

THE NUCLEUS

January 1992

Of the Northeastern Section of the American Chemical Society

Vol. LXX, No. 4

Monthly Meeting

*S.D. Fazio speaks on
Capillary Electrophoresis*

Environment Report

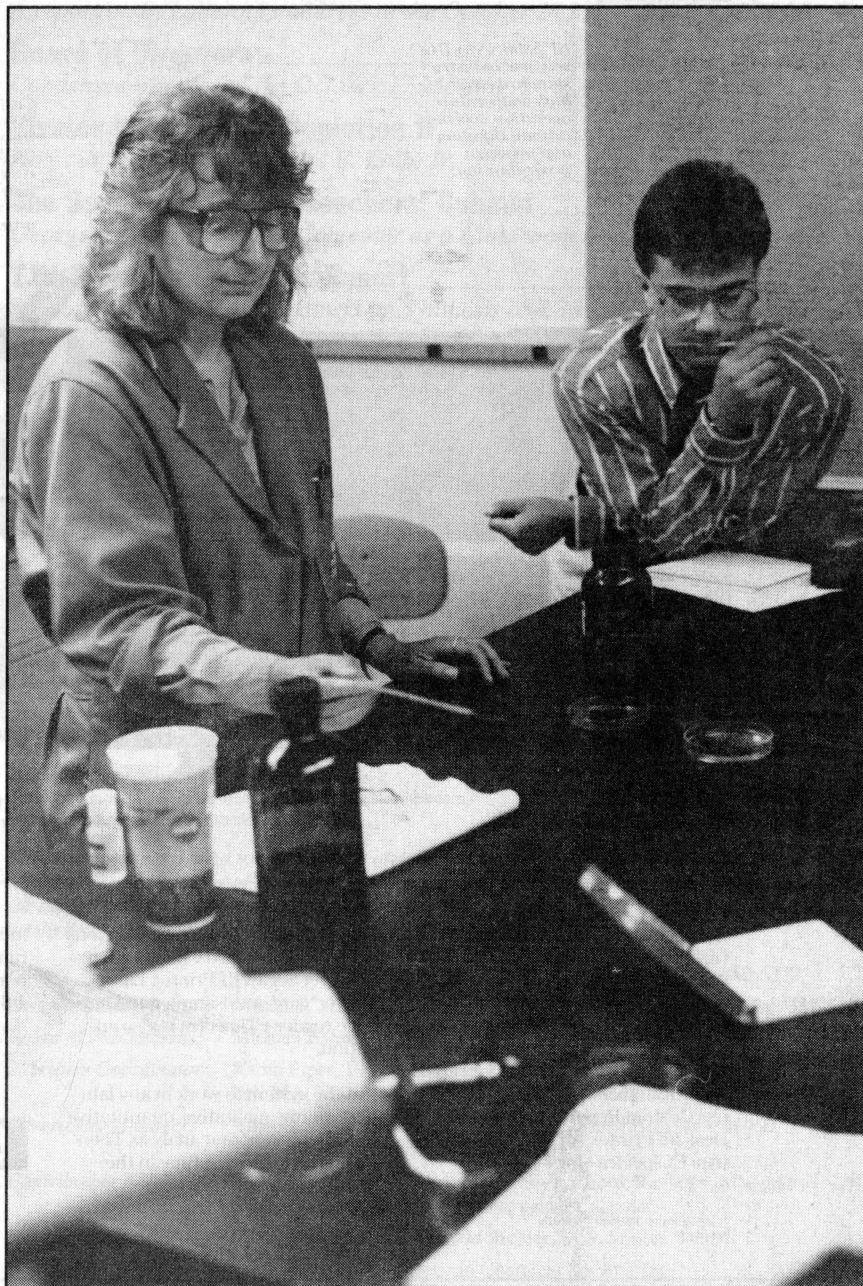
Holes at the Poles

Teachers' Column

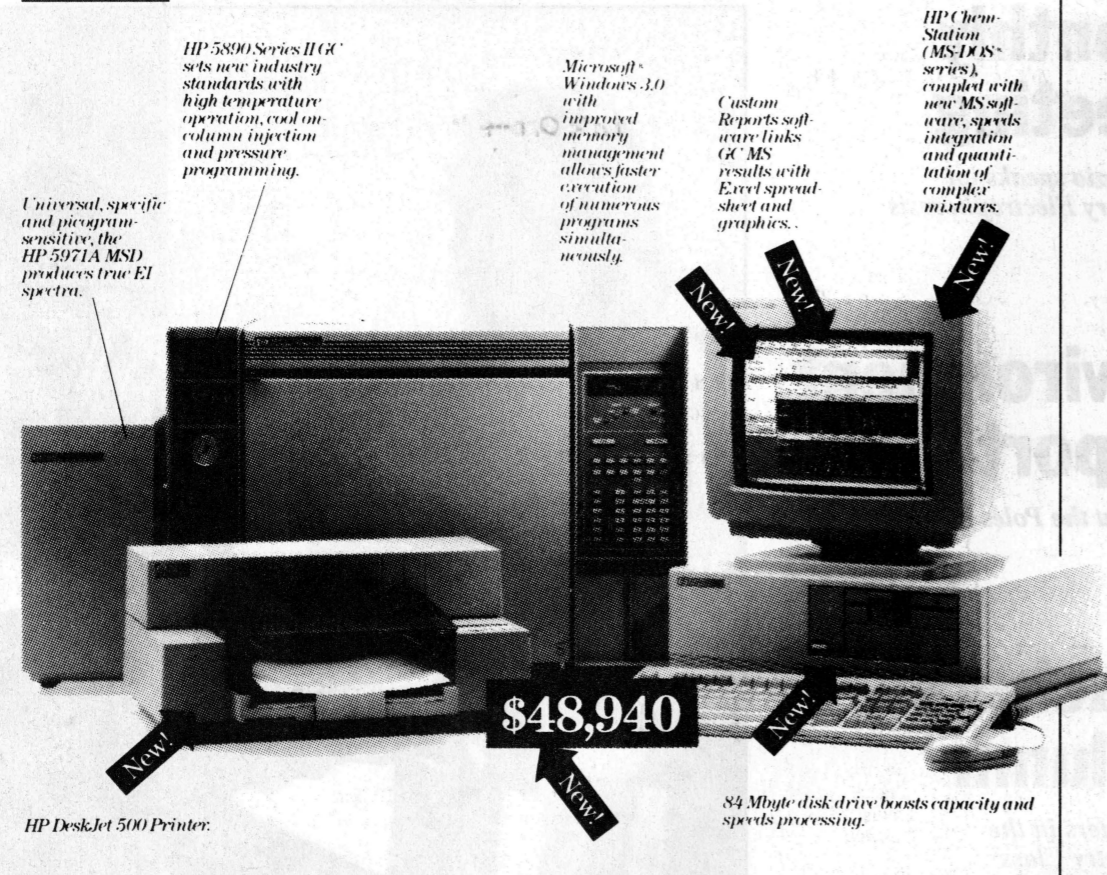
*Computers in the
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Richards Scholar's Report

*Luminescent Copper (I)
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Deadlines: <i>March 1992 issue: January 24, 1992</i>	

THE NUCLEUS

Dedicated to the Memory of James Flack Norris
Published monthly from October to May by the Northeastern Section of the American Chemical Society, Inc.



