EMERSON CENTER Newsletter

A Publication of the Cherry L. Emerson Center for Scientific Computation, Emory University
http://www.emerson.emory.edu
Volume 11, February 28, 2003

Inside This Issue . . .

In the News

◆ ***EC Short Course***

The Emerson Center will offer a special short course on "Introduction to Practical Computational Chemistry" that is open to everyone on campus. The course starts on March 20 and runs continuously every Thursday, from 1:30-3pm, for six weeks. See the inserted flyer for details.

◆ ***Emory Report***

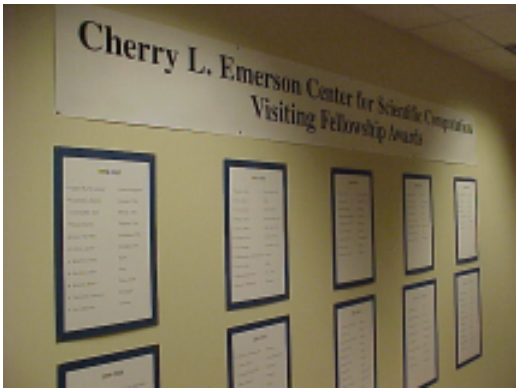
The Emerson Center was featured on the front page of the Dec. 2, 2002 issued of the Emory Report. Eric Rangus of the Emory Report wrote the report after his visit to the Emerson Center and interviews with the center's Director, Prof. Keiji Morokuma, and the center's Manager, Dr. Jamal Musaev.

◆ ***Computational Chemistry Conference***

Prof. Joel M. Bowman, a major subscriber to the Emerson Center, is organizing a conference on "Frontiers in Computational Chemistry," which will be held on April 12, 2003. Details on the inserted announcement.

TEN YEARS OF VISITING FELLOWSHIP PROGRAM BRINGS 100 SCHOLARS TO EMERSON CENTER

The names of ten awardees of the 2003-2004 Emerson Center Visiting Fellowship awards have been announced recently (see page 2 of this newsletter for the names and affiliation of the recipients). This marks the tenth anniversary of the center's Visiting Fellowship Program that started in 1993. Conceived in the earliest stage of negotiation for establishment of the Emerson Center among Drs. Cherry Emerson, Billy Frey (Provost) and Joel Bowman (Chemistry Chair) in 1991, the Visiting Fellowship Program, in addition to the high-power computational facilities, rich software libraries and technical expertise, constitutes one of the backbones of the activities of the Emerson Center and is surely a front runner in Emory's efforts in internationalization. The program is announced in prominent scientific journals every year, as well as on the Emerson Center web site. Although substantial financial resources have been placed in the program, the selection process each year remains extremely competitive.



Emerson Center Visiting Fellowship Awards, 1994-2004

Ten years of the program brought approximately 100 Fellows from all over the world to the Emerson Center. The countries represented by the Fellows include Australia, Brazil, China, France, Germany, Japan, Korea, Poland, Russia, Thailand, Turkey, the United Kingdom, to name just a few. Some of the fellows are world-renowned senior scientists, such as Professor William H. Miller from Berkeley, who spent a semester at the Center. Some are professors from colleges and universities in the United States, who become involved in intensive research during the summer months. Most of the Fellows collaborate with Subscribers of the Center, and are

--Continued on page 4

NEWS FROM THE ECEC MEETING

The 14th meeting of the Emerson Center Executive Committee (ECEC) was held on Tuesday, February 11, 2003. On the agenda were administrative issues, technical reports, and the selection of the Visiting Fellowship awards for 2003-2004. Issues related to the upcoming major computer upgrade with the remaining NSF funds were discussed while a technical report was presented by the Center's scientific staff about the current condition and recent updates on the hardware and software requisitions at the Center. The technical staff members proposed an introductory short course series that is open to the public on campus. The ECEC also approved Visiting Fellowship awards to 10 scientists from various parts of the world. There was also discussions on the proposal to setup a special Emerson Center Lectureship Award.

Letters from Fellows

The application of peer-to-peer computing techniques (P2P) to the area of High Performance Computing is of increasing interest. Since joining Emory in early June my research has focused on developing new protocols for peer to peer (P2P) networks. For example, a protocol called findcast is under design, which, in the context of HPC, seeks to form a group of N computers with the desired resources to cooperate on one calculation. Each collaborating computer must advertise what resources it has and under what terms it is prepared to join with others. The idea is a generic one but the choice of HPC as an exemplar is rich enough in problems to be a suitable challenge to the design. Other protocols are under study to handle the interactions between group members which, potentially, will support data movement and management aspects.

