

*Abstracts omitted from the proceedings issue because of mail problems.*

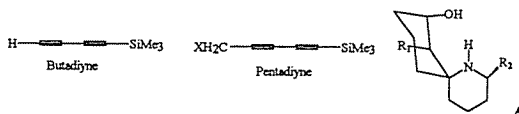
## Biology

### MODULATION OF PLANARIAN REGENERATION BY CAFFEINE

Sophia C. Worobec\* and Roman B. Worobec, Biomed. Res. Consults., POB 162, Mt. Vernon, VA 22121-0162. Exposure of a sexual variety of decapitated *Dugesia tigrina* to caffeine (11-220 mcg/ml) was shown to modify the course of regeneration as monitored by unambiguous eyespot appearance under 40X magnification. The most telling results were that regeneration was accelerated by constant exposure to 55 mcg/ml of caffeine, whereas 220 mcg/ml precluded regeneration. When caffeine exposure was limited to the first 4 h after sectioning, i.e., to the critical stage of cell activation, both the 55 and 100 mcg/ml caffeine concentrations were stimulatory. Under the same conditions 220 mcg/ml of caffeine delayed eyespot regeneration, while 11 mcg/ml was without effect. Constant exposure to caffeine in a concentration of 220 mcg/ml was particularly toxic to isolated heads, leading to complete disintegration of the eyespots and then of the entire head within 6-8 h. In about 40% of intact animals 200 mcg/ml of caffeine induced a reversible loss of one or both eyespots after 6-8 h of exposure. These observations were discussed in the light of cell activation mechanisms and photoreceptor susceptibility to methylxanthines.

## Chemistry

A SYNTHETIC STUDY TOWARDS AN ETHYNYLATED AZASPIROCYCLIC INTERMEDIATE OF HISTRIONICOTOXIN. Benjamin Ayida and Godson C. Nwokogu, Dept. of Chemistry, Hampton University, Hampton, VA 23668. Histronicotoxin (A:  $R_1 = cis\text{-CH=CH-C}\equiv\text{CH}$ ;  $R_2 = cis\text{-CH}_2\text{CH=CH-C}\equiv\text{CH}$ ), an alkaloid isolated from the skin secretion of the from *Dendrobates histrionicus*, blocks trans-synaptic ion transport. A number of methods for assembling the azaspirocyclic framework and for total synthesis of the natural compound, however, have been reported due to the difficulty of creating the unsaturated side-chains through multi-step C-C bond formations and functional group transformations. In order to overcome this difficulty, we wish to adopt a strategy that introduces the side chains in a convergent way as diynes which later could be stereoselectively reduced to cis-enynes. As a result, we have been studying different methods of generating butadiynes and 1,3-pentadiyne derivatives as well as searching for optimal conditions for Pd(O)-catalyzed coupling of the butadiyne to model 2-bromoallyl acetates.



MULTINUCLEAR NMR INVESTIGATION INTO THE ACTIVATION OF SILICON-HYDROGEN BONDS BY A BINUCLEAR PLATINUM COMPLEX. Kimberly A. Brittingham and Serge Schreiner, Dept. of Chemistry, Randolph-Macon College, P. O. Box 5005, Ashland, VA 23005-5505. The secondary silanes,  $\text{Me}_2\text{SiH}_2$ ,  $\text{Et}_2\text{SiH}_2$ ,  $\text{Ph}_2\text{SiH}_2$  and  $\text{MePhSiH}_2$  react with the binuclear complex  $[\text{Pt}_2(\mu\text{-CO})(\text{CO})_2(\mu\text{-dppm})_2]$  (1;  $\text{dppm} = \text{Ph}_2\text{PCH}_2\text{PPh}_2$ ) to give zerovalent  $\mu\text{-SiRR}'$  complexes of the form  $[\text{Pt}_2(\mu\text{-SiRR}')(\text{CO})_2(\mu\text{-dppm})_2]$  ( $\text{R} = \text{R}' = \text{Me}$  (2),  $\text{Et}$  (3),  $\text{Ph}$  (4);  $\text{R} = \text{Me}$ ,  $\text{R}' = \text{Ph}$  (5)). In the reaction of 1 with  $\text{Ph}_2\text{SiH}_2$  leading to 4, low temperature, multinuclear NMR data show that the reaction proceeds via an intermediate formulated as  $[\text{Pt}_2(\text{H})(\text{SiHPh}_2)(\text{CO})_2(\mu\text{-dppm})_2]$ , 6.