The Nucleus is distributed to the members of the Northeastern Section of the American Chemical Society, to the secretaries of the Local Sections, and to editors of all local publications. Forms close for advertising on the 1st of the month of the preceding issue. Text must be received by the editor six weeks before the date of issue.

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From the New Chairman

by Katie Stygall

It is with great pleasure that I welcome you to a new year of NESACS programs and activities. I look forward to serving you as your chair. Please do not hesitate to call me if you have ideas you'd like to share, questions or concerns.

I have three goals as chair for 1992:

1. I should like to see an expansion of our public outreach programs. The programs we have in place already are flourishing, but we can do more. In a time of rapidly advancing technology and of severe environmental problems, it is essential that we play our role in improving public awareness of scientific issues. I shall be continuing my work with the past chair, Charles Kolb, on the Education Task Force and I in-

tend also to continue our discussion on Science and Public Awareness that we began at the Nobel Laureate evening at Harvard University on October 17.

2. I am concerned that we do not attract new and active members to our section. We need people who will enrich our thinking and activities with a fresh perspective.

3. We have been performing a valuable education service for middle and high school students but I believe that we have yet to reach inner city students. I intend to work with officers of the Boston School District to facilitate work with these students.

I look forward to hearing from you and working with you.

I bid you peace and a very happy and productive New Year. ◇

National Chemistry Week

by Patricia L. Samuel

November 3 through 9 marked the celebration of National Chemistry Week, a time set aside for all of us to contribute to the public understanding of our science. Several events highlighted our Section's celebration:

On Saturday, November 2, some forty area teachers, ranging from middle school to university, attended an all-day program at Boston University, hosted by the Department of Chemistry. The speakers and workshop leaders represented the spectrum of chemical educators as well. "Chemistry for the 21st Century" featured a morning session of demonstrations; a lecture, "Understanding a Protein Associated with Alzheimer's Disease," by Peter Lansbury of M.I.T.; and a presentation on cooperative education in chemistry. Demonstrators were Monty Wells of Newton North High School, Katie Stygall of Bradford College, Patricia Samuel of Boston University, and Jerry Bell of

Simmons College. Speakers on cooperative education were Kathleen Dunn of Simmons and Phillip Veysey of Dearborn Middle School, Boston. In the afternoon, following a talk by Valerie Wilcox on chemical waste disposal, teachers had a choice of workshops: microscale chemistry by Peggy Corbett of Belmont Hill and Kathleen Skelly of Dana Hall School; computer chemistry by Harvey Gendreau of Framingham High, George Martins of Newton North High, and David Olney of Lexington High School; or ICE Box (Institute for Chemical Education) Demonstrations by Bette Bridges of Silver Lake Regional High School and Katie Stygall.

On Wednesday, November 6, a Student Science Symposium, "Oil and Energy for the 21st Century," was presented to almost 200 students and teachers at the Museum of Science, Boston. A popular feature was the award-winning electric car designed

and built by the students of St. Johnsbury Academy, Vermont, and their teachers. Speakers were Vladimir Haensel, Univ. of Massachusetts, Amherst; Lon Topaz, Sacramento (CA) Municipal Utility District; Bruce Burk, St. Johnsbury Academy; and Helena Chum, National Renewable Energy Laboratory, Golden, Colorado.

On Friday, November 8, a public forum on the new food labelling regulations was held at Framingham State College, hosted by the Department of Chemistry and Food Science. The program featured a lecture by Dr. Fred Shank, Director of the Center for Food Safety and Applied Nutrition of the United States Food and Drug Administration, and a panel of prominent local nutrition scientists. More than 150 persons attended.

These were the official offerings, designed and implemented by the Public Service Committee of the Section, but there were many other celebrations throughout the area. The University of New Hampshire welcomed more than 500 parents and children at their annual Halloween Chemistry Magic Show. Boston University's Chemistry Department and Student Affiliates hosted over 200 students and faculty from area colleges and universities for a lecture by

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January Meeting

The 740th Meeting of the Northeastern Section
of the American Chemical Society

Thursday, January 9, 1992

Boston College

5:30 Social Hour, Shea Room, Conte Forum (Athletic Center)

6:15 Dinner

8:00 New Chemistry Building, Rm. 130: Steven D. Fazio, Sandoz Pharmaceutical Corp., E. Hanover, N.J.: *Requirements of Capillary Electrophoresis in the Pharmaceutical Industry*

Refreshments will be served after the program.

Dinner reservations should be made no later than January 3. Please call Mrs. Karen Piper at (508) 456-8622 or (800) 872-2054 (MA or NH). Reservations not cancelled at least 24 hours in advance must be paid. Members, \$21.00; Non-members, \$23.00; Students and Retirees, \$8.00. **THE PUBLIC IS INVITED.** Free parking is available in the garage off Beacon Street.

February Meeting: February 13, 1992, Boston College: Dr. William Orme-Johnson (M.I.T.) His field of specialty is Nitrogen Fixation. Title to be announced.



Biography

Dr. Fazio is an Associate Fellow in the protein analytical research group at Sandoz Research Institute, E. Hanover, N.J. He received his B.S. in chemistry from Florida State University in 1978 and worked with microbial lipids and exopolysaccharides in the Biology Department at Florida State University from 1978 to 1981. In 1981 he went to

the Chemistry Department at Rutgers University and in 1985 received his Ph.D. in analytical chemistry. His present position at Sandoz involves methods development, stability, preformulation, and characterization of monoclonal antibodies and recombinant proteins. Part of his present work involves the basic development of capillary electrophoresis for the analysis of small molecules, peptides, and protein pharmaceutical products. ◇

Preliminary Notice 1992 James Flack Norris Undergraduate Summer Research Scholarships

Potential applicants, research directors, nominators and recommenders are advised that detailed guidelines and application forms should be reaching the respective departmental offices by mid-January.

Abstract

*Capillary Electrophoresis in
the Pharmaceutical Industry*

by Steven D. Fazio, Guy G. Yowell,
Richard V. Vivilecchia

Capillary electrophoresis analytical methods are presently being developed for pharmaceutical products. However, its potential use is limited in part by current UV detector technology and the inability to attain the traditional UV detection limits seen by HPLC. The current limits of UV detection for small molecules, peptides, and proteins which have been achieved in our laboratory will be discussed. An evaluation of commercially available techniques to improve these detection limits will be presented.

