kurashiki Station that is within a 10-minute commuter train ride from the Shin-Kurashiki and Okayama Stations, both of which are served by Shinkansen. For further details, please see the page of Travel Information of the Second Circular. Accommodations will be arranged by our official travel agent (JTB Corp.). JTB will also help you arrange personal excursions if you wish. Also, see the Second Circular.

We are planning two- to three-day field trips after the conference, half-day tours during the conference, and social events including the conference banquet. Social programs for accompanying persons will also be arranged during the week.

All the information you may need for Goldschmidt 2003 will be available on the conference website www.ics-inc.co.jp/gold2003. If you require information not available on the website, please e-mail help desk (gold2003@ics-inc.co.jp).

Goldschmidt 2003 is the first Goldschmidt Conference that will be held in the western Pacific region. This will provide a great opportunity to broaden research activities and increase the awareness for geochemistry and cosmochemistry worldwide. I look forward to seeing you in Kurashiki in September.

Yukihiro Matsuhisa
Chairman,
Organizing Committee for Goldschmidt 2003

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**Important Dates**

- **April 14, 2003**
  - Deadline for grant application (should be together with the abstract submission)
  - Deadline for paper submission of abstracts

- **May 5, 2003**
  - Deadline for electronic submission of abstracts

- **July 7, 2003**
  - Deadline for early registration with reduced rates
  - Deadline for guaranteed reservations of hotel rooms
Important Notice

SLIDE PROJECTORS WILL NOT BE AVAILABLE in lecture rooms. All oral presentations should be prepared for either PowerPoint or overhead projectors.

Goldschmidt 2003: List of Symposia

Detailed description of each symposium will be found in the page of Symposia of the Second Circular.

General Symposia
G01. Chemical Oceanography
G02. Climate Change
G03. Biogeochemistry and Organic Geochemistry
G04. Environmental Geochemistry
G05. Sedimentary Geochemistry
G06. Igneous/Metamorphic Geochemistry
G07. Planets and Meteorites
G08. Physics and Chemistry of Minerals
G09. Volcanic Gases, Fluids and Ore Deposits

Special Symposia
Marine and Atmosphere,
Geochemistry and Climate Change
S01. High-resolutional paleoceanography in the western Pacific during late Quaternary (IMAGES activity)
S02. Biogeochemical cycling of trace elements and isotopes in the ocean and applications to constrain the contemporary marine processes (GEOSECS II)
S03. Marine geochemistry of the rare earths, actinides and noble metals: The present and past oceans
S04. Long-range atmospheric transport of terrestrial materials over the ocean
S05. Atmospheric aerosols and reactive gases: Their impacts on atmospheric composition and air quality over the Asian and Pacific regions

Biogeochemistry
S06. Global Biogeochemical Cycles
S07. Advances in the Use of Stable isotopes to Study the Global Methane Cycle
S08. Assessing biogeochemical cycles using nitrogen isotopes
S09. Progress in subsurface microbiology and its development through Ocean Drilling; over bridging from ODP to IODP
S10. Biogeochemistry of Trace Metals in Shallow Estuarine Systems and Coastal Lagoons
S11. The role of bacterial surfaces in chemical processes of metal ions in the environment
S12. Weathering and the biosphere
S13. Geochemical Role of Available Humus or Dissolved Organic Matter (DOM) in soils and sediments

Origin and Evolution of Life
S14. Origins and distribution of life in the Universe
S15. Geochemistry of Biological Radiation and Extinction

Sedimentary Geochemistry
S16. Chemical Diagenetic Processes in Sediments and Sedimentary Geochemistry
S17. Biogeochemistry and paleoenvironmental implications of metals in marine sediments
S18. Multivariate methods and heterogeneity in geochemical/hydrochemical surveys

S19. Geochemistry of Seepage: subduction products from modern to past
S20. Geology, Geochemistry, and Microbiology of Natural Gas Hydrates and Related Methane Seeps

Isotope Geochemistry
S21. In Search of Isotopic Biosignatures
S22. Non-Traditional Stable Isotopes
S23. Molecular Isotope Geochemistry - From Natural to Anthropogenic
S24. New advances in high precision trace element and isotopic analysis
S25. Laser ablation ICP-MS and MC-ICPMS with applications in Earth Sciences
S26. Unraveling Geological Processes by Noble Gas Isotopes
S27. Lithium isotope geochemistry: from oceans to mantle
S28. Lanthane Tetrad Effect and New Trends in REE Geochemistry

Crustal Fluids, Mineralization, and Natural Hazards
S29. Following Giggenbach’s Rulers and Witnesses of Crustal Fluids: Volcanic, Geothermal and Ore Systems
S30. Geochronology of ore formation processes and ore genesis in relation to the magma generation
S31. Geochemistry linked to the reduction of natural hazards

Mineral Sciences and Waste Confinement
S32. Nano materials/minerals in geoscience by TEM
S33. Mineral-fluid interfaces: molecular-scale insights to macroscopic processes
S34. Geochemical Immobilization and Long-Term Isolation of Waste

Crust, Mantle, and Core
S35. Metamorphic Processes: Diffusion, Reaction and Fluid Flow
S36. Subduction zone processes and global material circulation
S37. HP to UHP Metamorphic Mass Transfer and Chemical Cycling in Convergent Margins
S38. Mantle heterogeneity and dynamics of mantle plumes
S39. Composition, Processes and Structure of the Mantle
S40. Hot Spots and Global Mantle Circulation
S41. Structure and properties of silicate melts and fluids
S42. Geochemistry of diamond, a window to the deep earth
S43. Mantle-Core Differentiation and Evolution from a Deep Magma Ocean

Early Earth
S44. New Views of Old Rocks: The Hadean and Early Archean Earth
S45. Co-evolution of the biosphere, atmosphere, hydrosphere, and lithosphere in the early Earth
S46. New insights into early Earth’s environments from the multiple sulfur isotope system

Meteorites and Solar System
S47. Early solar system processes
S48. Martian Meteorites and the Evolution of their Parent Body
S49. Cosmogenic Nuclides Produced in situ in Solar System Matter

Geochronology
S50. Hadean geochronology: Establishing the first 500 Ma of Earth history
S51. Thermochronometry: recent developments in calibrating (and intercalibrating) the thermal sensitivity of isotopic dating techniques
S52. Geochronological decay constants
S53. Dating methods for Quaternary Geochronology
S54. Archaeological Geochemistry: Isotopically decoding prehistoric human life and nature
An Interview with Alexandra Navrotsky
Winner of the 2002 Benjamin Franklin Prize
In Earth Science

Interview Recorded Dec. 5, 2002 by Mitch Schulte

Editors Comments: Dr. Alexandra Navrotsky is the Edward Roessler Chair in Mathematical and Physical Sciences and Interdisciplinary Professor of Ceramic, Earth, and Environmental Materials Chemistry at the University of California at Davis. Dr. Navrotsky has won numerous awards, most recently the highly prestigious Benjamin Franklin Medal in Earth Sciences. She graciously sat for the following interview with Geochemical News Associate Editor Mitch Schulte on December 5, 2002 in her office at UC Davis. More information about Dr. Navrotsky and her research can be found at her web site (http://navrotsky. engr. ucdavis.edu).

MS: I always like to start with your background. How did you get into science, [in] what are your degrees, where did you go to school?

AN: Ok. I’m a fake geologist. I have no degrees in geology whatsoever. In fact, I never actually took a geology course for credit, although after I passed my candidacy exams, I sat in on a few geology courses. So whenever people say you don’t know any geology, I have all sorts of excuses. I’m a chemist by training. All my degrees are from [the] University of Chicago. My Ph.D. specialization was physical chemistry.