BETWEEN TRUTH AND FICTION: WHAT DO YOU GET FROM THERMAL ANALYSIS? Lori Brock\*, Jeff Keister\* and Thomas C. DeVore, Dept of Chemistry, James Madison University, Harrisonburg, VA 22807. Several methods for extracting kinetic parameters from the thermal analysis data obtained for heterogeneous systems have been developed. Most use a best fit graphical method to determine intrinsic values for the kinetic parameters ( $A =$  pre-exponential factor,  $E_a =$  activation energy, and  $n =$  order of the reaction) and provide information about the reaction mechanism. However, Maciejewski has clearly shown that kinetic parameters determined depend on the experimental conditions used. No explanation for these differences was offered. Evolved gas analysis - Fourier transform infrared spectroscopy (EGA - FTIR) provides additional information about heterogeneous processes. EGA - FTIR has been used to investigate the reaction between  $\text{CCl}_4$  and  $\text{V}_2\text{O}_5$  and the thermal decomposition of  $\text{NH}_4\text{VO}_3$ . The results of these investigations indicate that equilibrium processes, not kinetic processes, limit the "rate of reaction." These results offer possible explanation to the paradox presented by Maciejewski.

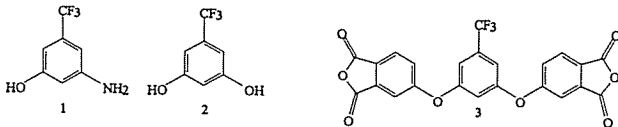
APPLICATIONS OF FLUORESCENCE TO BIOCHEMISTRY: INTERCALATION OF PROBES INTO DNA, Lisa Christianson and Benjamin A. DeGraff, Department of Chemistry, James Madison University, Harrisonburg, VA 22801. The intercalation of ethidium bromide into calf thymus DNA has been explored using various spectroscopic and fluorescent techniques. Shifts in peak positions and intensities were found in absorption and emission fluorescence spectra with addition of DNA. Emission polarization increased with addition of DNA in both buffer solutions and saturated sucrose solutions. Identical studies were performed using the ruthenium trisphenanthroline complex. The absorption spectrum of the solution displayed little change upon addition of DNA, while the peak intensities were increased in the emission spectrum. Quenching experiments were also performed, using the ruthenium trisphenanthroline complex as the intercalator and the ferrocyanide ion ( $[\text{Fe}(\text{CN})_6]^{4-}$ ) as the quencher. It was found that quenching of the  $[\text{Ru}(\text{phen})_3]^{2+}$  was minimized when it was intercalated into DNA, thereby protecting the metal complex from bulk solution environmental effects.

ESR STUDIES OF FREE RADICAL INTERMEDIATES IN THE ENZYMATIC OXIDATION OF SYRINGALDAZINE AND RELATED COMPOUNDS BY HORSE RADISH PEROXIDASE, Kelly A. Coggs and Herbert J. Sipe, Jr., Department of Chemistry, Hampden-Sydney College, Hampden-Sydney, VA 23943. ESR spectra were observed for three methoxy *ortho* di-substituted phenols. Syringaldazine, acetosyringone, and syringaldehyde were studied in a system of  $H_2O_2$ /HRP to produce phenoxy free radicals. A well resolved spectrum was measured for the acetosyringone radical, hyperfine coupling constants assigned, and a simulation reproduced for the experimental spectrum. The ESR spectrum of the radical from the syringaldehyde system was not fully resolved, although hyperfine coupling constants were measured for methoxy substituents. The syringaldazine system produced radicals but the ESR spectrum was not intense and was incompletely resolved.