Methods development for small pharmaceuticals and peptides has proceeded with little or no modifications to the capillary walls. However, the analysis of proteins in unmodified capillaries has shown little promise. Recent advances in capillary wall modifications to improve the separation of proteins at neutral pH will be presented. Bonding chemistries, coatings, and their effects on reproducibility and resolution are included. Finally, examples of where these modified capillaries are presently being used for the analysis of proteins will be presented. ◇

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At the November 7 Meeting

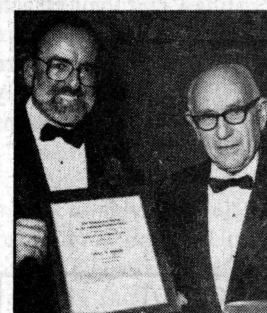
(Photos by A. Finland)



Drs. Robert Varnerin, Ernest Becker and Janet Perkins at the reception.



Dr. and Mrs. Moore and some of the meeting audience.



Dr. Moore and Dr. Robert O'Malley, Chairman of the Norris Award Committee.



Dr. Moore demonstrates "what we see" during his address.

Managing and Being Managed

A report of the talk given by Dr. Benjamin Luberoff on October 24 at the Professional Relations Meeting

To explain his definition of managing, Luberoff posed the question, "What gets managed?" His answer, Resources: 1. Things: materials, products, waste, devices; 2. Energy: kilowatts, BTU, nuclear energy, human energy, information; 3. Time. Managing requires making decisions, most easily done by assigning dollar values to choices.

Each of us manages. We manage our human energy, our equipment, people we are responsible for, vacations, our paycheck, our home, cars, boats, and other possessions, liquid assets, and our pensions. Luberoff stated that each of us manages over half a million dollars.

How do we manage? Taxes, paycheck, etc. We "manage by delegation," since we still have responsibility, although we may have no direct input. Our pension we "manage by neglect." We "manage by objective," a very popular concept, but, by whose objective, ours or theirs? We "manage by exception," "if it ain't broke don't fix it."

People have a hierarchy of needs, food, shelter, things, love, power, etc. What do the people in your team need? What motivates them?

What ways are there to manage others? "The Tishler Pancake" where Max Tishler was able to talk to and

lead 120 PhD's? It takes a genius to manage in this way, Luberoff concludes. More common is the hierarchy where the head talks to a few sub-heads who, in turn, each have a number of subordinates to talk to, and so on down the line. In military terms, this system works for the attacking force. In retreat, the lower echelons have to talk to those above them. Edwin Land used what Luberoff calls the Copernican Version of Management. The leader, the sun, is surrounded by satellites in the work team, but the system is flexible and today's satellite may be tomorrow's sun. Still another version is matrix management, but Luberoff noted that invariably this leads to two bosses, with the problems that this creates.

Motivation varies. The fear motive: If you don't solve the problem you get fired. Luberoff feels that the Japanese techniques of lengthy discussions without time limits generates genuine commitment.

People at the top often don't hear what they are supposed to hear, hence the value of the outside consultant, to whom they do listen.

Decisions are of three kinds: yes, no, let's not decide. Buy, sell, or hold. "Holding" can be a useful way to operate, it is decision of the third kind.

How to be managed in a situation with an uncomfortable level of ambiguity to the problem? Create a tickler file and follow up every week. Every Thursday tell the boss what's happening, and every three months tell the boss where you are. It's easier to make your mistakes on paper than in the lab, easier in the lab than in the pilot plant, easier in the pilot plant than in manufacturing. Ten percent of the value of a decision must be spent in figuring out the decision. Spend \$10,000 to decide on a \$100,000 item.

Reported by M.S. Simon ♦

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Board of Directors

Condensed Minutes, Meeting of October 17, 1991

by Michael J. Hearn

Chairman's Report: The ACS is active in seeking an increase for the National Science Foundation of funds for research and development. Volunteers from industry are sought to help with this effort; interested members should contact the Section office.

Treasurer's Report: The Section funds continue to be sound, but expenditures should be watched in the second half of the year. J. Piper MOVED and it was VOTED to increase budget lines 27 (Levins Award income) and 70 (Levins Award expenses) to reflect the figures. This award account is in balance. J. Piper reminded the Board that proposed budgets for 1992 are needed by November 7. The report was ACCEPTED.

Committee Reports:

Archivist: E. Garber reported that the archives can remain at Harvard through the spring of 1992, but that a new home would have to be found by then.

Board of Publications: The Board has had meetings in June, July, September and October. A. Heyn has received a contract for 1991-2. Vincent Gale is also continuing his excellent work as Advertising Manager. K. Piper has been appointed as Business Manager, now renamed as Executive Coordinator. Advertising has exceeded the budget predictions saving the Section up to \$1000 for the year.

Editor of the Nucleus: A. Heyn asked what policy the Section should pursue in respect to paid advertising for candidates to national ACS office. He was instructed to continue an even-handed policy.

Constitution and Bylaws: The vote on the amendments published in the October 1991 NUCLEUS will be voted at the November meeting of the Section.

Education: M. Schwartz reported on the "Chemical Career Insights-1991" program sponsored by the Younger Chemists Committee. 50 Students attended this event. She recommended that the Section might sponsor this program as a Section activity in the future. Past Norris Summer Scholars are being located in order to evaluate the impact of this program. Chairman D. Bagley recommended that there should be a budget so that some teachers can be sent to workshops next summer.

Nominations: E. Billo announced that D. Rickter will be an Alternate Councilor until the next annual election to fill a vacancy.

Norris Award Committee: R. O'Malley announced that the 1991 Norris Award Recipient for the Excellence in Teaching Award will be Prof. John W. Moore of the University of Wisconsin. He will address the Section at the November 7 meeting.

Professional Relations: M. Simon reported on the activities planned for the October 24 meeting. So far about 40 guests have registered for the dinner. Plans are under way for activating an *Employment Opportunities Task Force*, with Leon Rubin, chairman. M. Simon sees involvement of our Corporate Sponsors and Patrons as the next step. T. Light and V. Wilcox are assisting in the work of the Task Force.

Public Relations: William Schmid has been appointed to the chairmanship of this committee.

Other Committees:

Public Service: V. Wilcox announced the activities for National Chemistry Week with a Science Teachers' Day, a symposium on the 6th of November and a public lecture on the 8th.

Safety: F. Wagner described the

September Workshop held in conjunction with the Section meeting. Ten high school teachers attended and two speakers discussed laboratory accidents and their legal consequences.

