EMERSON CENTER Newsletter

A Publication of the Cherry L. Emerson Center for Scientific Computation
http://www.emerson.emory.edu
Volume 2, September 1, 1998

In This Issue . . .

New Chemistry Reference Database Installed!

The Emerson Center has recently installed an MDL Database per the request by EC subscriber, Prof. Al Padwa. This is a powerful chemistry reference database and includes SPORE (Solid-Phase Organic REactions), ACD (Available Chemicals Directory), RefLib (The Reference Library of Synthetic Methodology), CHC (Comprehensive Heterocyclic Chemistry), ORGSyn, ChemInform Reaction Library and more databases. This may be useful not only to chemists but also to people with biomedical and related interests. For more information, please read "Software upgrade news" on Page 3.

Letter from the Director

A NEW AGE OF COMPUTATION - IBM SP UPGRADED -

You may not notice by looking from the outside, but the central computer system of the Emerson Center, the IBM SP supercomputer system, has gone through a total face-lift during the summer. With this upgrade, the computer is running approximately 2.4 times faster than before. It is now loaded with faster P2SC (160MHz) processors, faster memory and faster switches. Virtually the only thing unchanged is the outside look, as the same outer cabinet is still used.

The Emerson Center provides the resources for the highest level of computational need for academic research in the Emory community. This means that the computer capacity has to be improved constantly. The SP supercomputer was fully saturated for the last year or so. The present upgrade, the first since the SP purchase in the summer of 1995, is expected to satisfy the ever-increasing needs for the new age of scientific computation, at least for a few years.

Keiji Morokuma

Come and Celebrate SP Upgrade!

Open House – 1-5pm, Friday, September 11

The Emerson Center is having an open house on Friday, Sept. 11, 1998 to celebrate the successful upgrade of both the hardware and the system software. The open house will be from 1:00pm to 5:00pm at the Emerson Center, 440C Atwood Chemistry Center. The ceremony will be from 1:00pm to 1:30pm, with Provost Rebecca Chopp participating. Refreshments will be served and everyone is invited to see Emerson Center and its upgraded SP computer.

BIMCORE joins Emerson Center as a subscriber

The Emerson Center Executive Committee has recently approved an application from BIMCORE to become a new subscriber of the Emerson Center. With this subscription, the members of BIMCORE can access the hardware and software resources and the visiting fellowship program of the Emerson Center. Prof. Morokuma, Director of the Emerson Center, welcomes this subscription and expects a stronger cooperation between the two academic computing facilities.

Want to Be a Subscriber? New Introductory Subscription Offered

At the recent Emerson Center Executive Committee meeting, an introductory subscription of $1250 per year was approved . This low-cost introductory subscription offers the subscriber access to all Emerson Center research resources, both hardware and software, except for the privilege of hosting visiting fellows.

A no-cost 3-month trial subscription of the Emerson Center is still available for those who want to try out the benefit of subscription. For further information, please contact Dr. Musaev (7-2382, musaev@euch4g.chem.emory.edu) or Dr. Irle (7-4658, sirle@emory.edu) at the Emerson Center.

1999-2000 Visiting Fellowship Offered

The Emerson Center offers visiting fellowships in computational chemistry/physics/sciences throughout the year. Scientists from academic institutions all over the world who want to perform intensive research in computational chemistry/physics/sciences for one to several months are encouraged to apply. We also accept faculty on sabbatical leave. Postdoctoral research associates are not supported through this program. Travel expenses (and stipends for long term stays) are available. Although fully independent research is not excluded, collaboration with an EC subscriber is desirable, and EC subscribers are encouraged to make recommendations. Deadline for application is February 1, 1999.

To Formally Apply, please submit:
- *1-2 page research proposal,*
- *CV including publication list,*
- *the amount of financial support needed and*
- *the length of stay and an approximate start/end date*

Applications should be submitted to the Emerson Center (address on p. 4).

DEADLINE TO APPLY IS FEBRUARY 1, 1999

Meet the EC Visiting Fellows

Dr. Kurt Christoffel

Dr. Kurt Christoffel is a second-time Emerson Center Visiting Fellow having previously collaborated with Prof. Joel Bowman during the summer of 1995. He will be spending his sabbatical year leave from Augustana College (IL) at the Emerson Center again working with Prof. Bowman. Current work underway involves the use of quantum mechanical calculations of molecular internal states for use in improved RRKM estimates of unimolecular reaction rates.

