THE GEOCHEMICAL NEWS

Newsletter of The Geochemical Society

in cooperation with The European Association of Geochemistry

In This Issue...

An Interview with David Des Marais

Geochemistry at Oak Ridge National Laboratory

January 2005
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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 ***G^3*** (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
January 2005

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From President Tim Drever,

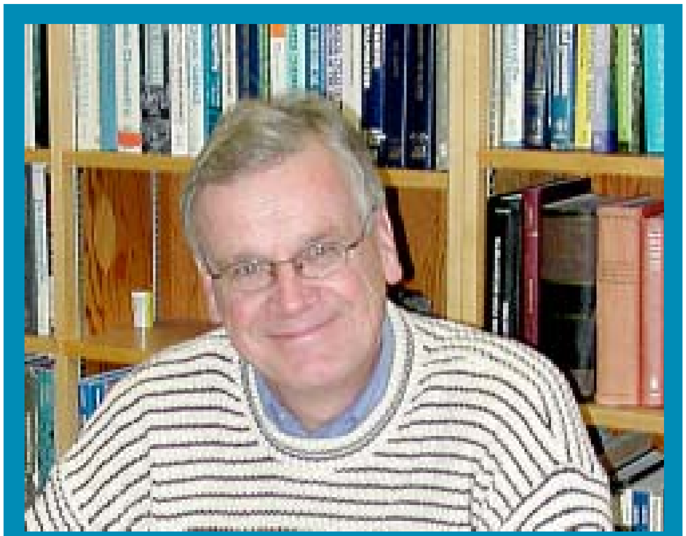
By now you should all have received the first issue of *Elements*—the new magazine sponsored by a group of mineralogical and geochemical societies in North America and Europe. I hope you are as impressed as I am. I would like to congratulate Rod Ewing, Mike Hochella, Ian Parsons and Pierrette Tremblay on a superb job: I look forward to seeing the next issues. *Elements* does not replace the *Geochemical News*, which Carla and Johnson have built into an attractive and successful publication over the last few years, but we are changing the format. Issues will be on-line only, with one printed issue which will focus on the Goldschmidt conference. Please let us know what you think of the new arrangement and give us your feedback and suggestions for both *Elements* and the *Geochemical News*.

At this point I would like to thank the officers of the Society whose terms have come to an end, and to welcome the newcomers. Becky Lange is retiring as Treasurer, having served us ably for the last four years. Youxue Zhang, also of the University of Michigan has taken over as Treasurer. Eric Oelkers and Erwin Suess are rotating off the Board of Directors, to be replaced by Laurie Reisberg (Vandoeuvre-les-Nancy) and Vincent Salters (Florida State University). The Society depends on the hard work and enthusiasm of the volunteers who serve as officers and committee members. Thank you all, particularly Becky, Eric, and Erwin. I am happy to report that Jeremy Fein will be continuing as Secretary and Scott Wood as Special Publications Series Editor.

I would also like to congratulate the 2005 medalists of The Geochemical Society and the newly-elected Geochemistry Fellows selected jointly by the Geochemical Society and the European Association for Geochemistry. The Goldschmidt Medal will be awarded to Bruce Watson (Rensselaer Polytechnic Institute), the Patterson Medal to Ken Bruland (U.C. Santa Cruz), the Clarke Medal to Jim Van Orman (Case Western Reserve University), and the Distinguished Service Award to Gunter Faure (Ohio State University). The new Geochemistry Fellows are Nicholas Arndt (Institut Dolomieu, Grenoble), Stein Jacobsen (Harvard University), Stuart Wakeham (Skidway Institute of Oceanography), and Lynn Walter (University of Michigan). Congratulations to you all on the well-deserved recognition and thank you to the selection committees for a job well done.

I am looking forward to seeing many of you in Idaho. It promises to be a great meeting, so come and join us and celebrate the 50th anniversary of our society!

Tim Drever, GS President



Tim Drever

Editors' Corner

This is the first totally digital edition of *The Geochemical News*, issued to our members in the form of a PDF emailed directly. This is an experiment of sorts, and we're not yet sure if this will constitute the "ultimate" form of *GN* or is just a transitional step to something else. Other models that we've considered include a web version, possibly with an emailed table of contents that includes links for each article. There are advantages and disadvantages with each format, and your next issue of *GN* may look very different from this one... or it may not.

One advantage to a digital format is that we can now publish longer articles and full color images. You'll see some of that in the current issue. The highlights this month are an interview with eminent geochemist David des Marais, by associate editor Mitch Schulte.

With this issue we also begin a new article series that showcases geochemical research at US National Laboratories, beginning this month with Oak Ridge National Laboratory.

We're always interested to hear about new and exciting events in the world of geochemistry, so please send us your ideas for articles. No good idea will be ignored, at least without a good reason.

Finally, we'd like to offer congratulations to the teams at NASA and the European Space Agency for their astounding success in the Cassini-Huygens probe's safe landing on murky Titan, the frigid moon of Saturn where methane rivers creep down to hazy, oil-dark seas. Or so we imagine. As the muddy Huygens lander stares out across Tartarean leagues of stygian gloom, and its brighter Earthbound puppeteers cheer their success, we wish everyone a happy and peaceful New Year !

Until next issue,

Johnson R. Haas (johnson.haas@wmich.edu),
Carla Koretsky (carla.koretsky@wmich.edu),
Editors

COVER: This oblique image taken by the Viking orbiter spacecraft shows a thin band of the Martian atmosphere. This image looks northeast across the Argyre basin. The Argyre basin is about 600 kilometers across with a rugged rim of about 500 kilometers in width. Image credit and caption text copyright © 1997 by Calvin J. Hamilton. http://www.solarviews.com

Greetings from the Business Office,

2005 Geochemical Society Medalists Announced

The recipients for the 2005 Goldschmidt, Clarke and Patterson Awards have been selected. They are: E. Bruce Watson (V.M. Goldschmidt Award), James A. Van Orman (F.W. Clarke Award) and Kenneth Bruland (C.C. Patterson Award). The presentation of these awards will occur at the 2005 Goldschmidt Conference.

2005 Geochemistry Fellows Announced

The recipients of the 2005 EAG and GS Geochemistry Fellows Awards have also been selected. They are: Nicholas Arndt, Stein Jacobsen, Stuart Wakeham, and Lynn Walter. These awards will also be presented at the 2005 Goldschmidt Conference. Congratulations to all of our recipients.

Award nominations for 2006 may already be submitted. For more information, please visit our website at: http://gs.wustl.edu/archives/nominations.html

2004 Membership by Country

Country	# of Members	% of Total
United States	970	40.2%
Germany	198	8.2%
United Kingdom	187	7.8%
France	149	6.1%
Japan	118	4.9%
50 Other Countries	789	32.7%

Elements Magazine

By now, members should have their first issue of Elements Magazine. If you did not receive one, I have a limited number of extra copies available upon request. Also, so we can improve the content of the magazine we are looking for your opinion about what you like and don't like about it. Please send your comments to me at: office@gs.wustl.edu.

Elsevier Books Discount

Just a reminder that the Geochemical Society has negotiated with Elsevier to provide a 25% discount and free shipping to Geochemical Society Members on all Elsevier books. Note this does not include electronic products nor major reference works (e.g. Treatise on Geochemistry). An order form may be found elsewhere in this newsletter. Elsevier has an on-line newsletter with the latest on their Earth & Planetary Sciences publications at:
http://www.extranet.elsevier.com/listman/earth/earthjan.html

GSA – Denver

GSA-Denver was a successful event for the Geochemical Society.
The 2004 Ingerson Lecturer, Roberta Rudnick, presented her talk on Geochemical Probing of Continental Dynamics. Marty Goldhaber and Daniele Cherniak worked diligently to produce excellent geochemical programming. Further, the MSA/GS reception was well catered and provided people the first opportunity to see the new Elements magazine. And the GS booth was well received. In 2005, the GS exhibit will be appearing at the 2005 Goldschmidt Conference in Moscow, Idaho, and then again at the GSA – Salt Lake City Meeting.

The Geochemical Society – A Truly International Society

In 2004, the GS membership reached an unprecedented level of 2,411 members in 55 countries.

Have a great 2005,

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Review

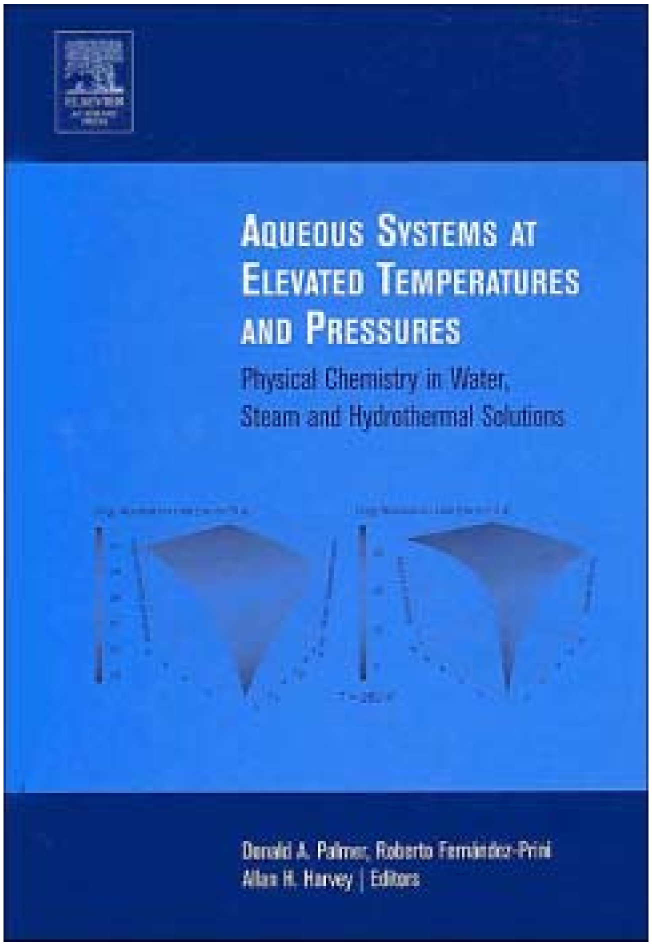
AQUEOUS SYSTEMS AT ELEVATED TEMPERATURES AND PRESSURES, PHYSICAL CHEMISTRY IN WATER, STEAM AND HYDROTHERMAL SOLUTIONS

Edited by Donald A. Palmer, Robert Fernndez-Prini, and Allan H. Harvey

Elsevier Academic Press, 2004. ISSBN: 0-12-544461-3. 752 pp. $180

BY THOMAS J. WOLERY

AQUEOUS SYSTEMS AT ELEVATED TEMPERATURES AND PRESSURES was produced by the International Association for the Properties of Water and Steam (IAPWS) for the purpose of providing "an accessible, up-to date overview of important aspects of the physical chemistry of aqueous systems at high temperatures and pressures." The book is primarily aimed at physical chemists, chemical engineers, and geochemists. It contains eighteen chapters plus a Foreword by Professor E.U. Franck, and has no appendices. Each chapter is a self-contained review article on a major topic, with limited cross-referencing to other chapters. Each was written by one to six experts drawn from the targeted technical disciplines. The total number of contributors is about fifty, with some authors contributing to more than one chapter. The book is aimed at the upper postgraduate and professional levels (the preface says that and I concur).


AQUEOUS SYSTEMS AT ELEVATED TEMPERATURES AND PRESSURES
Physical Chemistry in Water, Steam and Hydrothermal Solutions
Donald A. Palmer, Roberto Fernández-Prini
Allan H. Harvey | Editors

What this book mainly addresses is well summarized by its subtitle, *Physical Chemistry in Water, Steam and Hydrothermal Solutions*" Most of the chapters emphasize the measurement of thermophysical or thermodynamic properties and the theoretical interpretation thereof, much like the classic Robinson and Stokes (1965) *Electrolyte Solutions*, though the present work is more inclusive of the vapor phase. In addition to discussions of rigorous theoretical framework, there is also plenty of discussion of approximate representations exemplified by Pitzer's equations for aqueous electrolytes and the HKF equation of state for the aqueous ions. Thus, there is plenty of material here for both experimentalists and modelers. The book does not stop here. Other chapters address such topics as stable isotope partitioning, kinetics, solubility, surface adsorption, and phase equilibria. Only the final two chapters are oriented toward specific end applications, Dooley et al., *Water chemistry in commercial water-steam cycles*, and Suchanek et al., *Hydrothermal synthesis of ceramic materials*. Despite the lack of any chapters specifically devoted to geochemical applications, the book as a whole shows the influence of geochemists in this field of endeavor, and most of what is in the book is applicable in geochemistry.

The book is physically appealing with an attractive hardcover and excellent, very readable printing on high-quality paper. It weighs in at 3.4 pounds and 725 pages. It packs a lot of content. The editorial team did an outstanding job editing the contributions, or perhaps they just chose well in picking contributors. The book has a nearly seamless feel to it, despite the numerous contributors. As review articles, the chapters are uniformly very high quality, very readable, summarizing the current states of their topics and offering useful judgments. Most include a large number of references, which readers will find useful. This book is not a handbook (no steam tables, for example), but it does include a lot of useful data that is less likely to be found in an engineering handbook.

So what's not to like? My main criticism is that it is not as easy as it should be to find things in this book. The table of contents only gives the chapter titles and authors. It would have been more useful had it included sectional titles or subtitles to a first or second level. Suppose you wanted to bone up on pH at elevated temperature. Where would you go? The answer is Chapter 11, Lvov and Palmer, *Electrochemical processes in high-temperature aqueous solutions*. That isn't very obvious from the title, which in this instance probably should have been *pH in high-temperature aqueous solutions*, given the chapter's actual focus. You could readily find this material using the index, but that strikes me as a step that shouldn't be necessary. Another one: suppose you wanted to check out models for activity coefficients of aqueous ions? The answer to that one is Chapter 8, Simonson and Gruszkeiwicz, *Solute concentration effects on reaction thermodynamics in steam cycle fluids*. Here the main title is appropriate given the overall focus, but the index is less helpful in pointing to this material. This illustrates that the sectional titles should have been included in the table of contents.

Given the explosive growth of information on this topic in the past decade, the appearance of this book is very timely. However, that growth has also made it difficult to produce a single volume (even at 725 pages) that is as comprehensive as one might desire. I commend the editorial team for the nice balance that has been struck, but feel I should note for the reader's sake that in my opinion at least a few areas could have used more extensive treatment. For example, the discussion of activity coefficient models for aqueous ions in Chapter 8 seems overly limited to me, and this probably should have been the subject of its own chapter. Various models used in geochemistry and chemical engineering are discussed, but I found it glaring that some of the models now receiving a lot of attention in the chemical engineering literature (e.g., Mean Spherical Approximation and Extended UNIQUAC) are not mentioned.

Only one chapter (5, Seward and Driesner, *Hydrothermal solution structure: experiments and computer simulations*) makes a significant connection to the world of molecular dynamics and *ab initio* calculations. I would like the book to have included more on this topic. At my institution I periodically run into colleagues who do those sorts of calculations, and when I explain how I need data from new measurements (as for Pitzer interaction parameters at high temperature), they smile indulgently and say that such measurements are now obsolete and we can now calculate everything. It would appear that this is not quite so, as I cannot seem to find the relevant data, which you would think someone would have calculated by now and published somewhere. A good review of the state of the art here (what has been done, what can be done now, what problems need to be overcome) would be welcome indeed.

Despite these few points of criticism, I enthusiastically recommend adding this volume to the bookshelf or library of any geochemist interested in the physical chemistry of aqueous solutions. It is a valuable, up-to-date reference book on a breadth of topics on the physical chemistry of aqueous solutions, and most any of the review article chapters can make for a pleasant evening of technical reading.

Thomas J. Wolery
Environmental Sciences Division,
Earth & Environmental Sciences Directorate,
Lawrence Livermore National Laboratory

MEETING REPORT

SPECIATION AND TOXICITY CONFERENCE LONDON, UK

13-14 SEPTEMBER, 2004

A successful meeting on the theme of 'Speciation and Toxicity' was held at the Research School of Earth Sciences at UCL-Birkbeck on the 13th and 14th of September 2004. The meeting was sponsored by the Geochemical Society (via the GS MAP fund), the UK Mineralogical Society, The Environmental Mineralogy, Applied Mineralogy and Geochemistry Groups of the Mineralogicial Society, the Society of Environmental Toxicology and Chemistry (SETAC) and CAMLAB.

Ecotoxicological studies are concerned with determining structural and functional changes in ecosystems under the influence of environmental chemicals, which include mineralogical and geochemical species, in water, soil, sediment and air. The toxicity of these species varies according to the nature of their complexing agents, solubility, oxidation state, co-ordination environment, and other factors. This meeting brought together geochemists, mineralogists, biologists, ecologists and toxicologists to discuss these issues and identify avenues for future research and collaboration. Sixty-three participants and 8 keynote speakers (total of 71 people) attended the meeting.

The three main meeting themes were:

1. Speciation. Studies on the mineralogical and geochemical properties of toxic species, and measurement and monitoring.

2. Ecotoxicity. Studies on the fate and effects of toxic substances on organisms, especially on populations and communities within defined ecosystems, and methods of monitoring and measuring these effects

3. Integrated Studies. Studies linking toxic element mineralogical and geochemical speciation with toxicity to plants and biota (including humans).

The meeting was structured around eight keynote addresses on speciation and toxicity. The speakers were John Duffus (Edinburgh Centre for Toxicology), Willie Peijnenburg (RIVM, The Netherlands), Jerome Nriagu (University of Michigan, USA), Peter Goering (US-FDA), Bill Davison (University of Lancaster, UK), Vala Ragnarsdottir (University of Bristol, UK), Iain Thornton (Imperial College, University of London, UK) and Sean Comber (WRC-NSF, UK). All speakers gave excellent 45-minute presentations that were enthusiastically received, and generated many questions.

A plenary poster session was held in the afternoon of the first day of the meeting. Over 35 posters were presented, including 14 student posters. The latter were judged by the 8 keynote speakers, and a prize of £80 of book tokens was awarded by Dr Graeme Paton, Vice President, SETAC-UK (Society of Environmental Toxicology and Chemistry) on Tuesday 14th September AM, to the best student poster (Imad Ahmed from the University of Nottingham, UK).

Workshops were held in the afternoon of the second day of the meeting. Three groups were formed to discuss (1) determining toxicity in the field, (2) how do we set regulatory limits for contaminants in soils and (3) measuring speciation. The notes generated from these discussions were compiled and sent to all registrants.

A special issue of *Mineralogical Magazine* on the meeting is currently being prepared. Feedback from participants was extremely good, and we hope the meeting will generate future research, discussion and collaboration in this area. We are very grateful to all our sponsors for support of the meeting.

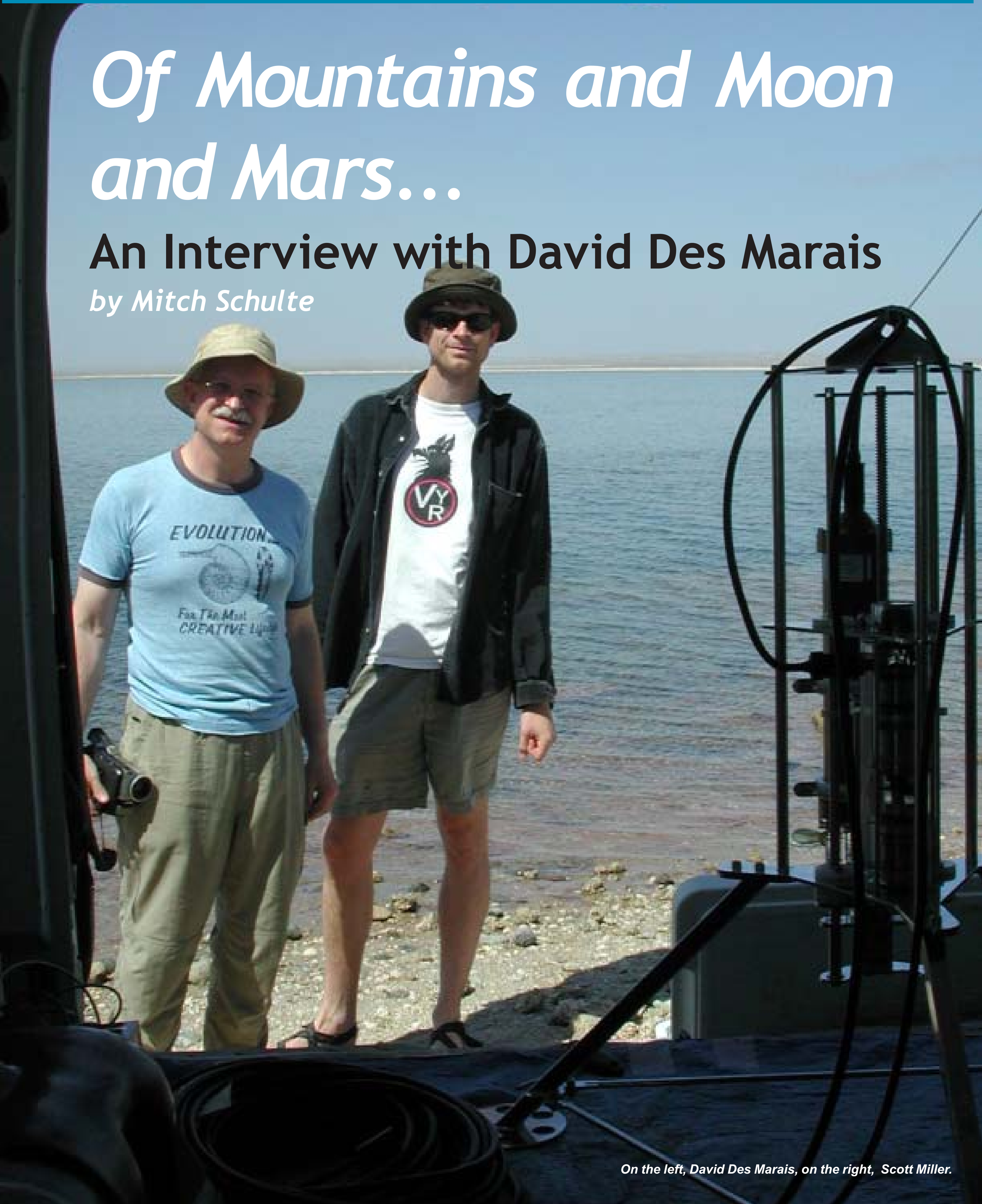
Karen Hudson-Edwards
Birkbeck, University of London, UK

Mark Hodson
University of Reading, UK

Of Mountains and Moon and Mars...

An Interview with David Des Marais

by Mitch Schulte



On the left, David Des Marais, on the right, Scott Miller.

Dr. David Des Marais is a research scientist at NASA Ames Research Center in Moffett Field, CA. He is a fellow of the Geochemical Society and the European Association of Geochemists and a member of the science definition team for the Mars Exploration Rovers. He received the H. Julian Award for best scientific paper at NASA Ames for the year 2000. He was instrumental in the development of the Astrobiology program at NASA and was the chief architect of the most recent version of the Astrobiology Roadmap, which serves as the science definition for the program. He has served as associate editor for *Geochimica et Cosmochimica Acta*, the *Journal of Geophysical Research – Planets*, and *Biogeochemistry*. He currently serves on the editorial boards of the journals *Geobiology* and *Astrobiology*.

Dr. Des Marais was interviewed on September 1, 2004 in his office at NASA Ames by Geochemical News Associate Editor Mitch Schulte.

MS: OK, the first thing I like to do is start with a person's background to give people a sense of where you're coming from, so what is your undergraduate degree, where is it from, what is your graduate degree, where it's from, whether you did any postdocs, who you worked with during your graduate [school] years and undergraduate, undergraduate if appropriate and then if you did a postdoc, or whatever. So... if you wouldn't mind just, you know, filling us in on where you've been to school.

DD: My undergraduate degree's in chemistry from Purdue University. While I was there... probably in my sophomore year, is when I first got interested in geology. And that's because I was involved in the outing club, and one of their activities was to go into caves in southern Indiana.

MS: Good part of the world to be a caver, right?

DD: Exactly. I'm sure having spent time in Missouri, you know what we're talking about.

MS: Sure, yeah. Well, we of course used to keep beer [in them].

DD: Oh, did you? If 55º F is what you like your beer at, it's the thing to do. I stayed with chemistry and got that undergraduate degree. I got accepted into Indiana University and did a Ph.D. there in geochemistry and my thesis project addressed the carbon, nitrogen and hydrogen in lunar samples. I worked with lunar soils and rocks.

MS: So this must have been early 70s?