MS: Physical chemistry... and that was your undergraduate degree as well?

AN: My undergraduate degree was just chemistry. Undergraduate degrees are just chemistry. I think I started off, as did a lot of people, in the early 60s... you sort of had the feeling that your were either going to be a physicist doing nuclear physics or a biologist who would cure cancer in three years at the beginning of your career and get the Nobel Prize. And of course, none of those things happened and I sort of drifted from biochemical things to physical chemical things, from low temperature to high temperature, all by a set of coincidences and accidents and opportunities. I don’t think there was [a] grand plan to it. And now I’m sort of drifting back down to low temperature and watching all the biogeochemistry and everything. I’m suddenly thinking, “You know, it’s a good thing I went through organic chemistry and first year graduate biochemistry before switching to high temperature p-chem.”

MS: So how did you drift into the geosciences at all? Just because of the nature of the things you were working on?

AN: The nature of things I was working on at the time, and again, [to put it] in perspective, that was around the time when inorganic chemists had discovered crystal field theory and what transition metal ions do in octahedral and tetrahedral coordination, and why they turn pretty colors and all those exciting things. It’s textbook stuff now, but it was brand-new stuff in the 1960s. So, in consultation with my thesis advisor, Ole Kleppa, we hatched up the idea that spinels would be a wonderful testing ground for these ideas of crystal field theory, because they have octahedral and tetrahedral sites, cations go into them and if we could do some thermochemical measurements before switching to high temperature p-chem, we’d get quantitative data and correlate with all the wonderful spectroscopic measurements. So the thesis became the thermodynamics of spinels. The end result of it was that crystal field effects were minor factors in the stabilization of spinels for a whole variety of reasons that we now understand and that other things were more important. I do remember at one point going over to the old geology building at Chicago, which was on the fourth and fifth floor of an ancient building [and] meeting up with J. V. Smith, who gave me some spinel samples that he had. And I think that was the start of the realization that spinels are indeed minerals. And then I started reading some of the papers on high pressure work, and sort of hobnobbing over with the geologists in Bob Newton’s high pressure lab, and I think ever since then I’ve been sort of a hybrid chemistry-geology type person.

MS: So you weren’t sort of dragged into it kicking and screaming; it was a natural extension of what you were doing.

AN: It was a natural, and it was sort of intriguing at that point to realize that what I’d initially gone into for theoretical chemistry reasons, in a way had planetary implications, in the same sense that it’s nice to see that things have practical applications. Some of these same materials are used as everything from moisture sensors to ceramics to goodness knows what.

MS: But your primary interest in studying these materials is more from a purely scientific standpoint?

AN: I think that’s right. The thing that holds the huge variety of things I’ve done together is to address the fundamental question of solid state chemistry, which is: given a bunch of atoms, a pressure and a temperature, why they form a particular structure, what other structures can form, and why, in a chemical bonding sense. Whether that’s an oxide superconductor or magnesium silicate perovskite in the lower mantle, the basic physical chemistry or physics and chemistry (or whatever you want to call it) of the same. So that’s what’s in it for me. Of course, the way one gets this variety of things funded is to realize that the same sort of data [that] thrill me provide things that people are actually interested in that have to do...
with petrology, or environmental geology, or materials compatibility, or corrosion, or space shuttle reentry or you name it.

MS:  Sure, or even things that make people money.

AN:  Right.  Semiconductors and the like.

MS:  [Y]ou’ve also mentioned that these [studies] are applicable to a large planetary scale, and so you’ve run the gamut now between thinking about larger questions on the planetary scale and really small things.  So not only have you done [a wide] temperature range, but you’re also doing [a wide] scale range as well.

AN:  That’s right.

MS:  So what interested you in trying to do very small [or] nanoscale technology kinds of things?

AN:  Well, I think two things.  In a way, and it’s going to sound funny, [it was] the high pressure mineral physics game, which is using high pressure and high temperature as a tool for studying relatively simple structures.  There are a few ultra-high pressure materials that are very complicated, but a lot of them are spinel, perovskite, rock salt, rutile structure, etc.  There are relatively simple solid state compounds, and of course because the temperature is high, equilibrium is reached fairly quickly.  Well, sometimes it isn’t, but relative to low temperature things, relative to sedimentary materials, relative to nanomaterials, high PT materials are simpler.  One has a more exotic technology for studying them, but you can get important information in diamond anvil cell experiments that last a couple of minutes, or even in shock wave experiments that last less than a second, whereas if you talk about nanomaterials, or you talk about sediments, they’re more complicated, they’re much more sluggish to react, the structures they form are much more complex:  the effect of small particle size is something you usually don’t have to consider in igneous and high pressure work, so in a way the mineral physics adventure was almost a rehearsal for going to more complicated systems.  So the logical level of complexity is to go down in temperature [where there are] more open architectures of materials, more hydration and more complexity.  I think things that have made the ‘nano’ revolution possible for everybody is the ability to make materials in a controlled fashion, and the tools for studying them.  [For example], as long as you lumped all manganese oxides together by some sort of derogatory name like “wad,” you weren’t going to learn much about them [chuckles].  When you realize that you have tools to study seven different crystal structures, all present in the same thumbnail-sized specimen, then you begin to learn something, and it’s having those tools and realizing the complexity of those materials that offers the challenges.  So I think the time is right, the tools are right, and the money is there.

MS:  How important do you think the nanomaterials studies are going to be, and what do you see as the more geochemical and geological applications of those?

AN:  Well, I think from the geological point of view, we’ve only begun to come to grips with the fact that some very large percentage of chemical reaction on this planet or on any planet occurs at the nanoscale, in small particles and [on] mineral surfaces in what we sometimes nowadays call the critical zone and that the reactivity is really governed by reactions at that scale and by reactions on small particles.  And certainly anything related to life is governed that way, whether you’re talking about transferring ions through a membrane, or bacteria interacting with oxide particles.  So realizing that most of the chemical action in fact is nanoscale action I think is really changing the way we think about process, because we no longer think about process as homogeneous, in the whole body of a rock.  We think about process as occurring at an interface at the sort of level that you see by electron microscopy or other probe techniques.  For the most part, most of the material is a bystander until it gets brought into the action by having it move toward the surface or the surface move toward it.  And that realization that chemical reaction, that everything we think of as geology, petrology, diagenesis, is fundamentally heterogeneous and fundamentally localized in a few areas where everything’s going on, comes as no surprise if you think about your everyday world.  But it’s not the sort of macroscopic way we used to think about things, when we just [did] whole rock chemical analysis or whole rock isotope analysis.

AN:  Oh, it’s certainly easier than it was.  But I think it’s more difficult in three senses; one, the equipment is more expensive.  If the hand lens is replaced by the electron microscope, that’s an order of 10^8 in cost, and somewhat similar in learning curve as well.  The second is you need to know so many more things if you’re going to solve Earth and planetary science problems.  You need all the insight about structures on a geologic scale and about what one thinks of as geology, and yet you need to be an increasingly sophisticated chemist and physicist and materials person as well.  So you really need to link knowledge in those different length scales and understand how something at one length scale affects something in another.  The example I like to cite is the idea that, any earthquake originates somewhere, so you could argue that a particular earthquake originates with the breaking of one chemical bond somewhere.  And of course, you would have the breaking of that kind of chemical bond many, many times but only one time in 10 to the something or other will the sequence of events eventually lead to a hundred kilometer rupture, and yet you need to understand that playback of length scales and time scales.  So it’s a challenge.

