Chemistry Department
Annual Report
July 1, 2005 – June 30, 2006

The Chemistry Department continues to make excellent progress in all three mission areas of Education, Research and Service/ Outreach. As data in the following sections will show, the Chemistry Department teaches more students than in 2001 while increasing sponsored research awards and engaging in high levels of service and outreach. These accomplishments are particularly remarkable in light of an inadequate operational budget which dates back to budget cuts in 2001-2002. A successful chemistry department is critical for the university to achieve the goals set forth in its strategic plan. One amazing highlight is that total sponsored research awards for the university increased to $143,665,258 in FY06 from $142,440,688 – a change university-wide of $1,224,570. Yet, during that same period, chemistry saw a change from $5,176,485 to $7,410,660 – an increase of $ 2,234,175!!! In addition, Virginia Tech data indicate that the Chemistry Department is the third highest ranked academic department in terms of grant awards behind two engineering departments that have twice the faculty of the Chemistry Department and without the high service teaching load that Chemistry has. This is a testament to the excellence and determination of the chemistry faculty – qualities that are endangered and will be lost if the proper level of support is not provided to the department. With a restoration of base funding and further investment to bring the department to adequate funding levels, the Chemistry Department can and will reach new heights of excellence.

The following sections give further information about the accomplishments of the department during the past fiscal year.

Research: The Chemistry Department continued its performance whish places it among the top chemistry departments in the country. NSF rankings for the latest period available (FY 2003) list the Chemistry Department ranked # 29 based on research expenditures. This is a remarkable trajectory which has the department showing ranking changes in FY 2001- 2003 of 53 to 39 to 29.

In an ever increasingly competitive environment, the department is proving to be adept at attracting research funding in that environment. In FY 06, the Chemistry Department received sponsored research awards totaling $7,410,660 an increase of over $2, 2M from FY05 . Some specific highlights in research funding:

- Karen Brewer obtained funding in the amount of $581K for catalytic production of hydrogen - an important part of alternative energy production. At the same time, she attracted over $320K for anticancer research.

- Harry Dorn and Harry Gibson received over $800K to fund research in nanotechnology.

- John Morris received over $600K from the Army to study important reactions at surfaces.
- It is interesting to note that one of our "retired" faculty, Harold McNair, received over $300K from the Transportation Safety Agency to develop more sensitive methods to detect explosives.

- The future of the department lies with our new faculty. Professor Diego Troya is a shining example he was awarded the prestigious NSF Career Award on his first application, but he also received a competitive award from the Air Force Office of Scientific Research.

- The department also strives to put forward proposals for the common good. We received an award of $300K to upgrade the department's solid-state NMR instrument and have received word that a proposal for anew 600MHz NMR spectrometer will be funded.

Chemistry faculty serve on the editorial boards of seven journals and serve on seven national society committees. (Of particular note is that Tim Long is a member of a National academy of Sciences Committee assessing the status of U.S. Chemistry in the world.) The Chemistry faculty published 127 articles in refereed journals, 25 reviews and book chapters, four books, and received nine patents in the calendar year 2005. Faculty presented 24 talks at professional meetings and were invited to present 41 lectures at other universities.

2005-2006 was a year for many transitions involving Chemistry faculty. Dr Neal Castagnoli retired in the Fall of 2005 and is now Harvey Peters Professor Emeritus. Dr. Jimmy Viers also retired to become Professor Emeritus.

2006 has proven to be a very successful year for faculty recruiting. Three new faculty have been hired to join the department in the fall of 2006. Dr. Edward Valeev adds to our growing strength in computational chemistry. Along with Daniel Crawford and Diego Troya, the department has a core of computational chemists unrivalled by most departments. The synergism with the remaining College of science computational scientists will make the College preeminent in computational sciences.

Dr. Lou Madsen will join the department and establish a research program in NMR instrumentation and methods development. Lou Madsen, Sungsool Wi and Daniel Capelluto form a powerful cluster in the increasingly important area of NMR methodology.

Dr. Webster Santos will add investigations into infectious diseases to the Department's strong efforts in drug discovery for treatment of cancer, depression and other diseases.