THE REACTION BETWEEN BIS(2,4-PENTANEDIONATO)LEAD(II) AND WATER VAPOR: A THERMODYNAMIC STUDY, Melissa A. Crouch and Thomas C. DeVore, Department of Chemistry, James Madison University, Harrisonburg, VA 22807. Evolved Gas Analysis-Fourier Transform Infrared Spectroscopy was used to investigate the reaction between bis(2,4-pentanedionato) lead(II) and water vapor from 300 to 600 K. 2,4 pentanedione, acetone, and carbon are the principle gaseous products produced. Powder X-ray diffraction indicated that lead oxide and lead metal were the principle solid products. The equilibrium concentrations of all products and reactants were determined as a function of temperature. This enabled the enthalpy of formation for bis(2,4-pentanedionato)lead to be estimated. The value determined is  $855 \pm 10$  kJ/mol.

SYNTHESIS AND STUDIES OF  $(\eta^5-C_5H_5)(CO)_xM(CH_2C_6H_3-15-crown-5)$  Andrew Dattelbaum, Audra Wright, Donna S. Amenta and John A. Mosbo, Department of Chemistry, James Madison University, Harrisonburg, VA 22807. The purpose of this research was to synthesize, characterize and study the reactivity of transition metal complexes whose ligands contain crown ethers. One of the target molecules,  $(\eta^5-C_5H_5)(CO)_2Fe(CH_2C_6H_3-15-crown-5)$  (**1**), was prepared from  $[(\eta^5-C_5H_5)(CO)_2Fe]$  and  $ClCH_2C_6H_3-15-crown-5$  (**2**). The synthesis of **2** was accomplished from the reaction of 3,4-dihydroxybenzaldehyde with the dichloride of tetraethylene glycol, followed by  $NaBH_4$  reduction of the resulting aldehyde to yield 4'-HOCH<sub>2</sub>-benzo-15-crown-5. Treatment of this alcohol with thionyl chloride gave the desired **2**. All intermediate products have been characterized by NMR spectroscopy. The conversion of **1** into an acyl complex has been attempted using external phosphine ligands via carbonyl insertion reactions. The products from these attempts have been characterized by IR and NMR spectroscopy.

SYNTHESIS OF A NEW TRIFLUOROMETHYLATED DIANHYDRIDE FOR HIGH PERFORMANCE POLYIMIDES. Michael S. Hines and Roy F. Gratz, Dept. of Chemistry, Mary Washington College, Fredericksburg, VA 22401-5358. New synthetic routes have been developed for the preparation of 3-amino-5-hydroxybenzotrifluoride, 1, and 3,5-dihydroxybenzotrifluoride, 2. The syntheses begin with 3,5-dinitrobenzotrifluoride, which is converted first into a monobenzyl ether and then into a dibenzyl ether by nucleophilic displacement of the nitro groups. Catalytic hydrogenations of the ethers lead to 1 and 2. Attempts to convert 2 into an arylene ether linked dianhydride, 3, by reaction with 4-fluorophthalic anhydride will be described.



COMPUTER SIMULATION OF PEPTIDE PROPERTIES. Tamaki Kurusu and David R. Bevan, Dept. of Biochemistry & Anaerobic Microbiology, Virginia Tech, Blacksburg, VA 24061-0308. It is generally accepted that lipophilic compounds diffuse through cell membranes more readily than hydrophilic compounds. However, diffusion requires desolvation of molecules prior to their passing through the lipid bilayer. We used the computer programs MOPAC, POLARIS, and AMSOL to simulate the solvation properties of a series of phenylalanyl peptide chains for which the permeability and lipophilicity were known experimentally. Our results clearly show that as the peptide length increases, the free energy of solvation ( $\Delta G_{\text{solv}}$ ) becomes more negative, suggesting that the free energy of desolvation ( $\Delta G_{\text{desolv}}$ ) is less favored and therefore the permeability decreases. Also, with increased methylation of backbone amide nitrogens, the  $\Delta G_{\text{solv}}$  becomes less negative, favoring  $\Delta G_{\text{desolv}}$ , and so increasing permeability. These results are consistent with experimental data obtained from the literature. Therefore, our computer simulations suggest that both  $\Delta G_{\text{solv}}$  and lipophilicity of peptides must be considered when evaluating the permeability of bilayer membranes.