Dr. Ryza Musin

Dr. Ryza Musin comes to the Emerson Center from the Novosibirsk Scientific Center of the Russian Academy of Sciences. Dr. Musin's current project in collaboration with Emerson Center subscriber, Prof. M.C. Lin, deals with quantum chemical study of the series of pseudocubic silicon-carbon nitrides with composition $Si_xC_{3-x}N_4$ (x=0,1,2,3) to predict structural characteristics and physical properties of these hypothetical superhard crystalline materials.

Dr. Yoshihiro Osamura

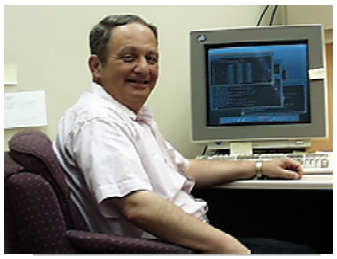
Dr. Yoshihiro Osamura is Professor of Chemistry at Rikkyo University in Tokyo, Japan. His current projects collaborating with Prof. Morokuma at the Emerson Center involve: a) development of the full variational method to optimize electronic and nuclear wavefunctions and geometries simultaneously; b) molecular structures and interactions of the hydrated clusters of strong and weak acids; and c) reaction mechanisms of the formation processes of interstellar molecules.

Dr. Brian Yates

Dr. Brian F. Yates spent one month as an Emerson Center visiting fellow in the summer of 1998. He collaborated with Prof. Morokuma on the application of the new computational methods (IMOMM and IMOMO) to large organometallic complexes. The treatment of these real experimental systems is beyond the capabilities of normal molecular orbital methods. Dr. Yates will apply these techniques to research in homogeneous catalysis back at the University of Tasmania, Australia and will revisit Emory this winter.

My Year at the Emerson Center

Prof. Harold Basch, Bar Ilan University, Israel



Dr. Harold Basch

I have to say how much I've enjoyed my year at the Emerson Center. I don't remember such a scientifically productive period of time since I was a postdoctoral fellow many years ago. The congenial atmosphere of the staff and other visitors, their creativity and openness, all combine to produce an almost ideal atmosphere and surroundings that are conducive to productivity and excellence in research.

Such conditions don't arise spontaneously. The leadership of Prof. Keiji Morokuma and the generous support of the Center's Benefactor, Dr. Cherry L. Emerson, provide the scientific and material means upon which the Center flourishes. To Prof. Morokuma we must credit the organizational skills for orchestrating the various activities, scientific and otherwise, of the Center. His boundless energy imparts a dynamics to the many research activities which is essential to maintaining momentum on a daily basis.

The list of projects that I have been involved in is impressive:

A. The reaction of molecular hydrogen with binuclear metal complexed molecular nitrogen (in its free form, 80% of the air we breath).
B. The reaction of the greenhouse gas methane with the oxygenase enzyme.
C. Ligand-assisted reaction of Ti^+ to activate chemical bonds.
D. Cluster cations of Pt as activators of the chemical bonds.

The Emerson Center certainly brings out the best in people.

Harold Basch

**Prof. Basch stayed at the Emerson Center from July 1997 to August 1998.*

Report on Research Activities from EC Subscribers

The Emerson Center is supported, in part, by "subscribers" or faculty members who purchase shares in order to gain access to its resources for their research projects. The following are research activity reports from some subscribing groups of the Emerson Center.

Our Recent Research Activities

Prof. Joel Bowman
Department of Chemistry

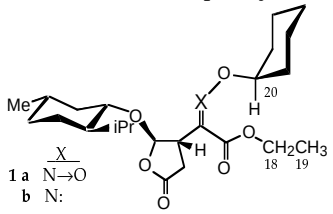
During the past year several Emerson fellows worked with my group. Dr. Vladimir Mandelshtam from UC Irvine spent one week helping us develop a 'filter diagonalization' program to efficiently calculate all the bound states and many resonance states of HOCl. This code has been re-written by Dr. Sergei Skokov, who is my postdoc, and interfaced to 'MULTIMODE'. This code, which was developed by former Emerson fellow, Dr. Stuart Carter, has been used to calculate anharmonic/coupled transition state theory rate constants for two important reactions in combustion chemistry. This work is being done by a new visiting fellow, Prof. Kurt Christoffel, from Augustana College, who will be working on a variety of projects in reaction rate theory during the coming year. Others involved in the rate calculations are graduate student Heather Shnider and undergraduate student Gabe Weinberg (MIT).