Graduate Education: The Chemistry Graduate program had 110 students pursuing advanced degrees in Chemistry during the 2005-2006 academic year. In addition, 25

students pursuing graduate degrees in other disciplines (e.g. MACRO) conduct their dissertation research in the laboratories of Chemistry faculty. Of the 112 students, 28 began their graduate studies during the fall 2004 semester. 4% of the current graduate student population are African American and 37% are women. Recruiting efforts during the spring 2006 semester focused on increasing the diversity and the size of the graduate student population, in concert with the goals of the PhD 2010 initiative. A total of 33 students accepted our offer of admission. Of these, three students are African American, 1 is Hispanic, and 16 are female. The department was successful in attracting a very good applicant pool, and we anticipate that the entering class for fall 2006 will be a strong group of students. This is reflected in the awarding of a Cunningham fellowship, a Dean's Diversity Assistantship, and two PhD 2010 Assistantships to four of the entering students.

Nine students earned a PhD in Chemistry and one student earned a MS in Chemistry during the 2005-2006 academic year. These numbers are consistent with previous years and reflect the department's transition to increasing the number of PhD students and decreasing M.S. students

Undergraduate Education: The number of chemistry majors remains steady and healthy at approximately 200. Record numbers of students presented at the departmental Undergraduate Research symposia during 2005-06, indicating that the students are reaching a high level of achievement. The recently completed five-year outcomes assessment indicates that alumni appear to be very satisfied with the chemistry program and with the quality of instruction by the chemistry faculty. Assessment of individual courses was obtained from senior exit interviews conducted during Spring 2005. Overall the senior interviews are consistent with the alumni survey: students view the quality of instruction and their interactions with the Chemistry Department faculty very favorably. The core courses in our baccalaureate program; general, organic, and physical chemistry; and the faculty members who teach these courses are rated highly. Even conceptually difficult courses are appreciated for the knowledge learned. Most critical comments are directed at the workload for low-credit labs or courses, which has increased with the requirement for writing-intensive courses, and with class size or composition. A consistent comment was "the only thing I would change is that you should provide better space for undergraduate labs, and you did that."

Service Student Credit Hours continue to be greater than 80% in the Department of Chemistry and the imbalance between the fall and spring semesters presents additional challenges. Enrollments in most lower-level chemistry classes continue to increase gradually. General Chemistry lab increased by 200 students during Fall 2005 (compared with Fall 2004 which, in turn, was already greater than Fall 2003) leading to significant overcrowding in the laboratories.

The stress on our undergraduate program from unsupported increases in enrollment cannot be overemphasized. In the Fall of 2000, the chemistry Department taught approximately 20,000 undergraduate student credit hours. The following year, the

department had to absorb a significant budget cut. According to the Teaching Load Report, that number has increased steadily to 23,568 in the Fall of 2005.

Even with a large service load, the deportment places a great deal of emphases on quality education and concern for the students. In the Fall of 2005 and Spring of 2006, the average student response for ALL chemistry classes in various areas were (on a scale of 1 to 4):

Knowledge of Subject: 3.73
Concern and Respect: 3.51
Overall Rating: 3.46

Service and Outreach: The inactivity of the Mobile Chemistry Laboratory is a disappointment to the department. There is an indication that funding from a private foundation maybe available in 2006-2007. Residual funds from the National Science Foundation are being used to prepare the MCL for a return to the road should this funding materialize.

Alumni Development: Several of our recent graduates were recognized for their accomplishments this past year. Notable was Dr. William Bryant (Ph.D. 1999) who received the Virginia Tech College of Science Young Alumni Award.

Our alumni advisory counsel continues to be very active. A total of 29 alumni sit on the council, at the fall meeting of 2005, 16 alumni attended and in the spring of 2006 we had 10 members of the council in attendance. The spring meeting of the council was held to coincide with our undergraduate research symposium to give our alumni a chance to interact with our juniors and seniors. Our commencement speakers for 2006 were Dr & Dr Andy & Heather Brink.

Giving to the Department has continued to show significant increases. The Friends of Larry Taylor Fund (a discretionary fund for the department chair is fully endowed. Gary Cools has also derided to endow the annual faculty research and teaching awards. The research award will be known as the John Schug Research Award and the teaching award as the Jimmy Viers award.

“The Elements” ‘the chemistry department Alumni Magazine is produced twice a year (Fall and Spring) and is received well by alumni and friends.