Dr. Roger Loader

Regards, Roger
School of Comp. Science, Cybernetics & Elec. Engineering
The University of Reading
United Kingdom

Dr. Roger Loader visited the Math & CS Department of Emory as an Emerson Center Visiting Fellow from June to November 2002.

Emerson Center Visiting Fellowship Awards for 2003-2004

Dr. Stefano Boccaletti
Physics, Ins. Nazionale di Ottica Applicata, ITALY
Dr. Sylvie Ducki
Medicinal Chemistry, Univ. of Salford, ENGLAND
Dr. Jacob C. Koella
Evolutionary Parasitology, Univ. P&M Curie, FRANCE
Dr. Jerzy Moc
Chemistry, Wroclaw University, POLAND
Dr. Kichisuke Nishimoto
Chemistry, Osaka City University, JAPAN
Dr. Piotr Paneth
Chemistry, Technical Univ. of Lodz, POLAND
Dr. Seung C. Park
Chemistry, Sungkyunkwan University, KOREA
Dr. Andrea Tafi
Medicinal Chemistry, Univ. of Siena, ITALY
Dr. Mark M. Tanaka
Bioinformatics, Univ. New South Wales, AUSTRALIA
Dr. Zhen-Feng Xu
Chemistry, Emory University, USA

The Emerson Center offers visiting fellowships to interested scientists throughout the year. Please refer to the Emerson Center homepage at http://www.emerson.emory.edu for application details and deadlines, or send email to clec@euch4e.chem.emory.edu.

My Stay at the Emerson Center as a Visiting Fellow

Prof. Han Zuilhof, Wageningen University, The Netherlands

The advantages of a sabbatical leave include the privilege to live and work in a completely new environment, which is as stimulating for scientific aspects in life as for all others! From October 2002 to December 2002 I joined the Morokuma group, to familiarize myself more with the ONIOM method that Prof. Keiji Morokuma developed over the last decade. The goal of the research was the prediction of enantiomeric separation of D and L amino acids, via the formation of diasteromeric complexes. This goal had hitherto been too far to reach, largely because the size of the systems under scrutiny did not allow high-level ab initio computations of the whole system. Using a stepwise approach, the factors were delineated that determine the relative diasteromeric stabilities. In practice this means that the efficiency of enantiomeric separation can be better predicted, which enhances the applicability of the experimental research that is also going on in my group in Wageningen in the Netherlands. All in all, the discussions with Keiji, the support of the complete Morokuma group and Keiji's secretary Jianli Zhao, and the excellent computational facilities kept up-to-date by Jamal Musaev & Stephan Irle made this a very fruitful research period for me. The presence of a child section in the Botanical Gardens, and of pandas in the Zoo also made Atlanta memorable for the rest of my family!

Dr. Han Zuilhof

Dr. Han Zuilhof stayed at the Emerson Center and Prof. Keiji Morokuma's group from October to December 2002.

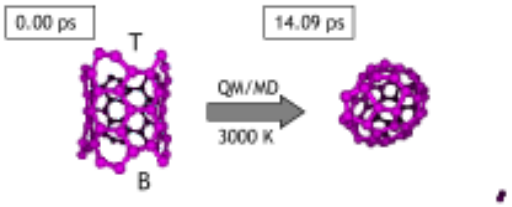
Report on Research Activities at the Emerson Center

The Emerson Center is supported, in part, by "subscribers" - faculty members, research groups or departments that purchase shares in order to gain access to its resources for their research projects. EC scientific staff members are also encouraged to conduct scientific research in their own areas of specialty. The following are two research reports from the Emerson Center.

