Volume 4, Number 3 Summer 2005

Journal of Undergraduate Chemistry Research

ISSN: 1541-6003

CONTENTS

GUAIOL EPOXIDES: NEW CHEMISTRY OF MEDICINAL PLANT DERIVATIVES AND POTENTIAL XENOBIOTIC ACTION IN HUMANS
Robert A. Craven*, Nathan W. Arp*, Elizabeth Johnson*, and Thomas G. Waddell† 81

STUDY OF THE PHOSPHORESCENT TRIPLET STATE OF 2-INDANONE-d_1: USE OF A MICROCONTROLLER BASED PHOTON COUNTER AND PULSE TRAIN GENERATOR
D. Carroll*, R. Broadus*, J. Hanson*, T. Conant* and A. M. Nishimura† 85

OPTICAL METHODS AS PROBES OF THE SURFACE DYNAMICS DURING DISORDER-TO-ORDER TRANSITION IN NAPHTHALENE ADLAYER ON Al_2O_3(0001)
T.S. LeDoux*, M.A. Evans*, K.E. Howard*, A.D. Louie*, and A.M.Nishimura† 91

EXTRACTS FROM KUDZU LEAVES INHIBIT CANCER CELL GROWTH
Angelina M. Dorman†*, Shabana Khan‡ and Luther Elrod 97

OPTICAL STUDIES OF THE DISORDER-TO-ORDER TRANSITION IN 1,4-DICHLORO-NAPHTHALENE ADLAYER ON Al_2O_3 (0001)
J.S. Brigham,* D.R. Hoss,* A.J. Bishop*‡, K.A. Martin‡ and A.M. Nishimura† 101

CHEMICAL COMPOSITION OF MINOR, COPPER-BASED COINS OF THE BYZANTINE EMPIRE VIA ENERGY DISPERSIVE X-RAY FLUORESCENCE SPECTROMETRY
Irice Ellis* and Mark Benvenuto† 107

METHANOL AND WATER CLUSTER AB-INITIO STRUCTURE DETERMINATION
Maxwell Merkle* and Leon L. Combs† 113

THE DESIGN AND SYNTHESIS OF NOVEL CHAETOMELLIC ACID A ANALOGUES
Mark F. Mechelke†, Jacquelyn C. Webb*, and Jessica L. Johnson* 117

The *Journal of Undergraduate Chemistry Research* publishes papers of original research performed by undergraduates on all aspects of chemistry including analytical, organic, inorganic, physical, polymers and biochemistry. Articles about laboratory experiments to be used in the teaching of chemistry are not applicable. The *Journal of Undergraduate Chemistry Research* is issued quarterly and indexed once per year by Dr. Daniel Y. Pharr Editor, Chemistry Department, Virginia Military Institute, Lexington, VA 24450. Subscriptions price per year U.S.A.: institutional $ 120.00, individual $ 50.00 all other countries US $ 150.00. Claims for missing issues will not be honored after four months of issue date. Duplicate copies may not be sent due to the change of address when the publisher was not notified in a timely manner. The *Journal of Undergraduate Chemistry Research* can be contacted via phone (540-464-7244), fax (540-464-7261) or e-mail (PharrDY@vmi.edu) through Dr. Daniel Y. Pharr Editor. No responsibility is assumed by this journal, editor, reviewers or sponsors for any injury and/or damage from products, negligence, experiments, instructions or ideas contained in this journal that result in damage to persons or property. **POSTMASTER**: Send change of address to: Journal of Undergraduate Chemistry Research, Dr. Daniel Y. Pharr Editor, Chemistry Department, Virginia Military Institute, Lexington VA 24450.

GUAIOL EPOXIDES: NEW CHEMISTRY OF MEDICINAL PLANT DERIVATIVES AND POTENTIAL XENOBIOTIC ACTION IN HUMANS

The common and widely distributed sesquiterpene alcohol guaiol [1] is a likely xenobiotic substance toward humans where after ingestion it may be metabolized to an electrophilic epoxide derivative which can react with cellular DNA. In this study, the guaiol epoxides [2,3] are prepared and the reactions of the α-epoxide [2] with protic (trifluoroacetic acid) and Lewis acids (Al isopropoxide, BF_3) are described yielding cyclic ether and new diene-ol products. The characteristic "guaiol color reaction" is observed in these reactions. The sterically hindered, tetrasubstituted epoxide unit of [2] and [3] is unreactive toward a variety of model DNA nucleophiles.