Appendix 1.

Undergraduate Education

Awards and other noted achievements of undergraduate students

Academic Excellence Award: **Stephanie Moore and Stuart Dunn**

James Lewis Howe Award (presented by the Virginia Blue Ridge Section of the American Chemical Society): **Clark Ramsey**

Hypercube Scholar Award: **Julie Heineckeer**

The Merck Index Award: **Jennifer Loman**

Phi Lambda Upsilon Award: **Mary Spencer**

Undergraduate Research Award: **Erika Bechtold**

Analytical Chemistry Award: **Joseph Zadrozny**

CRC Freshman Chemistry Achievement Award: **Wesley Morris and James Mills**

Viers Achievement Award**: Courtney Baskeyfield. Nina Comorian, Amanda Edwards, and Stephanie Vashell**

McGrath Award for Excellence in Polymer Chemistry: **Matthew Green**

The "Stars of Excellence" awards are given to the top 1% of students in the CHEM 2545/2546 and 2565 organic laboratory courses. This year's awards, which consist of a certificat and $100, go to: **Samuel Faith, Catherine Hendershot, Shun Mayumi, Jon Meade and Yinhua Qi**

Names of students participating in undergraduate research

Department of Chemistry
Fall 2005 Undergraduate Research Symposium
Friday, Dec 2, 2005
2:00 PM – 4:00 PM
Davidson 303
Virginia Tech Chapter of the ACS Student Affiliates Presiding

2:00 PM *Load presentations onto computer.*

2:10-2:30 **The Family of Allenes: Ab Initio Predictions of Optical Rotations Observed in Allene Derivatives** Tom Alongi and Prof. T. Daniel Crawford

Abstract

Dimethyl allene and 1-ethyl, 3-methyl allene are chemical systems containing a chiral axis. Because previous data has shown coupled cluster theory to have more success in accurately predicting the optical rotation of systems containing a chiral axis, ab initio calculations were performed to predict the optical rotation of these compounds.

2:30-2:50 **Magnetic Coordination Polymers: Manipulations of $V[TCNE]_2$** Joseph M. Zadrozny and Prof. Gordon T. Yee

Abstract

Modifications to the room temperature coordination polymer magnet, $V[TCNE]_2$, where TCNE = a bridging tetracyanoethylene radical anion, have been made. Replacement of one cyano group on the TCNE molecule with a substituted phenyl ring has permitted experiments aimed at tuning the magnetic coupling between vanadium ions. In particular, chlorine substitution on the ring has allowed for the exploration of the effects of the pi electron donating and sigma electron withdrawing characteristics of the chlorine atom on the magnetic ordering temperature. It appears that the stability of the radical anion correlates with the ordering temperature.

2:50-3:10 **Creation of Ligands for Zinc Phosphate Topologies** Doug Gross and Prof. Brian Hanson

Abstract

Metal phosphates can be used in ion exchange, catalysis, absorption and ionic conduction. These zinc phosphate sheets are linked by organic ligands, giving each sheet unique properties that can be used in the processes above. Creation of the dibromobenzene ligand will the focus of the presentation.

3:10-3:20 *break*

ONCCNOOONCCNOO+ $MnCp^{*2+}$ $CrCp^{*2+}$ $MnCp^{*2+}$ $CrCp^{*2}$di-n-butyl dicyanofumaratedi-iso-butyl dicyanofumarate

3:20-3:40 **Dialkyldicyanofumarte Diesters as Acceptors for Charge-Transfer Molecule-Based Magnets** Alexis Wells and Prof. Gordon T. Yee

Abstract

Dicyanofumarate diesters are made by replacing two nitrile (CN) groups on tetracyanoethylene (TCNE) with ester functional groups. These compounds are relatively easy to synthesize and also to reduce by one electron, making them good acceptors for charge-transfer salt production. Charge-transfer salt magnets arise upon the reaction of dialkylfumarates with decamethylmetallocenes, MCp^*_2, where M = Cr, Mn. By varying the length in the alkyl chains of the ester, structure-property relationships can be analyzed to reveal information concerning magnetic coupling. Presented here is the synthesis of two new acceptors: di-n-butyl dicyanofumarate and di-iso-butyl dicyanofumarate, along with their reactions with $CrCp^*_2$ and $MnCp^*_2$ to form salts. Complete magnetic measurements of the salts have been made, which reveal the nature of the magnetic coupling.