Unlocking the Mysteries of Fullerene Formation by Quantum Chemical Molecular Dynamics Model Calculations

Research Report by Dr. Stephan Irle
Emerson Center

Despite the fact that fullerenes have been around for some time and are being heavily researched for new chemical and physical properties as well as building blocks of larger nano structures, the actual mechanism to fullerene formation still remains one of the best kept secrets of nature. For a practical computational investigation of the formation mechanism one has to resort to molecular dynamics approaches due to the high dimensionality of the problem. However, it is clear that even modern reactive molecular force fields like REBO are inappropriate for reaction dynamics, since π-conjugational effects are not taken into account. Therefore, we chose to run quantum chemical molecular dynamics using DFTB, a new extended Huckel type method which has been demonstrated to give fast and reliable in the context of fullerene isomers and derivatives. Both chiral and achiral open-ended nanotubes of different lengths were chosen as precursor molecules. Temperature is the most important factor. Above 4000 K, the systems falls apart into fragments. At 3000 to 3500 K, we observe that the hexagons of the nanotube open ends open and create C_2-chains that wobble at the end of the openings. Some of them recombine and form pentagons which causes the open ends to curl inside. At the curled end, a wobbling C_2 chain suddenly binds to the other side of curl and forms a new ring, narrowing the opening. This occurs repeatedly and preferably at 5/7 ring combinations with broken bond in their center, forming a bridge like structure in the opening. Eventually the openings will close, leaving octagons as the largest cyclic structures observable at the ends. When this happens at both ends of the nanotubes, the tube is fully closed and a fullerene molecule is formed. Actual movies of these processes are available on the web at http://euch4m.chem.emory.edu/nano.



More realistic studies starting with C_2 units are underway and show promising preliminary results for the formation of substantial large carbon clusters on a computationally feasible time scale.

On the Mechanism and Kinetics for the Reaction of Phenyl Radicals with Acetylene

Research Report by Dr. Igor Viktorovich Tokmakov
M. C. Lin Group, Chemistry Department

The mechanism of the $C_6H_5 + C_2H_2$ reaction has been investigated by the G2M composite method. Electrophilic addition to the triple CC bond is found to be the only important mode of the phenyl radical attack on acetylene. The initially formed chemically activated $C_6H_5C_2H_2$ adducts may follow a H-elimination and several isomerization pathways (see Fig. 1) in competition with collisional stabilization. Our calculations provide accurate thermochemistry for various decomposition and isomerization channels. The energetic parameters predicted by the G2M(RCC5) method agree with the best available experimental and theoretical data within 1.2 kcal/mol. For the key intermediates, the following isodesmic enthalpies of formation (at 298 K) have been found: 94.2±2.0 kcal/mol (C_6H_5CHCH), 86.4±2.0 kcal/mol ($C_6H_5CCH_2$), and 95.5±1.8 kcal/mol (o-$C_6H_4C_2H_3$).

The kinetics and product branching of the $C_6H_5 + C_2H_2$ reaction have been evaluated by weak collision master equation/RRKM analysis of the truncated kinetic model which included only kinetically important transformations of the isomeric C_8H_7 radicals. Available experimental kinetic data can be quantitatively reproduced by calculation with a minor adjustment of the C_6H_5-addition barrier from 3.7 to 4.1 kcal/mol. Our predicted total rate constant, $k_1(T) = 2.29\times10^{10} T^{0.834} \exp(-2320/T)$ $cm^3\ mol^{-1}\ s^{-1}$, is weakly dependent on pressure and corresponds to the phenylation process under combustion conditions ($T > 1000$ K). At low T, three wells (isomers **1**, **3** and **8**) effectively compete for the reactive intermediates. The fraction of C_8H_7 radicals reaching the pentalene branch (over **TS13**) increases with T but does not exceed 0.1% even at 2000 K.

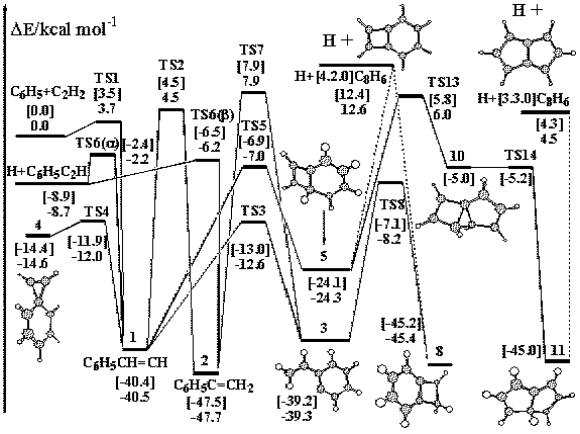


Figure1. Truncated potential energy diagram for the $C_6H_5 + C_2H_2$ reaction. Relative energies (kcal/mol) are calculated by the [G2M(RCC6)] and G2M(RCC5) methods using the geometries optimized at the B3LYP/6-311++G(d,p) level.