DEVELOPING A COMPUTER MODEL FOR SIMULATING THE CRYSTALLIZATION OF A MELT INTO A POLYCRYSTALLINE SOLID: OVERVIEW AND SOME GEOMETRIC PROBLEMS. Michael Leopold,\* Dept. of Chem., Roddy V. Amenta, Dept. of Geol. and Geog., James Madison University, Harrisonburg, Va. 22807. Igneous rocks are naturally occurring polycrystalline solids that form the bulk of our planet. The fabric of an igneous rock, i.e. the spatial arrangements and chemical compositions of its crystals, contains the clues to its evolution over time by the slow cooling and crystallization of a melt. The inverse problem of interest to geochemists is determining what likely crystallization processes produced the resultant rock fabric. As with most inverse problems a unique solution model is rarely possible. Computer simulation of fabric development in polycrystalline solids would help in finding possible models for complex, non-linear, crystallization processes. The present study deals with one aspect of this problem, that of simulating the growth of crystals in a confined space and of resolving the competition for space among growing crystals in two dimensions. Specific efforts deal with methods for calculating and minimizing the overlap areas among adjacent crystals. Future efforts will deal rates of crystal nucleation and growth.

PYRIDINES IN FLAVORINGS AND FUELS: SYNTHETIC APPROACHES TO THE 2,5-DIALKYL PYRIDINES. David L. McElfresh and Wayne M. Stalick, Chemistry Department, George Mason University, Fairfax, VA 22030. 2,5-Dialkylpyridines occur widely in nature, from the essential oils of citrus fruits to the unrefined oil from oil shale and lower rank bituminous and lignite coals. The thrust of the current research is to find an efficient method for the synthesis of 2-methyl-5-alkylpyridines, 2-alkyl-5-methylpyridines and 2,5-dialkylpyridines, where the alkyl group would vary from five to fifteen carbon atoms. The original starting material was 2,5-lutidine, which upon reaction with sodium amide in ammonia give 5-methyl-2-pentylpyridine when reacted with 1-bromobutane. Dianion formation was assumed to be the ideal pathway into the 2-methyl-5-alkylpyridine series of compounds. Since the anion on the 5 position would form more slowly, it should react more readily such that with a limited amount of alkyl halide, substitution would preferentially occur at the 5 position. The use of excess  $\text{NaNH}_2$  or  $\text{KNH}_2$  in ammonia or LDA in THF resulted in alkylation or dialkylation on the 2 position only. New experiments have been performed using the "super base" system of potassium *t*-pentoxide and 1-ethylhexyllithium with 2,5-lutidine and with methylolithium, pentyl bromide and pyridine.

ANALYSIS OF THE SUBUNIT STRUCTURE OF THE GUANINE-7-METHYLTRANSFERASE. Joelle M. Onorato and Thomas O. Sitz, Dept. of Biochemistry and Anaerobic Microbiology, Virginia Tech, Blacksburg, VA 24061. Previous kinetic studies have defined three domains in the active site of the guanine-7-methyltransferase: S-adenosylmethionine domain, cap (GpppG) binding region, and the RNA binding domain. We have been successful in labeling (by UV cross-linking) the combined cap-RNA region of the enzyme with a  $^{32}\text{P}$ -labeled capped RNA that was synthesized *in vitro*. Using native polyacrylamide gel electrophoresis we have characterized the size of the labeled protein as 107 K molecular weight and what appears to be a monomer of 55 K molecular weight. This agrees with earlier studies from this laboratory that characterized the subunit structure of purified enzyme as a homodimer with a molecular weight of 95 K (gel-exclusion chromatography) with a subunit molecular weight of 46 K (SDS-PAGE). Gel exclusion chromatography with HR-Sephacryl S-300 also showed a labeled enzyme with a molecular weight of 107 K. These data support our model for the subunit structure of the guanine-7-methyltransferase.

ESR SPECTROSCOPIC STUDIES OF THE ANTIOXIDANT PROPERTIES OF DIMETHYLTHIOUREA BY THE SPIN TRAPPING TECHNIQUE, Matthew T. Ranson and Herbert J. Sipe, Jr., Department of Chemistry, Hampden-Sydney College, Hampden-Sydney, VA 23943. Hydroxyl radical, formed by the Fenton reaction of hydrogen peroxide with  $\text{Fe(II)-EDTA}$ , is scavenged by dimethylthiourea. When the resulting radical species is spin trapped by 2-methyl-2-nitrosopropane (MNP), a single long-lived spin adduct is observed. The nitroxyl radical ESR spectrum consists of a triplet pattern (g-value ca.  $2.00638 \pm 0.00001$ ) and is consistent with hydroxyl radical attack at the C=S with MNP trapping of the resulting S' radical. Given the high reactivity of  $\cdot\text{OH}$ , it is likely that other transient radicals are formed as well, but we do not observe them under our conditions.