3:40-4:00 **Examination of Branched Amphiphiles at the Air/Water Interface and Determination of Structure using Theoretical Chemistry** Erika Bechtold, Prof. Rich Gandour, Prof. Alan Esker, Woojin Lee, Richard Macri, Whinny Sugandhi, Lauren Neeley, and Brett Kite.

Abstract

A series of tri-headed and two-tailed, carbamate-linked amphiphiles with anti-microbial properties were synthesized with varying hydrophobic chain length to observe the microbial activity as a function of increasing hydrophobicity. A two-step synthesis, with purification of the intermediates, provided high purities and yields for the target compounds. Because of their surfactant-like behavior at the air-water interface, Langmuir film studies of the interfacial properties of these amphiphiles was also investigated using the Wilhelmy plate technique and a pH ≈1 acid subphase. All of the amphiphiles formed liquid-expanded (LE) monolayers; lift-off, extrapolated limiting areas and collapse concentrations gave values on the order of A= 115, A= 95, and A= 60 Å/moleculerespectively for the carbamate linked series. A similar urido-linked series gave A= 80, while A= 60 Å/molecule as with the carbamate-linked series. Theoretical studies were preformed using Hartree-Fock Self-Consistant Field Method in order to determine the most energy stable conformations of the hydrophillic region of these branched amphiphiles. $_{\text{liftoff 0 collapse}}^{2}$ $_{\text{liftoff collapse}}^{2}$

4:00 PM *adjourn*

Virginia Tech Department of Chemistry
Spring 2006 Undergraduate Research Symposium
Friday, April 28, 2006
2:30 PM – 5:30 PM
Davidson 3
Virginia Tech Chapter of the ACS Student Affiliates Presiding

2:30-2:45 **Purification and characterization of the recombinant serine hydroxymethyltransferase from the human parasite Trypanosoma cruzi**

Shivan Desai, Kamran Shahzad, Brittany Gettleman, and Dr. Daniel Capelluto
Department of Chemistry, Virginia Tech

Trypanosoma cruzi is the causal agent of the Chagas disease, an illness with no effective drug treatment. Serine hydroxymethyltransferase (SHMT) generates precursors for the synthesis of folate. Our previous studies indicate that T. cruzi SHMT presents structural differences compared with the mammalian counterpart. However, the native T. cruzi SHMT is unstable and thus making difficult its characterization as a target for drug design. We have cloned and expressed the T. cruzi SHMT in E. coli. Initial purification yielded a highly stable and soluble protein. Folate analogs will be tested as potential T. cruzi SHMT inhibitors using circular dichroism, X-ray crystallography, and NMR spectroscopy.

2:45-3:00 **Synthesis of the Lithium Salt of Trisulfonated Triphenylphosphine oxide and its Ionic Conductivity**

William Henderson and Prof. Brian Hanson
Department of Chemistry, Virginia Tech

Triphenylphosphine was sulfonated using 30% fuming sulfuric acid. Two methods were explored for the workup of the trisulfonated product to form lithium triphenylphosphine oxide trisulfonate, LiTPPTSO. It is difficult to obtain pure LiTPPTSO due to similar solubilities of Li_2SO_4 and LiTPPTSO. Thus, a workup from the commercial synthesis of NaTPPTSO was used to minimize the formation of Li_2SO_4. Preliminary results showed the material to have good lithium ion conductivity. Additionally the phosphine polymer, JandaJel, was also sulfonated using fuming sulfuric acid and ion conductivity testing is in progress.

3:00-3:15

Development of Ru-Rh-Ru Supramolecular Assembles Applicable in Solar H_2 Production

Geoff Lewis and Prof. Karen Brewer

Department of Chemistry, Virginia Tech

A new light absorber was developed as a subunit in a supramolecular complex for the purpose of hydrogen production. The formula of the light absorber is $[(phen)_2Ru(dpp)](PF_6)_2$, where phen = 1,10-phenanthroline and dpp = 2,3-bis(2-pyridyl)pyrazine. Two of these light absorbers are attached to a rhodium core to yield the trimetallic complex, $[\{(phen)_2Ru(dpp)\}_2RhCl2](PF_6)_5$. Redox and spectroscopic properties of the monometallic and trimetallic complexes were studied. This complex looks promising in the application of photo-initiated hydrogen production.