Summerthing: M. Chen was thanked for her excellent work in organizing the successful 1991 program in Salem.

Old Business: C. Kolb reported on the activities of the Education Task Force. A curriculum is being developed. To date three one-hour segments with demonstrations, activities and lectures have been produced, to be tried out in the schools of Fairhaven, Lawrence and Beverly, grades 4-6. The next step will be a grant application to the NSF.

New Business: It was announced that Joseph E. Bunnett of the Univ. of California, Santa Cruz, will receive the national Norris Award in Physical Organic Chemistry at the San Francisco meeting in April, 1992. This award is sponsored by the Northeastern Section. ♦

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Stratospheric Ozone Depletion

II. Holes at the Poles

C.E. Kolb, Jr.
Center for Chemical and Environmental Physics
Aerodyne Research, Inc.

In early October of last fall the National Aeronautics and Space Administration (NASA) announced that the spring ozone level over the Antarctic continent had reached a new low. Their Total Ozone Mapping Spectrometer (TOMS) instrument aboard the Nimbus 7 satellite had measured column ozone levels as low as 110 Dobson units, about one third of the normal average ozone level over the polar region. (One Dobson unit is equal to 0.01 mm of gaseous O₃ at standard temperature and pressure or about 2.7 x 10¹⁶ molecules per cm².) These were the lowest column ozone levels ever measured.

Two weeks later at the United Nations, NASA and other scientists on a UN assessment panel announced that

mean ozone levels over the mid-latitude regions of the Earth had clearly been falling at an accelerating rate during the 1980's. Previous assessments had determined that between 1969 and 1986 the mean ozone level had probably decreased 2 to 3 percent in the Northern Hemisphere's 30 to 65 degree latitude band. This covers a large fraction of the world's population. However, most of this earlier decline was in the winter months, when ozone levels are highest and the exposure of people and plants to any extra ultraviolet radiation is minimal. New data, gathered from 1987 through 1990, clearly indicated that serious ozone depletion is now evident during the spring and summer when people, crops and other

components of the biosphere are most susceptible to increased UV irradiation caused by ozone loss. The UN panel predicted a further stratospheric ozone decline of 3 percent during the 1990's. The next day, DuPont announced an acceleration of its previously adopted phase-out rates for CFC-11, CFC-12 and related compounds.

Neither the massive loss of ozone over the southern pole in spring nor the current rate of ozone loss at mid-latitudes is predicted by atmospheric models based solely on the gas phase catalytic ozone destruction cycles, presented in the last Environmental Chemistry Column (Stratospheric Ozone Depletion I. Freezing Out Freons®). Something else is accelerat-

ing ozone loss at unanticipated rates.

Much to the surprise of most atmospheric chemists the missing, mysterious "something else" appears to be heterogeneous (gas/surface) reactions which occur on very small acid ice and/or liquid acid aerosol particles found in the stratosphere.

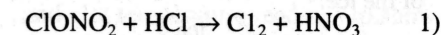
The elucidation of these heterogeneous stratospheric processes results from a very recent set of events. The discovery of the Antarctic ozone hole was not published until 1985, although we now know that serious depletions in spring Antarctic ozone levels occurred as early as 1976. The discovery is credited to Joseph Farman of the British Antarctic Survey who has been making ozone column density measurements from the British base at Halley Bay, Antarctica, for over 35 years. His measurements began showing serious and increasing depressions in the late September and October ozone levels nearly every year in the late 1970's. Farman waited until 1985 to publish in order to establish the trend unambiguously. He had been concerned that no other re-

searchers, including those associated with NASA's TOMS instrument, were announcing such serious (and unpredictable) ozone losses. (It turns out that the TOMS data reduction software was constructed to treat very low ozone readings as data artifacts and NASA scientists were blissfully unaware that their satellite instrument was recording massive seasonal O₃ depletion over the Antarctic.)

Once Farman's data were published and confirmed by re-analysis of the TOMS satellite data, atmospheric scientists scrambled to concoct theories to explain the low O₃ levels. Physical meteorologists insisted that the ozone was merely displaced by vertical atmospheric motions associated with the strong polar vortex winds which prevent the air over the winter southern pole from easily mixing with the rest of the atmosphere. Other atmospheric scientists insisted that massive levels of NO_x were drawn down into the polar stratosphere from the upper atmosphere, possibly driven by variations in the solar cycle. However, in 1986, at-

mospheric chemists (including Susan Solomon of the National Oceanic and Atmospheric Administration's (NOAA) in Boulder, CO with co-workers and Michael McElroy and colleagues at Harvard University) noted that if the chlorine normally locked up in the relatively unreactive ClONO₂ and HCl "reservoir" species were to be transformed into more reactive chlorine species, the massive springtime Antarctic ozone loss might be explained.

This could be accomplished by a direct reaction between chlorine nitrate and hydrogen chloride:



While the gas phase rate constant for reaction 1 was known to be very small, the reaction did seem to proceed fairly rapidly on the walls of laboratory apparatus. Solomon and co-workers and McElroy et al. hypothesized that reaction 1 would also occur on the surfaces of tiny ice crystals, clouds of which were known to form in the polar

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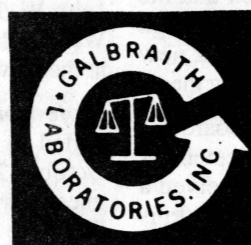
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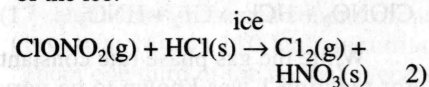
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Stratospheric Ozone

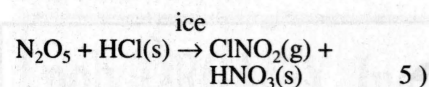
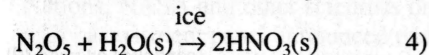
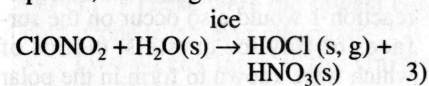
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stratosphere on the coldest days of the polar winter.