DD: I got my degree in '74. But the research group of John Hayes, who was my thesis advisor, was into biogeochemistry so I got exposed to that also. The geobiology was happening all around me while I was doing the lunar work. I stayed on there for a year after the degree to add carbon isotope measurements to my thesis project on the lunar materials. And that's when I got into developing technology for microanalysis for isotopes. We developed the methods to analyze submicromolar amounts of carbon or nitrogen. Of course I was motivated to develop this to perform the lunar analyses, but it also became a method that John and others used until small lab computers could support the new GC-IRMS methods that John and others later developed. Then I became a postgraduate research fellow at UCLA with Ian Kaplan, an early pioneer in biogeochemistry, [especially with regard to] sulfur, microbiology, and, frankly, a lot of things! [Laughs] Ian was also involved in lunar analyses. I continued to develop an interest in biogeochemical cycles, because Kaplan was a pioneer in the microbiological and oceanographic aspects of the cycles. I came to [NASA] Ames in 1976 and was then able to pursue a variety of aspects of carbon biogeochemistry.

MS: Well, let's continue the story. The first thing I was going to mention was that you're perhaps best known for your work on biogeochemical cycles and how they've changed or evolved through Earth's history. Why is it particularly important to know that, and what kinds of things does that tell us?

DD: Basically in those years, and then later, I was involved with the geochemistry of carbon in igneous rocks, in [the] mid-ocean ridge (MOR) system. That was an outgrowth of the lunar basalt [and] regolith work that I had done. Jim Moore (U.S.G.S.) and I found that the primary carbon in MOR basaltic glasses was remarkably uniform along the ridge system. In 1984, we published the first accurate estimate of the global flux of carbon from the mantle into the deep ocean. We achieved this by relating our carbon measurements to the mantle ^{3}He flux. At that time I also got interested in carbon isotope fractionation by microorganisms. Neal Blair was the first postdoc in my lab; he is now on the faculty at North Carolina State. He examined isotope discrimination by *E. coli* and heterotrophic bacteria in general. I joined the Precambrian Paleobiology Research Group (PPRG), led by Bill Schopf,. The first PPRG project occurred in the late 1970s, and led to that incredible 1983 book "Earth's Earliest Biosphere. " That project got me very much involved in the sedimentary rock record and carbon isotopes. We addressed the ways that life interacts with its planet, including the biogeochemical cycles of those elements that are important for life. Carbon is important in many ways: life, atmospheric greenhouse effects, pH buffering, mineral stabilities, magmas, and more. Carbon provides a perfect focal point for studying how the biosphere interacts with the host planet. The significance of the biogeochemical carbon cycle for astrobiology is that it allows you to relate planetary processes in a very fundamental and broad way to potential biospheric processes, not only on Earth but maybe elsewhere. We can infer more about how other rocky planets might function from a planetary [or geochemical] perspective than we are able to do from the biological perspective. Given that that the geologic processes of the Earth probably affected strongly the evolution of our biosphere, our understanding of these processes can assist our search for evidence of life elsewhere.

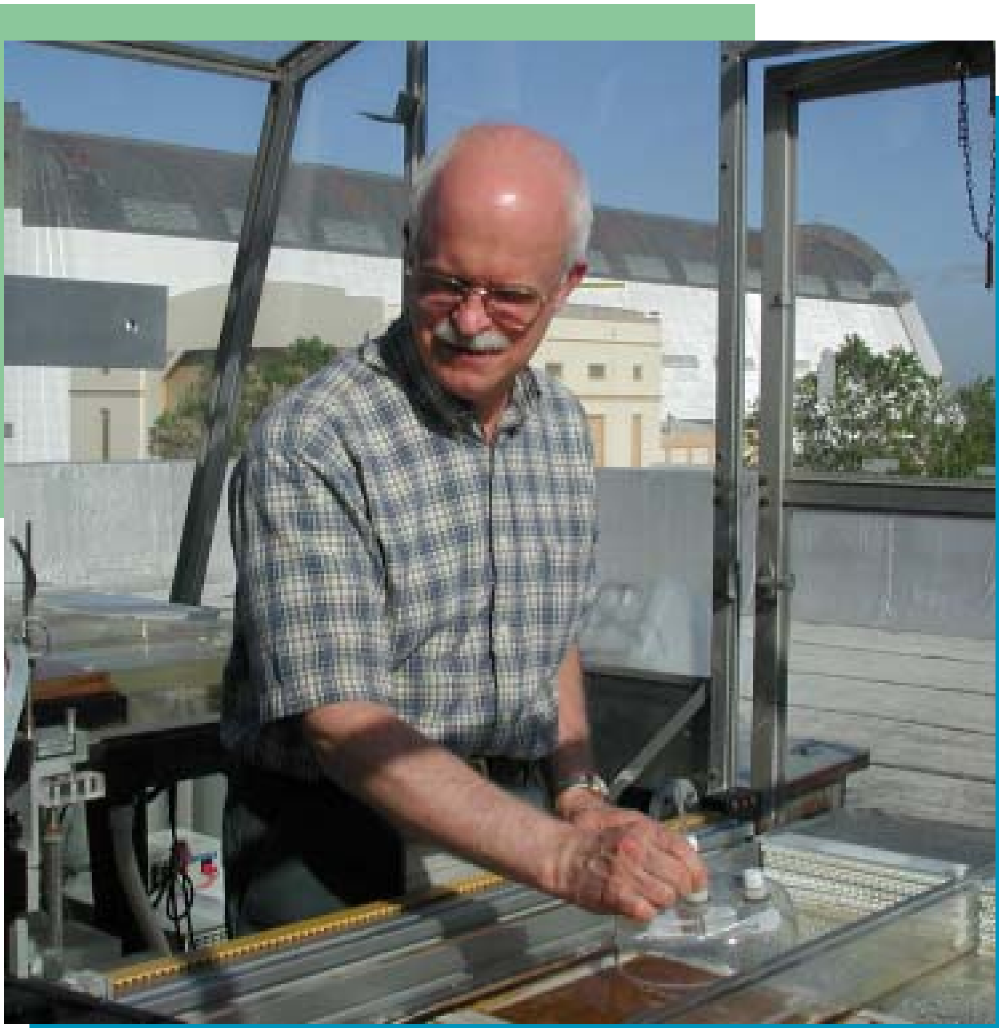
MS: There's some controversy that's developed lately about the validity of using [the] carbon isotope record to establish [the] biogenicity of organic material, especially on the early Earth [where] the record's largely been skewed. I'm thinking in particular of the recent controversy over the Steve Mojzsis paper in which he claims to have demonstrated that the carbon he's found in rocks from Akilia [Island] in Greenland are firm evidence of life at 3.8 billion years [ago]. Is there room for figuring [that] maybe this isn't quite as definitive as we thought that it is?

> *"I am part of the sea and stars*
> *And the winds of the South and North;*
> *Of mountains and Moon and Mars,*
> *And the ages sent me forth!"*
> *- Edward H.S. Terry*

DD: The fundamental value of carbon isotopic patterns is that they provide insights as to which key processes have been involved in the formation of geological materials. And these include both nonbiological and biological processes. I started my career by addressing abiological processes involving carbon in lunar samples.

MS: It doesn't get any more abiologic than that!

DD: Probably not! Another important perspective that came out of [the initial work we did in mid-ocean ridge basalts] is that some of the isotopically light carbon that people were seeing in the basalts was probably just contamination; that carbon did not come from the mantle as some had thought. So I have tried to remain objective about what the isotopes are telling us. Now when you look at more recent rocks, especially in aqueous sedimentary environments, the evidence for biological control of isotopic patterns is pretty overwhelming. As you go back in time, the evidence of life moves inexorably towards a kind of gray zone because geological processes start to obscure the biological signals. Also, if you could explore back in time to the transition between prebiotic chemistry and life, by definition you're going to be in a very ambiguous situation if you try to evaluate the former presence of life. I would contend that even if these light isotopes that we see in the early rocks turn out to be not conclusively biological, they may tell us about non-biological processes that are of significance to life's development. I don't think that the Fischer-Tropsch mechanism is very relevant to the early rock record because the oxygen fugacity of virtually all crustal materials was too high. But perhaps various other kinds of abiotic processes might offer insights about the origins of the organic matter that led to life. So I think if we just use isotopes as a window into processes and try to entertain a variety of possible scenarios, we will eventually figure out what the early carbon isotopic record is trying to tell us.



"Understanding the origins of life is the ultimate scientific challenge. We will probably have to discover a lot more about the nature of life and its host planet(s) before we will comprehend how life began."

MS: That brings up Bill Schopf's fossils, alleged microfossils apparently now. So there's controversy surrounding that now too. It would be interesting to hear your opinion about [that] controversy.

DD: Well, first I must admit is that I have not personally studied those rocks and looked at those features.

MS: Fair enough.

DD: So everything you hear here from me is a second-hand opinion at best. Some of the features that Bill has reported from those rocks look very biological to me, in particular the long filaments that are about one micron in diameter. Those don't seem to be discussed nearly as much during this controversy, if at all, in contrast to the larger elongate features that exhibit segmentation. What is good about a controversy is that people get motivated and they go out and they do things. The debate about the Allan Hills meteorite ALH84001 is a great example of that. Bill had told me a few years ago that he was disappointed that there wasn't more follow-up work by others in the years after he and Bonnie Packer published the Apex Basalt microfossil study the early 1990s. I imagine that Bill doesn't enjoy ALL of the reasons why there's a lot of follow-up work today on those Archean microfossils, but the point is people are looking at that field locality and we're going to learn a lot from it.

MS: So do you think that we'll ever actually really figure out when life started? Is that sort of an irrelevant question for a lot of what we're talking about?

DD: Well, my first reaction when Bill first came out with these reports on these fossils in the early '90s was that we probably wouldn't, because the rock record doesn't go back far enough in time to preserve evidence of the origin of life. One of the motivations for going to Mars is that we actually might find deposits that did witness the origins of life, or at least did witness earlier stages of life than what the Earth's rock record has preserved for us. It might well be harder for us to understand how life began on the Earth than to understand how life can begin as a general phenomenon elsewhere in the universe. If life began prior to 4 billion years ago, and especially if it moved around from planet to planet, the Earth might be one of the [least] prospective places for understanding that early history. Then, of course, if you find evidence of life elsewhere in the solar system, the big question is, does it share a common origin with life on Earth? In which case, asking how life began on Earth just might be the wrong question because life didn't begin on the Earth! Understanding the origins of life is the ultimate scientific challenge. We will probably have to discover a lot more about the nature of life and its host planet(s) before we will comprehend how life began.

MS: Let's move on to something perhaps more tractable with which you've also been associated. You've been working with photosynthetic bacterial mats, for example, and how [they] relate to the rise of oxygen. When did oxygen become a significant factor in Earth's atmosphere?

DD: Oh, I'd say for sure oxygen was a significant component in the Earth's atmosphere by 2 to 2.1 billion years ago. Oxygen probably was becoming a major constituent between 2.4 and 2.1 billion years ago. Thus oxygenic photosynthesis exerted a major geochemical impact during the Paleoproterozoic and it left its mark on the carbon isotope record. We showed that the long-term net oxidation of the surface environment probably occurred in a step-wise fashion.

MS: So what do the studies of the [microbial] mats tell us?

DD: The important thing about microbial mats is that they represent an ecological lifestyle that goes back billions of years. The analogy for terrestrial plant ecosystems would be tropical rainforests, which have been remarkably stable for millions of years and which therefore have developed and maintained incredible biological diversity. At high latitudes, climatic disturbances [and] movements of continents created instability. There, animals and plants live much closer to the edge of oblivion. Photosynthetic cyanobacterial mats are the original example of durability and incredible diversity, having developed though billions of years of evolution. Such mats are important to study; first because they are billions of years in age. The biosignatures you find within living mats are excellent potential examples of biosignatures you might expect to find in ancient rocks. Microbial mats might reveal biosignatures that we hadn't even thought to look for in the rock record. Another important perspective is that the mat environment probably hosted major evolutionary developments. These might include the development of photosynthesis and the subsequent diversification of ecosystems that probably was triggered by the huge increase in productivity associated, first from the rise of anoxygenic photosynthesis, and, later, from the rise of oxygenic photosynthesis. Perhaps the radiations within the bacterial lineages that we infer from the ribosomal RNA "tree of life" might be tied to the rise of photosynthesis. And maybe those major events actually occurred within photosynthetic microbial mats. We may find new evidence of ancient lineages in these mats, or at least information that helps us to reconstruct ancient lineages that will be incredibly important for learning how life actually developed over billions of years. These mats probably contain

This Mars Global Surveyor (MGS) Mars Orbiter Camera (MOC) image shows erosion gullies likely formed from geologically young groundwater seepage out of the walls of a Noachis Terra impact crater. Photo credit NASA.

living evidence of early evolution that is much more accessible and much more diverse than you can hope to find anyplace else.

MS: So that was a significant event in Earth's history, or at least the history of life on Earth, because [there was] a consortium of microbes that figured out how to photosynthesize. And that's responsible for a lot that's happened since.

DD: I think there were lots of major consequences, even for anaerobic microorganisms. I once asked Bill Reeburgh, who [is an] expert on methane biogeochemistry, how he thought methanogens would respond to long-term evolution of the biosphere. Bill responded that, even though molecular oxygen is toxic to methanogens, the rise of oxygenic photosynthesis probably greatly increased the rate of methanogenesis. This is because oxygenic photosynthesis created a huge source of electrons for methanogens to utilize. Methanogens had to avoid the oxygen, but [there was suddenly] so much organic matter being created. Before sulfate [accumulated] in the oceans methanogens could have been a major sink for all of the electrons provided by oxygenic photosynthesis. And so even obligate anaerobes like methanogens could have diversified because of oxygenic photosynthesis. So, when Victoria Orphan was an NRC fellow with me at Ames, she investigated methanogens in hypersaline mats. Methanogens are indeed present, even though cyanobacteria produce oxygen in there and the mat pore waters contain abundant sulfate. This kind of work could lead to some important insights about early evolution.

Microbial mats can defy our intuitions. When Don Canfield was working in my lab in the early 1990s on the cyanobacterial mats from Baja California, he discovered the highest rates of bacterial sulfate reduction ever measured... and in the oxygenated layers of the mats! The microbial sulfate reduction process is "supposed" to be inhibited by molecular oxygen, so some kind of ecological effect is in play here. Our lab and others also have shown how the microenvironments within mats are very different from the surface environment. Their characteristics have been important for their microbiota for billions of years. And we have a lot to learn about them.

These mats provide a guide to the biosignatures that we might seek in the rock record. And mats retain a living record of early evolution. The dynamics of the mat ecosystem also provide a template for understanding the roles of microorganisms in our modern biosphere. These microbial consortia are very accessible and amenable to studies of symbiotic relationships between organisms.

MS: This is a good place for geochemistry to come in because obviously it's the environment that these things are living in and what kinds of microenvironments they're creating [for] themselves that [allows them to thrive].

DD: Thanks for reminding me about how we can get back to carbon isotopes with that because isotopes really are an emerging property of an ecosystem. Interactions between organisms give rise to the isotopic patterns that one sees. As we now go back and try to figure out how to interpret isotopes in the rock record, we have to remember that there's a major ecologic component to the patterns that we see. [We have to] interpret that component once we have some sense about how it works in ecosystems where [we have] a more complete picture of the processes involved.

MS: Let's [talk about] what's consuming your life these days, which of course is the Mars Exploration Rovers (MER). You've been a big part of the science team for [which of them]?

DD: Principally for Spirit at Gusev crater.

MS: What are we finding out about Mars from these rovers, that you can talk about right now without letting any cats out of the bag?

DD: Well, let's just start at Viking and [then get into] what [the] expectations were going into MER and then where we are now. Viking went to Mars with the idea [that] you just land anywhere on the surface [with] this wonderful array of instruments, all you have to do is reach out with the arm and pull up stuff and, my gosh, maybe you'll find organic matter, maybe you'll even find organisms living on the surface. Now, of course, we all know in retrospect that was, quite bluntly, very naive.

DD: I think it's also interesting to [note] that Chuck Klein [Editor's note: Chuck Klein was the science lead for the life detection experiments on the Viking mission] realized that searching for life was a long shot even before the mission began. But Chuck felt that we'd learn a lot just by being on the surface and that all in all it was an adventure well worth the effort and cost. But Viking basically told us that we weren't going to find evidence of life or even learn much about liquid water just by examining unconsolidated material that we would access just by touching down on a [random] spot. The MER mission demonstrated that the basic techniques of the field geologist provide an excellent template for the design of a spacecraft that explores the surface of Mars.

MS: [Didn't that] start with Pathfinder?

DD: Yes. The central objective with Pathfinder was to develop and verify a robust entry, descent and landing (EDL) system. Interestingly, the Pathfinder EDL system was probably more amenable to visiting rocky landing sites than Viking was because the Pathfinder air bags were somewhat resilient to an encounter with a rocky surface. And Pathfinder cost a lot less than Viking. Of course, the little Sojourner rover was the other significant attribute of Pathfinder. But MER really represents a huge step beyond the Viking lander because MER deployed a pretty comprehensive set of capabilities of a field geologist. And MER focused upon a more attainable goal, namely search for and evaluate the evidence for liquid water on Mars.

MS: That is the primary stated goal.

DD: Exactly. Part of the reason that the Viking lander didn't find evidence of life or liquid water was that the samples analyzed by the lander were unconsolidated surface materials whose properties were shaped largely by modern environmental processes (impacts, volcanism and aeolian activity). These processes have acted to obscure or destroy any evidence of liquid water and life that might have existed. Those materials that could be reached by the fixed lander were so extensively altered by recent energetic processes that Viking did not have a chance to answer questions about life or liquid water. MER was a step beyond Viking in two respects. One is the "field geologist" capabilities of MER that I just alluded to, and secondly the goal set for MER was far more realistic. Let's not look primarily for life in the first stages of exploration. Let's first look for evidence of a very important attribute of habitable environments, namely liquid water. If we can establish how liquid water chemically altered martian crustal materials, then we have gained a much better perspective about the potential for life-sustaining environments. Therefore we are better prepared to take that next step to look for evidence of life. The success of MER is a classic example of the importance of a sound intellectual approach.

MS: If you had your pick of a single instrument to fly to Mars, what would it be? That we haven't flown already.

DD: I'd vote for an instrument that can really provide a comprehensive and definitive assessment of the minerals in the rocks and soils.

> *"[Microbial] mats probably contain living evidence of early evolution that is much more accessible and much more diverse than you can hope to find anyplace else."*

You would learn a lot about martian crustal evolution, and you'd learn a lot about water and habitability considerations. Mineralogical assemblages record evidence of the processes that created them. A visible-near IR camera is incredibly valuable. The MER panoramic camera accounts for, and I'm probably being conservative here, over 90% of the data volume of the MER mission. But beyond that, being able to do definitive mineralogy I think is really good. Now of course we also think about the rovers' wheels and other mechanical devices as instrument of a sort. Measured motor currents help us to understand the physical properties of surface materials. But your question I think is more like where would we go beyond MER.

MS: Right. [Would you say] XRD?

DD: I've been trained pretty [well], as you know, not [to] mention specific instruments, just measurement capability. [Laughs]

MS: Now if you could put a mass spec[trometer up] there!

DD: Well, that's the other one. But see, even there, I would focus on the measurement. We need the capability to analyze volatile constituents in the broadest sense, which would include organic matter and also non-organic volatiles.

MS: [That's] very diplomatic.

DD: Yeah, [laughs]. But I have to agree that XRD and mass spectrometry are excellent examples of the kinds of capabilities that we really haven't put on a rover yet and which would be an important step for the next mission to take. Capabilities like that are pricey, but they are essential for the next stage of exploration.

MS: How hard is it to convince people to put "the right instruments" on these missions?

DD: I feel that the community has bought into the idea that you need a strong capability for mineralogic identification and a strong capability for volatile constituent identification. If a single instrument, such as a mass spectrometer, can analyze the volatile and organic constituents, then so much the better. The instruments on MER that have had the greatest impact are the ones that are really the most versatile in their application. When you're dealing with a resourceconstrained environment, that kind of versatility coupled with sensitivity is critical.

MS: How important would it be to bring a sample back? Would that be worth the expense rather than trying to figure out how to get a mass spec flown there?

> ***"I think the experience I've had in looking at biogeochemical cycles of carbon and other elements has helped me to grasp the breadth of astrobiology and to contribute to the Mars mission.***
>
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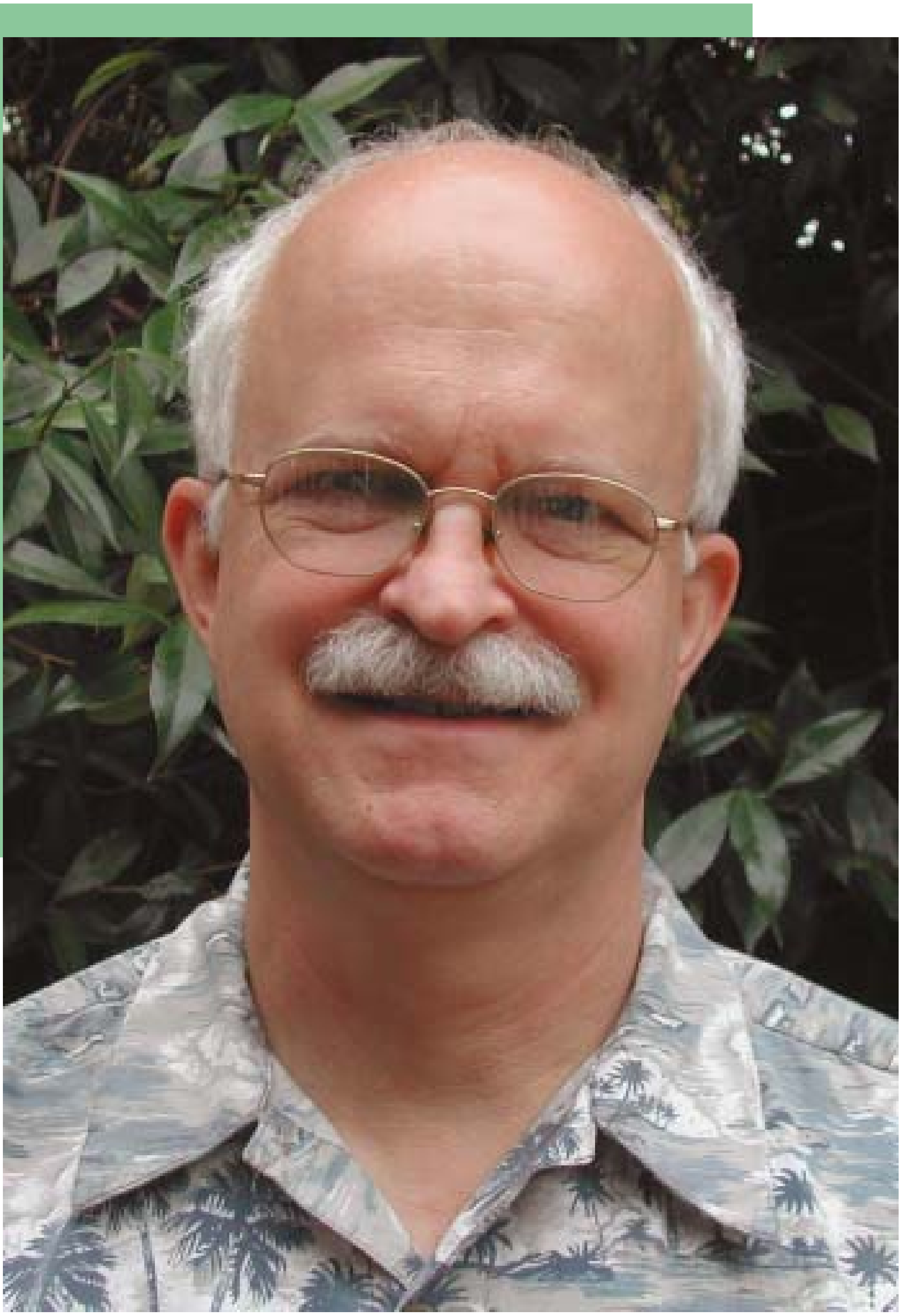

DD: Well... bringing a sample back just takes you to a whole new level of capability.

MS: How close are we to being able to do that?

DD: It's largely a financial consideration. I don't think anybody has shown yet that we can do a sample return mission for less than $2 billion. We just did the two rovers on Mars for about $840 million. Another key question with sample return then is how good do you want your sample [to be]? I think it's fundamentally important that we usea rover to collect the returned samples because we must move around to collect samples worthy of the great expense of the mission. On one hand there's the quality of the instruments that you can bring to bear on the samples, which is undeniably important and of course returning the samples gives you the ultimate quality of instruments. But then there's the quality of the samples [chuckles]. The significance of the mission depends upon product of the quality of the samples that can be accessed and the quality of the instruments that determine which samples are the most valuable candidates for sample return.