AB INITIO MODELS OF METAL CHELATION SITES IN POLYIMIDES Donald D. Shillady, V. Kincaid and K. Esperdy, Virginia Commonwealth Univ., Dept. of Chemistry, Richmond, VA 23284-2006. It has been shown that  $\text{Na}^+$  ion enhances electrical conductivity in polyimides. Work in this laboratory by Guillem proved that  $\text{Er}^{3+}$  ions undergo ligand exchange and are chemically bound to typical polyimides by analyzing the magnetic circular dichroism (MCD) spectral changes in the hypersensitive bands. Recent work by Esperdy has shown that  $\text{Ho}^{3+}$  and  $\text{Gd}^{3+}$  will react with DuPont Pyre-mL to bind up to 8% (w/w) of total dry solid film using IR, MCD and UV spectroscopy. The question addressed here is how metal ions are chelated within amic-acid sites of an incompletely imidized polyimide. The GAMESS ab initio program has been used to optimize the geometry of an interesting new "tetradentate site" postulated to exist in polyamic acids and incompletely imidized polyimides. STO6G\* (\* = d orbitals on C, O, N) basis calculations are reported for the geometry and vibrational frequencies of a model compound, Aluminum N-phenyl phthalamate. Calculations show that such a tetradentate site could bind metal ions in Polyimides. The vibrational frequency analysis is compared with experimental IR data.

SYNTHESIS AND SPECTROSCOPIC CHARACTERIZATION OF METAL COMPLEXES OF BUCKMINSTERFULLERENE ( $\text{C}_{60}$ ). Harvey E. Smith and Serge Schreiner, Dept. of Chemistry, Randolph-Macon College, P.O. Box 5005, Ashland, VA 23005-5505.

Organometallic derivatives of  $\text{C}_{60}$  can be prepared by using dehydrochlorination of chloro hydrido transition metal complexes to generate coordinatively unsaturated metal fragments for subsequent reaction with  $\text{C}_{60}$ . The compound  $[\text{Pt}(\eta^2\text{-C}_{60})(\text{PPh}_3)_2]$  has been prepared from  $[\text{Pt}(\text{H})(\text{Cl})(\text{PPh}_3)_2]$  in refluxing ethanol/benzene in the presence of ethanolic NaOH and  $\text{C}_{60}$ . Elemental analysis and spectroscopic data of this compound are consistent with its previously reported preparation by reaction of  $[\text{Pt}(\eta^2\text{-C}_2\text{H}_4)(\text{PPh}_3)_2]$  with  $\text{C}_{60}$ . The new compound  $[\text{Ir}(\text{H})(\text{CO})(\eta^2\text{-C}_{60})(\text{PPh}_3)_2]$  has been prepared in a similar fashion from  $[\text{Ir}(\text{H})_2(\text{Cl})(\text{CO})(\text{PPh}_3)_2]$  and has been characterized spectroscopically.

METHIONINE METABOLISM AND mRNA METHYLATION. Darrin R. Sorokti and Thomas O. Sitz, Dept. of Biochemistry and Anaerobic Microbiology, Virginia Tech, Blacksburg, VA 24061. Methionine is an important amino acid required for protein synthesis and the formation of S-adenosylmethionine (SAM). SAM is an important cellular methylating agent used to modify macromolecules such as protein and nucleic acids. We have been studying the methylation of mRNA cap structure, particularly the important guanine-7-methylation. By using the enzyme, guanine-7-methyltransferase isolated from Ehrlich ascites tumor cells, we can quantitate the amount of hypomethylation found in mRNA cap structure. We have been able to lower the level of methylation found in the cap structure of mRNA by restricting the level of methionine in the culture media of normal rat kidney (NRK) cells. Cycloleucine, an inhibitor of SAM synthetase, also was shown to have a similar effect. A combination of low methionine media and cycloleucine caused the greatest level of inhibition of cap methylation. Thus, by lowering the levels of cellular SAM, the guanine-7-methylation found in mRNA cap structure can be reduced.