MS:  Is it more difficult to do [studies on a small scale], or [has] it come to the point where the technology is there that makes it a little easier to do?

AN:  That’s right.

MS:  That’s right.

AN:  That’s right.

AN:  Well, I think from the geological point of view, we’ve only begun to come to grips with the fact that some very large percentage of chemical reaction on this planet or on any planet occurs at the nanoscale, in small particles and [on] mineral surfaces in what we sometimes nowadays call...
tion is how applicable are those studies on that scale of those particular materials to Earth science in general?

AN: Well, there certainly have been numerous examples; a good example is silicon carbide, moisesite, which had been a well-known ceramic material for a century or more and was discovered as a mineral relatively recently.

MS: In meteorites.

AN: In meteorites. Carbon nanotubes exist as combustion products. The rules of nuclesynthesis give you certain elemental abundances, and [determine that] the Earth is this kind of mixture and it’s usually not going to make pure yttrium barium copper oxide. Let’s take the oxide superconductors, ordinary perovskite, calcium titanate, and the lead zirconate titanate materials that are important ferroelectric materials, that among other things are resonators and enabled the microwave and cell phone revolution[s] and finally magnesium silicate perovskite, with all of its presumed impurities in the mantle. I think the proper question to ask is, what does studying all of these materials at once tell you that studying one of them doesn’t? That’s been our approach and I think it gives you some systematic comparisons. Also, if you have a certain phenomenon you want to study, sometimes that phenomenon is more accessible in one system than in another. So you understand what you should be studying, what is important in a model system that is tractable and then you can go and look for similar sort of effects in the complex natural system. It’s much the same as saying that the biologist does in vitro experiments and then does in vivo experiments not because the laboratory experiments are a complete analog to the mouse experiments but because you can begin to home in on what you’re looking at and what your important parameters are. And I think in a sense the application of materials science to Earth science is the same sort of thing. The other thing that you don’t have in materials science that you do have in Earth science is the time scale. So you can turn that one around. A good example is in nuclear waste disposal, attempts at formulating appropriate waste forms, the use of or the study of natural minerals that have contained radioactive elements for millions or billions of years. Things like zircons become quite important because here nature has done an experiment, a long term experiment for you that you have some ways of mimicking in the laboratory, mainly by raising temperature so that reactions occur faster, or raising radiation doses so somehow you get more damage in a shorter time. But looking at the natural system that has had the long time will give you information which will be important when fed back into the materials context. So it’s a two way street.

MS: What’s next? What do you see as the next big research area from your perspective? What kinds of questions can we start answering?

AN: I think right now, at least for our perspective, our thermochemical studies [are] taking in several different directions. One is we’re continuing the nanomaterials studies [by] thinking about how differences in polymorphs [that] form and their relative surface energies will stabilize and destabilize a different mineral. Those effects can be quite significant and I think we’ve done some pioneering work in that but there’s a lot more that can be done. For example, [there is] the realization that, in general, hydrous phases have smaller surface energies, especially in an aqueous environment, than anhydrous phases, so you have sedimentary or environmental processes in which you simply don’t have particle growth. [Y]ou simply don’t have coarsening; then [the] phase equilibria constrained to be at very small crystal sizes can look very, very different. [Y]ou can play a thermodynamic “what-if?” game. What if all of your particles are constrained to be 100 nm in diameter? What would your phase relations look like? And that might be a better way of looking at geochemical problems. You have, in a sense, another variable. I know where we’re going in the materials context, [but] I don’t know quite where we’re going yet in the geological context, but I think another area where we’re beginning to do more than I ever thought we’d do is [in] organic-inorganic interactions; the strength of chemical binding, the ability to make all sorts of organic-inor-

“...If the hand lens is replaced by the electron microscope, that’s an order of 10^6 in cost, and somewhat similar in learning curve...”

There are still some very interesting issues particularly having to do with the water budget of the Earth and water in the mantle and water in silicate perovskite, [like] how much water [there is], what happens to water during subduction. Although we’re doing less high pressure work than we were at the height of being involved with CHiPR, there’s still a lot of really pretty much first order problems there that I think we’re going to continue working on. And we’re doing quite a bit of environmental material[s] [such as] sulfates, and we’re sort of drifting toward sulfides. Sulfides are a good case in point; a lot of the ordered sulfosalts and complex sulfides cannot be replicated in the laboratory because they are ordered materials that order over geologic time and so far [no] one has been successful at making many of them. So if one wants look at their energetics, first of all we don’t quite have the techniques yet down to where we would like, and secondly it’s going to be a real balance between natural samples and synthetic samples as has been the case with the feldspars. You could not synthesize an ordered feldspar, only nature can. Graduate students don’t stick around that long. Well, that’s not quite true. There’s a window of pressure/temperature space where you can get substantial ordering, but for the most part it’s almost true.

MS: You’ve actually touched on a subject that’s a little close to my heart, actually, which is interactions between organic and inorganic systems, and it’s always occurred to me and my colleagues that [there] is an artificial division between inorganic and organic things. I think this is becoming apparent especially when we start talking about things like sulfur, because sulfur chemistry is so diverse because of its oxidation states, its size, and its place in the periodic table.

AN: Yes, absolutely. Well, it is likely to go into both organic and inorganic.

MS: Exactly. And that might be a good bridge between these realms as they currently exist.

AN: Exactly. There are diverse groups of people that are looking at various aspects of it... the origin of life people, I think are onto some very interesting things.

MS: That’s me!

AN: That’s right, but so are the self-assembled monolayer people who put down a layer of some sort of thiol on a metal surface, on typically a gold surface, and then put something on the end of the thiol and create little local microenvironments. Finally, as those alkyl chains curl up or spread out, you’ve got an artificial membrane, and then you say "is this
MS: Well, there is. In fact, I don’t know if you are aware of Mike Russell’s work. He’s at the University of Glasgow. One of his models for the origin of membranes, is iron sulfide bubbles that are encapsulated as they exhale from hydrothermal fluids.

AN: Yeah. Sure. And of course that whole thing then gets you back even into some traditional fields. You know, the beautiful bubbles you make, putting everything you need inside the system. Some of those things look absolutely alive!

MS: Indeed they do. Of course, we still haven’t even defined life to our satisfaction. But that’s another whole issue.

AN: That’s a whole other issue related to nanotechnology in the broadest sense.

MS: Exactly, yeah, especially mineral surfaces and how those play a role in that whole scheme of things as well.

Let’s switch gears for just a minute and talk about your path to Davis. You have quite an operation going here at Davis. What led you here to take this position and do the work here rather than, for example, staying at Princeton or wherever else you’ve been.

AN: I think my career has gone, and it’s easier said in retrospect, in 12 to 15 year pieces. So I spent... I guess it was 15 or 16 years at Arizona State. And at that point I felt I had sort of explored the phase space there, let’s say, because you kind of know what’s possible and how things are going.

MS: In terms of resources?