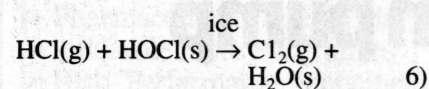
Studies performed on cold ice surfaces in the laboratories of Mario Molina (then at the Jet Propulsion Laboratory, now at M.I.T.) and David Golden (at SRI, International) soon showed that reaction 1 did proceed rapidly, with the Cl_2 product being released into the gas phase, while the HNO_3 remained behind on the surface of the ice:



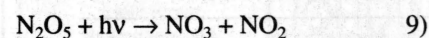
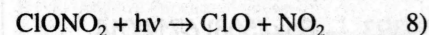
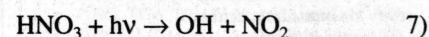
Soon other lab studies uncovered other important heterogeneous reactions of stratospheric "reservoir" species, including:



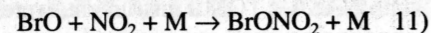
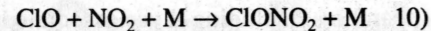
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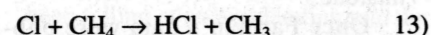
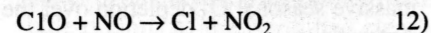
All of those reactions either produce an easily photolyzable chlorine compound which can release atomic Cl much more quickly than ClONO_2 or HCl and/or they sequester nitrogen oxides in the form of condensed phase nitric acid. This latter effect is important because nitrogen oxides tied-up in condensed HNO_3 cannot be photolyzed to produce NO_2 , reducing the impact of processes such as:



The resulting decrease in NO_2 sources in turn reduces the scavenging of the ozone destroying radicals ClO and BrO:



If enough NO_x and water vapor are removed from the gas phase, ClO and BrO cannot easily reform the more inert nitrate compounds. The reformation rate of relatively inert HCl is slowed by the following two reactions:

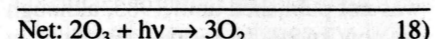
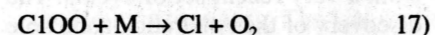
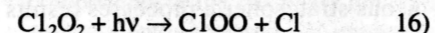
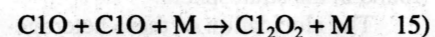
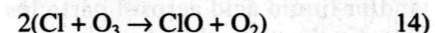


The resulting chemistry greatly increases the chemical chain lengths for catalytic reactions involving ClO and BrO, enhancing their ability to destroy ozone.

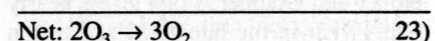
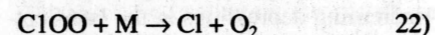
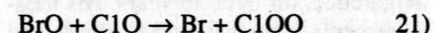
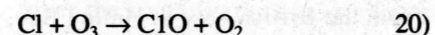
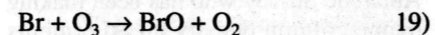
Gas phase nitric acid, formed from NO_x in the stratosphere, also helps create the ice particles which allow reactions 2-6 to proceed. At typical stratospheric HNO_3 and H_2O vapor levels, nitric acid trihydrate ($\text{HNO}_3 \cdot 3\text{H}_2\text{O}$ or NAT) condenses at temperatures several degrees higher than H_2O vapor alone. Thus, clouds of small NAT ice particles can form, allowing reactions 2-6 to occur to some extent, even at temperatures above those necessary for ice clouds. If the stratospheric air parcel cools further, the NAT particles grow as they serve as condensation centers for stratospheric water vapor. If they grow large enough, the resulting ice particles fall to lower altitudes, dehydrating and denitrifying their original air parcel. These polar ice cloud microphysical subtleties were first described by McElroy and his co-workers Stephen Wofsy and Ross Salawitch at Harvard, along with atmospheric scientists at NASA's Ames and Langley Research Centers and Germany's Max Planck Institutes.

However, in addition to the effects of the surprising gas surface reactions listed above, explaining the Antarctic ozone hole also demanded some novel gas phase chemistry. The ozone destruction cycles presented in Part I of this series require the participation of atomic oxygen, which arises from O_3 photodissociation. However, the initial Antarctic O_3 loss occurs early in the spring when the returning sunlight is too feeble to provide enough atomic O.

In 1987 Luisa and Mario Molina pointed out that the very cold polar stratosphere would allow the formation of a ClO dimer species, in turn permitting O_3 destruction through a new cycle:



McElroy and co-workers then pointed out that a dark cycle involving Br would also work:



In order to confirm the proposed ozone hole explanations, direct measurements in the polar stratosphere had to be made. The theory predicted that a large fraction of the Cl (and Br) in the Antarctic stratosphere had to be released into the reactive ClO and BrO forms by the results of reactions 2-6 and the suppression of reactions 10-12.

The "smoking gun" was found during a NASA/NOAA sponsored airborne mission to Antarctica during August and September of 1987. The most critical measurements were made by NASA's ER-2 aircraft (a research version of the U-2 spy plane). On-board instruments measured NO_x , O_3 , ClO, BrO and other stratospheric trace species. The critical ClO and BrO measurements were made with an instrument designed and built in James Anderson's laboratory at Harvard.

Flying out of southern Chile, the ER-2 penetrated the polar vortex structure over the Antarctic continent. The ClO mole fraction increased from about 100 ppt (parts-per-trillion-by volume) north of the vortex edge to 1000 to 1200 ppt inside the vortex. By mid-September the ClO levels were strongly inversely correlated with the ozone con-

centrations inside the vortex, as required by the reaction cycles 14-17 and 19-22. The BrO concentration was also significantly enhanced inside the vortex. Detailed analyses by Anderson and co-workers have shown that the observed levels of BrO and ClO can explain the measured O_3 loss levels. The data indicates that about three quarters of the ozone is destroyed through the reaction cycle 14-17 and one quarter is lost through 19-22.

ER-2 flights over the Arctic in 1989 with the same instrumentation showed that, although the Arctic polar vortex is much weaker than the Antarctic vortex and the temperature falls low enough for polar stratospheric cloud production much less often, highly elevated levels of ClO and BrO also form during the Arctic winter and spring. These radicals do not stay localized to cause a massive ozone hole like that in the Antarctic, but mix out fairly continuously to lower latitudes, depleting ozone as they go. This process may well explain a significant portion of the observed northern hemisphere mid-latitude winter and spring ozone loss. Anderson of Harvard is the Mission Scientist for a second Arctic airborne study spanning this winter and early spring, which is designed to further quantify this possibility.

While polar stratospheric ice clouds do not occur over Boston and other mid- and low-latitude areas, sulfuric acid aerosol droplets do occur. Their level is greatly enhanced by occasional large volcanic eruptions like that of El Chichon in 1982 and the even bigger eruption of Mount Pinatubo in 1991. A modest level of measured ozone loss has been associated with El Chichon's sulfuric acid cloud.

Laboratory studies of heterogeneous reactions on sulfuric acid surfaces by an Aerodyne Research/Boston College team lead by Douglas Worsnop and Paul Davidovits, a NOAA Aeronomy Lab team lead by A.R. Ravishankara, and an SRI, International team lead by Margaret Tolbert and David Golden have shown that reactions 2 and 5 are slow on sul-

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The Secondary School Teachers' Column

The Computer as a Classroom Demonstrator

by George F. Martins, Newton North High School, Newtonville, MA 02160

The 1980's have introduced a new tool into the high school chemistry classroom. Beside the *sine qua non* of live chemical demonstrations and a variety of visual aids, the teacher now has the computer. Together with a large monitor or projection device, e.g. an overhead projection panel, the computer (Apple IIe or IIc) can provide an array of stimulating experiences for the student. As examples, seven uses with short descriptions follow. Software has been developed by the author and obtained from Seraphim and some commercial suppliers.