Robert A. Craven*, Nathan W. Arp*, Elizabeth Johnson*, and Thomas G. Waddell†

Department of Chemistry, University of Tennessee at Chattanooga, 615 McCallie Ave., Chattanooga, TN 37403 Thomas-Waddell@utc.edu

STUDY OF THE PHOSPHORESCENT TRIPLET STATE OF 2-INDANONE-d_1: USE OF A MICROCONTROLLER BASED PHOTON COUNTER AND PULSE TRAIN GENERATOR

The lowest electronically excited state of 2-indanone is $^3\pi\pi^*$, with a nearby $^3n\pi^*$ state that plays a large role in facilitating the intersystem crossing into the triplet manifold (1-5). The phosphorescence emission is of sufficient intensity to allow the probing of very subtle intramolecular interactions, such as the deuterium isotopic substitution of the hydrogen α to the carbonyl. One method by which the excited triplet state of molecules can be probed is optically detected magnetic resonance, ODMR (1-4). For example, in the phosphorescent excited state, the oxygen of the carbonyl is out-of-plane (1-5). Hence in 2-indanone-d_1, the ODMR spectrum showed a doublet due to the two geometrical forms that the carbonyl may have relative to the deuterium and the assignment of the two peaks in the doublet to the two molecular structures was ambiguous (1). In this study, the 2-indanone-d_1 was synthesized. A microcontroller based pulse train generator and photon counter circuit was designed and fabricated with which pulse experiments were done. From the results of these experiments, the trends in T_2* and T_2 with deuteration was determined and the doublet was uniquely assigned to the two excited state geometries.

D. Carroll*, R. Broadus*, J. Hanson*, T. Conant* and A. M. Nishimura†

†Department of Chemistry, Westmont College, Santa Barbara, CA 93108-1099

OPTICAL METHODS AS PROBES OF THE SURFACE DYNAMICS DURING DISORDER-TO-ORDER TRANSITION IN NAPHTHALENE ADLAYER ON Al_2O_3(0001)

Amorphous naphthalene, prepared by vacuum deposition onto a cold Al_2O_3 surface, forms electronically excited dimers or excimers, when optically pumped, and their emission is characteristically red-shifted, broad and featureless compared to the monomeric fluorescence. The disorder-to-order transition can be caused by heating the surface. Since crystalline naphthalene fluoresces and does not exhibit excimeric features, the transition was studied by several optical methods by taking advantage of the changes in the spectral characteristics of the adlayer. These included emission from fluorescence and excimer, transmittance, and optical interference. The combination of these methods allowed a close look at the surface dynamics of molecules on the surface of Al_2O_3 as the adlayer was heated from deposition to desorption.

T.S. LeDoux*, M.A. Evans*, K.E. Howard*, A.D. Louie*, and A.M.Nishimura†

Chemistry Department, Westmont College, Santa Barbara, CA 93108, nishimu@westmont.edu

EXTRACTS FROM KUDZU LEAVES INHIBIT CANCER CELL GROWTH

In this experiment, the investigation covered the *in vitro* inhibitory effects of kudzu extracts on a panel of transformed cell lines including *KB, SK-OV-3, SK-MEL, BT-549, LLC-PK_1,* and *VERO* cells. The results show that the steam distilled kudzu extract had a greater effect on *KB, BT-549, SK-OV-3, LLC-PK1,* and *VERO cells*. The steam distilled extract did not show a remarkable impact on *SK-MEL* cells. All cell lines except for *SK-MEL* showed low IC_{50} values against cellular replication (e.g. *KB P-291*, IC_{50} = 60μg/mL; *BT-549*, IC_{50} = 80μg/mL; *LLC PK-1*, IC_{50} = 9μg/mL). In almost all of the cell lines, inhibitory action is clearly shown by the steam distillation. Methyl distillation showed high IC_{50} values and had very little effect on growth of cells. Although the extracts are cytotoxic to kidney cells *LLC-PK1* and *VERO*, it is possible that through a chromatographic column, the active compound can be isolated and have a safe effect on the cells.