MS: You want to be able to take a look around before you decide what to pick up.

DD: Exactly. If there's been one fundamental lesson from MER it's been how crucially important the roving capability has been for both spacecraft. Even in Eagle Crater if you couldn't have roamed you couldn't have been able to visit the key features of that outcrop that was visible from the lander... [that would have been] extraordinarily frustrating. So I think MER has set the standard for what you have to do when you go to the surface, at least to pursue questions for astrobiology, anyway. The 2007 Phoenix mission will land at a higher latitude. Phoenix is a stationary lander but that is fine because it is fundamentally a climate mission. The next steps in martian climate and atmospheric science can be done effectively without a rover.

Climate is one of the major aspects of Mars exploration and so it can stand alone on those merits. But an astrobiology mission to the surface of Mars requires rovers. Even with the rovers on MER, we've had to be creative and really iterate with the rovers' capabilities to get past this "prison of the present," namely the obscuring effects of impacts, volcanism and aeolian processes. So the spacecraft must mimic a field geologist.

MS: OK, well let's talk for a minute about what these missions have told us so far. We've of course all seen the press conferences where people get all excited about things, but in a broad geological sense what is significant about what we've found out from the MERs so far?

DD: Well the first order statement there is that MER has moved us beyond observations of just geomorphology and morphology into the domain of geochemistry and mineralogy of surface materials. And so MER really represents the opening foray into a new phase of Mars exploration. To a first order the crust of Mars is basaltic.

MS: We knew that.

DD: [Laughs] Yeah, that we knew. Water interacting with basalts causes elemental separations and mineralogic changes that are characteristic signatures of water. Both rovers now have demonstrated beyond any doubt that some of the observed compositions require liquid water for their formation. The rovers have offered very different, complementary scenarios about how liquid water has altered the martian crust. The Opportunity rover discovered rocks that represent an outcome of a weathering, erosion, and deposition cycle, one that is very reminiscent of sedimentary rock cycles on the Earth. Perhaps we are dealing with an aqueous system that was at least the size of the state of Oklahoma, if not bigger, so, that's very important. Spirit is showing us that.

MS: A standing body of water of that scale?

DD: Yeah, and so we can probably infer the presence of liquid water acting over a fairly extended period of time. But quantitative estimates are still elusive, still TDB, as to the time and system size needed to create the chemical separations that the sulfur-rich bedrock is revealing.

MS: That's fundamentally a chemical sediment.

DD: Before the MER mission, you could observe a channel network from orbit and indeed believe that liquid water was responsible. But, for all we knew, that channel feature might have developed in a decade or a thousand years. Now, Oppoortunity is examining geochemical features that I suspect required millions of years to develop. So it's not just the fact that liquid water existed sometime in the past, however briefly. Now it appears that water might have persisted long enough to create an opportunity for life to begin or at least to survive. Spirit has found extensively altered rocks that once might have been basalts. That rover earlier identified abundant olivine-rich basalts. On Earth, water can react with olivine-rich basalts to sustain the serpentization reaction and thereby provide a chemical energy source for life. And so we have *prima facie* evidence that, even if habitable surface environments on Mars have been very rare, subsurface environments were capable of sustaining life.

The environments revealed by Opportunity resemble those on Earth that have sustained the more familiar microbial mat ecosystems that we discussed earlier. Therefore the work our group has done in coastal hypersaline lagoons in Mexico perhaps offers a very relevant perspective on the environments at Meridiani Planum. Spirit's discoveries in Gusev crater potentially represent another kind of habitable environment, one that sustains subsurface ecosystems using chemical sources of energy. Such nonphotosynthetic ecosystems represent equally viable and significant models for understanding how life might have persisted on another planet.

MS: This is kind of a silly question, but if Opportunity were to roll across a desiccated mat, would you recognize that?

DD: Potentially.

MS: Really?

DD: Possibly, because one of the features of a microbial mat that are most robust is its rubbery coherent nature. If, during the course of its growth, the mat was torn, ripped up, or folded over, it created a fabric with folded or rolled-up layers that could have been preserved as carbonized films or it could be completely replaced by minerals. It would be pretty exciting to find evidence of a fossilized flexible and coherent (organic?) film. Anyway, we're in an environment where conceivably we might find it, if it ever existed. We might find it next week.

MS: What is the schedule these days for missions to Mars? What's been approved, what's on the books and what's planned?

DD: Well, the Mars Reconnaissance Orbiter will be launched in August 2005. It has a very high capability orbital camera that will get down to just tens of centimeters of resolution. It also has an instrument, CRISM, which is [a] near-infrared mapping spectrometer. CRISM has lot of capability for looking at the finer detail of the surface for geochemical evidence of processes. There are a number of additional important instruments on this complex spacecraft.

MS: And that's strictly an orbiter?

DD: That's an orbiter. The next lander , Phoenix, will be launched in 2007. Phoenix was selected as a scout mission that will conduct climate studies at a high latitude site. The Mars Science Laboratory (MSL) mission is scheduled for launch in 2009. MSL might be the true sequel to MER in the sense that it will deliver the capabilities that we discussed earlier regarding measurements of mineralogy, volatiles and organics. Beyond that, another scout mission might occur in 2011. A scout mission opportunity is an open competition for investigators. The specific objectives of a Scout mission are deliberately not established in advance of the competition because Scout missions offer a chance for the community to create novel initiatives that augment the core Mars program.

MS: So these are all approved missions so far?

DD: Yes. Missions beyond 2011 are being actively discussed, but they are still in their conceptual stages of development.

MS: They're allowed to compete the 2011 Scout mission at this point.

DD: Well, no. The announcement for that competition will occur next year. So in a sense it's approved as an opportunity. There's been some talk about 2013 being potentially a sample return mission. The alternative to that would be something called the Astrobiology Field Laboratory, which in many respects might be an improved version of the MSL 2009 mission. We once thought it would be really great if MSL and AFL could survive for longer than one Earth-year. We thought that maybe that would be possible, but only if they are nuclear powered! [Laughs]

MS: Yes, those MER rovers have performed remarkably well just relying on the sun, haven't they? They're still kicking aren't they?

DD: They sure are.

MS: That's why you keep getting called back to JPL.

DD: That's right yeah, hopefully... [for] the next 8 to 10 months.

MS: Have they requested funding to keep them going for that long?

DD: The nominal mission was basically the first three [to] four months of this year. The extended mission was May 1st to September 30th. The proposed "extended extended" mission is October 1st to September 30th, '05. At this point (September 2004), the "extended extended" mission has been approved for six months.

There's another key point that I had wanted to make earlier. Even with the ability to move around, to dig trenches, to choose the most interesting rocks and to grind into those rocks, we have now clearly encountered samples that probably did not preserve organic matter, had it originally existed. And so the capabilities of MER might not be enough to reach organic-rich samples. We probably need a longer-range rover that can drill more deeply.

MS: Is there a target for how far we think we would have to go to find that kind of information?

DD: Well we can consider our experiences on Earth. The drill should penetrate as deeply as four to ten centimeters into a rock to really get past that alteration rind. We're finding rocks in Gusev crater that Spirit can't grind deeply enough to get past their alteration rinds. The rocks that the water has affected most extensively are the ones that are also so altered that they may not preserve organic matter. So we must step up to at least two challenges in future missions. One is to develop the ability to go deeper into rocks and the second one is to include the capability to drive far enough to visit compositionally different parts of a sedimentary basin, such as an evaporitic basin. For example, we must be able to visit the part of an evaporitic basin where silica-rich minerals were deposited. On Earth, silica can preserve organic matter very well.

MS: As you pointed out we have the same problem here in terms of preservation so doing it from millions of miles away is even harder.

DD: Exactly. So beyond MER, we have to meet several challenges if we want to study the chemistry of carbon on Mars. We still haven't characterized carbonates in martian crustal materials! And I'm firmly convinced that it's not because they're not there, it's because we haven't put it all together yet to a point where...

MS: ...We're looking in the right place?

DD: Yeah, we need to look in the right places. In the final analysis, there weren't a lot of places that MER could have gone, given the constraints imposed upon its entry, descent and landing. If we really do reduce further the size of the landing ellipse, we will have hundreds of sites to choose from, which is good. But then the Mars science community will have to come together and choose from among all of these possible sites, which will be hard!

MS: It was bad enough deciding with MER, right?

DD: It was challenging enough. But you need to choose from a menu of a hundred or more possible sites if you're going to find and access the right places. And the lessons we've learned studying the early record of the Earth will help to point us in the right direction.

DD: If I were to make a "closing statement," it's that astrobiology is mostly what I do these days and it involves a combination of microbial ecology, planetary science, and chemical and biological evolution. I think the experience I've had in looking at biogeochemical cycles of carbon and other elements has helped me to grasp the breadth of astrobiology and to contribute to the Mars mission. We're training a whole new generation of scientists who will become much more capable than we were in the interdisciplinary domain of astrobiology. What has been really great about the MER mission is that many of the hundreds of people who were involved have adopted interdisciplinary approaches in their science and engineering. And the results speak for themselves.

MS: I want to conclude with one personal item.

DD: Oh, OK.

MS: There's a picture in the hallway of you throwing out the first pitch at a Giants game. How did that happen? And what was it like?

DD: A technology exposition called NexTech is held in San Francisco every year. People present new ideas in technology. One of the key aspects is human-machine interaction. They had a number of technology demonstrations at the Giants-Phillies game to publicize the exposition. They decided to tip a hat to the Mars Exploration Rover mission, which has indeed been a successful example of human-machine interactions. They contacted Ames to invite a member of the MER team to throw the first pitch. What I found most remarkable about the experience was all of the photography and the attention. One key preparation that I made was to play a little game of catch with Mike Kubo, a colleague here at Ames, the day before the game. The distance from the mound to the plate, which is 60.5 feet, is a little further than I would normally stand to play catch with somebody. And other "first-pitch veterans" advised me NOT to throw from top of the mound, because a forward AND downward step could cause a total amateur like myself throw the [ball] in the dirt. And if the ball hits the ground before it reaches home plate, the crowd will boo. Fortunately, I was able mostly to tune out the presence of some 30,000 people. I figured that the catcher was just like Mike Kubo with whom I practiced the day before. You just throw the ball.

MS: Otherwise it's just a little more intimidating than giving a talk at a national meeting.

DD: It's interesting how that scales with the crowd size. At some point the crowd gets so big and so far away...

MS: ...that you just don't even notice?

DD: Yeah. It's not like most of them are looking at me. Quite frankly I figured that a lot of the people in the stands were chatting and drinking beer [Laughs].

MS: Well, that's what I'm doing.

DD: Yeah, that's right [laughs]. That first pitch was quite an experience. Everybody involved is very professional, even the field is impeccable. It's not an experience you can count on having in your life, but once is enough for me.

MS: Thank you again for [talking with me today].

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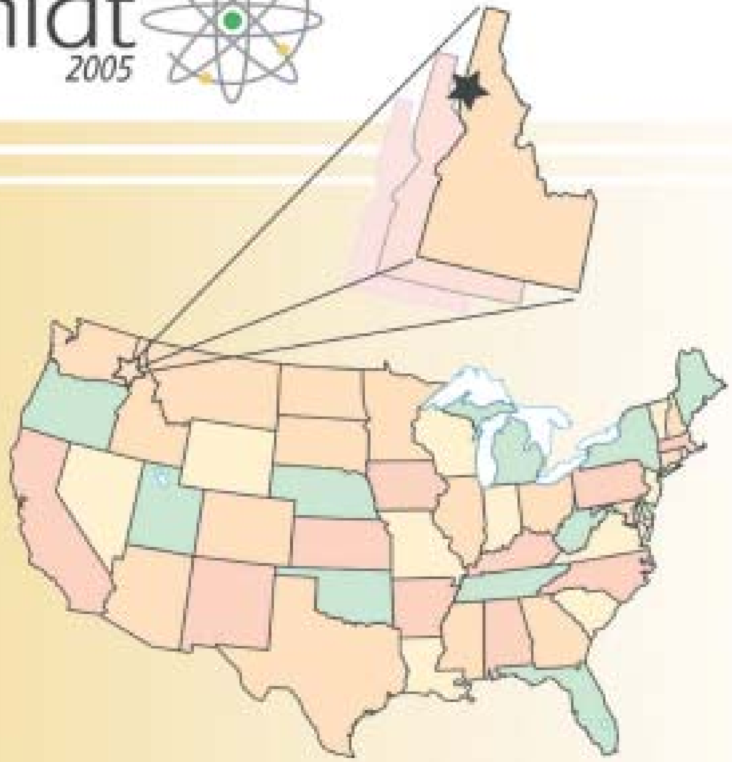
15th Annual

V.M. Goldschmidt 2005

Moscow, Idaho



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Voyage of Discovery

50th Anniversary of the Geochemical Society

Geochemistry at U. S. National Laboratories

OAK RIDGE NATIONAL LABORATORY

David R. Cole, David J. Wesolowski, James G. Blencoe, Juske Horita,
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INTRODUCTION

Oak Ridge National Laboratory (ORNL) is the U. S. Department of Energy's largest science and energy laboratory (www.ornl.gov). Managed since April 2000 by a partnership of the University of Tennessee and Battelle, ORNL was established in 1943 as a part of the secret Manhattan Project. During the 1950s and 1960s, ORNL was an international center for the study of nuclear energy and related research in the physical and life sciences. The creation of the Department of Energy in the 1970s led to an expansion of ORNL's research program into areas of energy production, transmission, and conservation. The laboratory's six major core competencies include neutron science, energy, high performance computing, complex biological systems, advanced materials, and national security. The laboratory is comprised of a number of research divisions, as well as numerous centers and institutes. Consistent with the national scientific trend of an emphasis in genetics, nanoscience, and advanced computing, ORNL is undergoing an expansion involving the completion of several new facilities including the Functional Genomics Center, the Center for Nanophase Materials Science, the Advanced Materials Characterization Laboratory, and the Joint Institute for Computational Science. Additionally, the $1.4 billion Spallation Neutron Source, slated for completion in 2006, will make ORNL one of the world's foremost centers for neutron science research.

The earliest roots of geochemical research at ORNL reach back into the 1940s and 50s in two distinct arenas; one involved issues of waste disposal, characterization of actinides in environmental systems, and radionuclide transport in both soil and groundwater environments, and the second involved the pioneering studies of the properties of high-temperature water and salt solutions as nuclear reactor coolants and geothermal energy sources. Despite the absence of a centralized Geosciences division, activities in these areas had a profound impact on waste mitigation policy/procedures and hydrothermal geochemistry, respectively. As one of the world's leading centers for experimental studies of the properties of hydrothermal fluids, including water and steam, it was inevitable that a geochemistry research program would grow from this fertile ground because water is the primary transporter of mass and energy in the crust. Similarly, a world-class program designed to quantitatively constrain the deleterious impact of toxic and radioactive contaminants on water quality and biological systems was spawned from the early pioneering efforts to assess the environmental consequences of both low- and high-level radioactive waste disposal.

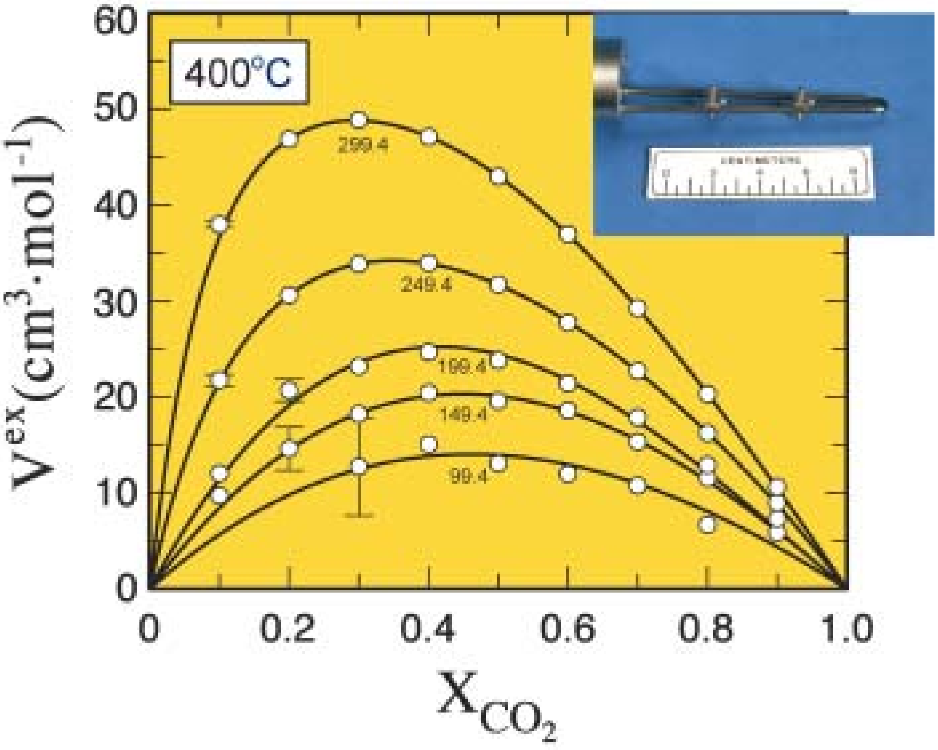


Fig. 1 Experimentally determined excess molar volumes (V^{ex}) of CO_2-H_2O mixtures at 400°C and pressures below (99.4 – 299.4 b) the critical isochore of pure H_2O. The plot symbols depict our experimental data (with error bars), and the curves represent interpolation functions used to illustrate the general trends of the isobaric data. The inset shows a close-up of the vibrating tube.

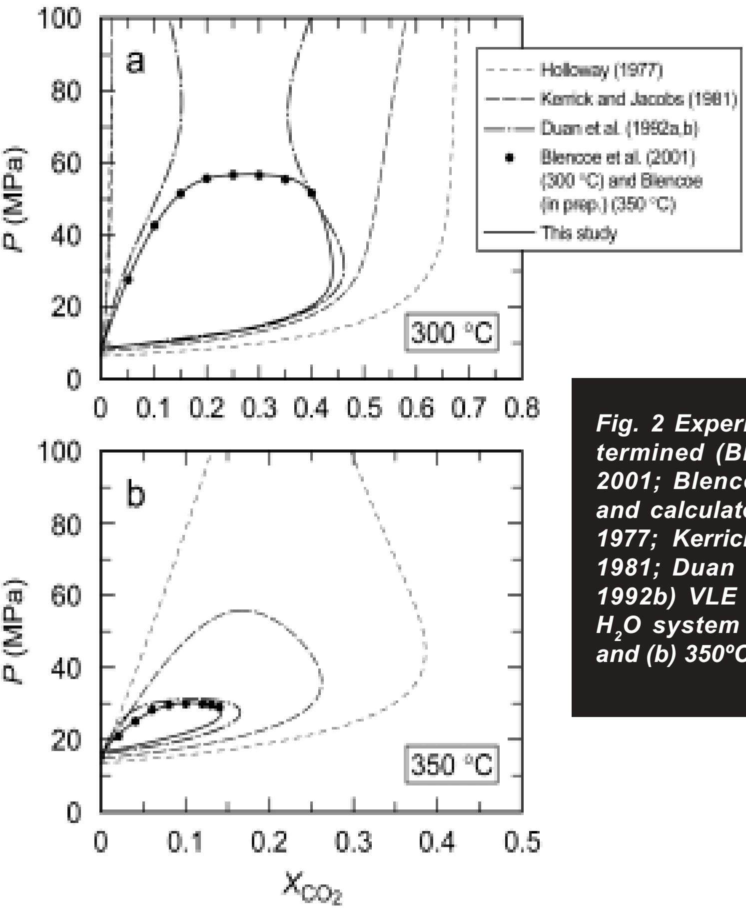


Fig. 2 Experimentally determined (Blencoe et al. 2001; Blencoe, in prep.) and calculated (Holloway 1977; Kerrick and Jacobs 1981; Duan et al. 1992a, 1992b) VLE for the CO_2-H_2O system at (a) 300ºC and (b) 350ºC.

Currently, geochemistry activities at ORNL are divided between the Chemical Sciences Division (CSD) and the Environmental Sciences Division (ESD). In CSD, the research staff focuses primarily on model systems involving complex natural fluids and their interactions and reactions with solids from ambient conditions to elevated temperatures and pressures. In this program, the effort can be subdivided into three thrust areas, each with its own unique problems and methods for addressing these problems.

- fluid-dominated processes involving complex geological fluids;
- the properties and processes uniquely associated with fluid/fluid and fluid/solid interfaces; and
- complex heterogeneous mineral-fluid reactions involving processes such as dissolution/precipitation, mineral replacement, grain boundary and lattice diffusion, and fluid confinement in nanoporous regimes.

Scientists in (ESD) focus on understanding processes and issues of importance to Earth's shallow environment and ecological systems. A subset of the Division's research portfolio can be grouped under the broad heading of Environmental Geochemistry. Research strengths in geosciences, environmental chemistry, hydrology, biogeochemistry, and environmental biotechnology are integrated to conduct research in the environmental sciences. Research efforts conducted at the lab to field scale provide a sound scientific basis for identifying problems, advancing remediation technologies, and evaluating the success of such approaches.

Below we present a number of scientific highlights from these four areas that best define the geochemistry activity at ORNL.

COMPLEX GEOLOGIC FLUIDS

Experimental studies of homogeneous aqueous chemistry at elevated temperatures and pressures has a long history at ORNL, beginning in the early days of the former Reactor Chemistry Division in the 1950's with the pioneering studies by M. Lietzke on the activity coefficients of the acid halides, the hydrolysis of cations by C. Baes, R. E. Mesmer and F. Sweeton, the vapor pressures of concentrated electrolytes by Mesmer and H. Holmes, the conductances of dilute electrolytes by W. Marshall and the high temperature heat of dilution calorimetry studies of Mesmer and R. Busey (see Mesmer et al., 1997 and references therein). This work has been continued in the Aqueous Chemistry and Geochemistry Group by physical chemists J. M. Simonson, D.A. Palmer and M. Gruszkiewicz and expanded to a very fruitful collaboration with geochemists D.J. Wesolowski, J.G. Blencoe, D.R. Cole, J. Horita and former group members S.E. Drummond and P. Bénézeth. Thus, the early interest in metal speciation and pH-control in steam generator systems has evolved into applications in geothermal energy, hydrocarbon resources, seafloor hydrothermal systems, ore deposits, CO_2 sequestration and the assessment of toxic and radioactive

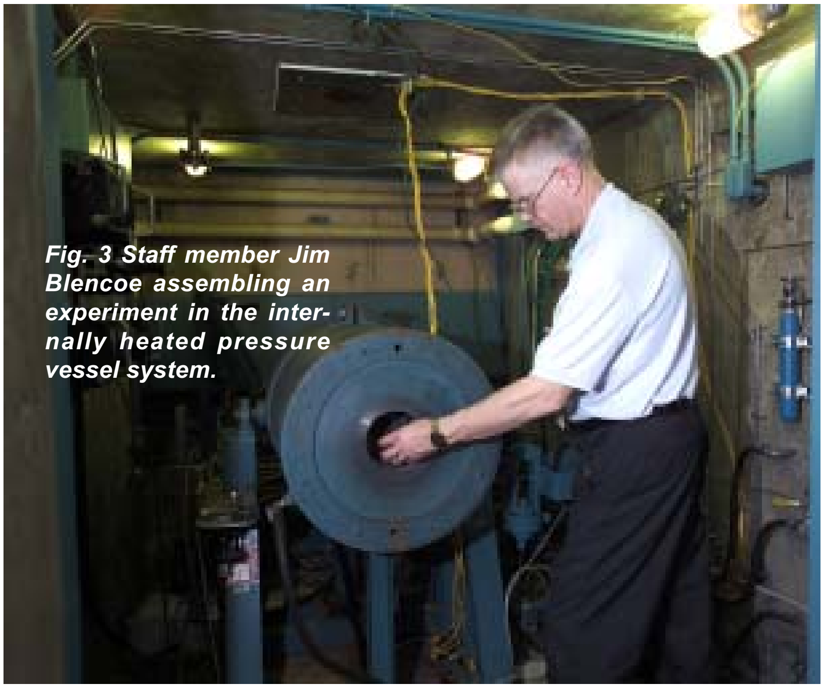


Fig. 3 Staff member Jim Blencoe assembling an experiment in the internally heated pressure vessel system.

waste disposal and remediation schemes. For a recent compilation of ORNL's high temperature aqueous chemistry and geochemistry studies and experimental techniques, the interested reader is directed to chapters in the recent book on *Aqueous Systems at Elevated Temperatures and Pressures: Physical Chemistry in Water, Steam and Hydrothermal Solutions* (Palmer et al., 2004).