1. *Computing Functions.* Historically, number crunching has been a major use of computers. Energy changes for the Bohr atom along with corresponding wavelengths can be quickly calculated from formulas. Molecular weights can be calculated from formulas. Complex calculations, such as cubic equation solutions for gaseous equilibrium systems, can be made using successive approximation methods.

2. *Drill and Practice.* "Balancing" chemical equations can be used for classroom review after students have tried textbook methods. Students may work on their own in the school library or at home if appropriate hardware is available. Significant figure drills reinforce students' treatment of data.

3. *Experiment Simulations.* Scientific equipment can be very expensive and complex. Chemicals may be hazardous. Software with graphics allow the viewer to pursue Rutherford's alpha scattering, collect data for a kinetics rate law, and follow a warming or cooling curve study. A bomb calorimeter experiment can generate heats of combustion data. (See Figure)

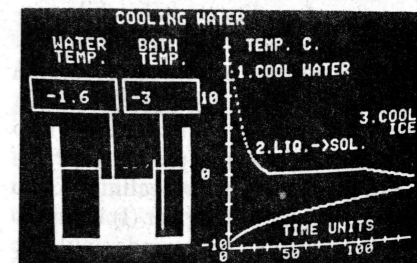
4. *Graphical Representations.* Density lines, vapor pressure curves, bar graphs of periodic table trends are

effective visuals. Graphical analysis of lab data is possible with slopes and statistical analysis. Even electron orbital plots can be appreciated.

5. *Interfacing Real World Data.* A thermistor and software can measure and plot temperature readings to show that evaporation is endothermic, and to give data for heats of reaction. pH measurements and titration curves can be plotted while the experiment is being done. Light absorption colorimetry can be carried out.

6. *Games.* Most students have already experienced the thrills of computer games and chemical games are no exception. Ordering the elements by periodic property, chemical hangman, acid-base mazes and element and compound searches are available.

continued on page 16



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T.W. Richards Scholar's Report

Synthesis and Structural Studies of Luminescent Copper (I) Laser Dye Clusters

by Richard Woudenberg* and Jerry P. Jasinski

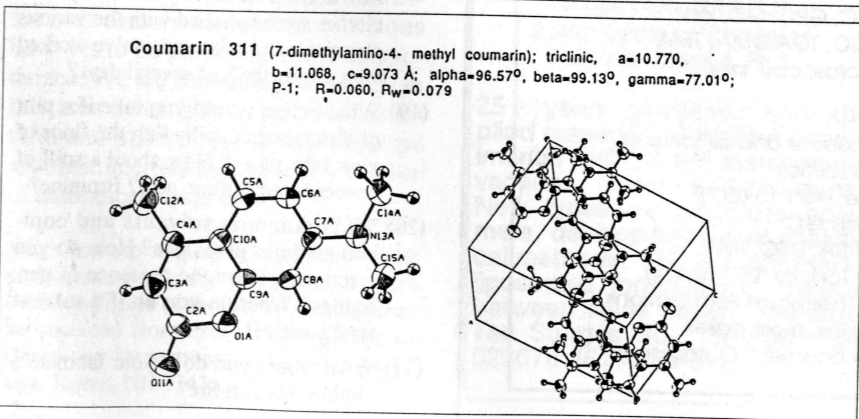
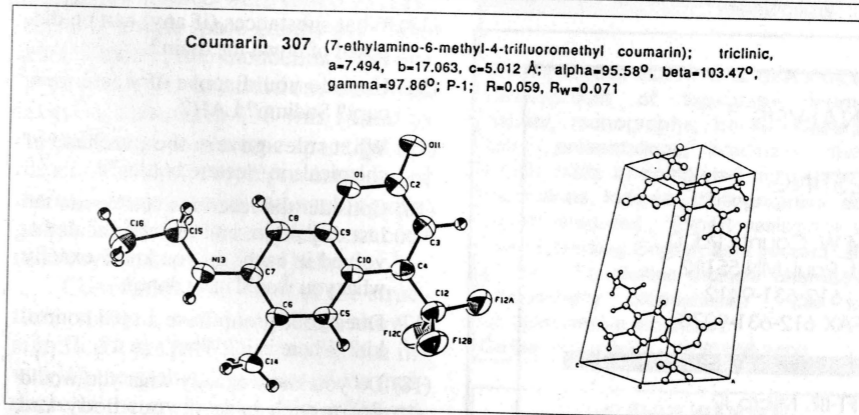
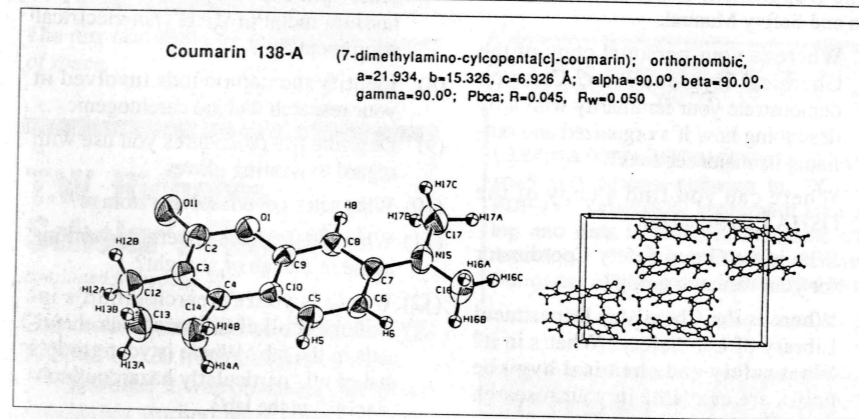
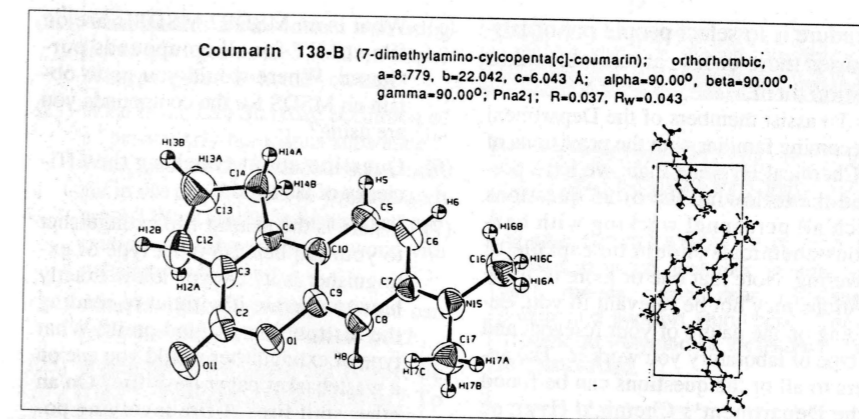
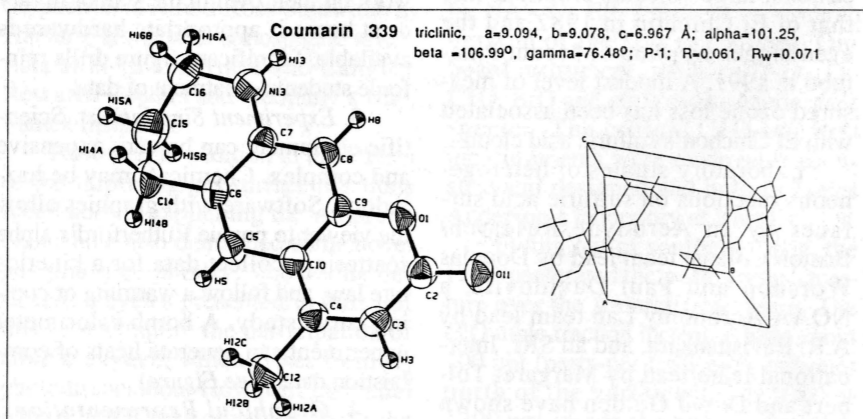
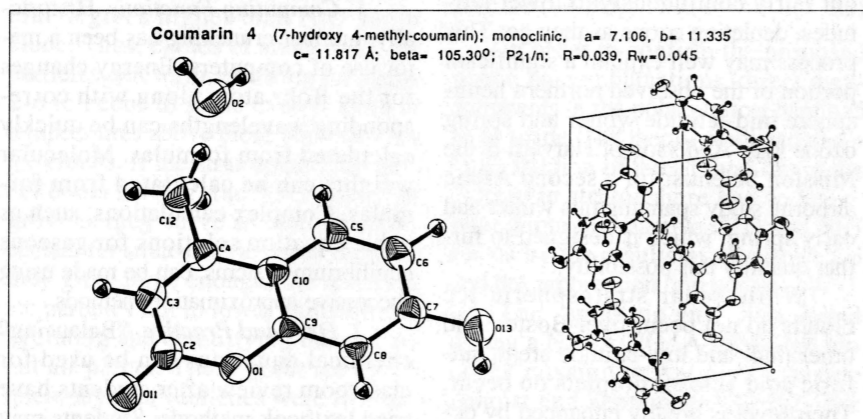
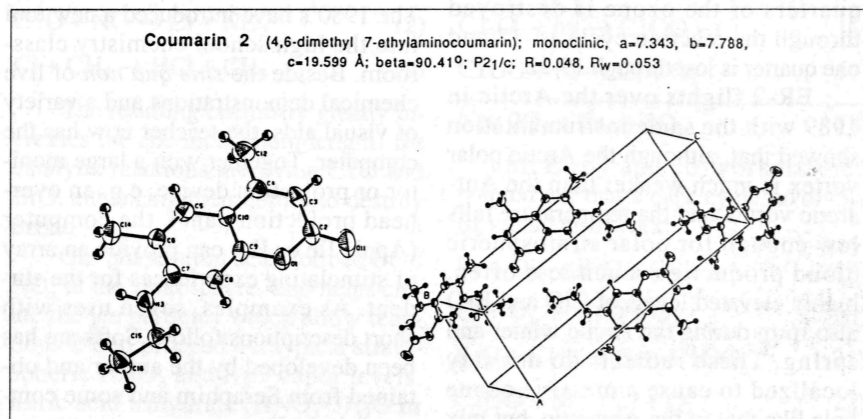
Chemistry Department, Keene State College, Keene, N.H. 03431