AN: In terms of resources, in terms of people, in terms of opportunities, just in terms of everything. Life becomes a little too predictable. And the limitations you have basically change slowly, so you know what they are. So at that point you begin to feel a little footloose when the right opportunity comes along. That happened to me in 1985. [And] I moved to Princeton. And then in 1996 [or] 1997 when I moved to Davis, the same sort of thing happened. I was sort of finally faced with the choice of well, I have another, something on the order of 15 [or] 20 years of career, until one retires these days. Do I spend it at the same place, doing what I was doing quite successfully, or is it time for one more reincarnation? And you know, I opted for a change. Of course Davis came up with some very unique and very wonderful opportunities. In a way, Arizona State is a very different place from Princeton, Princeton is a very different place from Davis, Arizona State and Davis are very different places. But of course, time marches on, so in a way, they’re not simple lateral moves from one very similar situation to another, and that to me is the adventure of the move. What I like about Davis upon having my own group set up, very nicely and successfully, is it’s such a diverse university in terms of what it has. It has the veterinary school, the medical school, the agricultural school, science and engineering, humanities, everything on one big campus. It’s probably, arguably, if not the most intellectually diverse in terms of fields covered, one the most intellectually diverse schools in the United States, simply because we have that whole spectrum. And it plays out intellectually in ways that you can’t imagine. One little idea from here jumps over to there and I always talk to a lot of people and we’re involved in initiatives that are campus-wide and building things related to nanomaterials. It’s sort of one idea coming back to another, so you end up collaborating on [one thing] and it gives you an idea for something else. I think it’s that breadth of field that was the big attraction to come here. And gee, there are no blizzards!

MS: Well, not yet anyway. So you feel rejuvenated?

AN: Essentially, absolutely. I’ve watched different people’s careers, and some people really do seem to be like me, that they need to move every so often, and some people are happy being where they are for their whole career and it’s just a difference in temperament, I suppose.

MS: And a change in climate never hurts.

AN: A change in climate. I think it’s fair to say that ever since I moved to Arizona I’ve loved the West, and in that sense I’m glad to be back west. That’s a factor, but certainly the dominant factor is putting a new intellectual challenge in front of me.

MS: But you’re clearly not from around here.

AN: No. I’m from New York originally.

MS: New York City?

AN: New York City. Like most Californians, I’m not from California.

MS: I’m not from California either. This actually brings up another question. You grew up in New York, and obviously you’ve been doing science a long time, since [you were an] undergraduate. Have you always been interested in science since you were young? What spurred that interest?

AN: I’ve always been interested in science, I think. My family’s always had an interest in nature and we had a country house, and my grandfather was an engineer. But my mother was a commercial artist [and] my father was oh, more or less a salesman, but I think we all always were interested in the world around us, and I suppose by the time I had any notion of careers or fields or anything like that I just always knew I was going to be in some aspect of science, I don’t think there ever was any question. It just seemed natural.

MS: You talked about your experiences during the 60s being in science, there couldn’t have been that many women in not only geology, but the physical sciences in general. Was that difficult for you or did you not even really notice that it was a little unusual at the time?

AN: Actually, at the Bronx School of Science, the entrance exam school in New York, we were about one-third women, two-thirds men. I think there was an actual quota; that is, you all took a competitive entrance exam, and I think they pretty much jockeyed the numbers to keep that ratio. And of the people that were at the top of the class, which I was... I think I graduated 7th or 8th in a class of 800, something like that. If I remember, it was about half and half men and women. We all took the same curriculum, everybody took a course in, I forget what they called it, but it basically was a machine shop course. Everybody took a mechanical drawing course. Thank goodness for computers [nowadays]. I don’t think what women did, what men did was a real issue there. And it was not an issue for me at Chicago. It seemed to be an issue for other people. I don’t know, I just always went and did what I wanted to do.

MS: So it didn’t really affect you in any way. You just sort of ignored all of that?

AN: Oh, I suppose.
MS: Let’s move on to some of your accomplishments. What do you consider to be your real big accomplishment and your real big contribution to physical chemistry and/or Earth sciences?

AN: Let me answer that in three different ways. First, I think the real accomplishment is, if you will, a world view of how crystal structures, thermodynamics and energetics fit together. And that’s sort of an all-encompassing kind of thing. If one gets more specific and thinks of two or three more specific things, probably the two that I would point out were the early work in the 1980s that led to the realization that the lower mantle phase transition, like the spinel to perovskite, generally negative pressure temperature slopes and why. I think that was a real high point; and then the second, which really grew out of work starting in the mid 1990s, and going on to now, so really in the last decade, is the concept that for small particles, one actually gets stabilization of differing polymorphs as a playoff between surface energy and polymorphic transitions and what those ramifications are. Now those ideas have been around in certain senses, but I think first of all we provided hard evidence for them, and second of all I think we’re beginning to realize just how far they go. So if we’re to point to two things, those would probably be the ones. There was a Gordon Conference in somewhere around 1980, give or take a couple of years, on silicate melts in geology, and we were all bemoaning how little we knew. And if you look at what we know twenty years later we know much, much more and certainly what my group has done is part of that knowledge and is totally intermingled with the structural work that other people have done. So I think the contribution to understanding silicate melts, although one can’t [point to] one thing like the negative P-T or the energy crossovers, but the general understanding of silicate melts is probably something that we’ve spent a lot of energy on and made a very significant contribution to. And then the last [thing] is the students and postdocs that I have influenced and who have come through the group that are going on to doing things that are obviously different from what I’m doing. I’m very proud of the number of people who’ve come through the group and equally of the fact that I’m in some sort of contact with probably a good 80-85% of the more than 100 people that have worked with us over the years.

MS: Are you still teaching? Do you still take students?

AN: Oh yeah. Right now I’ve got 8 Ph.D. students, about 6 post docs, a bunch of visitors, two undergraduates, and several technical people.

MS: And they’re in several different fields, I imagine, like chemistry, Earth science and materials science?

AN: Right now the majority of my students come from chemical engineering and materials backgrounds, but some of them are working on things that really are geological problems or environmental problems. But the backgrounds here are mostly chemical engineering and materials, in part because they have the quantitative background that they need, which few of the geology people have.

MS: I’m not sure the readers of the Geochemical News will be happy to hear that.

AN: Well, let me give you an interesting statistic, though, if you want to be provocative.

MS: Of course!

AN: A few years ago when I was still at Princeton, I went through an epidemic of being on advisory committees for Ivy League universities. We had a elite advisory committee, with National Academy members, fellows of the Royal Society, all the usual. We were sitting around at [a] breakfast one day and talking about our own backgrounds. Out of the group, all of whom then had [excellent] reputation[s] in the Earth sciences, something like 9 of us [out of 12] had our undergraduate degrees in something other than geology, and four of us had our Ph.D.s. in something other than geology. And this is a group of people who have all the kudos imaginable in the Earth sciences. So I’m not sure what that’s telling us, but it’s something to bear in mind.

MS: Yeah, well, I think it’s probably telling us that geology is much more interdisciplinary than a lot of other fields, and it attracts the best and brightest from all of these fields. How’s that?

AN: Perhaps.

MS: You’ve won a lot awards, the most recent of course [being] the Benjamin Franklin Award in the Earth Sciences. Just describe for us what your reaction was at hearing that you won what [is] consider[ed] to be the American Nobel Prize.

[Editors Note: “Her findings have established, convincingly, the identity of materials at hundreds of kilometers of depth in the earth that otherwise are inaccessible to direct observation,” according to the citation for the award. More information about the Benjamin Franklin award is available at the Franklin Institute’s website (http://sln.fi.edu/index.html).]

AN: Well, obviously I was thrilled. And I was all the more thrilled because when I heard who the other winners were, two of them were people that I have known for years. Sumio Iijima, the carbon nanotubes fellow, was actually a postdoc and then a junior faculty member at Arizona State about the time all the electron microscopy was starting out and John Cahn, the Bower Prize winner, is a metallurgist, thermodynamicist, whom again I’ve known, oh, certainly since the mid 70s. So that added to the pleasure and the thrill. It [is] probably fair to say that it was not absolutely out of the clear blue, because the person who had nominated me had asked for some some information, so I knew the award existed. But as with such things, you’re busy doing other things. All of a sudden from one moment to the next you get a phone call and your life changes.