CHARACTERIZATION OF A CYANOBACTERIAL GLOBIN. Marc V. Thorsteinsson and David R. Bevan, Dept. of Biochemistry & Anaerobic Microbiology, Virginia Tech, Blacksburg, VA 24061-0308. Potts et al. (*Science* 256, 1992), detected a globin, now known as cyanoglobin, in the nitrogen fixing cluster of the cyanobacterium *Nostoc commune* UTEX 584. Herein, we describe the large scale induction, purification, and partial structural characterization of recombinant cyanoglobin. Comparative studies using absorption spectroscopy and circular dichroism with sperm whale myoglobin and soybean leghemoglobin A reveal that cyanoglobin is atypical in its ability to bind exogenous ligands in the ferric form. The heme environment of cyanoglobin more closely resembles that of leghemoglobin A, although little sequence similarity exists. Cyanoglobin appears to possess a fast rate of autooxidation, which parallels the behavior of myoglobin isolated from *Tetrahymena caudatum*, with which it shares sequence similarities in the heme environment.

ESR SPECTROSCOPIC STUDIES OF THE REACTION OF NITRIC OXIDE WITH PHENOLIC ANTIOXIDANTS, Gresham T. Weatherly and Herbert J. Sipe, Jr., Department of Chemistry, Hampden-Sydney College, Hampden-Sydney, VA 23943. Nitric oxide (NO) has been reported to oxidize phenols and reversibly couple to the free radical produced. Since NO has recently been discovered to be an important biological messenger, its reaction with 2-*t*-butyl-4-methoxyphenol (BHA), a widely used food additive, was investigated to determine if NO would oxidize and reversibly couple to BHA. In order to optimize experimental parameters the BHA analog 3,5-di-*t*-butyl-4-hydroxyanisole (DTBHA) was also reacted with NO. NO was found to oxidize and reversibly couple to BHA and DTBHA. ESR hyperfine coupling constants taken from the literature could be used to simulate the BHA spectrum. However reported hyperfine coupling constants could not simulate the DTBHA spectrum. As yet the product of the reaction of NO with DTBHA is undetermined.

COMPUTATIONAL METHODS FOR COMPARING PREDICTED AND EXPERIMENTAL IR DATA. Robert H. Williams and Frank A. Palocsay, Department of Chemistry, James Madison University, Harrisonburg, Virginia 22807. A Visual Basic program has been written that enables the user to compare sample and predicted infrared spectroscopic data. Sample data is organized using Galactic Corporation's *Grams/386* while predicted spectroscopic data is created using Autodesk's *HyperChem*. Students construct molecules using *HyperChem* which then predicts the infrared spectrum of the molecule as drawn. The student next chooses a spectrum file saved by *Grams/386*. The peak heights and locations of the two data sets are then compared in a visual manner with both spectra displayed at the same time. The data sets can also be compared quantitatively by examining the tables of peak values. Easy to access on-line help has been added to aid the student's use of the program as well as improve the student's understanding of infrared spectroscopy.

THE SYNTHESIS OF ANALOGUES OF METHYL-*p*-HYDROXYPHENYLLACTATE (MeHPLA): POTENTIAL ANTIESTROGENIC AGENTS AND CANCER CELLS. R.L. Williams, Mark Elliott and K. Bryant, Enological Research Facility, Dept. of Chemistry/Biochemistry, Old Dominion University, Norfolk, VA 23529. Several analogues of the natural ligand MeHPLA found in normal and breast cancer cells have been synthesized in an attempt to generate potential antitumor agents for biological evaluation in human breast cancer cell in culture. MeHPLA was synthesized from commercially available *para*-hydroxyphenyllactic acid (HPLA) in 70% yield and characterized by IR and NMR analysis. MeHPLA was shown to exhibit a relatively high binding affinity for the type II estrogen binding sites in human breast cancer cell (MCF-7) in culture. Human breast cancer cells have been shown to produce a specific esterase which converts MeHPLA to the unreactive HPLA *in vivo*. In order to circumvent this phenomena, we have synthesized several nitrogen analogues of MeHPLA which should be resistant to this specific esterase and hopefully exhibit reasonable levels of type II binding affinity. The corresponding N-methyl analogue of MeHPLA has been evaluated and indeed does exhibit type II estrogen binding site affinity. The other compounds include the ethanol amine analogue and the benzyl analogue of MeHPLA. The synthesis and identification of these potential antitumor agents will be described in this paper.