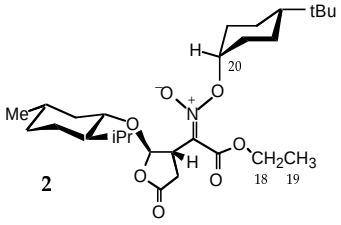
Postdoctoral associate, Dr. Sergei Skokov has developed a global potential for HOCl→Cl+OH in a collaboration with Prof. Kirk Peterson, and together with Drs. Chao-Yie Yang, Stephen Gray, and Vladimir Mandelshtam, has done a thorough analysis of the bound states of HOCl. He is also working on the calculation of the vibration/rotation states of twelve degree-of-freedom water dimer.

On Pure Axial Monosubstituted Cyclohexanes

A Report from Prof. Liotta's Laboratory
Department of Chemistry

Conformational analysis of six-membered rings occupies one of the cornerstones of organic stereochemistry. The two textbook features that characterize the structural class are the existence of axial (ax) and equatorial (eq) conformations and the predominance of equatorial conformers in the accompanying dynamic equilibrium. Very recently the ^{1}H NMR spectra of nitronic ester **1a** and O-cyclohexyloxime **1b** were interpreted in terms of a purely axial monosubstituted cyclohexane.





The unprecedented axial-oxygen conformation was presumed to be induced by steric effects arising from the presence of a rigid and planar π-system for the Z,Z,Z-configured $C_{20}O$-X=C-C(O)OC_{18} moiety. Ben Cornett, Matt Davis, Shaoxiong Wu, Neysa Nevins and Jim Snyder have evaluated these proposals by analysis of the coupling constants reported for **1a**/**1b** and by synthesis and ^{1}H/^{13}C NMR appraisal of the conformationally rigid *cis* and *trans t*-butylcyclohexanol derivatives **2** and (**3**). By comparison, the NMR spectra of **1a** and **1b** do not appear to represent a pure axial cyclohexane. The rigidity of the model nitronate MeO-NO=C(Me)CO_2Me was assessed by density functional (DFT) geometry optimizations (Becke3LYP/3-21G) and supported by fixed point energy calculations with higher basis sets (Becke3LYP/6-31G* and MP2/6-31G). While the nitronate moiety is planar, calculated energy barriers for isomerization around the CO-NC and NC-C(O)O bonds are less than 15 kcal/mol. The values are well below that necessary for rigidity at room temperature (18-20 kcal/mol). We conclude that compounds **1a** and **1b** do not constitute the first example of a purely axial monosubstituted cyclohexane, but that the systems are at best a complex average of conformations with a significant population of the equatorial diasteriomer.

Hardware & Software Upgrade News

Hardware & System Software Upgrade

A report from the Systems Manager

The last issue of this Newsletter on March 15 included a statement that "we plan to substantially upgrade our hardware in the near future." This article now reports a completed upgrade, which took place somewhat earlier than we expected, very much to the pleasure of our users. Before, the heavy load on our machines caused two to three days waiting time for a job in the queue, a situation which has improved quite nicely due to the upgrade.

Extensive price/performance comparisons for various types of supercomputers revealed that the best option was to replace all 14 CPUs in our IBM SP frame by new chips running at 160Mhz clock speed. Compared to the old processors with 66Mhz, this makes up for a speedup factor of roughly 2.4 which indicates a

-continued on page. 4

Application Software Upgrade

A report from the Application Software Manager

After successful installation of new SP nodes and upgrading of the Operating System (OS) of our computers from AIX-3.2.5 to 4.2.1, we have checked the comparability of our existing system and application software with the new OS. We are glad to report to our user community that our major application programs, such as GAUSSIAN-94, MOLPRO-96, GAMESS-96, CERIUS2, work very stably with the new OS and the new Fortran (version 4.1) and C++ (version 3.1) compilers.

Also, we would like to inform that the latest version of the EC's most popular program, GAUSSIAN-98, just arrived and will be in service very shortly. New methods and features of the program are:

- *MP2 and Raman Intensities,*

-continued on page. 4

Hardware, continued from page. 3

high level of performance as shown in the table below. Most other systems, like e.g. the SGI/Cray Origin2000 (O2K) do not reach the floating point performance on a per CPU basis, essential in scientific computing. The DEC 4100 server is somewhat faster, however it turned out to be twice more expensive than the IBM solution. Lately, off-the-shelf Pentium PC's have received a lot of attraction at educational sites due to their relatively strong numerical power and their comparatively low price due to the street market. However, these systems are still at an experimental stage, and among their weak points are lack of stability (typical reboot time 30 to 60 days) and lack of experience in the case of parallel computation, factors to be considered seriously at a service facility like the Emerson Center.