3:15-3:30

Serine-trans-proline Isostere stereo-selective synthesis of (E)-Alkene Mimic by Ireland-Claisen Rearrangement

Department of Chemistry, Virginia Tech

Stereo selective synthesis of a trans proline mimic was synthesized according the method described by Wang et al in 2002. The goal of this research was to provide a stock supply of trans mimic for further research and catalogue binding studies in the inhibition of the Pin1 enzyme. Starting with N-Boc-Ser(OBzl)-OH and carrying this as far down the synthesis line as the time in a semester would allow.

Lucas Tucker, Song Zhao, and Prof. Felicia Etzkorn

3:30-3:45 refreshment break (load presentations onto computer)

Session 2: Alexis Wells presiding

3:45-4:00

Silicon Dioxide Corrosion: A Kinetic, Spectroscopic, and Surface Structural Test of Classical Nucleation Theory

Enoch Dames[1], Nizhou Han[2], and Prof. Patricia Dove[2]

[2] Department of Geosciences

A recent study showed that classical nucleation theory developed for crystal growth also explains dissolution rates of crystalline SiO_2. Because dissolution kinetics of crystalline and vitreous SiO_2 are similarly dependent on solution composition, nucleation theory may also explain vitreous silica corrosion. Measurements of vitreous SiO_2 dissolution rate versus chemical driving force indicate an agreement with nucleation theory. Raman spectroscopy shows the glass contains three- and four-member ring structures, although length scale of their ordering is unclear. When vitreous silica is reacted in electrolyte solutions, AFM indicates that higher energy sites are removed, revealing surface features corresponding to the most-stable ring structures.

4:00-4:10 **Synthesis of a New Electron Acceptor to make Charge Transfer Salts** Mary Spencer and Prof. Gordon Yee Department of Chemistry, Virginia Tech Di(2,2,2-trifluoroethyl) dicyanofumarate was synthesized as a potential new electron acceptor for the synthesis of charge transfer salts. The two step synthesis is composed of synthesizing 2,2,2-trifluorocyanoacetate (60%) and then dimerizing the cyanoacetate, purifiying by column chromatography after each step. The acceptor was reacted with different donor decamethylmetallocenes to study the crystal structures and magnetic properties of the resulting charge transfer salts. By altering the acceptors, the critical temperature and hysteresis of the salts can be studied to learn more about what causes ferrimagnetism and antiferromagnetism.

4:10-4:20

Analysis of Low T_g Polyesters for Pressure Sensitive Adhesive Applications

Jacquelyn Evans, Gozde Ozturk, and Prof. Timothy Long

Linear and branched polyesters with low glass transition temperature (T_g) were synthesized as potential PSAs using diethylene glycol (DEG) and 1,4 dimethylcyclohexanedicarboxylate (DMCD) via melt polymerization. The polymers were characterized using size exclusion chromatography (SEC) and differential scanning calorimetry (DSC). The peel strength of the samples were measured using 90º peel test at a peel rate of 12 in/min at room temperature. The variation in peel adhesion with contact time, peel speed, weight percentage, and adhesive thickness were measured. The peel test results showed that the synthesized low-T_g polyesters had peel strengths comparable to that of commercial tape under applied test conditions.

[1] Departments of Chemistry and Engineering Science and Mechanics
Department of Chemistry, Virginia Tech

4:20-4:35

Adhesive Properties of Trisilanolphenyl-POSS

Department of Chemistry, Virginia Tech

Polyhedral oligomeric silsesquioxanes (POSS) have been an innovative area of research for the past twenty years. Recent studies showed that trisilanol-POSS derivatives form self-assembled monolayers at the air/water (A/W) interface. The purpose of this study was to improve adhesion between ceramics and metals and metals and polymers by preparing multilayer films with varying metal ion concentrations using trisilanolphenyl-POSS (TPP). These multilayer systems were prepared by spincoating to make the polymer (polystyrene) layer, the Langmuir-Blodgett technique to create the TPP layer, and physical vapor deposition to produce the aluminum layer. The resulting films were characterized for quality and stability using atomic force microscopy, optical microscopy, X-ray photoelectron spectroscopy, and dewetting experiments. Experiments demonstrated that TPP-aluminum ion complexes created a smooth aluminum film on silica while TPP alone caused a blistered aluminum surface. Dewetting experiments showed that the polystyrene layer completely dewet on TPP, but the TPP-aluminum ion complexes suppressed dewetting.