The overarching goal of this thrust area is to develop a comprehensive understanding of the thermophysical properties, structures, dynamics, and reactivities of complex geologic fluids and molecules (water and other C-O-H-N-S fluids, electrolytes, and organic-biological molecules) at multiple length scales (molecular to macroscopic) over wide ranges of temperature, pressure, and composition. This knowledge is foundational to advances in the understanding of other geochemical processes involving mineral-fluid interfaces and reactions. Our approach is to interrogate the macroscopic properties and molecular-level forces and interactions of geochemically relevant fluids at representative near-surface and crustal conditions. A quantitative understanding of the causative relationships between macroscopic properties and key molecular-level interactions will impact our ability to predict more complex geochemical behavior in natural fluids over wider ranges of environmental conditions.

Thermophysical Properties:

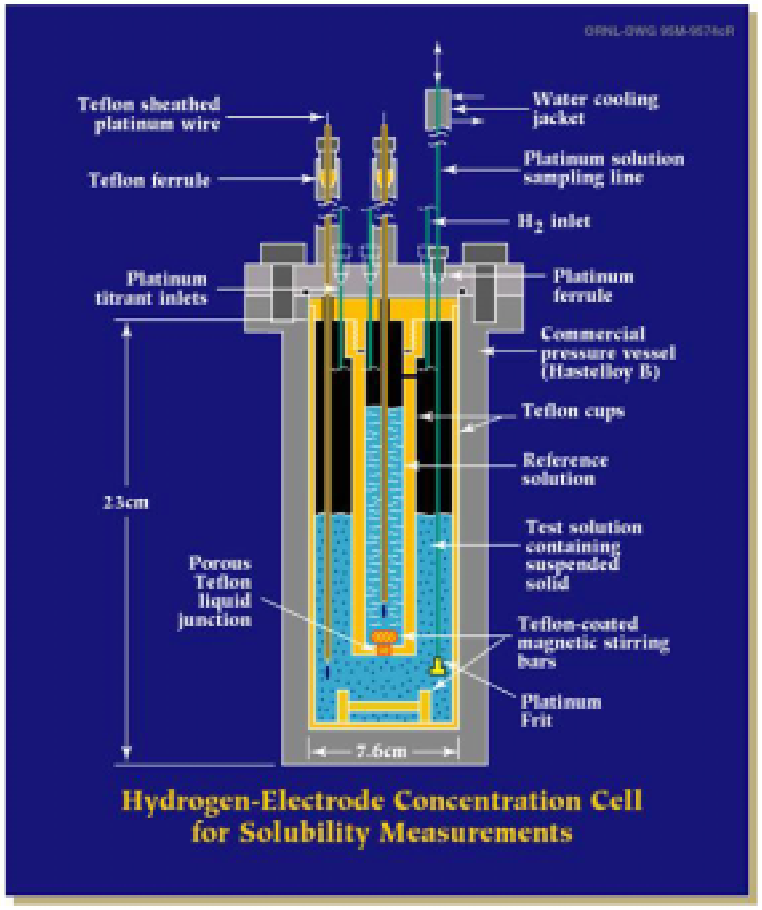


Fig. 4 Schematic of typical ORNL hydrogen electrode concentration cell configuration. A nested set of Teflon cups contain the reference solution (of known pH) and the test solution being studied. Teflon-sheathed platinum wires extend into each solution, serving as the rigorously-Nernstian electrodes. Both solutions are exposed to the same H_2 partial pressure, and there for the difference in potential is described by $DE = (RT/F)\ln(aH^+_{ref}/aH^+_{test}) - E_{lj}$ where E_{lj} is the potential drop across the liquid junction formed by a porous Teflon plug in the bottom of the reference cup. Both cups contain Teflon-coated magnetic stirring bars. One or more platinum capillary inlets are included, allowing addition of titrants from zircalloy positive displacement pumps. The cell shown contains a platinum dip tube with an in situ platinum submicron filter for removing samples during homogeneous or heterogeneous experiments.

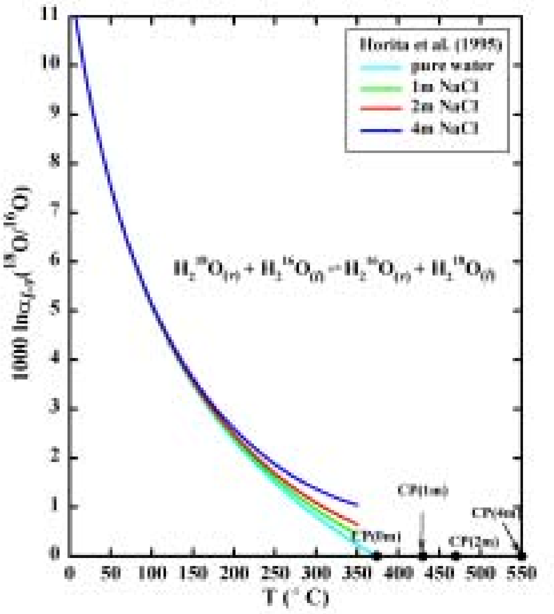


Fig. 5 The effect of dissolved NaCl on $^{18}O/^{16}O$ fractionation between liquid water and water vapor (Horita et al., 1995).

Jim Blencoe and his collaborators use state-of-the-art laboratory devices to determine the thermodynamics and phase relations of CO_2-CH_4-N_2-H_2O-NaCl fluids at elevated temperatures and pressures. Thermophysical properties and phase behavior are quantified with unsurpassed precision and accuracy. A unique, high temperature, high pressure, vibrating-tube

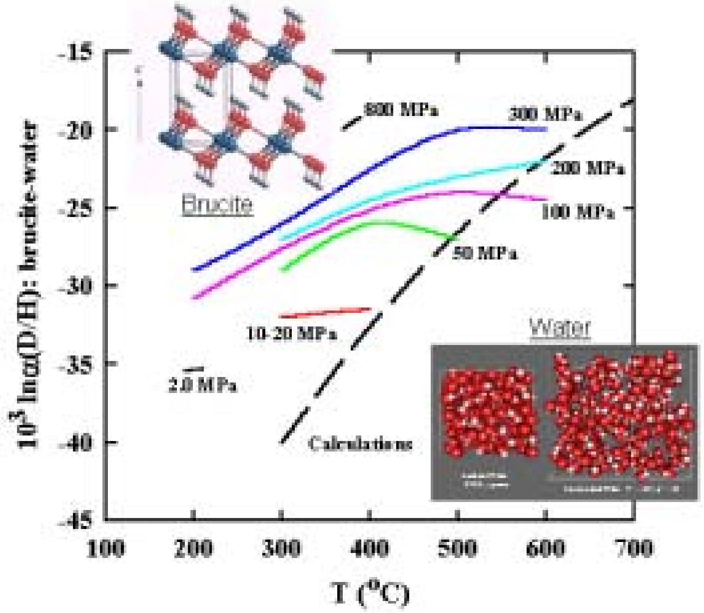


Fig. 6 The effect of pressure on D/H fractionation between brucite, Mg(OH)$_2$, and water (Horita et al., 2002).

densimeter (VTD) is employed to determine the volumetric properties of binary and ternary CO_2-CH_4-N_2-H_2O mixtures at 50-400° C (Fig. 1) (Blencoe et al., 1996). To date, results have been reported for binary and ternary CO_2-CH_4-N_2 gases, and for binary, aqueous CO_2-N_2-H_2O fluids (e.g. Seitz and Blencoe, 1999; Blencoe et al., 1999). An oscillating Inconel U-tube (Fig. 1) is the heart of the VTD. The tube is operable at *P*-*T* conditions as high as 120 MPa and 500° C. Properly configured and energized, the tube behaves as a harmonic oscillator, with the period of vibration varying monotonically with fluid density. Reported densities for pure fluids are believed to be accurate to ±0.0005 g/cm^{-3}. Estimated uncertainties for fluid mixtures range from ±0.0005 g/cm$^{□3}$(~1.0%) for low-density fluids to ±0.0010 g/cm$^{□3}$(~0.15%) for high-density mixtures.

The VTD can also be used to determine the upper baric stabilities of liquid-vapor assemblages (vapor-liquid equilibria, VLE) in fluid systems at high subcritical temperatures (Fig. 2) (Blencoe et al., 2001). The first step is to create an isobaric-isothermal, physically isolated and chemically homogeneous sample of "high-pressure" fluid of known composition. Fluid pressure is then lowered slowly at constant temperature. Pressure readings and matching values for (the period of vibration of the U-tube) are recorded at 1 or 2 bar intervals. When the fluid begins to separate into two phases (liquid + vapor), a distinct inflection is observed in the trend of *P* vs. *T*. Performing such experiments for mixed-volatile fluids at closely spaced compositional intervals produces a complete high-*P* liquid-vapor boundary curve/surface that is accurate to approximately ±2 bars.

The heterogeneous phase equilibria and activity-composition relations of binary and ternary fluid ± "salt" (CO_2-N_2-H_2O-NaCl) systems at 500-1000° C and pressures to 3000 bars are being determined with a custom-designed, hydrogen-service, internally heated pressure vessel (IHPV, Fig. 3) (Anovitz et al., 1998; 2004a). The IHPV is a unique apparatus for conducting experiments at moderate-to-high temperatures and pressures, and at low-to-very-high hydrogen fugacities. In its current configuration, the vessel can be operated routinely at temperatures between 22 and 1000ºC, and at hydrogen fugacities as high as 300 MPa. Many different kinds of samples (encapsulated rocks, minerals, gases, and liquids; pure metals and alloys; and numerous types of ceramics and polymer materials) can be reacted in the working cavity near the center of the vessel; therefore, the IHPV has great practical utility in numerous key areas of geochemical, petrologic, metallurgical, ceramic and hydrogen research, including: the activity-composition relations, multicomponent phase equilibria, and reaction kinetics of rock-forming crystalline solutions, mixed-volatile fluids, and brines at crustal temperatures and pressures; redox-sensitive, high *P*-*T* fluid/rock interactions; diffusion of hydrogen through solids; and production and consumption of hydrogen by solids and liquids. A key advantage of the ORNL IHPV is that it can be used to fix the activity of water in encapsulated samples. This is done by controlling the fugacities of hydrogen and oxygen (fH_2 and fO_2) inside each capsule, which automatically fixes water activity by the equilibrium: $H_2 + O_2 = H_2O$. Oxygen fugacity is fixed internally in each capsule by the addition of a solid buffer, usually Ni-NiO or Co-CoO. Hydrogen fugacity is mea-

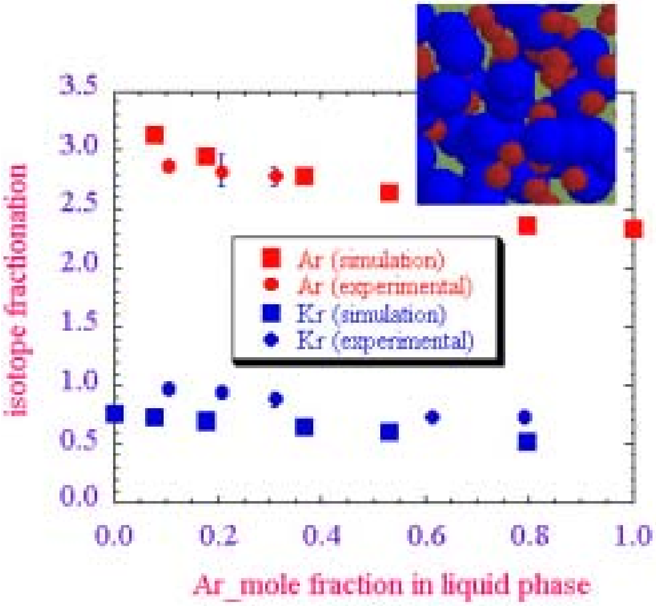


Fig. 7 Molecular-based simulations by means of advanced computing technologies are critical to our fundamental understanding of isotopic fractionation of various geologic-planetary systems. This figure presents the first ever simulations of mixtures (upper inset: Ar-red, Kr-blue) show good agreements of liquid-vapor fractionation of ^{40}Ar/^{36}Ar and ^{84}Kr/^{80}Kr in the system Ar-Kr with experiments in the literature (lower figure) (Chialvo and Horita, 2003).

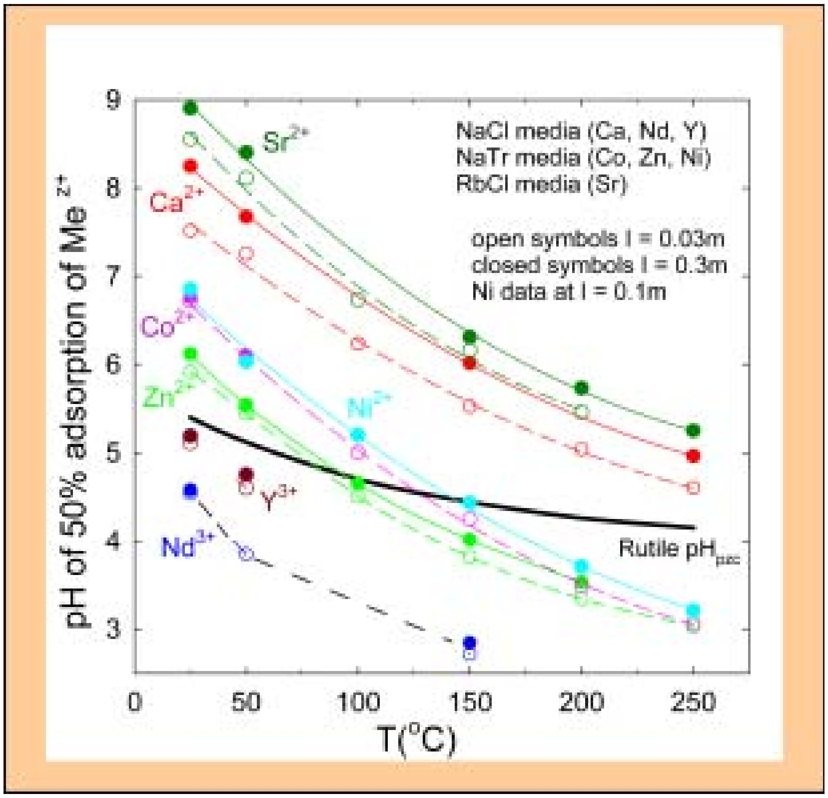


***Fig. 8** Plot of the pH at which 50% of a trace multivalent cation is sorbed on the surface of a rutile powder suspension in the pH-cell shown in Figure 4. In all of these experiments, approximately 50 grams of a solution containing 0.001molal Me^{z+} and 0.001 molal H$^+$ in the background electrolyte type and ionic strength indicated, was initially placed in the test cup along with about 1 gram of the rutile (Tioxide, Corp., 15m^2/g surface area, pretreated as described by Machesky et al., 2001). Samples were removed for analysis during titration to higher pH to establish the sorption isotherm and the 50% adsorption value. The pH of zero net surface charge of rutile is also shown as a function of temperature (Machesky et al., 2001).*

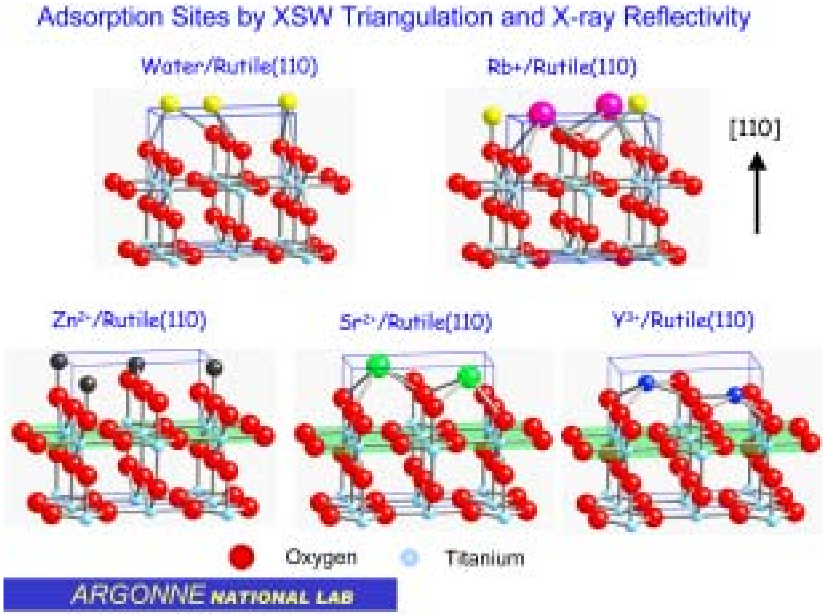
sured with a Shaw membrane. Use of a pre-mixed gas reduces hydrogen gradients in the vessel, allowing a constant hydrogen fugacity to be rapidly achieved and maintained until the experiment is quenched, and permits a range of water activities to be obtained.

The equations of state (EOS) developed from these experimental studies are used in predicting fluid behavior in a diverse range of environments such as oil, gas and geothermal reservoirs, volcanic systems, pipelines, high temperature treatment of wastes (supercritical oxidation processes), and CO_2 disposal in geological formations such as depleted oil and gas reservoirs and coal-beds (Blencoe et al., 2000; Labotka et al., 2002; Blencoe, 2004). The lower temperature results obtained by Blencoe and his colleagues have direct relevance to the use of CO_2 to displace CH_4 from unmineable coal seams, a value-added technology for CO_2 sequestration under serious consideration by DOE.

In Situ pH Studies:

Dave Wesolowski has made extensive use of ORNL's unique high temperature hydrogen electrode cells (Mesmer et al., 1970), which enable continuous, highly accurate and long-term pH-monitoring (Fig. 4) of both homogeneous and heterogeneous aque-

***Fig. 9** Inner sphere adsorption sites of ions on the rutile (110) surface determined by synchrotron X-ray standing wave and crystal truncation rod studies. These sites are in good agreement with similar sorption positions obtained in MD simulations, with the exception of Zn^{2+}, for which we are still working to optimize the MD simulations based on new ab initio studies that indicate a coordination change from 6- to 4-fold upon sorption. Not only do the ions occupy specific sorption sites relative to the underlying crystal structure, but the first layer of water molecules also occupy lattice-related sites and are observed by MD simulation to be highly oriented and essentially unable to diffuse away from the surface, at least in the simulation time frame.*



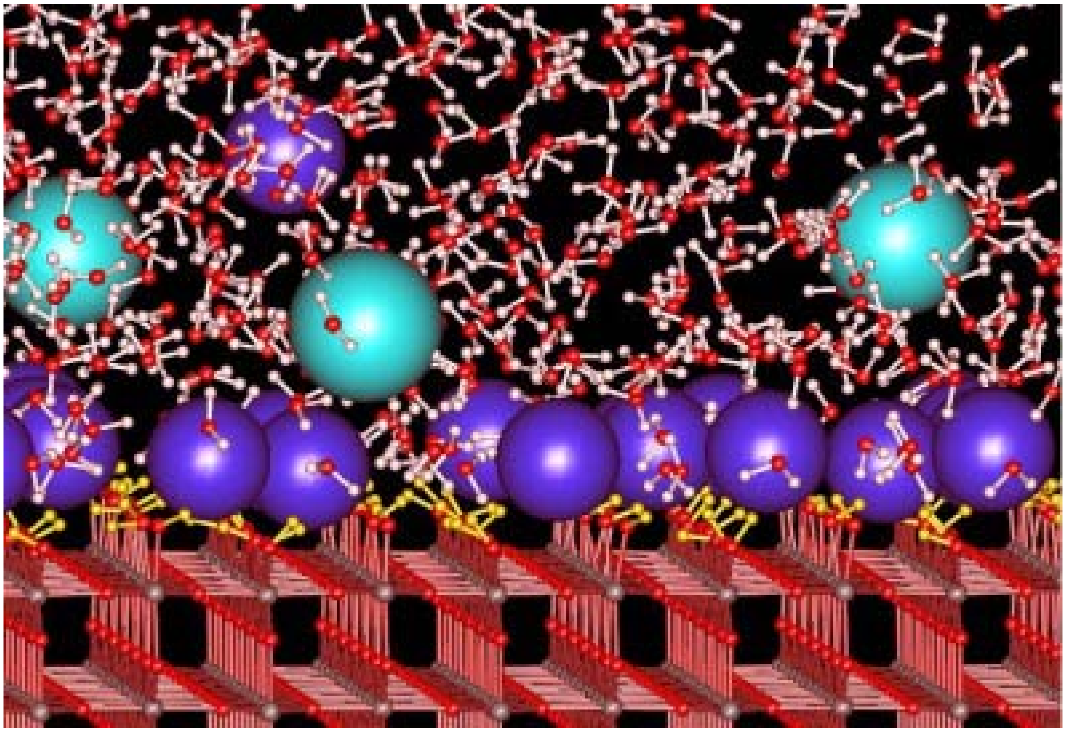
ous reactions from 0-300˚C at pressures near vapor saturation and hydrogen partial pressures from fractions of an atmosphere to approximately 100 atmospheres. This technique has enabled the definitive studies of the dissociation constants of nearly all of the major organic and inorganic weak acids and bases, including water itself, that control the pH of industrial and subsurface aqueous solutions, as well as the hydrolysis constants of many of the most important metals in NaCl and KCl brines. Numerous visiting chemists and geochemists have worked with Wesolowski and Palmer to extend our knowledge of even the most basic geochemical reactions. Just a few examples include the dissociation constants of HSO_4^- and citric acid (Dickson et al., 1990; Benezeth et al., 1997), the complexation of Al^{3+} by SO_4^{2-} (Ridley et al., 1999; Xiao et al., 2002) and the hydrolysis of Nd^{3+}, Cr^{6+} and W^{6+} (Wood et al., 2002; Palmer et al., 1987; Wesolowski et al., 1984). Similar facilities being developed by Scott Wood at the University of Idaho and Pascale Benezeth at CNRS, Toulouse promise to expand the impact of this powerful approach.

Salt and Pressure Effects on Isotopic Exchange:

Since their development in the early 1950's, stable isotope techniques have been extensively utilized to study the sources, fluxes, and paths of aqueous fluids, and the extent of phase separation and mineral deposition from aqueous fluids in active geothermal systems, ore deposits, metamorphic and magmatic rocks. The prerequisite to the successful application of stable isotope techniques to geothermal systems and other fluid-dominating geologic systems is basic knowledge of isotope fractionations between different phases and species (water, minerals, steam, gases, and dissolved species). It has usually been assumed that temperature is the sole variable controlling equilibrium fractionation of the stable isotopes of light elements (hydrogen, carbon, nitrogen, sulfur, etc.). Despite the discovery of the effect of dissolved salt on isotopic partitioning, "isotope salt effects," in the early 1950s, long-lasting controversy on the isotope salt effects at elevated temperatures was not resolved until the studies of Juske Horita, Dave Cole and Dave Wesolowski over the past several years (Horita et al., 1993a, 1993b, 1995) (Fig. 5). The same is true for the effect of pressure on isotope partitioning. Our recent studies unequivocally demonstrate that pressure indeed affects isotopic partitioning between fluids and solids far beyond analytical errors (Horita et al., 1999; Horita et al., 2002) (Fig. 6). Thus, the isotope fractionation factor is a function not only of temperature, but also of pressure and fluid composition.

Beyond accurate knowledge of the three variables (T, P, X_{fluid}) in macroscopic isotope fractionation, we are expanding our efforts to advance our understanding of fundamental causes of the isotopic effects in various fluids and minerals at atomic- and molecular - levels under geologic and planetary conditions, including those at high-pressures and high-temperatures. We are employing a synergistic approach of laboratory experiments, theory, molecular-based simulations (Molecular-dynamics, Monte Carlo), and neutron diffraction - scattering methods. A recent result stemming from this approach published in *J. Chem. Phys.* by Chialvo and Horita (2003) presented the liquid-vapor and solid-vapor isotope fractionations of noble gases (Ne, Ar, & Kr) by means of (classical) molecular dynamics and Gibbs Ensemble Monte Carlo simulations (Fig. 7).

Fig. 10 MD simulation of water containing dissolved RbCl in contact with the rutile (110) surface at pH 8 (Predota et al., 2004b). The near surface structure of the solid is ab initio optimized (Bandura and Kubicki, 2003). The surface oxygen bonds are permitted to move with fixed ab initio bond lengths. Oxygen (red), hydrogen (white in bulk water, yellow when bound to surface oxygens) and titanium ions (grey) are reduced in size for clarity. The dark blue Rb^+ ions and pale blue chloride ions are shown at close to 'real' ionic radius. The first layer of Rb^+ ions are specifically bound in the tetradentate site and in contact with two bridging and two terminal hydroxyl groups. Rubidium and chloride ions are present further out in the EDL, but they do not occupy specific sites relative to the surface crystal structure, and are essentially 'diffuse' layer ions.