ISOLATION AND CHARACTERIZATION OF PROCYANIDINS FROM GRAPE SEED EXTRACTS AND THEIR POTENTIAL BIOLOGICAL ACTIVITY. R.L. Williams, M. Elliott, J. Reddy and J. Recht, Old Dominion University Enological Facility, Dept. of Chemistry /Biochemistry, Old Dominion University, Norfolk, 23529. Crude grape seed extracts have been isolated from Virginia chardonnay grape seeds and the various bioflavonoids known as the procyanidin catechin, epicatechin, B1, B2, B3, and B4 have been separated and evaluated in various biological tests. Ten individual procyanidins have been isolated from the crude extract and identified by HPLC and TLC. These components of grape seed extracts have been tested in human fibroblast cells in culture with regard to their ability to affect cell growth. At reasonably high levels, several of the compounds apparently inhibit cell growth and are also effective in blocking cell damage due to high levels of free radicals produced *in situ* from a xanthine/xanthine oxidase study. These grape seed fractions as well as the crude seed extracts have now been shown to have some significant binding affinity to type II estradiol binding sites in MCF-7 human breast cancer cells in culture. The implications and significance of this latter study will be described in this paper as well as the methods of analysis of the separation of the various procyanidins.

SYNTHESIS AND CHARACTERIZATION OF LONG CHAIN ALKYLQUINOLINES. Nazdaneh Zahadat and Wayne M. Stalick, Chemistry Department, George Mason University, Fairfax, VA 22030. An important current goal in chemistry is to develop a better understanding of the decomposition pathways of alternate fuel sources such as oil shale and coal. A number of studies have been made demonstrating that studies of model compounds can give good extrapolations to the natural product. It has been estimated that nitrogen containing compounds constitute about 40% of the material found in crude shale oil and based on the GC/MS analysis of these compounds, long chain alkylquinolines along with alkylpyridines are the major constituents. In our continuing study of the pyrolyses of these compounds it became necessary to synthesize a series alkylquinolines. For this study, the isomeric undecylquinolines were selected. Considering that the  $pK_a$ 's of methylquinolines are about 5 units lower than those of the corresponding picolines, it was assumed that the synthesis of these compounds, by the Brown and Murphey technique using sodium amide in liquid ammonia, would be an easy task. Even though the 2- and 4-methylquinolines easily underwent alkylation, 3-methylquinoline was resistant to alkylation because of side reactions. The previously unreported compounds synthesized in this study were characterized by NMR, IR, GC/MS and elemental analyses.



**CARBON FIBER / POLYMER MATRIX ADHESION IN HIGH PERFORMANCE COMPOSITES.** Hong Zhuang and J. P. Wightman, Dept. of Chemistry, Va. Polytechnic Inst. & State Univ., Blacksburg, VA 24061. There is increasing use of fiber / polymer matrix composites worldwide today, for example, in automobiles and in recreational equipment. Further, high performance composites are used increasingly in aircraft construction as in the new Boeing 777. The strength and toughness of composites is controlled by fiber / matrix interfacial adhesion. The purpose of this work is to relate the measurements of fiber / matrix adhesion to properties of the carbon fiber and the polymer matrix. Single fiber fragmentation tests were carried out to evaluate the strength and temperature dependence of interfacial adhesion between carbon fibers and epoxy resins. The results were correlated with the carbon fiber surface properties. The surface composition of the fibers was determined by XPS (x-ray photoelectron spectroscopy), the fiber topography by SEM (Scanning electron microscopy) and fiber surface energy by DCAA (dynamic contact angle analysis). Increasing the surface energy of the carbon fiber by surface pretreatment increased the calculated interfacial shear strength. (Supported by McDonnell Douglas Aerospace)