MS: Speaking for myself, and talking to some other people, we really weren’t aware that such a thing actually existed.

AN: It’s funny. It’s true that somehow the publicity on the Franklin Awards [is] strange, it’s spotty. Some groups and people know of them, some do not, but it’s not sort of a household name. I don’t know why.

MS: How does it compare to some of the other things that you’ve been awarded?

AN: Certainly, by any scale, getting elected to the [National] Academy of Sciences and getting the Franklin Award are the two biggies. Now certainly the thing that came absolutely out of the blue for me was the first award I got, which was the Mineralogical Society of America Award in the early 1980s. I was not an MSA member at the time.

MS: You quickly joined.

AN: Well, actually I got a life membership as part of it [laughs]. But that really did come out of the blue. And of course, [it] being the first time that you sit up in public with the opportunity to spill salad dressing all over
AN: Ok. I’m a dog person, always have been. We have a group in California. No, let me backtrack. One of the problems all over the world, but in the United States certainly, is that there are continually a large number of unwanted dogs and cats. And something like 2 million dogs get killed in the shelters, euthanized, we’ll call it, for no better reason than that nobody wants them, and nobody bothered to spay and neuter them so they wouldn’t make puppies. A number of volunteer organizations try to place dogs from shelters or dogs that are given up by their owners, both for good [and bad] reason[s] and those organizations generally group themselves as breed rescue organizations just because it’s easier to deal with one kind of dog. And we have a very nice farmer’s market here in Davis on Saturday mornings, and there actually is a group that works at the market called Central California Labrador Retriever Rescue. I sort of knew they were there for a year, year and a half and finally I went up and said well, I’d like to help you but I travel a lot so there’s nothing I can do on an absolutely regular basis. They suggested I volunteer at their booth, and I’ve been doing that Saturday mornings when I’m in town, and that means you’re sort of a front-line person, talking to people who are coming to adopt dogs or to give up dogs sometimes, or just looking for advice on one thing or another. It’s a volunteer organization [and] the dogs that we take are all fostered in different people’s homes, so there’s a lot of logistics to be dealt with. I can’t foster because I have four dogs of my own. Last spring in fact, oh about two weeks before getting the Franklin Medal, our car had a little misunderstanding. It decided it wanted to go off the road for reasons which may have had to do with blowing a tire, although we’re not quite sure. The airbags decided they needed to save our lives [and] scraped up our faces. In two weeks I was going off to the Franklin Medal Awards, and the weekend after the accident I was working at Lab Rescue still with the biggest black eye imaginable and for reasons unknown a chocolate labrador’s big brown eyes got to me. That’s our fourth dog, whom we call Benjamin Franklin.

So I guess basically my message to people is for heaven’s sake, spay or neuter your pets and if you want a pet, adopt it from the huge reservoir of animals whose lives you’ll be saving.

MS: Do you have all labradors, or do you have a variety [of breeds]?

AN: No, I have a 14 [year-old] and he’s well over a hundred pounds, and... I would say he’s two-thirds labrador and one-third question mark. I have an eleven year old shepherd, who is a reject show dog, a shepherd built by a committee, from some shepherd breeder friends of ours in New Jersey. Then I have a two year old dog. I picked up [that] dog at the local animal shelter thinking that she was some sort of a short-haired mixed mutt, but I’ve realized in fact that she is an undersized ridgeless Rhodesian Ridgeback. There’s nothing else obvious in her. And then we got this chocolate lab last spring.

MS: They must take up a lot of your time when you’re not here.

AN: They take up time. They demand attention. They get it.

MS: I’m sure. Your colleagues over there were quite taken with your Lab Dog Rescue story, so they demanded that I ask you about that. So [now] everyone will know about... at least all the geochemists.

AN: All the geochemists will know, that’s right. Well, you know, Lab Rescue wouldn’t mind in the least if one put their web site in the article somewhere.

MS: We can certainly do that, if you tell me what it is.

[Editor’s note: The web site for Central California Labrador Retriever Rescue is http://www.cc-labrescue.org].

AN: Well, I just happen to have a brochure. Because after all, some people in California will read this and if we save one more, we’ve done something.

MS: Then I’ve done my job! Is there anything else you’d like to talk about or to mention?

AN: I suppose well, yeah, there is one other thing I should mention and that is that you know, for the most part, it has been and continues to be a heck of a lot of fun, and probably one of the best things about it is most of the time you get up in the morning sort of with the same feeling that my dogs have; what great wonderful thing’s going to happen next?

MS: That’s great. Thank you so much for your time and patience. I wish you continued luck and success here at Davis.

Central California Labrador Retriever Rescue
www.cc-labrescue.org
Meeting Report
Isotopes in the Environment

Is radiation a good or a bad thing? That's what the Environmental Chemistry Section of KNCV (The Netherlands’ version of the ACS) asked during its annual meeting at the University of Delft, just a few days before Christmas. The question hinted at the usefulness of radiation in research. The program spanned the entire globe: atmosphere, oceans and terrestrial soils and sediments. The day, however, started on a sad note as Wim van Raaphorst of the Royal NIOZ had been one of the intended speakers, but had suddenly passed away due to an accident (see previous issue of The Geochemical News).

The program's first presentation was by Greenpeace's Rianne Teule, who analyzed the radioactive-sludge problem of La Hague in France. Greenpeace has been sampling water, sediments and organisms from the vicinity of a waste discharge pipe of the reprocessing facility at La Hague, which reportedly releases over one million liters of liquid radioactive waste into the sea daily. Labs of the University of Bremen in Germany, the Royal NIOZ in The Netherlands, and ACRO in France were involved in this project. The research results show that the size of the particles in the released sludge is much larger than permitted (up to 63 micrometers instead of up to 25 micrometers). The concentrations of Pu-238, Pu-239, Pu-240, H-3, and other isotopes were also determined. The analyses reveal that the waste clearly qualifies as radioactive waste (according to Netherlands law - French law allows much higher values), necessitating a permit to transport or even possess the samples in The Netherlands. Greenpeace feels that Europe, including The Netherlands, should do something about it and states that the North Sea and Irish Sea are becoming increasingly radioactively contaminated. Pieter Kwakman of RIVM also discussed releases of radioactive materials into the environment, from various sources (mainly industry).

Arjan de Koning (University of Leiden) tackled the behavior of radioactive Cs in soils and sediments. The concentrations of Cs-137 in water, freshwater fishes and vegetation remain higher than expected, more than ten years after the accident at Chernobyl. This was in strong contrast to what was initially believed, namely that the Cs would be adsorbed onto illite like clay minerals (common in soils) and that only very little - <10% - could be removed again (and only at high concentrations - 0.1 or 1 M - of alkali ions). This has turned out to be an artifact: when Cs-selective ion exchangers are used in experiments, the desorption of Cs-137 is much larger. This helps to explain why the aqueous concentrations in water are still so high.

Michiel Rutgers van der Loeff, currently at RIKZ, was kind enough to step in for Wim van Raaphorst and gave a presentation on isotopes as marine particle tracers. It starts with U, the carbonate complexes of which dissolve well in seawater. U decays to a series of isotopes that either stay in solution (such as U) or are highly particle-reactive (such as Th). The former can be used as water mass tracers and the latter to monitor particle transport. Michiel's talk focused on Th isotopes, each of which has a very different half-life. Converting the results into transport rates of for instance C is not always easy (see also http://cafeouthorium.whoi.edu/).