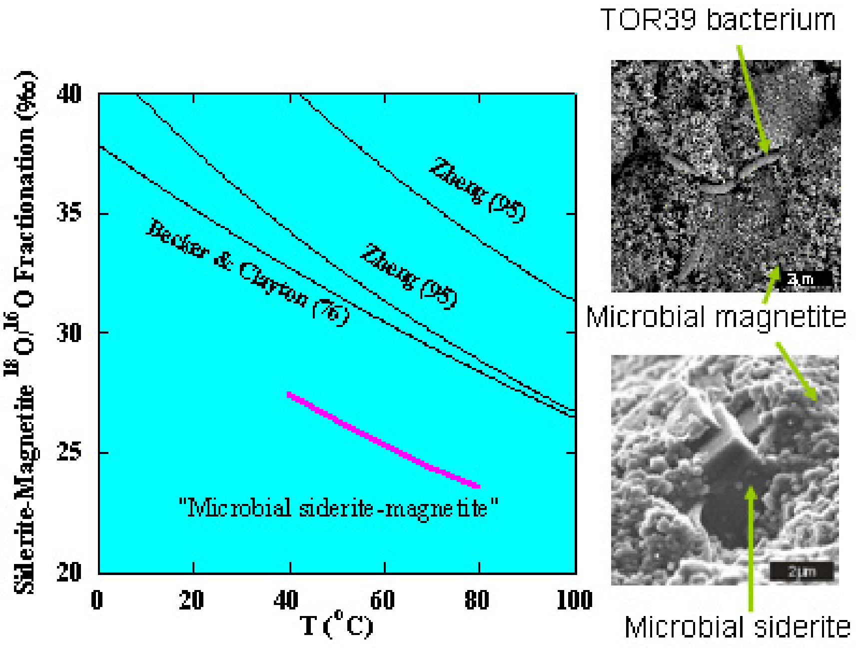


Fig. 11 $^{18}O/^{16}O$ fractionation between microbially precipitated magnetite and siderite (after Zhang et al., 2001).

INTERFACIAL PHENOMENA

Fluid/fluid and fluid/solid interfaces are regions across which all elemental transfers take place. Examples include water/gas, water/mineral, mineral/melt, coal/gas, gas/oil and water/oil interfaces. The complex structural and dynamic changes that occur at interfaces can profoundly affect hydrodynamics, reaction rates and reaction mechanisms. In this thrust area, we focus primarily on 'stable' interfaces, involving the juxtaposition of phases that largely retain their bulk characteristics at some distance from the interface. This enables us to isolate the unique features of the interface, which are controlled in part by changes in the compositions and state conditions of the bulk phases, whose structural and dynamic properties are often better understood.

Electrical charge develops on oxide and silicate surfaces in aqueous solutions due to the unsatisfied bond valence of the surface metal and oxygen atoms. Ions and water dipoles in solution are attracted to the charged surfaces, and the electrical double layer (EDL) thus formed influences the migration of dissolved species in subsurface brines as well as the stabilities and transport properties of colloids and the kinetics of dissolution and precipitation. Charge development and ion adsorption have been extensively studied by pH titrations and electrokinetic measurements of particle suspensions in aqueous electrolyte solutions. However, very few studies have been conducted at elevated temperatures, and almost none above 95˚C (Kosmulski 2001). Dave Wesolowski and Don Palmer, in collaboration with visiting scientists Mike Machesky and Moira Ridley have pioneered the first studies of the pH-dependent surface charge and pH_{pzc} (point of zero charge) of minerals at temperatures above 95˚C, including rutile (a-TiO_2) and magnetite (Fe_3O_4), by potentiometric titration (Machesky et al. 1998, Ridley et al. 2002, Wesolowski et al. 2000).

In the DOE Basic Energy Sciences project 'Nanoscale Complexity at the Oxide/Water Interface', Lead PI Dave Wesolowski is collaborating with a large group of ORNL and external researchers at Argonne National Lab, Illinois State Water Survey, Penn State, Vanderbilt, Texas Tech, St. Petersburg State University, University of South Bohemia (Czech Republic), Cardiff University, Wageningen in the Netherlands, and the University of Capetown to develop a molecular-level understanding of the EDL (Wesolowski et al., 2004). Figure 8 shows the point of zero charge of rutile as a function of temperature to 300˚C and the pH at which 50% of dissolved, multivalent trace ions in 1:1 electrolyte media are adsorbed on the mineral surface. This

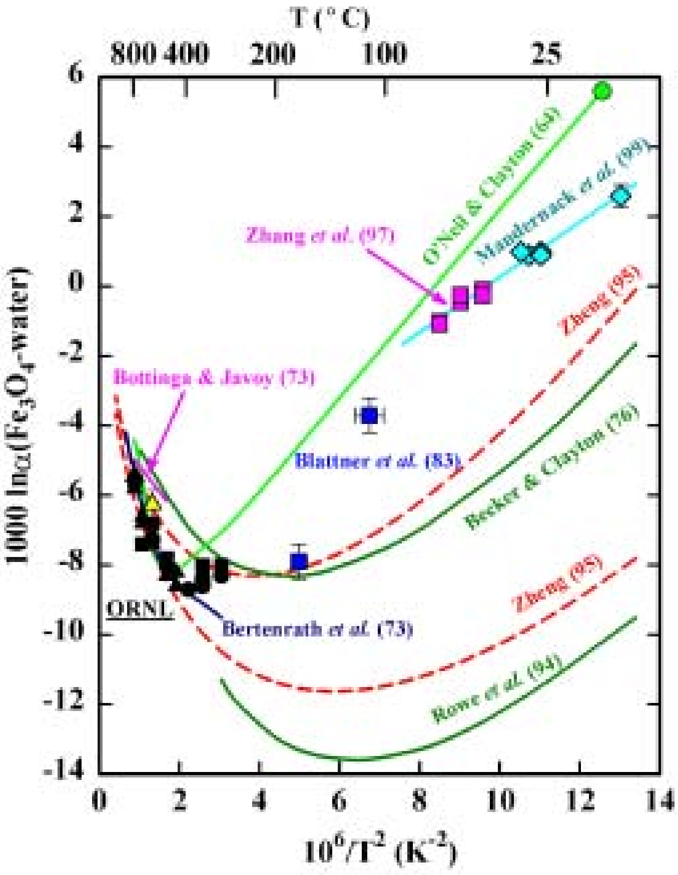


Fig. 12 Oxygen isotope fractionation between magnetite and water showing a comparison of high temperature data reported by Cole et al. (2004) with lower temperature results obtained in our studies using microbially- (squares) and inorganically-precipitated (solid circles) magnetite.

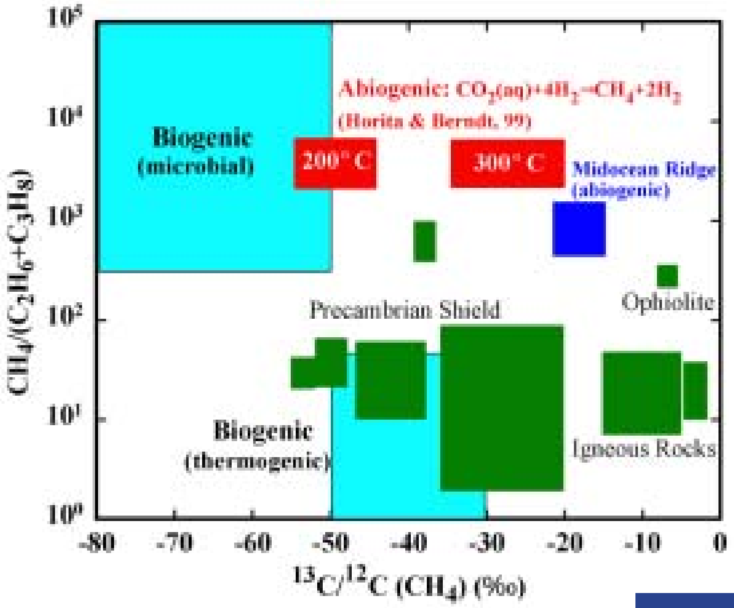


***Fig. 13** CH_4 and light hydrocarbons produced abiotically under hydrothermal conditions. $^{13}C/^{12}C$ values and $C_1/(C_2+C_3)$ values of abiogenic hydrocarbons are indistinguishable from those of microbial gases (Horita and Berndt, 1999).*

model-independent parameter gives a direct indication of the sorption affinities of these ions, which all increase with increasing temperature, at a rate considerably greater than the decrease in the point of zero charge with temperature, meaning that ion adsorption on mineral surfaces is even more important at elevated temperatures than at room temperature. Surface charge density for a given pH above or below the point of zero charge also increases with increasing temperature.

With support from this project, a high temperature zeta potential system has been developed by Serguei Lvov and co-workers at Penn State, and the pH_{iep} (isoelectric pH) of rutile and baddaleyite (ZrO_2) have been measured to 200˚C by microelectrophoresis (Fedkin et al. 2003). The team has also initiated a series of coordinated studies (cf. Zhang et al., 2004; Bandura and Kubicki, 2003; Ridley et al 2004; Predota et al., 2004a,b) in which pH-titration and electrokinetic data from powder suspensions are coupled with: 1) synchrotron X-ray standing wave (XSW) and crystal truncation rod (CTR) studies of single crystal surfaces in contact with electrolyte solutions; 2) neutron reflectivity and small angle scattering studies of organic ion interactions with colloidal particles and single crystal surfaces; 3) second harmonic generation at single crystal/water interfaces; and 4) *ab initio* quantum calculations and molecular dynamics simulations of the mineral-solution interface. Figure 9 shows the sorption site geometries of cations at the rutile (110) surface in contact with liquid water containing the ions shown. We have found that all cations studied, including multivalent ions Ca^{2+}, Sr^{2+}, Zn^{2+}, and Y^{3+} and the cation of the background medium (Na^+, Rb^+) bind as 'inner sphere' species in direct contact with the surface bridging and terminal oxygen atoms, and that

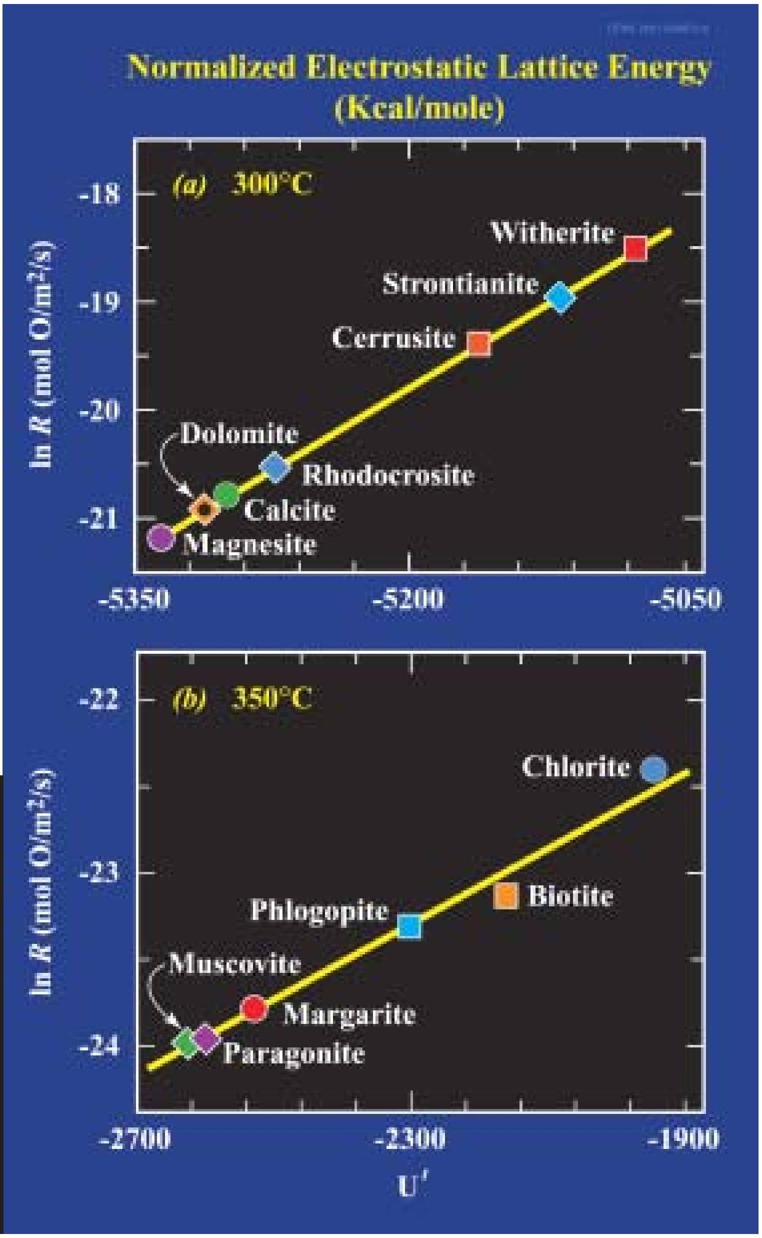
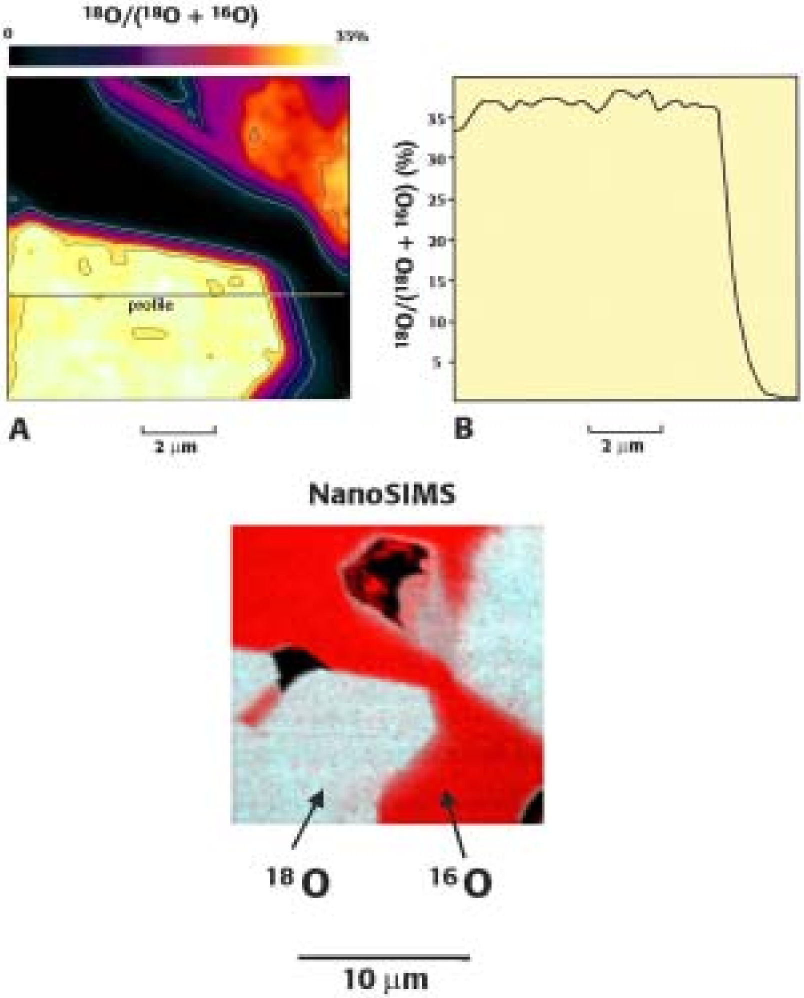


***Fig. 14** Oxygen isotope exchange rates for metal carbonates (a) and layer silicates (b) reacted with pure H_2O at 300 and 350°C, respectively, plotted against the normalized electrostatic lattice energy (U'). U' represents the sum of electrostatic site potentials for each cation and anion normalized by dividing by the number of cations per unit formula in each phase. Experimental data are given for calcite, strontianite, witherite, chlorite, muscovite and biotite (Cole, 2000). Lattice energies have been calculated for phases common to each mineral group for which rate data are lacking. These have been projected to the lines regressed through the experimental data.*

Fig. 15 (A) Contours of $^{18}O/(^{18}O+^{16}O)$ in replaced (via K-Na exchange) and unreacted albite, expressed as percent based on the detailed ion image given at the bottom. (B) Profile along the line shown in A. The ratio is uncorrected and is semiquantitative. The drop in the ratio occurs over a distance (several hundred nm) that is 5-10 times the spatial resolution of the NanoSIMS (Labotka et al., 2004b)



the radii of the ions largely dictate the specific geometry of their sorption sites, with the larger ions occupying 'tetradentate' sites involving two bridging and two terminal oxygens, and very small ions like Zn^{2+} forming mono- or bidentate complexes.

Figure 10 is based on an MD simulation of the interaction of Rb^+ with the rutile (110) surface (Predota et al., 2004b). We have determined that the revised MUSIC model of surface protonation (Hiemsta et al., 1996), when optimized using *ab initio* bond lengths, is consistent with our experimental observations of the pH_{pzc} (Fitts et al., 2004), and that classical simulations of the rutile/water interface, optimized using *ab initio* surface charges and ion-surface oxygen interaction parameters are fully consistent with the X-ray results and compatible with Guoy-Chapman-Stern models of the EDL (Zhang et al., 2004; Bandura and Kubicki, 2003; Predota et al., 2004a,b). Significantly, for this surface, the influence of increasing ionic strength of weakly-bound ions such as Sr^{2+} (Figure 8) is shown to be a result of direct competition with background electrolyte cations (Na^+, Rb^+) for binding *at the same 'inner sphere' site*, rather than evidence of "outer sphere" binding of fully-hydrated species.

MINERAL-FLUID REACTIONS

The overarching goal of this thrust area is to understand, at both the microscopic and molecular-levels, the chemical and isotopic phenomena engendered by complex mineral-fluid interactions occurring over ranges of temperature and pressure relevant to the evolution of continental and oceanic crustal systems. Our approach is to obtain a quantitative understanding of the effects of specific environments and time scales on geochemical reactions in mineral-fluid systems through laboratory-based studies of simple, geologically-relevant systems, complemented by investigation of appropriate natural analogs. Predictive understand-

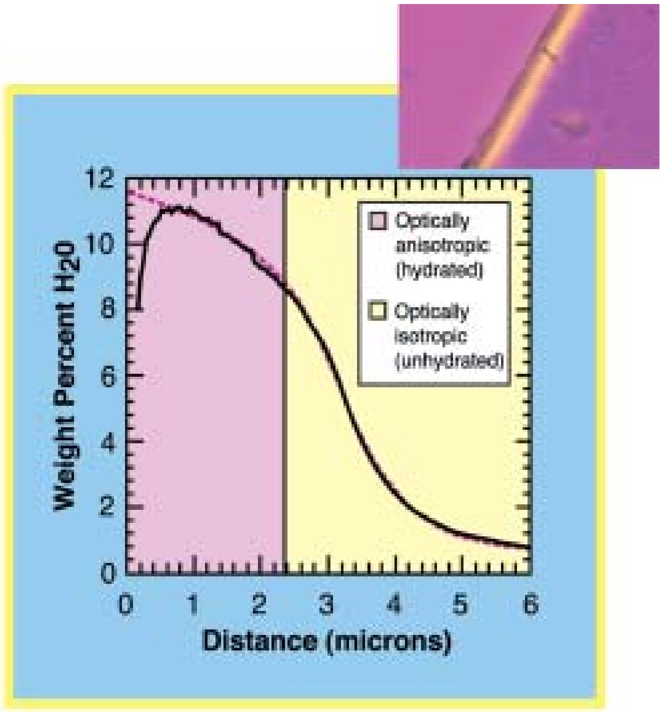
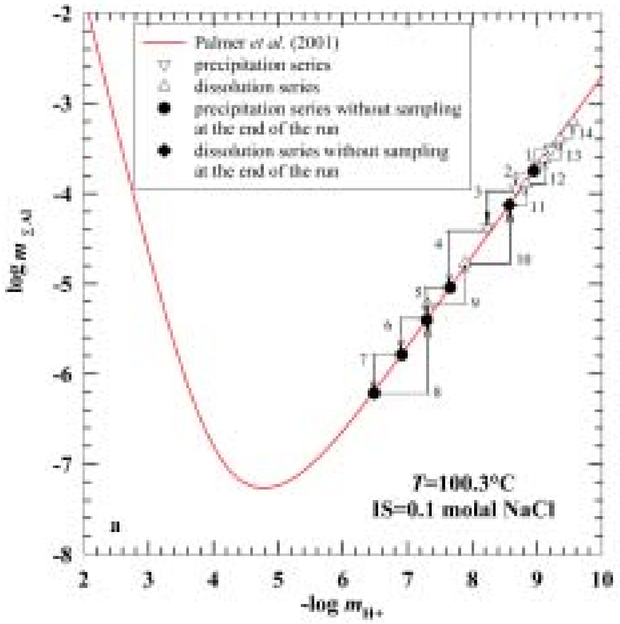
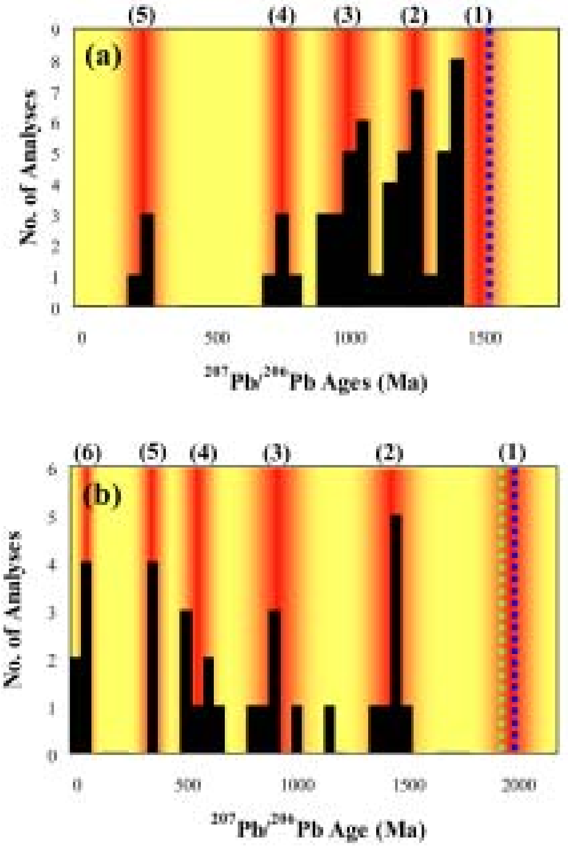


Fig. 16 Representative hydrogen diffusion profile in natural weathered Pachuca obsidian measured with ORNL's Camaeca 4f ion microprobe. The inset is a photomicrograph of the so-called "hydration rim" in a sample of weathered Pachuca obsidian. Note that this boundary is identified as a Becke line and is gradational, not sharp as assumed in the standard method of optical hydration dating (Anovitz et al. 1999).

(RIGHT) Fig. 17 Stepwise dissolution and precipitation rate studies of boehmite in equilibrium with a NaCl + NaOH + $NaAl(OH)_4$ solution at constant stoichiometric molal ionic strength of 0.1. The red curve is the equilibrium solubility of boehmite at this ionic strength and temperature reported by Palmer et al. (2001).





(LEFT) Fig. 18 Distribution of $^{207}Pb/^{206}Pb$ ages of uranium minerals determined by SIMS relative to major tectonic events that have affected (a) the Athabasca Basin region and (b) Francevillian Basin, host to the Oklo-Ok lobondo natural fission reactors. In (a), the black dash line represents the U-Pb age of the formation for the Athabasca uranium deposits (~1.6 Ga) and the numbers in parentheses mark the following tectonic events: (1) Accretion of Nena (~1.5.Ga); (2) Thermal emplacement of the McKenzie dike swarm (~1.3 Ga); (3) Accretion of Rodinia (~1.0 Ga); (4) Breakup of Rodinia (0.9-0.7 Ga); (5) Breakup of Pangea (~250 Ma). In (b), the dash line represents the U-Pb age of formation of the Oklo-Ok lobondo natural fission reactors (~2.0 Ga), the dotted line represents the U-Pb age for sustained fission reactions (i.e., criticality; ~1.95 Ga), and the numbers in parentheses mark the following tectonic events: (1) Accretion of Atlantica (~2.0 Ga); (2) basin uplift and carbonate diagenesis (~1.5 Ga); (3) Accretion of Rodinia (~1.0 Ga); (4) Accretion of Gondwana (~0.5 Ga); (5) Accretion of Pangea (~250 Ma); and (6) Breakup of Gondwana (~150-40 ma). These deposits represent one of the few areas in the world that have preserved a nearly complete neotectonic record of the continents over the past 1.5 Ga.

ing of these phenomena can contribute to the resolution of the long-standing problem of the inadequacy of simple assumptions of local equilibrium to represent accurately the observed geochemical record in natural systems. This thrust area is comprised of four sub-themes: isotopic fractionation in carbonate-, oxide- and silicate-fluid systems, mechanisms and rates of chemical and isotopic exchange, natural water-rock interaction analogs, and the influence of nano-confinement on fluid behavior.