Angelina M. Dorman†*, Shabana Khan‡ and Luther Elrod

Department of Chemistry, Piedmont College, PO Box 10, Demorest, GA 30535.

‡University of Mississippi Natural Products Division (NIH), PO BOX 1848, University, MS 38677.

OPTICAL STUDIES OF THE DISORDER-TO-ORDER TRANSITION IN 1,4-DICHLORO-NAPHTHALENE ADLAYER ON Al_2O_3 (0001)

Amorphously prepared 1,4-dichloronaphthalene on a dielectric Al_2O_3 surface exhibits very intense excimer emission. As the surface is heated, thermally sensitive non-radiative internal conversion process competes with the radiative decay and lowers the intensity of this emission. Annealing increases the stability of the excimer as indicated by the red-shift of the spectral peak. Continued heating of the surface causes what appears to be the disorder-to-order transition as evidenced by a maximum in the red-shift and a sudden increase in the excimer emission. Thermal relaxation continues until desorption, when the optical signal disappears, and is also detected by mass spectrometry. The surface dynamics observed optically afford a clearer picture of this complex transformation of the amorphous adlayer undergoing the transition to an ordered structure.

J.S. Brigham,* D.R. Hoss,* A.J. Bishop*‡, K.A. Martin‡ and A.M. Nishimura†
Department of Chemistry, Westmont College, Santa Barbara, CA 93108
‡ Permanent address: Point Loma Nazarene University, San Diego, CA 92106

CHEMICAL COMPOSITION OF MINOR, COPPER-BASED COINS OF THE BYZANTINE EMPIRE VIA ENERGY DISPERSIVE X-RAY FLUORESCENCE SPECTROMETRY

Nine Byzantine coins were analyzed via energy dispersive X-ray fluorescence (EDXRF) spectrometry for the following elements: iron (Fe), cobalt (Co), nickel (Ni), copper (Cu), zinc (Zn), arsenic (As), platinum (Pt), gold (Au), lead (Pb), palladium (Pd), silver (Ag), tin (Sn), and antimony (Sb). The composition of these samples was surprisingly high in copper, and low in alloying elements. These findings are significantly different than previous, published accounts.

Irice Ellis* and Mark Benvenuto†
University of Detroit Mercy, Department of Chemistry & Biochemistry, 4001 W. McNichols Rd., Detroit, MI 48219-0900, benvenma@udmercy.edu

METHANOL AND WATER CLUSTER AB-INITIO STRUCTURE DETERMINATION

A theoretical investigation into the geometry and properties of small water $(H_2O)_n$ (n=1-5) and methanol $(CH_3OH)_m$ (m=1-2) clusters is presented in this paper. Basis set effects were also investigated. Most of the variability in the results between basis sets occurred when the core functions were split. Although the structures of the clusters were qualitatively correct, basis set superposition error needs to be corrected before more quantitative results are available.

Maxwell Merkle* and Leon L. Combs†
Department of Chemistry and Biochemistry, Kennesaw State University, 1000 Chastain Road, MS 1203, Kennesaw, GA 30144, mmerkle@gmail.com

THE DESIGN AND SYNTHESIS OF NOVEL CHAETOMELLIC ACID A ANALOGUES

Chaetomellic acid A is an alkyl dicarboxylic acid isolated from the fermentation of *Chaetomella acutiseta*. Chaetomellic acid A has been shown to be a potent, highly specific inhibitor of RAS farnesyl protein transferase (FPTase). The association between RAS proteins and cancer has made chaetomellic acid A a potential chemotherapeutic agent. Two novel chaetomellic acid A analogues have been prepared that incorporate aromatic rings in the alkyl tail. It is anticipated that these compounds will bind more tightly to the FPTase active site than the natural product due to intermolecular interactions between the aromatic rings in the tail and the aromatic amino acid residues that have been shown to line the enzyme pocket.

Mark F. Mechelke†, Jacquelyn C. Webb*, and Jessica L. Johnson*
Department of Chemistry, St. Cloud State University, 720 Fourth Avenue South, St. Cloud, MN 56301, mfmechelke@stcloudstate.edu