In an effort to examine how structural design may be useful in obtaining new laser dye materials with improved lasing efficiency and photochemical stability, several coumarin laser dye compounds were crystallized in the solid state and analyzed through single crystal x-ray diffraction techniques. While the fundamental goal of the proposed research was to examine the interrelationships between the structural and photo-physical effects of copper (I) bound to various laser dye coumarin compounds in the crystalline state, only the native coumarins themselves were successfully crystallized and structurally characterized. The single crystal structure determinations for coumarins 2, 4, 138, 307, 311, and 339 are outlined below.

Experimental design: Slow evaporation of the target molecules in methanol and ethanol produced only small amounts of quality crystals while acetone worked well with coumarin 307. Acetonitrile as a solvent medium provided the best quality crystals in most cases. Coordination of copper (I) into the various coumarins proved to be difficult using the reflux technique. No suitable crystals of copper (I) bound to these laser dye compounds could be found as a result of this effort. X-ray data was collected on a RIGAKU AFC6S autodiffractometer at the New England Molecular Structure Center located in the Chemistry Department at Keene State College. Structure solution (Mithril), refinement (least squares) and graphical analysis (Ortep, Pluto and packing diagrams) for each of the crystalline systems were accomplished using the TEXSAN structure determination package (Molecular Structure

continued on page 15

*Theodore William Richards Scholar, 1991.



Health & Safety on My Mind

Concerning OSHA Inspections of Academic Laboratories

by M.A. Solstad

We are approaching the first anniversary of the OSHA Lab Standard. This summer the chemistry department at M.I.T. was awarded the DivCHAS award for excellence in academic chemical safety. This was due, at least in part, to the fine Chemical Hygiene Plan developed by the department under the leadership of Dr. Danheiser. The following article appeared recently in an inhouse chemistry department newsletter of M.I.T. Many of you may appreciate the reminder to review your own Chemical Hygiene Plan. Dr. Danheiser has given his permission to use it, but we both would like to remind you that the list of questions is not to be viewed as complete.

Concerning OSHA Inspections of Academic Laboratories

by Professor Rick L. Danheiser and the Chemistry Department Safety Committee

OSHA compliance officers have begun to inspect research laboratories to check for compliance with the new Lab Standard law. We have learned that between February and August, OSHA issued 95 citations to institutions not having an acceptable Chemical Hygiene Plan, and 108 citations for "inadequate" training of research personnel.

In a recent interview, OSHA representatives have described the format of their inspections which involve:

- (a) Review of the Chemical Hygiene Plan,

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Health and Safety on My Mind

continued from page 13

- (b) Inspection of records, especially training records and files of accident reports (which by law we must maintain),
- (c) Inspection of laboratories for safety violations, and
- (d) Interviewing randomly selected researchers to determine whether they understand and are following the provisions of the Chemical Hygiene Plan.