4:35-4:45

refreshment break (load presentations onto computer)

Session 3: Alexis Wells presiding

4:45-5:00

Modifications of the V[TCNE]$_2$ magnet

Sarah Huffer and Prof. Alan Esker
Joe Zadrozny and Prof. Gordon Yee
Department of Chemistry, Virginia Tech

Modifications to the room temperature coordination polymer magnet, V[TCNE]$_2$, where TCNE = a bridging tetracyanoethylene radical anion, have been made. Replacement of one cyano group on the TCNE molecule with a substituted phenyl ring has permitted experiments aimed at tuning the magnetic coupling between vanadium ions. In particular, chlorine substitution on the ring has allowed for the exploration of the effects of the pi electron donating and sigma electron withdrawing characteristics of the chlorine atom on the magnetic ordering temperature. It appears that the stability of the radical anion correlates with the ordering temperature. Substitution at the 2 and 3 positions generates higher ordering temperatures in the polymer than the un-substituted phenyl ring. This leads to an exceptionally high ordering temperature in the 2,6-substituted molecule, which orders near 285 K.

5:00-5:15

Proposed Mechanisms of the MAO-Catalyzed Oxidation of Cyclopropylamines

Department of Chemistry, Virginia Tech

Monoamine oxidases (MAO-A and MAO-B) are mitochondrial flavoenzymes that catalyze the oxidative deamination of the catecholaminergic neurotransmitters, including dopamine. These enzymes are important targets for drugs designed to inhibit their catalytic activities. MAO-B mechanism-based inactivators are effective in treating Parkinson's disease, and thus may possess neuroprotective properties. This study seeks a better understanding of the MAO catalytic pathway, which will be valuable in designing therapeutically effective inhibitors of these enzymes. Human MAO-A and MAO-B substrate and mechanism-based inactivator properties of a group of cyclopropylamine test compounds will be analyzed. The acquired partition ratios $[(V_{max}/K_m)/(k_{inact}/K_i)]$ will serve as structurally dependent parameters that will be used to evaluate results obtained from mechanistic and molecular modeling studies. The reaction proceeds via a two-electron α-carbon oxidation that transforms the aminyl substrate to the corresponding iminium metabolite. The principal pathways that have been proposed to account for the catalytic properties of MAO are the single electron transfer (SET) pathway, the polar pathway, and the hydrogen atom transfer (HAT) pathway.

5:15-5:30

Synthesis and Characterization of Iridium Hydride Amino Acid Complexes

Department of Chemistry, Virginia Tech

Rachel K. Piggott, Prof. Neal Castagnoli, Jr., Kay Castagnoli, Philippe Bissel, and Anthony Miller

Melissa Ritchie, Prof. Joseph Merola, and Dr. Michael Berg

We are studying the bonding modes of naturally occurring amino acids to the iridium center in the $[Ir(COD)(PMe_3)_3]Cl$ complex. We have previously obtained the crystal structure for the L-valine complex. Interestingly, it gives a helical extended lattice. Therefore, we wish to examine other amino acid complexes to see if they too give this phenomena, starting with the simplest of amino acids, glycine. This talk will present our efforts in synthesis and crystal structure of these compounds.

5:30 PM

adjourn

Graduate Education

Awards and other noted achievements of graduate students

Graduate Teaching Assistant Award

Each year the department recognizes excellence in teaching by our outstanding graduate teaching assistants. Professors in charge of laboratory courses, and the faculty in general, nominate GTAs for this award. The Chemistry Department Graduate Committee then chooses individuals from those nominated to receive the award, which consists of a certificate and an award of $100.00. The awards are made for service during the 2005-2006 academic year.