Astrid Fischer of the University of Delft was the next speaker. She studies iron uptake by marine algae. The basis of her project lies in the Southern Ocean, where phytoplankton growth is limited by light and iron. Her research addresses iron kinetics and she uses Fe-55 and Fe-59 in combination with various light conditions to try to chart these kinetics.

After the lunch break and the annual meeting, Carel van Eijk - also of the University of Delft - acquainted the audience with luminescence dating. Luminescence dating is a technique that enables timing of the last exposure to light or heat of minerals in sand and silt - mainly quartz but also feldspar and zircon. It is now widely used as a tool in geological and archaeological studies. All expertise on luminescence dating and related research in The Netherlands is brought together in NCL, Netherlands Centre for Luminescence dating.

Harro Meijer (CIO, University of Groningen) explained the application of radioactive and stable isotopes to study greenhouse gas budgets, particularly of carbon dioxide. Research on carbon dioxide cycling is high on the political agendas in Europe, in view of “Kyoto” (see also http://www.bgc-jena.mpg.de/public/carboeur).

Rob de Meijer, his colleague from a different institute at the same university, concluded the scientific part of the meeting. The Nuclear Geophysics Division of the KVI in Groningen has devised a method that measures gamma radiation from natural radionuclides. That has turned out to be a proxy for grain size and also carries information about provenance and history of the sediment. The technique was initially developed for marine sediment dynamics, but is also successfully applied for airborne charting of gold mines, agricultural purposes, to measure the thickness of specific layers on roads and to on.

The successful day was topped off with drinks and fruitful conversation, of course. Should you be interested in more details: most abstracts (and some PowerPoint files) of the presentations are available at http://www.milieuchemie.org/.

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Craig Harmon, continued from Page 5

methane, he analyzed the gases trapped in Greenland ice cores and showed that the methane content of the atmosphere has doubled over the past three hundred years, a finding which is important for studies of the atmospheric greenhouse gas effect. Craig and his wife and frequent collaborator, Valerie, had a long-term project that identified the various sources of marble in ancient Greek sculptures and temples using carbon and oxygen isotopes.

On recent expeditions, Craig had sampled volcanic rocks and gases in Yunnan, China, in the East African Rift Valley, in oceanic expeditions to six Pacific marginal basins, and in the north Pacific to the southernmost island of the Austral Chain. This work is concerned with delineating mantle hotspots and other regions where volatiles from the earth’s interior are emerging at the surface and are a part of continuing studies of deep circulation in the Pacific Ocean.

In recognition of his scientific achievements, Craig has received a number of honors. In addition to the 1998 Balzan Prize, he was elected to membership in the American Academy of Arts and Sciences in 1976 and the National Academy of Sciences in 1979. He received the V.M. Goldschmidt Medal of the Geochemical Society in 1979, the National Science Foundation “Special Creativity” Award in Oceanography in 1982, the Arthur L. Day Medal of the Geological Society of America in 1983, and the honorary degree of Doctor of the University of Paris (Pierre et Marie Curie) in 1983. In 1987 he was awarded the Arthur L. Day Prize and Lectureship of the National Academy of Sciences and was co-recipient of the Vetlesen Prize from Columbia University. In 1991 he was awarded an honorary doctorate degree from the University of Chicago, and in 1993 he was named an honorary fellow of the European Union of Geosciences.

Craig is survived by his wife of 55 years, Valerie, of La Jolla, daughters Claudia Craig Marek of Los Angeles, Calif., Cynthia Craig of East Lansing, Mich., and Karen Craig of Auckland, New Zealand, a brother John R. Craig III of Wittman, Maryland, and four grandchildren.

A memorial service was held on Friday, April 4, in the Martin Johnson House on the campus of Scripps Institution of Oceanography in La Jolla.
Canada Research Chair
Nitrogen Management in Agroecosystems

The Departments of Land Resource Science and Plant Agriculture, University of Guelph are seeking an outstanding individual to be nominated for a Canada Research Chair (Tier 1) related to Nitrogen Management in Agroecosystems. The successful candidate will be an established researcher who is internationally recognized as a leader in studies of soil/plant nitrogen dynamics and who has demonstrated superior capabilities in developing collaborative research programs. The successful candidate will hold a joint appointment in Land Resource Science and Plant Agriculture, and be housed in one or both of the departments. He/she will establish a strong, well-funded research program, and advise a significant number of graduate students. Accordingly, this position will have a reduced undergraduate teaching load. The candidate will be expected to develop innovative collaborative research programs in areas such as: transformation and transport of N in pedologic, groundwater, atmospheric or biological systems; development of management recommendations to enhance profitability in crop production and minimize environmental impacts on N on water quality and greenhouse gas emissions; modeling the fate of applied fertilizer, manure and sewage sludge N in agroecosystems; and, absorption and utilization of N by crop plants. These departments are developing a major new initiative on environmentally sustainable production of bio-based products in the emerging life sciences economy; the candidate will be expected to contribute research in this context.

The Canada Research Chair (CRC) program was established by the Government of Canada to enable Canadian universities to achieve the highest levels of research excellence in the global, knowledge-based economy. See www.chairs.gc.ca Tier 1 Chair candidates are expected to be world leaders in research in their field. The University of Guelph’s Strategic Research Plan is available at:

http://www.uoguelph.ca/research/programs/crc/

The University of Guelph is renowned for its strengths in agricultural, environmental and life sciences and is among the most research-intensive universities in Canada. The University offers a quality lifestyle and excellent career growth opportunities. Guelph is located in a region of intensive agriculture where the environmental impacts of agriculture, particularly on soil, air and water resources, are critical current issues. Research related to N in agroecosystems is emphasized in the Departments of Land Resource Science and Plant Agriculture with complementary research being conducted in several other departments. The Department of Land Resource Science has 19 faculty and 55 graduate students, the Department of Plant Agriculture has 50 faculty and 88 graduate students. Together these departments are planning the construction of major new research facilities. Additional information on the departments can be found at http://www.lrs.uoguelph.ca and http://www.uoguelph.ca/plant.

An application, with detailed statement of interests including potential research plans, a full resume, and the names of three persons who may be contacted for references should be submitted by July 15, 2003 to Dr. S.G. Hilts, Chair, Land Resource Science, University of Guelph, Guelph, Ontario, Canada N1G 2W1. Email: shilts@lrs.uoguelph.ca, fax: (519) 824-5730. All CRC appointments are subject to review and final approval by the CRC Secretariat in Ottawa. Our objective is to select a suitable candidate by the summer of 2003; the position will be available once approval is received from the Secretariat.

The University of Guelph is committed to an employment equity program that includes special measures to achieve diversity among its faculty and staff. We therefore particularly encourage applications from qualified aboriginal Canadians, persons with disabilities, members of visible minorities and women.

Postdoctoral positions in Environmental Microbiology and Geochemistry

Applicants are sought for two postdoctoral research positions at the Great Lakes Institute for Environmental Research (GLIER). The successful applicants will:

- Study the linkages between microbial ecology and the cycling and bioavailability of trace metals in the Great Lakes and other aquatic ecosystems.
- Develop new models for bacteria-metal-mineral interactions and microbially influenced processes in metals bioavailability.

Applicants should have a Ph.D. in microbiology, geochemistry, geomicrobiology, or related fields, and experience with utilizing molecular tools in microbial ecology (1) or geochemical modeling (2). The positions are renewable yearly for up to 2 years, based on performance. Salary is commensurate with qualifications and experience. Applicants, send a statement of research interests, CV, and names of three references to: Dr. David A. Fowle (fowle@uwindsor.ca), Great Lakes Institute for Environmental Research, University of Windsor, Windsor, ON, N9B 3P4 Canada.