Isotopic Fractionation:

In addition to the isotope salt and pressure effect studies described above, Cole and Horita have been involved in several studies designed to obtain accurate information on the partitioning of stable isotopes, both equilibrium and kinetic, for a number of key microbial and inorganic reactions, through systematic detailed laboratory experiments. For example, siderite ($FeCO_3$) was precipitated *in vitro* between 10 and 70˚C, mediated by thermophilic dissimilatory iron-reducing and fermentative bacteria sampled during deep subsurface drilling (Liu et al. 1997). Well-crystallized, nm-sized (10-100 nm), magnetite-rich (64-88 wt%) iron oxides were precipitated extracellularly after a few days of incubation. In the presence of CO_2(*aq*), thermophilic fermentative and iron-reducing bacteria facilitated the precipitation of well-formed rhombs of siderite (several m across). Siderite-magnetite $^{18}O/^{16}O$ fractionation factors obtained by combining results from separate studies of microbial magnetite (Zhang et al., 1997) and siderite (Zhang at al., 2001) differ substantially from those in the literature (Zheng, 1999) (Fig. 11). In a complementary study, Cole et al. (2004) determined the oxygen isotope fractionation factors between magnetite and water at temperatures between 300 and 800°C. These new results have been plotted in Fig. 12 along with the lower temperature fractionation data obtained from both microbial and inorganic magnetite precipitation pathways.

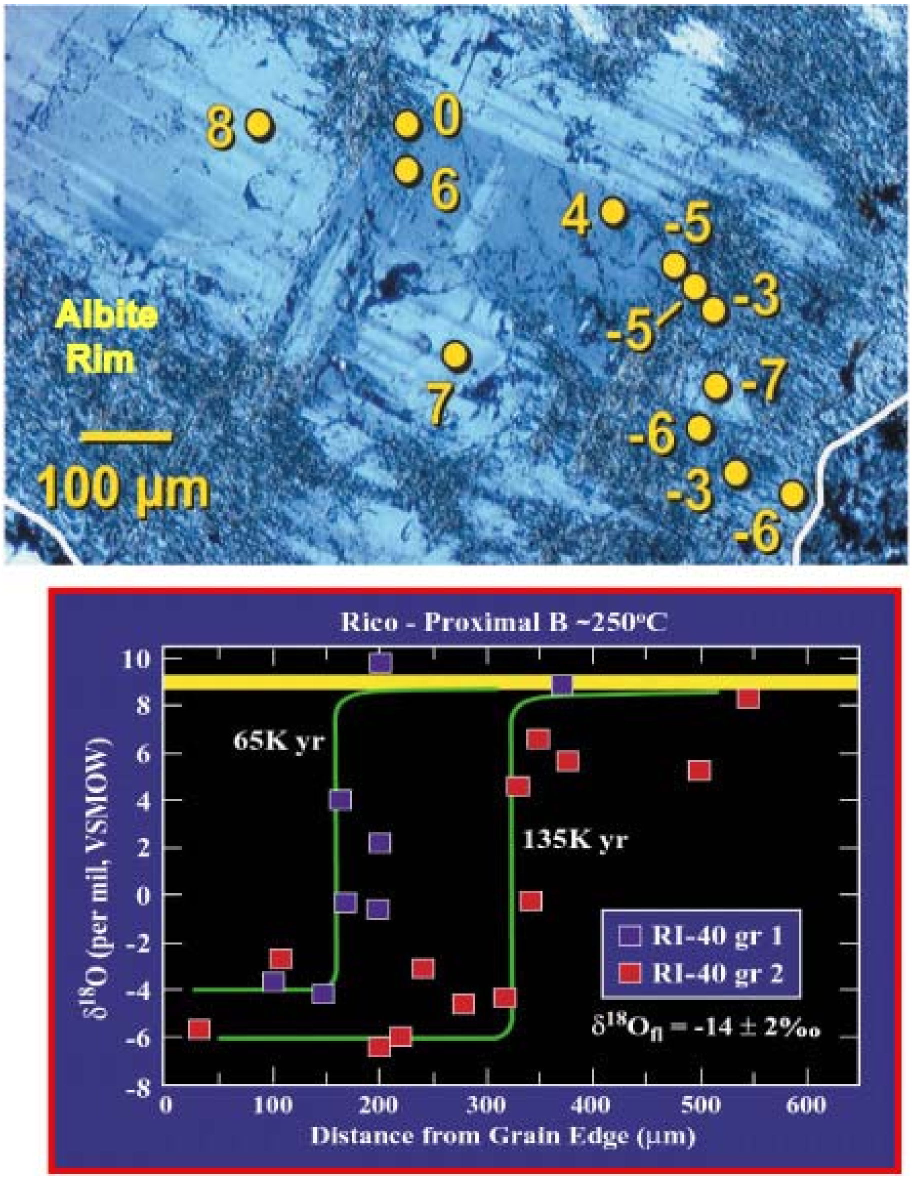


Fig. 19 (Upper) Representative photomicrograph of an altered plagioclase phenocryst from the intermediate temperature zone (200-250°C) in the Rico, CO paleo-hydrothermal system (Cole et al., 2004). Albite and minor muscovite compose mottled zones that typically rim unaltered plagioclase interiors. SIMS oxygen isotope data (rounded to the nearest per mil) are shown for spot sizes of ~25-30 mm in diameter. The value of 0ä near the interior is indicative of a case where isotopic exchange with isotopically light water (-14±2ä) can penetrate into the interior of grains along fractures. White lines in the lower left and right corners demarcate the grain edge. (Lower) Oxygen isotope compositions plotted versus distance from the grain edge for two different grains from the intermediate zone. Note the step function exhibited by both data sets indicative of an equilibrated rim and modestly sharp reaction front. The duration (in kyr) necessary to produce these fronts have been estimated with a coupled reaction-diffusion model that considers the position of the original grain edge fixed (pseudomorphic replacement).

Although the occurrence of deep-earth, mantle methane is still very controversial, there are an increasing number of reports suggesting the inorganic (abiogenic) formation of methane in the Earth's crust. We have experimentally investigated the mechanisms and isotopic fractionation during the abiogenic CH_4 formation from dissolved CO_2 under hydrothermal conditions (Horita and Berndt, 1999). Experiments were performed under conditions similar to those commonly encountered during the serpentinization of ultramafic rocks of the oceanic crust (200-400° C, 50 MPa). Our experimental results reveal that $\delta^{13}C$ values of abiogenic CH_4 formed from dissolved CO_2 can be very low, and may overlap values typical for microbial CH_4 (Fig. 13). In nature, Ni-Fe alloys, which are important phases in the paragenetic sequence of minerals that form during hydrothermal alteration of olivine-rich rocks, are rather widespread in nature (continental ultramafic settings, oceanic crustal environments, and meteorites). Thus, abiogenic methane formation via an awaruite/Ni-Fe alloy-catalyzed reaction may occur more commonly in the Earth's crust than is currently recognized.

Data on the oxygen and hydrogen isotope compositions of hydrous minerals provide a useful monitor of fluid-rock interaction in the Earth's crust. Rigorous interpretation of data generated from natural samples, however, requires accurate information of $^{18}O/^{16}O$ and D/H fractionation factors between minerals and water. Many of these have been summarized recently by Chacko et al. (2001) and Horita and Cole (2004). Using a variety of hydrothermal techniques we have reported on the fractionation factors between chlorite-water ($^{18}O/^{16}O$; Cole and Ripley, 1999), epidote-water (D/H; Chacko et al., 1999) and brucite-water (D/H; Horita et al., 2002).

Mechanisms and Rates of Isotopic Exchange:

A number of experimental, empirical and quasi-theoretical methods have been used to quantify the mechanisms and rates of isotopic exchange accompanying mineral transformations (growth, dissolution, chemical exchange), diffusion of light elements (O, C, H) in minerals, and transport of volatiles in glasses and melts (e.g. H_2O, SO_2). A detailed summary of the mechanisms and rates of isotopic exchange for many mineral and melt systems was given in Cole and Chakraborty (2001). We have investigated the dependency of rates of stable isotope exchange on temperature, pressure, fluid/volatile composition, fluid/solid ratios, and grain size for a number of mineral systems including calcite-H_2O-NaCl (Cole, 1992); calcite-CO_2 (Labotka et al., 2000,

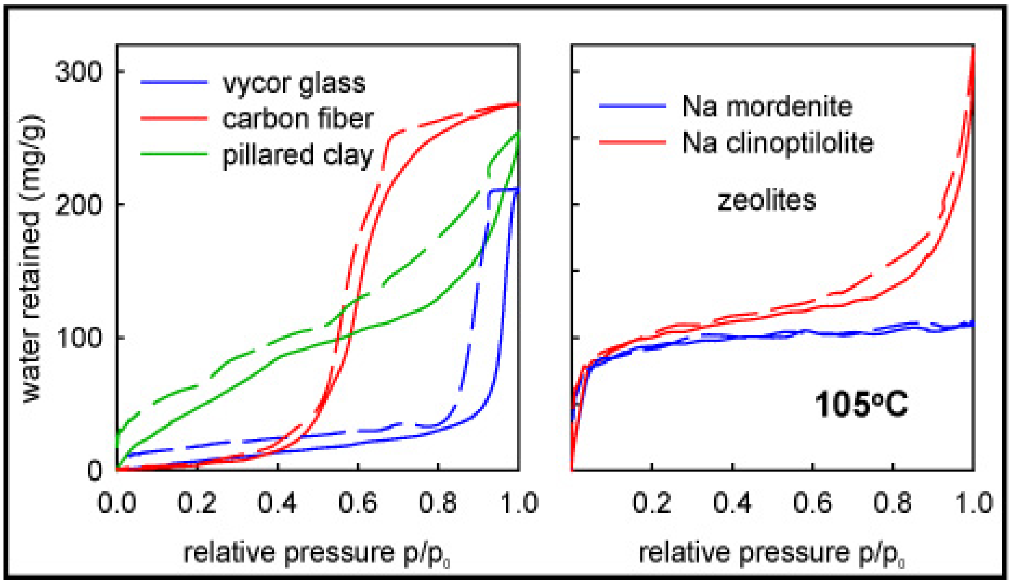


Fig. 20 Water adsorption (solid curves)-desorption (dashed curves) versus p/p_{sat} for a number of nano-porous solids (clay, silica, graphite, zeolites) at 105°C (Cole et al., 2004, Striolo et al., in press). ORNL's isopiestic apparatus was used to measure the water uptake and release as a function of temperature (up to 200°C) and pressure (vacuum to p_{sat} at a given T).

2004a); and metal carbonates [(Ca, Ba, Sr)-H_2O] and layer silicates (chlorite, muscovite, biotite-H_2O) (Cole, 2000). The influence of aqueous NaCl on oxygen isotope rates for calcite can be profound with an increase of nearly one order of magnitude (in units of moles O m^{-2} s^{-1}) with an increase in salinity of 1 molal. Pressure effect studies on calcite at a temperature of 500°C suggest that rate constants increase by about 0.4 log units per 100 MPa for the pure H_2O system, but only about 0.15 log units per 100 MPa at molalities between 1 and 4 (Cole, 1992). More recently, it has been noted by Cole (2000) that an increase in oxygen isotope exchange rates can be closely correlated with a decrease in the electrostatic lattice energies of select groups of minerals, i.e., carbonates and layer silicates (Fig. 14). By establishing an unambiguous relationship between rate, lattice energy, and ultimately, temperature, it should be possible to develop empirical equations useful in predicting rates of isotopic exchange for minerals for which experimental data are lacking.

We have used our Cameca 4f ion microprobe to measure the diffusivities of light elements in minerals and glasses via depth profiling. In collaboration with Ted Labotka at the University of Tennessee, Knoxville (UTK), diffusion of C and O has been measured in calcite reacted with pure $^{13}C^{18}O_2$ as a function of temperature at 100 MPa (Labotka et al., 2000) and pressure (0.1 to 200 MPa) between 600 and 800°C (Labotka et al., 2004). The ion microprobe has also been used to image the distribution of isotopic enrichments and depletions associated with chemical reactions. Amelia albite was reacted with 2 molal ^{18}O-enriched solution of KCl at 600°C and 200 MPa (Labotka et al., 2004b). In collaboration with Frank Stadermann at Washington University, we showed from NanoSIMS images that the interface is sharp in the distribution of ^{18}O and ^{16}O (Fig. 15). The combined electron microprobe and NanoSIMS analyses indicate that both cation and isotope exchange occurred during solution and precipitation of the feldspar. Use of ^{18}O rich H_2O was also effective in tracking the reac-

(Below) Fig. 21 Representative results from Grand canonical Monte Carlo (GCMC) and MD simulation of H_2O adsorption-desorption in graphite slit-pores (Cole et al., 2004; Striolo et al., in press). This example shows simulated sorption curves of H_2O at 498K for a simulation box 4.6 x 4.4 x 4.2 nm with pores 0.6, 1.0 and 2.0 nm wide (center box). The MD-derived distributions of H_2O at two different stages of water uptake are given in the lower left and right. The trajectories of water movement in these pores are shown in the upper right. The density profiles for O and H are shown in the upper right inset for a 1 nm slit pore with a p/p_{sat} value >0.4. Note that above this value we predict capillary condensation and the formation of two distinct water layers stabilized by hydrogen bonds. The general geometry and hysteresis behavior predicted by our simulations match quite closely what we observe experimentally, as seen in Fig. 20.

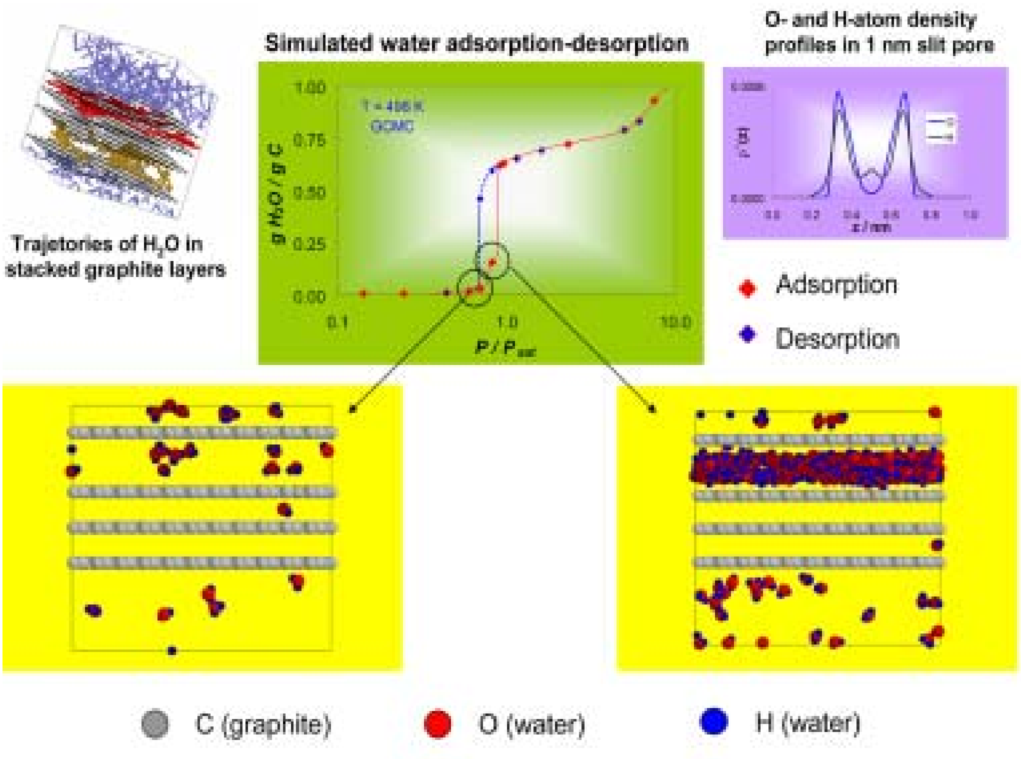
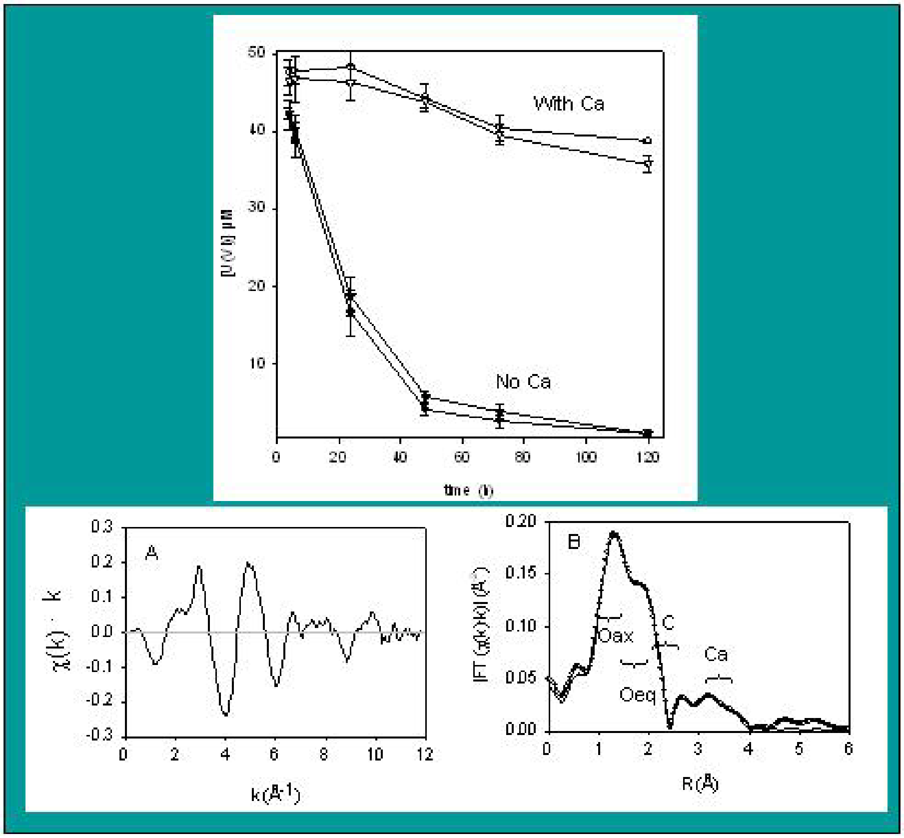


Fig. 22 Upper panel: Effect of Ca on U(VI) reduction by the obligate anaerobe* Desulfovibrio desulfuricans*; Lower panel: (a) XAFS* $\chi(k) \cdot k$ *data for Ca-containing base solution. (b) Magnitude of the Fourier transform of the data shown in Fig. 1a (open circles) and best-fit model (thick line). Data processed with Δk = 3.3-9.3* $^{-1}$*, ΔR = 0.9-4.0 , and a Hanning window with a full sill width of 1.0* $^{-1}$*. Oax = axial oxygen; Oeq = equatorial oxygen (Brooks et al., 2003).



tion progress in dolomite reacted at high temperatures and pressures (up to 700°C and 200 MPa) (DeAngelis et al., 2003).

In one other interesting application of the ion microprobe, Riciputi and Cole, along with Larry Anovitz, Mike Elam and Mostafa Fayek of UTK debunked the long-standing industry of dating ancient glassy artifacts by using optically measured hydration rims formed from weathering (Anovitz et al. 1999; Riciputi et al., 2002; Anovitz et al. 2004b). Our ion microprobe work demonstrated that the true position of the hydration front was not coincident with the optical front at all, as had been originally assumed (Fig. 16). Armed with new experimental diffusion data on water in glass, which determines the rate of water migration into the glass, and measurements of water's true distribution in the glass, a new, more reliable dating method was proposed that capitalizes on the sensitivity of the ion probe.

Dissolution and Precipitation Rates:

Combining ORNL's unique high temperature pH measurement cells (Fig. 4) with specially-designed flow-through and batch solubility facilities, Dave Wesolowski, Don Palmer and Pascale Benezeth have conducted definitive studies of the equilibrium solubilities of gibbsite – $Al(OH)_3$, boehmite – AlOOH, and zincite – ZnO at temperatures of 0-300˚C and pressures from vapor saturation to a few hundred bars (Palmer et al., 2001; Benezeth et al, 2001, 2002; Wesolowski et al., 1998). Recently, we have been focusing on the near-equilibrium dissolution and precipitation rates of aluminum oxyhydroxides, silicates and carbonates, and the redox-metastable transformation of magnetite – Fe_3O_4 – to hematite – Fe_2O_3 in acidic solutions under highly reducing conditions, the latter in collaboration with Dr. Hiroshi Ohmoto and his students at Penn State. Figure 17 is an example of pH-step experiments that enable determination of the rate of dissolution and precipitation of boehmite at near-equilibrium conditions over a wide range of pH, in a single batch experiment. For simple reactions, such as the dissolution of boehmite in basic solutions, $AlOOH_c + 2H_2O = Al(OH)_4^- + H^+$, simple monitoring of the pH and application of charge and mass balance equations are found to be sufficient to calculate the instantaneous rate of dissolution and precipitation over wide ranges of pH, temperature, ionic strength and degree of super- or undersaturation, without the need to take samples.

Natural Analogs:

The ORNL CAMECA ims 4f ion microprobe lab specializes in high precision isotopic analysis of light elements (H, B, Li, C, O, and S) as well as heavy element isotopes (e.g., U-Th-Pb). Major developments with the ion microprobe include heavy and light element isotope measurements in radioactive minerals. In addition, geochemists at ORNL along with their university affiliated colleagues have developed and utilized the unique capabilities of the Neptune laser assisted multi-collector ICP-MS (LA-MC-ICP-MS), Triton thermal ionization mass spectrometry (TIMS), and JEOL HRTEM imaging to study a number of fundamental processes associated with fluid-rock interaction at the nanoscale, including both cation and anion diffusion, hydrogen storage capabilities of various materials, and nano-scale uranium mineral precipitation on bacterial surfaces. These developments are the basis of long term ongoing projects concerning crustal scale fluid-rock interactions.

For example, high precision (±0.2‰) Cu isotopic analyses of turquoise associated with igneous activity from the southwestern United States, by LA-MC-ICP-MS, show regional trends and up to 10‰ variation. On-going research is attempting to elucidate the fundamental processes causing these trends and the wide range in Cu isotopic values (Evans et al., 2004). Exploiting the unique *in situ* capabilities of the secondary ion mass spectrometry (SIMS) by developing isotope measurement techniques has led to results at the forefront of scientific investigations of crustal scale fluid-rock interaction (Fayek et al 2002a, 2002b, 2003). Recent high spatial resolution (10-30 mm) *in situ* U, Pb, and O isotopic analyses, by SIMS, on U bearing minerals in sedimentary environments has revealed a wealth of detailed information corresponding to different paleo-fluid events associated with the large and economically significant sandstone basins including the age of orogenic events that resulted in large scale fluid events and mass transport. For example, *in situ* U-Pb and ^{207}Pb/^{206}Pb ages from U deposits indicate that uranium deposits can preserve a detailed record of large-scale fluid and thermal events, and may be sensitive to even larger tectonic events such as supercontinental cycles (Fig. 18). As most U deposits occur in sedimentary settings, these deposits offer one of the few approaches to developing a precise chronology of basin-scale fluid-rock events.

Similar ion probe studies have been conducted on the behaviour of oxygen isotopes in feldspars from different crustal settings. We have used oxygen isotope patterns in altered feldspars from the Rico, CO hydrothermal system (Fig. 19) to estimate the duration of fluid-rock interaction (Cole et al., 2004). The extent of albite rim formation and accompanying isotopic exchange vary across the system as a function of temperature, fluid isotope composition, and the local fluid-to-rock ratio. Formation times of reaction rims and associated isotopic patterns have been estimated with a coupled reaction-diffusion model that suggests that hotter (~250–350º C) hydrothermal circulation was active for ~100–300 k.y. in the center part of the system, perhaps only while the igneous "heat-engine" was still magma. Cooler (~150–200º C) circulation was widespread, lasting for >1,000 k.y. In collaboration with Claudia Mora at UTK, we have also determined the micro-spatial distribution of oxygen isotopes in feldspars from the Boehls Butte anorthosite, Idaho (Mora et al., 1999). The very large variations (up to ~15 per mil) with systematic gradients have been modelled as diffusive exchange between light meteoric water and original igneous feldspar at temperatures >500^{o}C and pressures of 200-400 MPa.