Will Alexander-Physical Chemistry
Joe DeGuzman-Organic Chemistry
Jason Harmon-General Chemistry
Bingbing Li-Physical Chemistry
Jessica Lu-Analytical Chemistry
Suolong Ni-Physical and General

Graduate Research Award

It is certainly fair to say that the lifeblood of any chemistry department is the graduate students who perform the great majority of research in the department. The Chemistry Department has had a long tradition of excellence in research. Students are nominated by the research supervisor. We recognize the following students for their excellence in graduate research. Each will receive a certificate and a $100 award.

Larry Fiegland - Prof. Morris
Ran Miao - Prof. Brewer
Jennifer Russ - Prof. Dorn
Afia Karikari - Prof. T. Long

Clifford Faculty Service Award

Given to a Chemistry faculty for extraordinary service in behalf of the Department of Chemistry and in honor of Professor Alan Clifford who untiringly served as Head of the Department from 1966 to 1981. A picture of Alan and his wife, Shirley, hangs in the atrium between Davidson and Hahn Halls. The recipient of this award is **Joe Merola**.

McNair Staff Service Award

Given to a Chemistry staff member for meritorious service in behalf of the Department of Chemistry. Professor Harold McNair is the initiator and sponsor of this award. The recipient of this award is **Bill Bebout**.

Jimmy Viers Award for Excellence in Teaching: Alan Esker

John Schug Award for Excellence in Research: Paul Carlier

Appendix 2

A Few Highlights from 2005.

- **Paul Carlier** is a co -PI on a Bill and Melinda Gates Challenge Grant to investigate new materials for mosquito (and, thus malaria) control

- **Tim Long** led a proposal team that was successful in attracting an Army Materials Center at V. T.

- **Tim Long** had a paper on new biocompatible materials published in Science.

- **Tim Long** was asked to set on a National academy of Science's committee to assess the state of U.S. science.

- **John Morris and Joe Merola** hosted a visit by Richard Pretty who was interested in research being done on a new gasoline additive.

- Two proposals were funded that improve and modernize departmental NMR facilities.

- Record level of sponsored research awards**: $7,410,000**

- **Harry Dorn** won Alumni Award for research**.**

- **Richard Turner** was named The Northeast Tennessee Section ACS Speaker of the Year for research in specialty polyesters. Professor Turner was also named Editor of the Americas for Chemistry and Synthesis of POLYMER

- Professor Emeritus-**Harold McNair**-was invited to give a plenary lecture at a Gordon Research Conference (September 2005) in Switzerland. The conference title was "Detecting Illicit Substances:Explosives and Drugs."

- **Feihe Huang** wonVirginia Tech's 2006 Outstanding Dissertation Award - Science and Engineering**.** Feihe's advisor was **Prof. Harry W. Gibso**n.

Appendix 3

Annual Statistical Information:

Summary of Research and Related Scholarly Activities

Articles in Refereed Journals	112
Presentations at Professional Meetings	56
*Invited Lectures (Off-campus)	43
Research Funding	9.4 million
Books and Monographs	3
Patents	8
Review Articles and Book Chapters	26
Memberships on Journal Editorial Boards	8
Memberships on National Committees	9
Short Courses Taught	18
Students pursued Masters & Ph.D. degrees in 2004-2005 academic year	112
Students received Ph.D. degrees during the 2004-2005 academic year	9
Students received M.S. degrees during the 2004-2005 academic year	4
Students received BA/BS degrees during the 2004-2005 academic year	31

*Does not include invited presentations at professional meetings, which are included in the previous category.

Appendix 4

Chemistry Endowments

Fund	March 2004	May 2005
Hopper Harvie Endowment	25,911	26,641
Chemistry Friends Scholarship	91,338	102,569
Keyser Chemistry Endowment	28,846	29,659
Walker Scholarship	27,818	28,602
Bilisoly Scholarship	108,540	111,599
McNair Fund Endowment	8,273	9,017
Dallas Kinser and R. T. Johnson	29,161	33,502
McGrath Professorship Endowment	9,300	44,468
J. P. Wightman Scholarship[a]	33,939	36,280
John Dillard Scholarship[a]	16,252	112,917
TOTAL	$379,378	$535,254

[a] Administered by the Center for Adhesive and Sealant Science now MII (these are included because they recognize Chemistry Faculty)