For further information see: http://biogeo.uwindsor.ca

The Society for Organic Petrology (TSOP)

invites applications for graduate student research grants. The purpose of the grants is to foster research in organic petrology (which includes coal petrology, kerogen petrology, organic geochemistry and related disciplines) by providing support to graduate students from around the world, who demonstrate the application of organic petrology concepts to research problems.

Grant Size: Monetary awards up to a maximum of $1,000.00 US will be granted. TSOP will also provide Merit Awards, in the form of certificates redeemable for TSOP publications, to top-ranking applicants not receiving grants. The program awards a maximum of two grants each year.

Use of Grant: Grants are to be applied to expenses directly related to the student's thesis work, such as summer fieldwork, laboratory analyses, etc. A portion (not to exceed 25%) of the funds may be used to attend TSOP Annual Meetings. Funds should not be used to purchase capital equipment, to pay salaries, tuition, room, or board during the school year. Funds must be spent within 18 months of receipt of the award.

Application Deadline: TSOP graduate student research grant application deadline is May 1, 2003. Grants will be awarded in September, 2003. Detailed information and an application form on the TSOP web site http://www.tsop.org/grants.htm or applications may be obtained from S. J. Russell, Shell UK Exploration and Production, 1 Altens Farm Rd., Nigg, Aberdeen AB12 3FY, United Kingdom; fax: +44(0)1224 884 418; e-mail: suzanne.j.russell@shell.com

Information for Contributors

Geochemical News publishes timely and informative articles, announcements, letters, and reviews relevant to geochemists and geochemistry. Contributions are welcome from professionals, students, and other interested parties. Please send all communications to geochemical-news@wmich.edu.

Text contributions should be in Microsoft Word format. Graphically-designed contributions (i.e. advertisements, announcements) should be submitted as PDF files, and must fit within one page having the dimensions 18.4 cm wide by 22.9 cm tall (or smaller).

Graphics files submitted as figures to accompany articles MUST be in one of the following formats only: PDF, GIF, JPG, or TIFF.

Thanks again for your contributions!
7th International Conference on the Biogeochemistry of Trace Elements (7th ICOBTE)

An interdisciplinary conference dedicated to link biosphere phenomena to physical & chemical reactions in the pedo-and lithosphere.

Uppsala, Sweden
June 15-19, 2003

We are pleased to invite you to participate in the 7th ICOBTE, which will take place for the first time in Sweden, at the Swedish University of Agricultural Sciences, Uppsala. This highly successful conference series began in Orlando (1990) and has been held in Taipei (1993), Paris (1995), Berkeley (1997), Vienna (1999) and Guelph (2001).

The 7th ICOBTE is dedicated to examining contemporary and emerging research in the biogeochemistry of trace elements. Biogeochemistry has developed into an interdisciplinary science, linking phenomena observed in the biosphere to physical and chemical reactions in the pedo- and lithosphere. The conference provides a forum for professionals, regulators, and students to present their most recent findings and to discuss with colleagues from around the world state-of-the-art methodology, analytical techniques, and process development.

The conference is sponsored by: Swedish University of Agricultural Sciences (SLU), Uppsala, Sweden International Society of Trace Elements Biogeochemistry (ISTEB)

For more information see:
http://www-conference.slu.se/7thICOBTE/

The Organic Geochemistry Division of the Geochemical Society plans a symposium for the Annual GSA Meeting in Seattle, Washington November 2-5, 2003

Quantitative Modeling of Petroleum Systems and Basin Processes

Organizers:

K.E. Peters
U.S. Geological Survey, Menlo Park, CA
kpeters@usgs.gov

M. B. Goldhaber
U.S. Geological Survey, Denver, CO
mgold@usgs.gov

Quantitative modeling can be used to reconstruct the temperature and fluid-flow histories of subsurface sediments. This symposium will provide a timely update of the concepts and methods used to model petroleum and mineral systems.

For more information:
http://www.geosociety.org

Newsletter of the Geochemical Society
**Meetings Announcements**

**SHORT COURSES 2003**

**MINERALOGICAL ASSOCIATION OF CANADA**

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**Analysis and Interpretation of Fluid Inclusions**

**Vancouver GAC-MAC-SEG 2003**

**May 24 and 25, 2003**

**Organizers**

- IAIN SAMSON (University of Windsor),
- ALAN ANDERSON (St. Francis Xavier University),
- DAN MARSHALL (Simon Fraser University)

**Objectives**

- Introduce participants to both basic and advanced tools for the analysis and interpretation of fluid inclusions (including melt inclusions).
- Teach the participants about what fluid inclusions are, what types of data can be obtained from fluid inclusions, the approaches and techniques that can be used to analyze fluid inclusions. How such data are processed and interpreted, and where the limitations and pitfalls lie in the various techniques.
- Examples using the various techniques will also be called upon.
- There will be demonstrations.

Detailed list of topics can be viewed at www.mineralogicalassociation.ca

**Presenters**

- Alan Anderson (St. Francis Xavier University);
- Fred Anderson (University of Chicago);
- Ronald Bakker (University of Leoben, Austria);
- Robert Bodnar (Virginia Tech);
- Philip Brown (University of Wisconsin);
- Robert Burruss (USGS);
- Laryn Diamond (University of Leoben, Austria);
- Brian Fryer (University of Windsor);
- Joel Gagnon (University of Windsor);
- Sarah Gleeson (University of Alberta);
- Robert Goldstein (University of Kansas);
- Stefano Salvi (CNRS, France);
- Iain Samson (University of Windsor);
- Anthony Williams-Jones (McGill University).

For more information, contact Iain Samson at ims@uwindsor.ca

To register: www.vancouver2003.com

**Registration fee**

- CDN$290 (students CDN$165)

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**Environmental Aspects of Mine Wastes**

**MAY 24 and 25, 2003, Vancouver**

**Conveners**

J.L. Jambor, D.W. Blowes & A.I. Ritchie

This two-day intensive short course, to be held at Robson Square in the heart of downtown Vancouver, will cover a wide spectrum of environmental issues dealing with mine-waste solids and effluents. Individual presentations will be given on environmental regulations and compliance, mine-waste geology, hydrology, mineralogy, geochemistry, microbiology, drainage prediction, remediation, advances in ARD modelling, and case studies. The course will ensure not only entry-level familiarization with the various topics of primary concern in studies of mining-related wastes, but will also provide exposure to the advances that have been made in these and related fields over the past decade.

**Presenters**


**Registration fee**

- CDN$375 (students CDN$250)

**Early registration (prior to April 15, 2003):**

- CDN$325 and CDN$200.

**Payable to**

MAC Short Course.