Nanoporosity and Fluid Behavior:

Hydrocarbons, aqueous solutions, and gaseous species (e.g. CO_2, CH_4) can occupy the pores or fractures of numerous types of complex heterogeneous solids. The size, distribution and connectivity of these confined geometries, the chemistry of the solid, the chemistry of the fluids and their physical properties collectively dictate how fluids migrate into and through these micro- and nano-environments, wet and ultimately react with the solid surfaces. In order to assess key features of the fluid-matrix interaction at the nanoscale, a multidisciplinary approach was taken that employed neutron and X-ray scattering, simulations, and thermodynamic measurements to quantitatively describe the molecular properties of pure water, aqueous electrolytes and simple hydrocarbons confined to well-characterized porous media that serve as analogues to natural materials (Cole et al., 2004). Results have been obtained in four separate, but interrelated areas. Various types of microscopy (SEM; TEM) and scattering (SAXS, SANS) have been used to characterize a number of porous silicas, carbon fiber monoliths, zeolites and clays prior to interaction with fluids. Water adsorption/desoprtion isotherms have been determined on these materials up to 200^{o}C (Fig. 20). FTIR, NMR and quasielastic neutron scattering (QENS) spectra have been obtained on water and, in the case of QENS, on electrolyte solutions (LiCl, $CaCl_2$, $NdCl_3$) confined in silica pore glass.

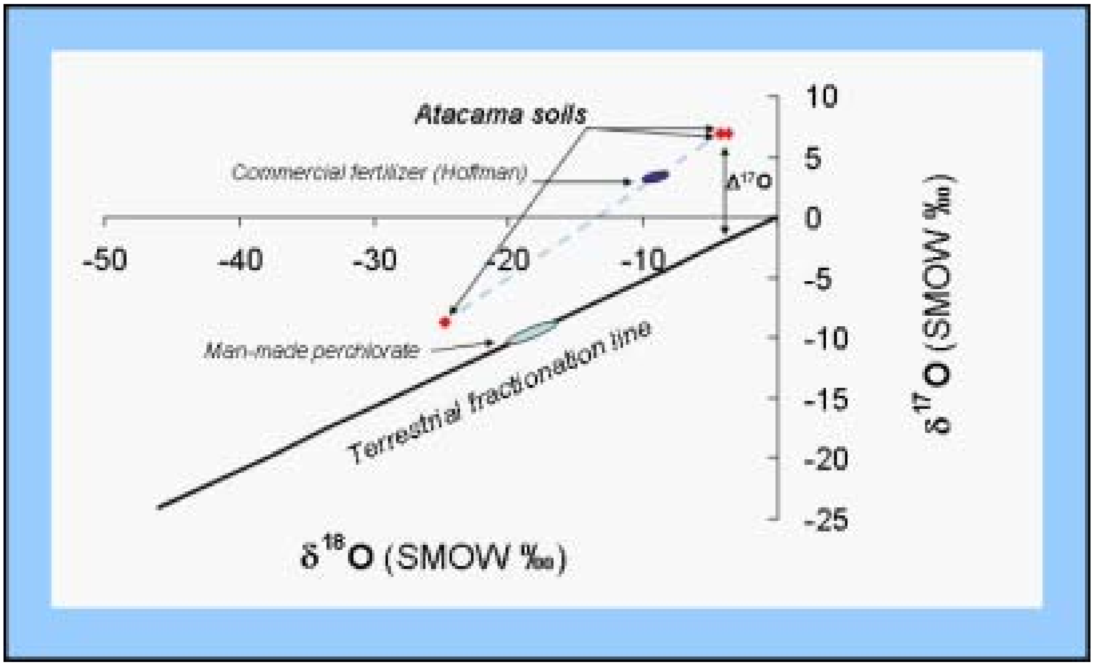


Fig. 23 $\delta^{18}O$–$\delta^{17}O$ plot for perchlorate from various man-made or natural sources including five reagent perchlorate salts, three different soils from the Central Depression of the central Atacama Desert, and a commercial nitrate fertilizer derived from Chilean salt deposits. Terrestrial fractionation line follows the mass-dependent fractionation relationship $\delta^{17}O = 0.52 \cdot \delta^{18}O$. The ^{17}O is the measure of the vertical deviation from this line (Bao and Gu, 2004).

SANS has been used to quantify the structural aspects related to critical phenomena of CO_2 confined to porous silica (Melnichenko et al., 2004; in press). Our simulation efforts (Grand canonical Monte Carlo; classical MD) thus far have focused on the adsorption and transport behavior of water and other volatiles such as CO_2 and CH_4 in slit pores geometries as a function of temperature (Fig. 21) composed of either carbon or mica (e.g., Striolo et al. in press). These studies conducted in concert are providing an understanding at the molecular level of how intrinsically different fluids behave in confined geometries compared to bulk systems. If properly calibrated and scaled, an atomistic or molecular understanding of fluid-solid interaction may provide quantitative insight into the behavior of systems at the macroscopic scale.

ENVIRONMENTAL GEOCHEMISTRY

Contaminant Transport:

The Environmental Sciences Division at ORNL has a rich history of research in the area of contaminant transport – basic research to provide an improved understanding and predictive capability of the mechanisms governing the fate and transport of radionuclides and heavy metals in subsurface environments. Traditional methods such as batch and miscible displacement experiments are now complemented with a new generation of analytical capabilities to provide new insights into aqueous and water-mineral reactions. For example, the codisposal of radionuclides with anthropogenic chelating agents (e.g., EDTA) has been recognized as a factor contributing to the undesirable movement of radionuclides away from disposal areas. The stability of cobalt-EDTA (Co-EDTA) complexes, and thus the fate and transport of ^{60}Co in the subsurface, is strongly dependent on the oxidation state of Co (log $K_{Co(II)EDTA}$ = 18.3; log $K_{Co(III)EDTA}$ = 43.9). Oxidation of Co(II)EDTA to Co(III)EDTA by manganese oxides present in aquifer solids has been described but the identity of the reduced Mn product remained unresolved (Jardine et al., 1993; Jardine and Taylor, 1995). Using a novel hydrodynamic flow cell coupled with X-ray absorption near edge spectroscopy (XANES) we determined both the solution and solid phase species of cobalt and manganese in real time (Fendorf et al., 1999). Co(III)EDTA is produced while Mn(IV) in pyrolusite (β-MnO_2) is reduced to Mn(III) which forms an α-Mn_2O_3 layer on the pyrolusite. Consequently, this layer passivates the surface limiting the production of Co(III)EDTA after an initial reaction period. The XANES spectra clarified that Mn(III) is formed rather than Mn(II) resulting in the formation of a stable Mn(III) solid.

Biogeochemistry:

In recent years, a significant body of work has shown that dissimilatory metal-reducing bacteria (DMRB) can also reduce a number of toxic metals and radionuclides of environmental concern such as Cr(VI), U(VI), and Tc(VII). From the perspective of remediating contaminated environments, the bacterial reduction of these contaminants is desirable as the lower oxidation state species are less mobile and have a lower solubility than when present at higher oxidation states. Despite the promise of bioreduction as a remediation strategy, the factors that enhance or inhibit the rate and extent of biogeochemical U(VI) reduction under representative environmental conditions are not well defined. Only recently has the quantification of a few key interactions been established. For example, we recently reported the inhibition of bacterial U(VI) reduction by DMRB in the presence of environmentally realistic concentrations of soluble calcium (Ca) (Fig. 22) (Brooks et al., 2003). X-ray absorption fine structure (XAFS) measurements confirmed the presence of an aqueous Ca-U(VI)-CO_3 complex. Calcium, at millimolar concentrations, caused a significant decrease in the rate and extent of U(VI) reduction by both facultative and obligate anaerobic bacteria, putatively through the formation of the Ca-U(VI)-CO_3 complex. The results are consistent with the hypothesis that U is a less energetically favorable electron acceptor when the Ca-U(VI)-CO_3 complexes are present. By understanding these key reactions, more predictable and effective approaches can be established for in situ bioremediation of U under realistic field conditions.

Environmental Forensics:

Perchlorate, or ClO_4^-, disrupts the thyroid gland that regulates metabolism in adults and physical development in children and is increasingly being found in soil and water. It is used to make solid rocket propellant and explosives but also occurs naturally, as in nitrate soils from Chile used to make fertilizers, making the source sometimes difficult to trace. An award-winning system developed at Oak Ridge National Laboratory to clean up perchlorate pollution is now also helping scientists determine whether the contamination is natural or man-made (Bao and Gu, 2004). The process of removing perchlorate also purifies it, allowing the isolation and examination of trace quantities of the compound. Using stable isotope analysis, investigators compared naturally-occurring perchlorate from Chile's Atacama Desert to synthetic or manufactured samples. The natural type had a distinctly high and positive ^{17}O anomaly but a lower ^{37}Cl value (Fig. 23). The ORNL treatment system provides a tool for the identification and forensics of perchlorate contamination in the environment. In addition, the results provide evidence to support the hypothesis that oxidation of volatile chlorine by O_3 with the subsequent formation of $HClO_4$ can be a minor sink for atmospheric chlorine.

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MEETINGS ANNOUNCEMENTS

Gordon Research Conference on Inorganic Geochemistry and Ore Deposits

Proctor Academy, Andover, New Hampshire
July 31 – August 5, 2005

The Gordon Research Conference on Inorganic Geochemistry traditionally addresses the geochemistry of metal-rich systems, and has been held every three to four years over a period of 36 years. The meeting serves as one of the premier conferences for international scientists with differing levels of experience in ore deposit research. A major theme of the conference is to promote increased communication and collaboration between industry, academia, and government. The next Gordon Research Conference will be held at Proctor Academy in Andover, New Hampshire, July 31 - August 5, 2005 and the organizers are seeking expressions of interest from those who wish to participate. Students are encouraged to attend and subsidies for students and junior level participants are anticipated, particularly for those presenting posters. We also seek the participation of women and members of minority groups.

The theme of this 5-day conference is *"Metals in ore-forming systems: Sources, transport, and deposition."* The focus of the meeting is on ore-related processes, which will highlight linkages between factors involved in the concentration of metals in the earth's crust and the resultant economic beneficiation of ore. The meeting will be interdisciplinary, with invited speakers who are experts in the fields of biogeochemistry, tectonics, structural geology, experimental geochemistry, and numerical modeling. A preliminary speakers program and conference details are available at the website: www.grc.uri.edu/programs/2005/inorgeo.htm.

To increase industry involvement, the organizers have included the opinions of corporate scientists to create a program that will appeal to industry as well as academic researchers. The introductory session will outline some of the problems that corporate researchers recognize from their field-based work, and set the tone for discussions throughout the meeting. During the final overview session, a group of scientists from industry and academia will review key discussion topics, highlight important ore-forming processes, and outline critical topics for future research.

The 2005 Gordon Conference organizers are Jean Cline (cline@ccmail.nevada.edu), Steve Garwin (steve.garwin@geoinformex.com) and Chris Heinrich (heinrich@erdw.ethz.ch). Those who wish to participate should contact Britt Meyer by e-mail at meyer@erdw.ethz.ch. Poster space will be available and those who wish to present a poster are invited to send a brief abstract together with your expression of interest. Students and other participants who wish to apply for funding to attend the meeting should contact Jean Cline.

The Dr. Denis Shaw Memorial Award

has been established at McMaster University to commemorate Denis's long and distinguished service to the University and profession, and particularly to the Geochemical Society. The terms are

"Established in 2004 by friends, colleagues and former students in memory of Dr. Denis Shaw. To be awarded to a graduate student in the School of Geography and Geology to attend the annual meeting of the Geochemical Society or a similar organisation. Selection will be made by the School of Graduate Studies on the recommendation of the Director of the School of Geography and Earth Sciences. Preference will be given to a PhD student in Geochemistry."

Donations to the Dr Denis Shaw Memorial Award may be made by sending a cheque with a note stating that it is for the award to:

Office of Advancement Services
McMaster University
DTC, 1st floor
1280 Main Street West
Hamilton, ON L8S 4K1

MEETINGS CALENDAR

Feb 10-11, 2005: seismic geomorphology, Westchase Hilton Hotel, Houston, Texas, US. Contact: Jessica Canfor, Geological Society of London, Burlington House, Piccadilly, London W1J 0BG, UK; Phone: +44 (0)20 7434 9944; Fax: +44 (0)20 7494 0579; E-mail: jessica.canfor_AT_geolsoc.org.uk; Web site: http://www.geolsoc.org.uk/seismicgeomorphology

Feb 13-17, 2005: Annual Meeting and Exhibition The Minerals, Metals & Materials Society, San Francisco, CA, USA. E-mail: mtgserv_AT_tms.org

Feb 24-25, 2005: 7. Geokemian Paivat 2005: Jarj. Vuorimiesyhdistyksen Geologijaosto, Geologian tutkimuskeskus, Espoo, Finland. E-mail: mari.lahti_AT_smoy.fi and reijo.salminen_AT_gtk.fi

Feb 25- March 2, 2005: Aluminium: Lithosphere to Biosphere (and Back), Sixth Keele Meeting on Aluminium, Bu aco, Portugal. Contact: Dr. Christopher Exley; E-mail: c.exley_AT_keele.ac.uk; Website: http://www.keele.ac.uk/depts/ch/groups/aluminium/meeting2005/meeting2005.htm

March 15-18, 2005: 1st International Conference on Environmental, Industrial and Applied Microbiology (BioMicroWorld-2005), Badajoz, Spain. Web site: http://www.formatex.org/biomicroworld2005

Apr 3-7, 2005: International Conference on the Biogeochemistry of Trace Elements (ICOBTE), Adelaide, Australia. E-mail: 8thICOBTE_AT_csiro.au; Web site: http://www.clw.csiro.au/conferences/8thicobte/

April 6-9, 2005: 10th IAEAC Workshop on Progress in Analytical Methodologies in Trace Metal Speciation, Luxembourg. Web site: http://chemspec2005.crpgl.lu

April 7-9, 2005: International MoMar Implementation Workshop, Lisbon, Portugal. Hosted by the Group for Deep Sea Research, Interministerial Oceanographic Commission, Ministry of Sciences (Portugal), and supported by the Monitoring and observatories Working Group of InterRidge, Ridge 2000 (USA), MOMARNET and EXOCET/D (EU), and MoMAR (France). Web site: http://ridge2000.bio.psu.edu/NewR2kSite/mw/MOMAR/MoMar_MeetingInfo.php

Apr 14-20, 2005: 5th International Symposium on Eastern Mediterranean Geology, Thessaloniki, Greece. Web site: http://geonet.geo.auth.gr/5thISEMG/

Apr 24-29, 2005: World Geothermal Congress - 2005, Antalya, Turkey. Web site: http://www.wgc2005.org/

Apr 25-29, 2005: European Geosciences Union (EGU) XXX General Assembly, Nice, France. Sponsors: EGU, AGU. Contact: EGU Office, Max-Planck-Str. 13, 37191 Katlenburg-Lindau, Germany; Phone: +49-5556-1440; Fax: +49-5556-4709; E-mail: egu_AT_copernicus.org; Web site: www.copernicus.org/EGU/EGU.html

May 2-6 2005: 37th International Liege Colloquium on Ocean Dynamics: Gas Transfer at Water Surfaces, Liege, Belgium. Web site: http://modb.oce.ulg.ac.be/colloquium/2005.html

May 5-7 2005: The Fourth International Colloquium "Magmatism, Metamorphism and Associated Mineralizations", Agadir, Morocco. Organization: The Department of Geology of the Faculty of Sciences of Agadir, under the auspices of the Minister of Scientific Research. Contact: Secretariat du colloque 3MA, Departement de geologie, Facult Des Sciences, Agadir B.P. 8106 Cit Dakhla, Agadir – Maroc; Phone: + 212 48 22 09 57; Fax: +212 48 22 01 00; E-mail: Colloque3ma_AT_esta.ac.ma or Colloque3ma_AT_yahoo.fr; Web site: http://3ma.esta.ac.ma

May 15-18, 2005: Window to the World, John Ascuaga's Nugget, Sparks, Nevada, USA. Contact: Geological Society of Nevada, P.O. Box 13375 Reno, NV 89507, USA; Phone: +1 775 3234569; Fax: +1 775 323 3599; E-mail: gsnsymp_AT_unr.edu; Web site: http://www.gsn2005.org/

May 15-18, 2004: Halifax 2005, Dalhousie University, Halifax, Canada. 2005 joint meeting of the Geological Association of Canada, the Mineralogical Association of Canada, the Canadian Society of Petroleum Geologists and the Canadian Society of Soil Sciences. Web site: http://www.halifax2005.ca/

May 18-20, 2005: Eurock 2005, International Symposium, Brno, Czech Republic. Contact: Dr Pavel Konecn˝, Inst. of Geonics AS CR, Studentsk‡ 1768, CZ-70800 Ostrava-Poruba, Czech Republic; Phone: +420 69 6979111; Fax: +420 69 6919452: E-mail: konecpa_AT_ugn.cas.cz

May 20-24, 2005: Fifteenth Annual V.M. Goldschmidt Conference, Moscow, Idaho, USA; Web site: http://www.uidaho.edu/gold2005

May 23-27, 2005: AGU Joint Assembly, New Orleans, Louisiana, U.S.A. Contact: AGU Meetings Department, 2000 Florida Avenue, NW, Washington, DC 20009 U.S.A.; Phone: +1-202-777-7333; Fax: +1-202-328-0566; E-mail: meetinginfo_AT_agu.org; Web site: www.agu.org

June 2005: Acid Rain 2005 7th International Conference on Acid Deposition, Prague, Czech Republic. Contact: E-mail acid2005_AT_chmi.cz

June 5-9, 2005: XIII International Conference on Heavy Metals in the Environment, Rio de Janeirio, Brazil. Web site: http://www.rioconventionbureau.com.br/rcvb_ingles/congressos/con_frames.htm

June 5-9, 2005: 105th General Meeting American Society for Microbiology, Atlanta, GA, U.S.A. Web site: http://www.asm.org/Meetings/index.asp?bid=470

June 13-17, 2005: 67th Annual International Conference & Exhibition European Association of Geoscientists & Engineers (EAGE), Madrid, Spain. E-mail: eage_AT_eage.org: Web site: http://www.eage.nl/conferences/index2.phtml?confid=17

June 19-24, 2005: ASLO Summer meeting, Santiago de Compostela, Spain. Contact: Helen Schneider Lemay, Registration Coordinator and Meeting Manager, ASLO Business Office, 5400 Bosque Boulevard, Suite 680, Waco, Texas 76710-4446, U.S.A.; Phone: +1 254 399 9635 or toll-Free: 800-929-ASLO; Fax: +1 254 776 3767; E-mail: business_AT_aslo.org; web site: http://aslo.org/santiago2005/

June 27-29, 2005: Advances in Marine Ecosystem Modelling Research (AMEMR), Plymouth, U.K. Web site: http://www.amemr.info/

June 27-July 1, 2005: International Conference on Mining and the Environment and Metals and Energy Recovery: Securing the Future, Skellefteå, Sweden. Contact: Expolaris Kongresscenter, Skellefteå, SE-931 78 Skellefteå, Sweden; Phone: +46-919-736000; Fax: +46-910-736010; E-mail: kongresscenter_AT_skelleftea.se or tomas.from_AT_metallgruppen.se or manfred.lindvall_AT_boliden.se or helena.ornberg_AT_kongresscenter.skelleftea.se

July 17-21, 2005: 17th Caribbean Geological Conference, San Juan, Puerto Rico. Contact: J.H. Schellekens, Dept. of Geology, University of Puerto Rico, P.O. Box 9017, Mayaguez, Puerto Rico, 9017; Phone: +1 787 265 3845; E-mail: Geoconf _AT_uprm.edu

MEETINGS CALENDAR

July 3-9, 2005: 7th International Eclogite Conference, Seggau, Austria. Contact: iec-7_AT_uni-graz.at; Web site: http://www.uni-graz.at/IEC-7

July 7-9, 2005: Belomorian Mobile Belt and Its Analogues: Geology, Geochronology, Geodynamics and Metallogeny (BMB_2005), Petrozavodsk, Russia. Web site: http://geoserv.karelia.ru/Rus/conf/BMB/bmb_e.html

July 17-22, 2005: 14th International Symposium on Carotenoids. Edinburgh, U.K. Contact: Prof. Andrew J. Young, School of Biological and Earth Sciences, John Moores University, Byrom St. Liverpool L3 3AF, U.K. Phone: +44 151 231 2173; Fax: +44 151 207 3224; E-mail: a.j.young_AT_livjm.ac.uk

July 31-Aug 8, 2005: Fifth International Dyke Conference IDC5, Pohtimolampi Wilderness Hotel, Polar Circle, Rovaniemi, Finland. Contact: Rovaniemi-Lapland Congresses, University of Lapland, PO BOX 122, FIN-96101 Rovaniemi, Finland; Phone: +358 (0)16 341 2799; Fax: +358 (0)16 317 843; E-mail: congres_AT_ulapland.fi; Web site: http://idc5.gsf.fi/

July 31-Aug 5, 2005: Gordon Conference on Inorganic Geochemistry, Metals in ore-forming systems: Sources, transport, deposition, Proctor Academy, Andover, New Hampshire, U.S.A. E-mail: Steve.Garwin_AT_geoinformex.com or christoph.heinrich_AT_erdw.ethz.ch or cline_AT_ccmail.nevada.edu; Web site: http://www.segweb.org/GordonConf.pdf

Aug, 2005: IUCr-20 - XX Meeting and General Assembly of the International Union of Crystallography, Florence, Italy.

Aug 7-11, 2005 10th International Platinum Symposium: "Platinum-Group Element - from Genesis to Beneficiation and Environmental Impact", Oulu, Finland. Contact: Congress Oulu, P.O. Box 56, Fin-90015 Oulun kaupunki, Finland; E-mail: congressoulu_AT_ouka.fi; Web sites: http://www.congressoulu.fi/ and http://platinumsymposium.oulu.fi/

Aug 8-11, 2005: Earth System Processes II, Calgary, Alberta, Canada. Ancient earth systems, modern earth system processes, and earth system futures. An interdisciplinary, integrative scientific meeting exploring the interactions among Earth's lithosphere, atmosphere, hydrosphere, cryosphere, and biota. Organization: Geological Society of America and Geological Association of Canada. Web site; http://www.geosociety.org/meetings/esp2/

Aug 18-21, 2005: The 8th Biennial SGA (the Society for Geology Applied to Mineral Deposits) Meeting "Mineral Deposit Research: Meeting the Global Challenge", Beijing, China. Contact: 8th SGA Biennial Meeting, Secretary: Dr. Jingwen Mao, Institute of Mineral Resources Chinese Academy of Geological Sciences, 26 Baiwanzhuang Road, Beijing, 100037 China; Fax: +86-10 68 33 63 58; E-mail: mail_AT_sga2005.com; Web site: http://www.sga2005.com

Aug 22-26, 2005: 13th International Symposium On Placer And Weathered Rock Deposits (PWR-2005) "Placer And Weathered Rock Deposits in Activated Platforms and Orogenes", Perm, Russia. Contact: Prof. Natalia Patyk-Kara, IGEM RAS; Phone +7-095-230 8427; Fax: +7-095-230 2179; E-mail pkara_AT_igem.ru; Dr. Vladimir Naumov, Perm' State University: E-mail naumov_AT_psu.ru, Prof. Boris Osovetsky, Perm' State University, E-mail minmuseum_AT_psu.ru

Aug 23-27, 2005: GES-7, 7th International Symposium on the Geochemistry of the Earth's Surface, Aix-en-Provence, France. Web site: http://www.cerege.fr/GES7/index.htm

Aug 28-Sept 1, 2005: American Chemical Society annual meeting, Washington, DC.