--ECVF, continued from page 1

stationed either in the subscribers' research groups or in the comfortable Visiting Fellow area of the Emerson Center facilities. All Visiting Fellows have access to the use of the computers and the software and technical expertise provided by the Center. There are over one hundred known papers published by the Visiting Fellows and their collaborators during their stay at Emerson Center. Many of the Fellows come back for continuation of collaboration, finding other sources of funding and sometimes with a second fellowship.

The length of stay varies from a few weeks to a year, but most visitors stay from one to three months. In order to accommodate lodging needs of visiting fellows, the Center has maintained a furnished apartment in the vicinity of the University. Since last fall a two-bedroom apartment is leased at the Clairmont Campus of the University (see page 4 about the apartment) and Visiting Fellows are given the top priority to reserve rooms.

The Emerson Center Apartment

The Emerson Center has received much positive response from its visiting fellows who have stayed at the new EC Apartment at the Clairmont Campus of Emory. Dr. Han Zuilhof, Professor of Chemistry at Wageningen University, The Netherlands , wrote in his email to us that "this new apartment is a big step forward! You have made a good choice! The campus is nice for me given the internet access (just submitted 7 jobs while sipping a cup of tea here), the excellent transport to the Emerson Center, etc.; it is nice for my wife, given the additional sports facilities in the high tower, and the fact that this is close to other families (easier to make contacts with other moms), and a lot safer for David, our son. All in all: three thumbs up & thanks for all your efforts!"

The Center also makes the apartment available to other short-term visiting faculty on campus when there is a vacancy. The apartment is a fully furnished 2-bedroom/2-bathroom apartment with cable TV and internet access. The rent, which includes all utilities and local telephone service, is $660 per room per month, or $35 per day if less than 30 days. Please call 727-0867 for more information.

Cherry L. Emerson Center for Scientific Computation

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This issue of the Emerson Center Newsletter is designed and edited by Jianli Zhao

Report on EC Operating System & System Software Upgrade

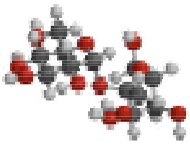
Jamal Musaev & Stephan Irle, Emerson Center

The Emerson Center is pleased to report that the operating system was successfully upgraded from AIX 4.3.3 to AIX5L Version 5.1 during the end of last year/beginning of 2003. AIX5L has a high degree of Linux affinity (therefore "L") which means that specific features of Linux are now integrated into the AIX kernel, such as the /proc file system for process monitoring or Linux type extended file systems ext2. Also included in standard AIX software are GNU type utilities such as make, bzip2, gtar, etc. But while these utilities have been provided already previously, it is more important that 64bit type applications can now be compiled and run on our SP3 and euch4e. More and more application software packages such as GAUSSIAN and MOLPRO are now written for 64-bit mode which provides performance enhancement and support for large memory addressing beyond 2GB. After almost 10 years of being available on Digital/COMPAQ and SGI platforms, we are glad to offer this functionality now also on our IBM systems.

Along with AIX5.1 we upgraded LoadLeveler, our queuing system software, from Version 2.2 to 3.1. This upgrade provides queuing system support at the AIX5.1 level, while being virtually indistinctable from its predecessor, so that old scripts are running just fine (except for one small detail, namely the AIX51 keyword has to be specified instead of AIX43).

At the same time as the operating system upgrade, we installed IBM's latest compilers: XL FORTRAN 8.1, Visual Age C++ Version 6.0, and Java Version 1.3. The compilers are available on euch4e and in special cases sp2.chem.emory.edu for compilation of large memory applications. They come bundled with IBM's graphic debugger "idebug" which provides for debugging High Performance Parallel Applications and allows to look at allocation of real time memory. Along with the compilers came an upgrade of IBM's mathematical library ESSL (Engineering and Scientific Software Library) Version 3.3. It now provides an O(N) algorithm (Divide and Conquer) for matrix diagonalization, which should proof to be extremely useful for some problems of our subscriber community. Moreover, the library provides support for automatic SMP-type parallelism, which can be made use of on our special queues (sp5, sp6).

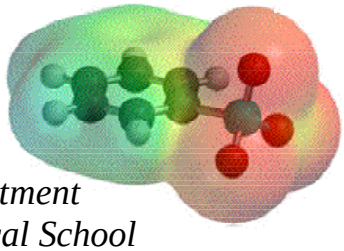
While for the average user AIX5L seems to no different from AIX 4.3.3, we are now glad to provide small but distinct improvements such as 64bit capability in a more robust environment.