We were somewhat surprised to learn that the most important part of the inspection is the interviewing of randomly chosen researchers. The Lab Standard is a "performance based standard"; apparently OSHA is not particularly interested in whether we have an elegant bound Chemical Hygiene Plan, they are more concerned whether people know what's in it, and whether they are abiding by it. It appears that their

procedure is to select people out of laboratories more or less at random and to question them.

To assist members of the Department in becoming familiar with the provisions of the Chemical Hygiene Plan, we have prepared the following list of 25 questions which all personnel working with hazardous chemicals should be capable of answering. Note that one or more of these questions may not be relevant to you, depending on the nature of your research and the type of laboratory you work in. The answers to all of the questions can be found in the Department's Chemical Hygiene Plan and Safety Manual.

- (1) Where is your personal copy of the Chemical Hygiene Plan? Can you demonstrate your familiarity with it by describing how it's organized and outlining its major sections?
- (2) Where can you find a copy of the OSHA Lab Standard?
- (3) Who is the Group Safety Coordinator for your research group?
- (4) Where is the Chemistry Department Library of Lab Safety? What's in it? What safety and chemical hygiene books are available in your research group library?

(5) What is an MSDS? MSDS's are on file at MIT for all compounds purchased. Where would you go to obtain an MSDS for the compounds you are using?

(6) Question about checking the efficiency of lab hoods.

(7) Where is the nearest fire extinguisher to your lab bench? What type of extinguisher is it? Do you know exactly how to operate it without re-reading the instructions printed on it? What type of extinguisher would you use on a wastebasket paper trash fire? On an ether spill fire? A fire involving potassium metal or LAH? An electrical equipment fire?

(8) Identify the compounds involved in your research that are carcinogenic.

(9) Describe the procedures you use with regard to wearing gloves.

(10) What rules govern solvent storage?

(11) What are the rules governing working alone in the lab or at night?

(12) Where is your research group's inventory of all of the hazardous chemicals in the lab? Where is your group's list of all "particularly hazardous substances" in the lab?

(13) What substances (if any) can be disposed of down the drain?

(14) How do you dispose of waste mercury? Sodium? LAH?

(15) What rules govern the purchase of chemicals in "lecture bottles"?

(16) Consider the reactions you've run the last day or so, and the chemicals involved in each: do you know exactly what you would have done?

(17) Does your group have a spill control kit? Where is it? What's in it?

(18) Do you know exactly what you would do in each case if your body and clothes were splashed with the various chemicals and mixtures you've worked with during the past several days?

(19) What action would you take if a pint of diethyl ether spilled on the floor of your laboratory? How about a spill of concentrated sulfuric acid? Bromine?

(20) What common solvents and compounds form peroxides? How do you test a sample for the presence of peroxides? What do you do if a solvent tests positive?

(21) What would you do if your labmate's clothes were on fire?

(22) What hazards are associated with using liquid-nitrogen cooled vacuum traps? What precautions should you take?

(23) What is the Lab Standard definition of a "particularly hazardous substance"? What particularly hazardous substances are in use or are stored in your research group? What special measures and precautions are associated with work with such substances?

(24) What is a designated area? What can and cannot be done in such an area?

(25) When must an accident report be filed? What does it consist of? To whom does it go? ◇

The text has been abbreviated for reasons of space.

T.W. Richards Scholar's Report

continued from page 12

Corporation) installed on a DEC VAXSTATION 3520 minicomputer system.

Results: It was observed that all six coumarins studied were found to crystallize in centric space groups with three being triclinic, two monoclinic, and one orthorhombic. In addition, a second motif of coumarin 138 was found to crystallize in an acentric space group. Structural parameters, representations of the asymmetric units and packing diagrams for each of the six different coumarin systems are outlined below:

Conclusions: In most of the structures studied, packing effects show a significant parallel layering pattern involving the aromatic portion of the molecule in the crystalline array. The effects of these structural interactions have yet to be photophysically characterized. We are continuing our efforts in this area investigating both the structural and photophysical relationships and their interrelationships for a number of luminescent laser dyes. ◇

Note: Because of space limitations, the table of data accompanying each figure has been omitted. Copies of the complete paper may be obtained from Prof. Jerry P. Jasinski, Chemistry Department, Keene State College, Keene, NH 03431.

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Monday, January 13

Professor Keisuke Suzuki
(Keio University)
Title TBA
Harvard University
MB-23 at 4:15 pm

Monday, January 27

Professor Ernst Bayer (Institut für Organische Chemie, Tübingen)
Title TBA
Harvard University
MB-23 at 4:15 pm

Professor Juliette T. J. LeComte
(Pennsylvania State University)
“Heme Binding Proteins”
Brandeis University
Gerstenzang 122 at 4:00 pm

Thursday, January 30

Professor Robert Weis
(UMass Amherst)
“Transmembrane Signalling by the Aspartate Receptor of Escherichia Coli”
Boston College
New Chemistry Building,
Room 127 at 4:00 pm

Notices for the Nucleus Calendar should be sent to:

Chris Arumainayagam
Department of Chemistry
Wellesley College
Wellesley, MA 02181
(617)235-0320 x3326
Fax (617) 237-1571
e-mail: CARUMAINAYAG@LUCY.WELLESLEY.EDU

National Chemistry Week

continued from page 4

Dudley Herschbach. Dartmouth College, Gordon College, M.I.T., South-eastern Massachusetts U., Polaroid Corp., W.R. Grace, and many other institutions presented programs in local schools. High school teachers were very active. More than one thousand buttons, balloons, and pamphlets were distributed, as well as over one hundred posters, ACS reprints, videotapes, and “NCW Activities Guaranteed to Succeed” booklets. Twelve thousand chemistry activities tabloids were placed in the hands of area students! ◇

Stratospheric Ozone

continued from page 11

furic acid droplets, but reactions 3 and 4 are quite fast.

Recent model calculations by Jose Rodriguez and colleagues at Atmospheric and Environmental Research have shown that reaction 4 may play a very important role in controlling NO_x , and therefore O_3 levels at mid-latitudes. In the meantime, the TOMS data will be closely examined to see if Mount Pinatubo's stratospheric sulfuric acid cloud causes a significant ozone loss as it spreads north over us. ◇

Secondary School Teacher's Column

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7. *Data Base And Spreadsheet.* The periodic table is one of chemistry's handiest data bases. Numerical data of periodic properties can be displayed and trends can be shown on the table. Spreadsheets are useful in the lab to record experimental data and compute results. Teachers can maintain their record book of test scores and assignments by computer spreadsheet. Ideally, a computer system permanently installed in the classroom, or one easily and quickly assembled, is desirable. An 80-column display may be too small for monitors and requires projection. Student work sheets can be prepared for most demonstrations. Students who develop computer expertise may even generate software for classroom use. ◇

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