System	Integer SPECint95*	Floating Point Performance SPECfp95*
SP 39H 66MHz (old)	3.31	9.35
SP P2SC 160MHz (new)	8.61	25.8
Intel PII 300MHz	11.7	8.15
SGI O2K R10000	10.3	19.0
DEC 4100 5/600	18.8	29.2
DEC AlphaStn 500/500	15.0	20.4

*** the higher, the better**

The good price/performance ratio for the upgrade of the SP as compared to the purchase of a completely new system is also related to the fact that IBM was willing to trade in our old nodes.

The upgrade turned out to be much more laborious than just to switch the CPUs. In fact, everything except hard drives and the frame itself had to be replaced, which was done around June 1st. The downtime associated with this part was only 5 days. However now the most user-unfriendly and tedious part of the upgrade had to be done: bringing IBM's operating system AIX to the latest stable level at 4.2.1. IBM's decision to discontinue any support for AIX 3.x since January 1 made this painful migration necessary, and we are glad to report that this upgrade is finished. We implemented the new operating system as close as possible to the old configuration, which caused a downtime of another 3 weeks. During this time, we also upgraded the workstation cluster of RS/6000 standalone machines to AIX 4.2.1, in order to achieve consistency in our setup. Along with the operating system, the C++ and FORTRAN 90 version 3.1.4 and 4.1 compilers are now available, and last but not least, we are now running a "Year 2000" safe system!

Stephan Irle
Systems Manager, Emerson Center

Cherry L. Emerson Center for Scientific Computation
Atwood Hall, 1515 Pierce Dr.
Atlanta, Georgia 30322
Phone: (404) 727-2380
Fax: (404) 727-6586
Email: clec@euch3g.chem.emory.edu
http://www.emerson.emory.edu

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

PLEASE VISIT US AT OUR WEB PAGE:
http://www.emerson.emory.edu

The Emerson Center web page gives the most up-to-date information about the Emerson Center operations. You will have access to information about the center's Mission Statement, the current list of the centers subscribers and their research interests, our Visiting Fellows Program updates, software and hardware upgrade information, news on conferences and other programs that the center initiates, tutorials, and links to many other exciting sites.

Software, continued from page. 3

- *Enhanced version of the Polarized Continuum (overlapping spheres) model (PCM) of Tomasi and coworkers for SCRF solvent effects,*
- *Trajectory calculations,*
- *Reaction path optimizations,*
- *The ONIOM facility of Morokuma and coworkers,*
- *ZINDO and TD excited state energies,*
- *Analytical ECP second derivatives Morokuma and coworkers,*
- *Forces, optimizations and frequencies with background point charges,*
- *Additional basis sets: Davidson's modified cc-pDVZ, Stuttgart/Dresden ECP, MIDI, Stevens-Basch-Krauss ECP,*
- *The IRCMax method for locating/optimizing transition states,*
- *Molecular mechanics methods using the AMBER, DREIDING and UFF force fields.*

The efficiency of several methods has been improved, e. g.,

(a) CASSCF calculations may now use an active space of up to 12 orbitals. CASSCF calculations may now use Davidson diagonalization in addition to Lanczos and full diagonalization.

(b) MP2 frequencies require less disk space.

(c) DFT frequencies speed improvements.

(d) Improved efficiency of parallel Hartree-Fock and DFT calculations.

(e) Linear-scaling performance for large semi-empirical and DFT calculations via the fast multipole method (FMM) and sparse matrix techniques.

We have installed (in collaboration with Prof. Padwa's group) on the Emerson Center computers a new chemistry reference database, a product of the MDL Information Systems Inc., which may be useful not only to chemists but also to people in biomedical and other research fields. This database actually consists of various databases, such as ORGSYN, Available Chemical Directory (ACD), Solid-Phase Organic Reaction (SPORE), ChemInform Reaction Library, Reference Library of Synthetic Methodology and Comprehensive Heterocyclic Chemistry (CHC), and includes information about chemical reactions, chemical references, chemical suppliers etc. up to the first half of 1998 (to be updated regularly). At the Emerson Center we have installed the ISIS/Host 3.0 software on one of our fastest workstations, euch3f.chem.emory.edu. In order to access this database, you should run ISIS/Base 2.1.4 software on your local computer, and set up a communication link between ISIS/Host and ISIS/Base. This is a relatively simple process. For more detail on how to use this database, please contact Chris Stroub, 7-6630, cstraub@emory.edu.

Jamal Musaev
Application Software Manager, Emerson Center