EMERSON CENTER
SHORT COURSE ANNOUNCEMENT

Introduction to
Practical Computational Chemistry

From March 20th through April 24th, 2003
1:30 pm – 3:00 pm, Every Thursday for Six Weeks at the
Cherry L. Emerson Center for Scientific Computation
E510 Emerson Hall

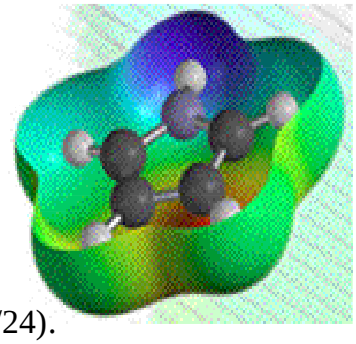


Lecturers:	*Dr. Jamal Musaev, Emerson Center*
	Dr. Stephan Irle, Emerson Center
Visiting Lecturers:	*Dr. James Snyder, Chemistry Department*
	Dr. Kim Gernert, BIMCORE, Medical School

This course is intended to teach newcomers in Computational Chemistry (a) how to use the Center's facilities, and (b) how to apply the existing electronic structure and molecular modeling software to their own research fields. Everybody who plans to use the Emerson Center's facilities and computational methods for their research is encouraged to attend.

1. Overview of the Center's Computational Facilities (3/20)

(a) Available Hardware, system software and application software at the Emerson Center; (b) Unix utilities; (c) Interactive machines and file server; (d) Batch jobs, Loadleveler queuing system, and Loadleveler commands.



2. Most Popular Quantum Chemistry Software (3/27, 4/3)

A. Introduction to the Gaussian program package (3/27);
B. Introduction to MOLPRO program package (4/3).

3. Molecular Modeling Software (4/10, 4/17, 4/24)

A. Homology Modeling (Dr. Kim Gernert, 4/10);
B. Molecular Modeling (Dr. James Snyder, 4/17);
C. TINKER: Molecular Mechanics/Dynamic Software (4/24).

Contact Information: Dr. Jamal Musaev, Emerson Center, E518 Emerson Hall
Phone: 7-2382, Fax: 7-7412, Email: dmusaev@emory.edu

EMORY UNIVERSITY

Frontiers in Computational Chemistry

Saturday, April 12, 2003
Mathematics and Science Center
Emory University, Atlanta

Symposium Speakers:

Joel M. Bowman
(Emory University)

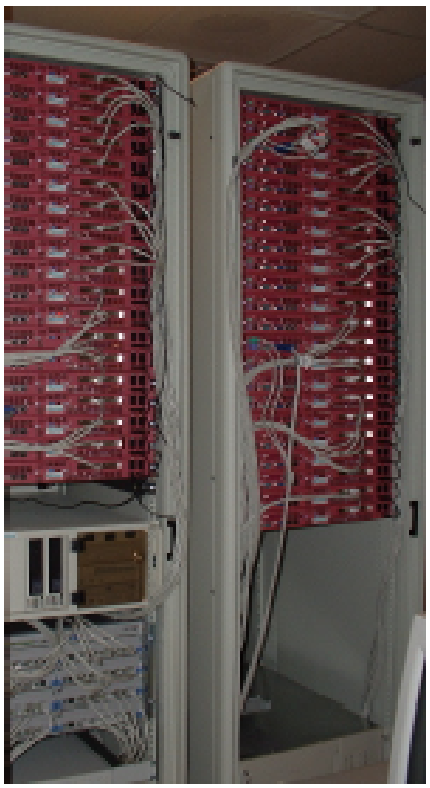
Stuart Carter
(University of Reading)

Nicholas C. Handy
(Cambridge University)

William H. Miller
(U.C. Berkeley)

Keiji Morokuma
(Emory University)

Henry F. Schaefer, III
(University of Georgia)



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Session Chairs:

Rigoberto Hernandez
(Georgia Tech)

James Kindt
(Emory University)

Peter Schmidt
(ONR)

David Sherrill
(Georgia Tech)

There is no fee
but space is limited.
If you plan to attend please let us know.

To register or
for more information
contact Susan Browne
sebrown@emory.edu
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(404) 727-6628 (fax)

http://www.emory.edu/CHEMISTRY/faculty/bowman/symposium/frontiers