**Remittances**

MAC business office

For more information: John Jambor (jljambor@aol.com) or the MAC website (www.mineralogicalassociation.ca)

To download a registration form or to register online, www.mineralogicalassociation.ca
Apr 2-4, 2003: 18th Himalaya-Karakoram-Tibet Workshop (IKTW), Ascona, Monte Verita, Switzerland. Website: http://www.geology.ethz.ch/sfg/Himalaya/default.htm

Apr 3-4, 2003: U-Series Geochemistry - A two-day short course presenting advances in the application of U-Series geochemistry across the earth Sciences, Paris, France. Website: www.mnsoac.com/MSA/SCU_Series_sc.html


Apr 6-11, 2003: EGS-AGU-EUG Joint Assembly, Nice, France. Website: http://www.copernicus.org/egsagueu.html

Apr 14-17, 2003: Uranium Geochemistry - 2003 - Ore deposits - Natural Analogy - Rehabilitation, Nancy, France. Contact: Uranium Geochemistry 2003 UMR-6292 - CEGUI, Henri Poincare University, BP239, 54606 Vandoeuvre les Nancy Cedex, France; Fax: +33 - 3 83 91 38 01; E-mail: Michel.Cuney@gr2.uphp-nancy.fr. Website: http://www.gl.rhbnc.ac.uk/geo/Registration.html

Apr 24-26, 2003: 15th Argentine Geological Congress. El Calafate, Santa Cruz Province, Southern Patagonia, Argentina. Contact: President Dr. Miguel Haller or Secretary Dr. Roberto Page, Asociacion Geologica Argentina, Maipu 645, 1 er Piso, Buenos Aires, Argentina; Phone: +54 11 4325 3104; Fax: +54 11 4325 3104; E-mail: haller@centau.edu.ar or fomicruz@internet.siscone.com.

May 5-8, 2003: 3rd JGOGS Open Science Conference, Washington DC, USA. Contacts: Roger Hanson, JGOGS International Project Office, SMR, University of Bergen, PO Box 7800, 5020 Bergen, Norway: Phone: +47 555 84244; Fax: +47 555 89667 or Ken Busseller, Department of Marine Chemistry and Geochemistry, WHOL MS 25 Woods Hole, MA 02543, USA; Phone: +1 508 289 2309; Fax: +1 508 457 2193.

May 8-10, 2003: Third Meeting on Magmatism, Metamorphism and associated Mineralizations (3MA), Hassan II Ain Chock University, Casablanca, Morocco. Website: http://www.colloque3ma.com

May 9, 2003: International Coalbed Methane Symposium, Tuscaloosa, AL, USA. Contact: College of Continuing Studies, University of Alabama, Box 870388, Tuscaloosa AL 35487-0388, USA; Fax: +1 205 348 9276; E-mail: gholm@css.ua.edu

May 12-17, 2003: GEOFLUIDS IV - on fluid evolution, migration and interaction in sedimentary basins and orogenic belts, University of Utrecht, Utrecht, The Netherlands. Contact: J. Verweij, Driehuis, Dr. J. Verweij@nitg.nrl.nwo.nl; Fax: +31 30 256 46 55; E-mail: j.verweij@nitg.nrl.nwo.nl. Website: http://www.nitg.nl/english/gofiuflids2.pdf

May 13-15, 2003: Using Science to Assess Environmental Vulnerabilities, Valley Forge Hilton, King of Prussia, PA, USA, by the US EPA. Contact: TPMC, Mill Wharf Plaza, Suite 208, Scituate, MA 02066, Phone: +1 781 544 0423; FAX: +1 781 544 3086; E-mail: conference@tpmc.com.

May 18-22, 2003: 103rd General Meeting American Microbiology Society for Microbiology, University of Maryland, Website: http://www.asmusa.org/mtgs/gm2003/prelimiprogtempgate.htm

May 18-24, 2003: 39th Forum on the Geology of Industrial Minerals, John Ascuaga’s Nugget Hotel & Casino, Sparks, Nevada, USA. Contact: Terri Garuda, NBG/MGS 178, University of Nevada, Reno, NV 89557-0088; Phone: +1 775-784-6691 ext 126; Fax: +1 775-784-1709; E-mail: tgaruda@unr.edu. Website: http://www.nbmg.unr.edu/imf2003.htm


May 19-23, 2003: International Symposium on Tectonics (IST) - IX National Symposium on Tectonics (SNET), Armação dos Búzios, Rio de Janeiro State, Brazil. Contact: Prof. Remi Blansko, Czech Republic; Phone: +420 385 959 4473; E-mail: rz@so.soton.ac.uk; Web site: http://www.geomin.unibo.it/snets/erice/highpres.htm

May 20-23, 2003: EUSTONE 2003 - Forum for stone, Natural stone congress, University of Joensuu, Joensuu, Finland. Organization: Geological Survey of Finland. Contact; Mr Hannu Luodes, P.O.Box 1237, 70211 Kuopio, Finland; Phone: +358 20 550 3528; Fax: +358 20 550 13; E-mail: hannu.luodes@gsf.fi; Website: http://www.gsf.fi/events/eustone2003


June 16-17, 2003: Biogeochemistry and Biodiversity of Chemosynthetic Ecosystems: Planning for the future, Southampton Oceanography Centre, U.K. Contact: Dr. Eva Ramirez Llodra; Phone: +4 (0)2380 596446; E-mail: ezl@soc.soton.ac.uk; Website: http://rds2000.bios.ps.u.edu/developer/index.php?prews=england03


June 22-26, 2003: Euroclay 2003, Moderna, Italy. Website: http://www.unimo.it/euroclay2003/

June 22-27, 2003: 8th International Kimberlite Conference, Victoria, British Columbia, Canada. Contact: Dr. Roger H. Mitchell, Geography Department, Lakehead University, Thunder Bay, Ontario, Canada; Phone: +1 807343 8237; Fax: +1 807-623-7526; E-mail: Roger.Mitchell@lakeheadu.ca. Website: http://www.venuwest.com/8IC/6


July 5-9, 2003: Workshop: Teaching Petrology in the 21st Century, Montana State University, Bozeman MT, USA. Deadline has passed. Website: http://serc.carleton.edu/ NAGWorkshops/petrology03/index.html


July 21-25, 2003: Ultra-high pressure metamorphism, 5th EMU School in Mineralogy, Eotvos L. University, Budapest, Hungary. Website: http://www.lcm3b.u-nancy.fr/ecasi5g/Activity.htm#EMU5

July 26-21, 2003: 66th Annual Meeting of the Meteoritical Society, Münster, Germany. Contact: EK@wz.uni-muenster.de (subject: 66MetSoc); Website: http://www.geomin.unibo.it/orgv/erice/highpres.htm

Jul 30-Aug 01, 2003: IX Colombian Geological Congress. Medellin, Colombia. Contact: Michel Hernandez, M.Sc. E-mail: mher亨@colciencias.edu.co; Website: http://www.congressocolombianodegeologia.org

Aug 10-14, 2003: GeoSciEd IV, University of Calgary, Alberta, Canada, by the International Geoscience Education Organization. Contact: Godfrey Nowlan, 3300 - 33rd Street NW, Calgary, AB, T2L 2A7, Canada; Phone: +1 403 292 7079; Fax: +1 403 292 6014; E-mail: gnw@ucalgary.ca. Website: http://www.geoscied.org


Aug 10-16, 2003: XVII International Congress on the Carboniferous and Permian (XV ICCP) and 56th Meeting of the International Committee for Coal and Organic Geochemistry
**Mineralogical Society of America**

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- (1) Analytical geochemistry
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- (4) Cosmochemistry and meteorites
- (5) Crustal mineralogy, petrology, trace elements
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- (8) Geochemical education
- (9) Low-temperature & interface geochemistry
- (10) Mantle mineralogy, petrology, trace elements
- (11) Marine geochemistry & chemical oceanography
- (12) Ore deposit and hydrothermal geochemistry
- (13) Organic geochemistry
- (14) Planetary geochemistry
- (15) Radiogenic and stable isotope geochemistry
- (16) Bio-geochemistry

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- (A) Yes, I wish to be a member of the Organic Geochemistry Division (OGD) at no extra charge.
- (B) Yes, I would consider being an officer, committee chair, or committee member of the Geochemical Society.

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