Aug 29-29, 2005: STOMP - Structure, Tectonics and Ore Mineralization Processes, Economic Geology Research Unit, James Cook University, Townsville, Australia. E-mail: Timothy.Baker_AT_jcu.edu.au or Thomas.Blenkinsop_AT_jcu.edu.au; Web site; http://www.es.jcu.edu.au/STOMP/

Sept 2005: MAEGS-14 Natural hazards related to recent geological processes and regional evolution, Association of European Geological Societies, University of Turin, Torino, Italy. E-mail: marco.giardino_AT_unito.it

Sept 4-20, 2005: IAGOD - Metallogeny of the Pacific Northwest: Tectonics, Magmatism & Metallogeny of Active Continental Margins, Vladivostok, Russia. Web site: http://www.fegi.ru/iagod/

Sep 5-9, 2005: 7th symposium on the Cretaceous, University of Neuchatel, Neuchatel, Neuchatel (Karl F llmi and Thierry Adatte, Geological Institute, University of Neuch‰tel, Phone: 41-32-7182655 FAX: 42-32-7182601 EMail: karl.foellmi_AT_unine.ch, thierry.adatte_AT_unine.ch Web: http://www.unine.ch/geologie/isc7/)

Sep 7-11, 2005: 6th International Conference on Geomorphology, Congress Hall-Auditorium of Zaragoza, Zaragoza, Spain. (Organizing Secretariat Geomorfologia, Facultad de Ciencias, Universidad de Zaragoza, C/Pedro Cerbuna 12, Zaragoza 50009, Spain; Fax: +34 976 761106; E-mail: iag2005_AT_posta.unizar.es; Web site: http://wzar.unizar.es/actos/SEG/index.html

Sept 11-16, 2005: AIG-6 - 6th International Symposium on Applied Isotope Geochemistry, Prague, Czech Republic. Web site: http://www.aig6.cz

Sept 11-15, 2005: 12th International Meeting on Boron Chemistry, Sendai, Japan. Contact: Prof. Xibai Qiu, IUPAC-2005 Secretariat c/o Chinese Chemical Society, P.O. Box 2709, Bejing 10080, China; Phone: +86 (10) 6256 8157; Fax: +86 (10) 6256 8157; E-mail: qiuxb_AT_iccas.ac.cn

Sept 12-16, 2005: 22nd International Meeting on Organic Geochemistry (22nd IMOG), Seville, Spain. 12-16 September 2005. Web site: http://www.imog05.org

Sept 12-16, 2005: 68th Annual Meteoritical Society Meeting, Gatlinburg, Tennessee, USA; web site: http://geoweb.gg.utk.edu/2005/metsoc2005.html

Sept 14-19, 2005: International Conference on Environmental (Geoecological) Problems in Karst, IAH, Belgrade, Yugoslavia. E-mail: jemcov_AT_ptt.yu

Sept 19-23, 2005: 22nd International Geochemical Exploration Symposium (IGES): "From Tropics to Tundra", Perth, Western Australia. Web site: http://www.promaco.com.au/conference/2005/iges/

Fall, 2005: Short course Neutron Scattering applied to Earth Sciences, San Francisco, California. Organizers: Rudy Wenk, University of California - Berkeley, California. Sponsors: Mineralogical Society of America and The Geochemical Society

Sept 20-24, 2005: 2nd International Congress of Seas and Oceans, Szczecin - Swinoujscie, Poland. E-mail: icso_AT_wsm.szczecin.pl; Web site: http://www.wsm.szczecin.pl/iirm/kongres/

Sept 26-29, 2005: MRS 2005 Scientific Basis for Radioactive Waste Management XXIX, Gent, Belgium.

MEETINGS CALENDAR

Oct 2005: Short course Low-Temperature Thermochronometry: Techniques, Interpretations, and Applications, Snowbird, Utah. Organizers: Todd A. Ehlers (University of Michigan) and Peter Reiners (Yale University). Sponsor: Mineralogical Society of America and Geochemical Society of America

Oct 16-19, 2005: GSA 2005 Annual Meeting & Exposition - with Mineralogical Society of America, Salt Lake City, Utah. Web site: http://www.geosociety.org/

Oct 17-19, 2005: International Lead-Zinc Processing Symposium 2005, Kyoto, Japan. E-mail: akiofuwa_AT_waseda.jp

Nov 6-11, 2005: International Gondwana 12 Conference, Mendoza, Argentina; Web site: http://cig.museo.unlp.edu.ar/gondwana

Nov 7-11, 2005: 20th World Mining Congress & Expo 2005, Tehran, Iran. Contact: Mr. A. Almasi, Chief of Executive Committee, No. 25, Ostad Nejatollahi Avenue, Tehran 1599913717, Iran; E-mail: info_AT_wmce2005.com,; Web site: http://www.20wmce2005.com/index.php?page=home

Nov 13-15, 2005: Geology Forum 05, Cape Town, South Africa. Topic: metalliferous ore deposits. Contact: Jon Wills; E-mail: jon_AT_min-eng.com; Website: http://www.min-eng.com/geologyforum05/index.html

Nov 30-Dec 2, 2005: 5th Fennoscandian Exploration and Mining Confernece, Rovaniem, Finland. Contact: Regional Council of Lapland, Ms. Riitta Muhojoki, Project Secretary, P.O. Box 8056, Fin-96101 Rovaniemi, Finland; Phone: +358-16-3301230; Fax: +358-16-318705; Web site: http://www.lapinliitto.fi/fem2005

Dec, 2005: 6th European Meeting on Environmental Chemistry, Belgrade, Yugoslavia. Contact: Dr. Branimir Jovancicevic, Department of Chemistry, University of Belgrade, Akademski trg 12-16, POB 158, 11001 Beograd, Yugoslavia; E-mail: bjovanci_AT_chem.bg.ac.yu; Web site: http://www.science.plym.ac.uk/ace/Meetings.html

Dec 5-9, 2005: AGU Fall Meeting, San Francisco, California, U.S.A. Contact: E. Terry, AGU Meetings Department, 2000 Florida Avenue NW, Washington, DC 20009 U.S.A.; Phone: +1-202-777-7335; Fax: +1-202-328-0566; E-mail: eterry_AT_agu.org; meetinginfo_AT_agu.org; Web site: www.agu.org/meetings

Dec 16-22, 2005: 13th International Conference of the Geological Society of Africa, Cairo, Egypt, 16-22. Contact: Dr Mahmoud Abdeen, GSAf Vice-President (North Africa); E-mail: m_m_abdeen_AT_hotmail.com; Web site: http://gsaf.narss.org/

Feb 20-24, 2006: AGU Ocean Sciences Meeting, Honolulu, Hawaii.

July, 2006: IMA-2006 - XIX General Meeting of the International Mineralogical Association, Kobe, Japan.

July 16-23, 2006: 7th International Conference on the Occurrence, Properties, and Utilization of Natural Zeolites (Zeolite '06), Socorro, New Mexico, USA. Contact: Dr. Bowman: E-mail bowman_AT_nmt.edu

July 23-28, 2006: 19th General Meeting of the International Mineralogical Association, Kobe, Japan. Contact: Prof. T. Yamanaka, E-mail b61400_AT_center.osaka-u.ac.jp; Web site: http://www.congre.co.jp/ima2006/index_e.html

Aug 27-Sept 1, 2006: 17th International Mass Spectrometry Conference (IMSC), Prague, Czech Republic. Web site: http://www.imsc2006.org/

Oct 22-25, 2006: GSA 2006 Annual Meeting & Exposition - with Mineralogical Society of America, Philadelphia, Pennsylvania. Web site: http://www.geosociety.org/

Dec, 2006 - 7th European Meeting on Environmental Chemistry, Brno, Czech Republic. Contact: Dr. Josef Caslavsky, Institute of Analytical Chemistry, Czech Academy of Science, Veveri 97, 61142 Brno, Czech Republic; E-mail: caslav_AT_iach.cz: Web site: http://www.science.plym.ac.uk/ace/Meetings.html

Dec 11-15, 2006: AGU Fall Meeting, San Francisco, California, U.S.A. Contact: E. Terry, AGU Meetings Department, 2000 Florida Avenue NW, Washington, DC 20009 U.S.A.; Phone: +1-202-777-7335; Fax: +1-202-328-0566; E-mail: eterry_AT_agu.org; meetinginfo_AT_agu.org; Web site: www.agu.org/meetings

Sept 2007: International Congress ICAM V 2007, Tromsø, Norway. Organized by International Council for Applied Mineralogy and Geological Society of Norway. Web sites: http://www.geologi.no/cgi-bin/geologi/imaker?id=1909 or http://www.icamv.org

Oct 28-31, 2007: GSA 2007 Annual Meeting & Exposition - with Mineralogical Society of America, Denver, Colorado. Web site: http://www.geosociety.org/

Dec 10-14, 2007: AGU Fall Meeting 2007, San Francisco, CA, U.S.A.

Aug 5-14, 2008: 33rd International Geological Congress (IGC 2008): Nordic Countries: Norway, Sweden, Denmark, Finland and Iceland, Oslo, Norway. Web site: http://www.ngu.no/igc2008

Oct 26-30, 2008: Annual Meeting Geological Society of America - with Mineralogical Society of America, Chicago, Illinois, U.S.A. Web site: http://www.geosociety.org/meetings/index.htm

Dec 15-19, 2008: AGU Fall Meeting, San Francisco, CA, USA. Web site: http://www.agu.org/meetings

Aug 5-15, 2012: 34th International Geological Congress (IGC 2012, Australia), Brisbane, Australia.

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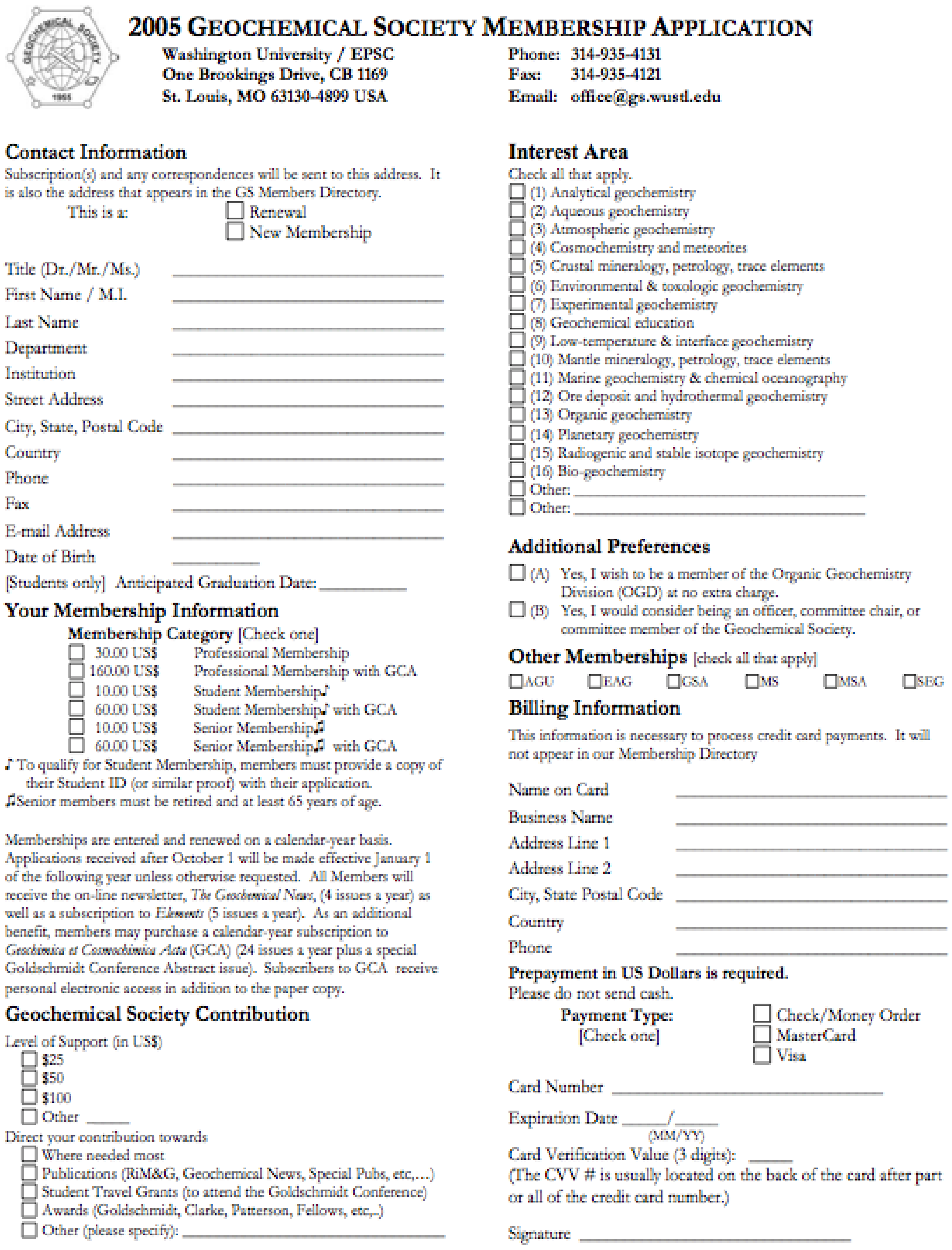

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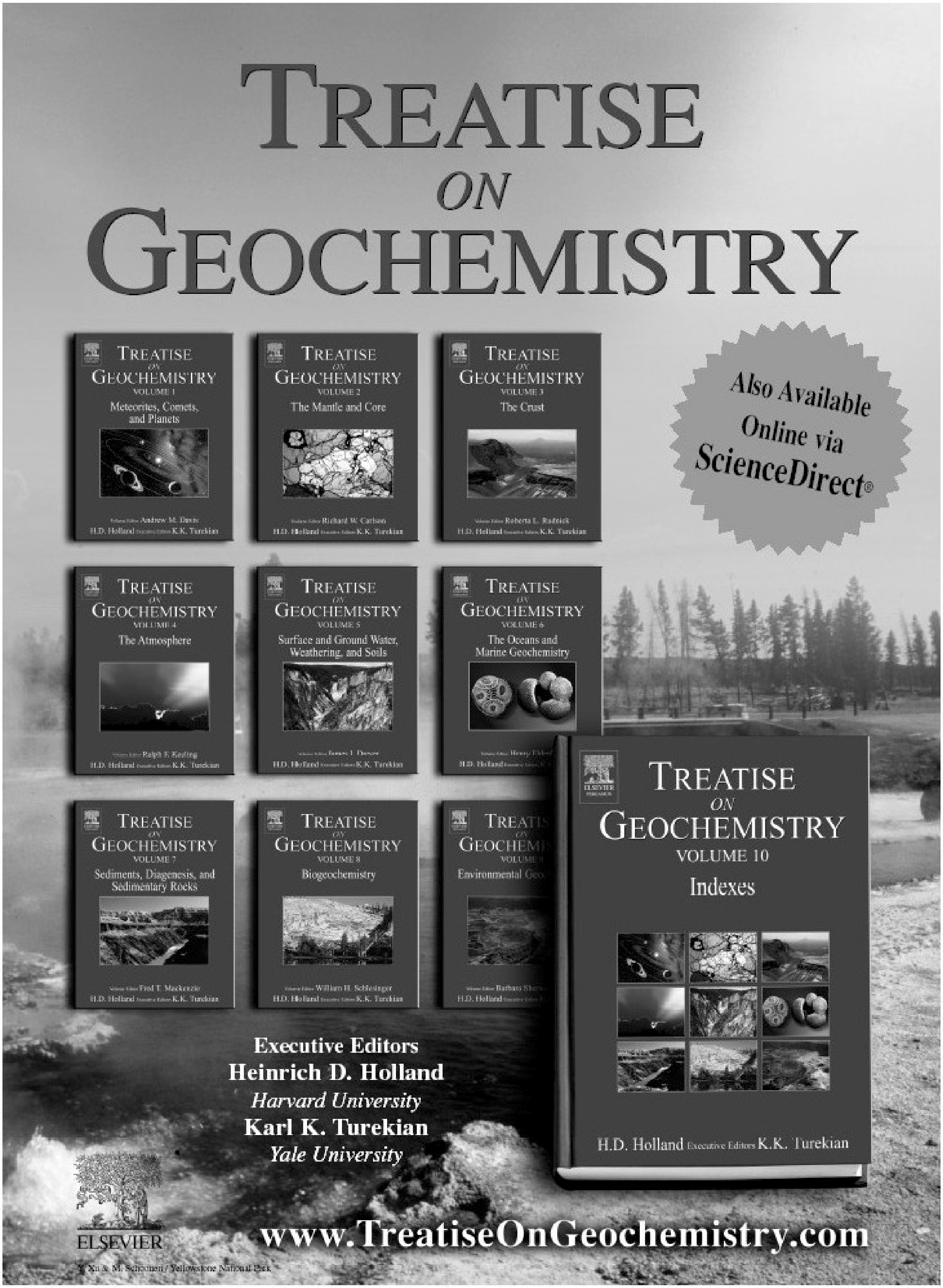
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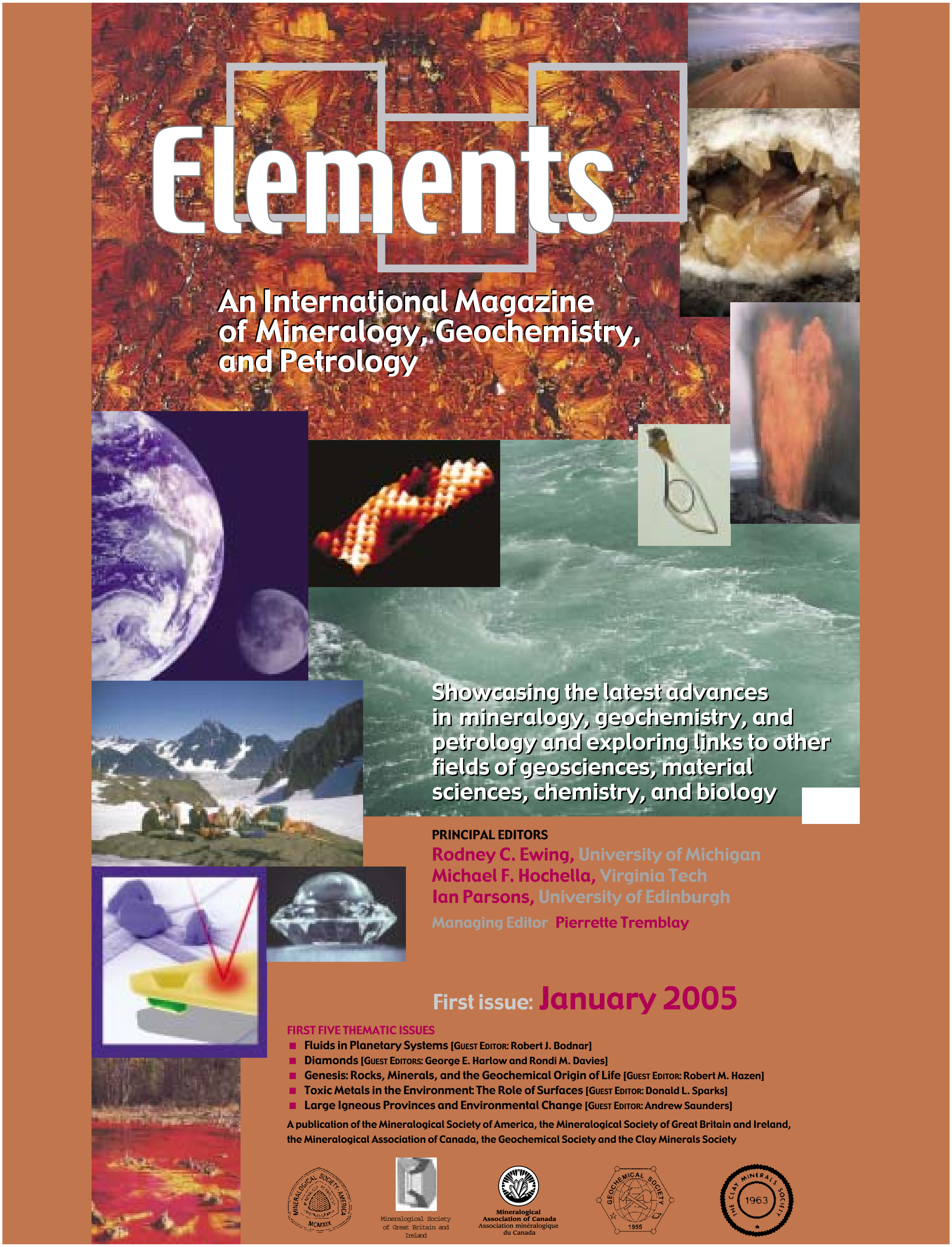

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Showcasing the latest advances in mineralogy, geochemistry, and petrology and exploring links to other fields of geosciences, material sciences, chemistry, and biology

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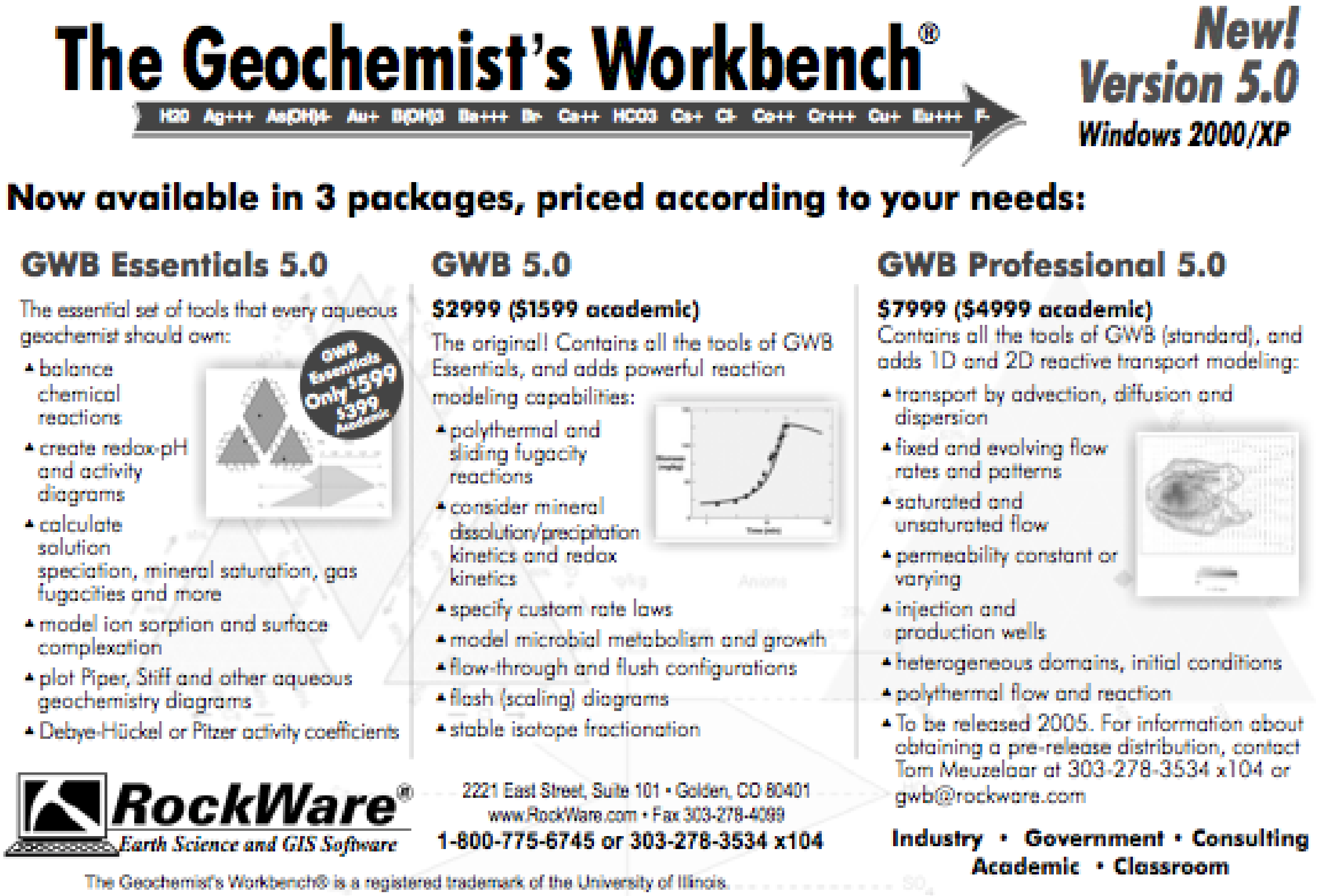
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ANNOUNCEMENT

Nominations for the **Pieter Schenck Award**

The Pieter Schenck Award is given every second year to a scientist normally under 35 years of age who has made a major contribution in any specific area of organic geochemistry or a related field. The previous awardees were Jaap Sinninghe Damst in 1993; Mark McCaffrey in 1995; Katherine H. Freeman in 1997, Stefan Schouten in 1999, and Kliti Grice in 2001.

The seventh award will be attributed at the 22nd EAOG International Meeting on Organic Geochemistry, Seville, Spain, September 2005.

Proposers should send details of their candidate(s) including CV, full list of publications, and a written justification (ca. 2000 words) to the Chairman of the Award Committee before May 31st 2005. The selection will be made by the Pieter Schenck Committee composed of Prof. Walter Michaelis (Chairman, michaelis@geowiss.uni-hamburg.de), Katherine H. Freeman, Roger E. Summons, Joseph A. Curiale, and Richard P. Evershed. Nominations submitted (as pdf, MS Word, or text files) by email to the committee chair are encouraged.

THE GEOCHEMICAL NEWS
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