UNIVERSITY OF MINNESOTA DULUTH

DEPARTMENT OF CHEMISTRY

SUMMER UNDERGRADUATE RESEARCH PROGRAM

1994

Director's Summary

A total of 19 students participated in the 1994 Summer Undergraduate Research Program. Each of these students worked on a research project for ten weeks under the supervision of a faculty member in the Department of Chemistry or Department of Biochemistry and Molecular Biology. Most students were supported by stipends provided by a UMD alumnus and several agencies. Support for equipment and supplies was provided from faculty research grants and departmental funds.

This booklet includes a list of the student participants, their home institutions, faculty advisors, and details of the research projects, including an abstract of each research project. Also included are a photograph of the participants and an acknowledgement of financial support.

Donald Poe

Donald Poe
Program Director
August 1994

UMD Chemistry Summer Undergraduate Research Participants
Summer 1994

Student	Institution	Advisor/Project Title/Funding
Ruslen Arbit	Moscow State U.	R. Caple. NSF.
Mike Barnes	UMD	R. Caple. Synthesis of carbon glycosides via the stepwise Ad_E approach. Swenson award.
Steven Berry	UMD	L. Thompson. Adducts of rare earth complexes. ACS-PRF
Craig Byersdorfer	UMD	D. Eide. Cloning of the human heart Fe(II) transporter gene. Research grant.
Jason Bolz	UMD	V. Zhdankin. Perfluoroalkyl iodonium compounds: new, promising reagents for organic chemistry. ACS-PRF.
Sara Duesterhoeft	UMD	D. Eide. 3192.
Brad Enerson	UMD	L. Drewes. 3192.
Mark Formaneck	U of M, Morris	V. Zhdankin. The preparation and study of organic derivatives of xenon(II). Swenson award.
Dan Gregory	UMD	R. Caple. NSF.
Stacy Kramer	UMD	J. Prohaska. Identification of the endogenous inhibitor of brain dopamin-β-monooxygenase. 3192.
Wade Kubat	UMD	J. Prohaska. Ascorbic acid determination in organs of copper-deficient rats determined by HPLC with electrochemical detection. Swenson award.
Yuri Kryschenko	Mendeleev Univ., High Chem. College, Russian Acad. Sci.	R. Caple. Synthesis of carbon glycosides via the stepwise Ad_E approach. NSF.
Hung Pham	Concordia College	V. Magnuson. X-ray structural determination of inorganic complexes. Swenson award.
Dana Reed	UMD	R. Carlson. Rearrangements of Allylic sulfonium salts. Research grant.

Dan Rutherford	U of M, Morris	R. Carlson, R. Caple, G. Rapp, G. Glass. Distribution of mercury in selected northern Minnesota lakes and rivers.
Angela Simonsen	UMD	V. Zhdankin. New reagents and synthetic procedures based on the organic chemistry of polyvalent iodine. Swenson award.
Joe Thorman	UMD	L. Thompson. Adducts of rare earth complexes. ACS-PRF.
Tricia Tomlinson	UMD	D. Poe. Efficiency in liquid and supercritical fluid chromatography. ACS-PRF.
Tim Zenson	UMD	P. Siders. Monte Carlo model of feldspar crystallization. ACS-PRF.

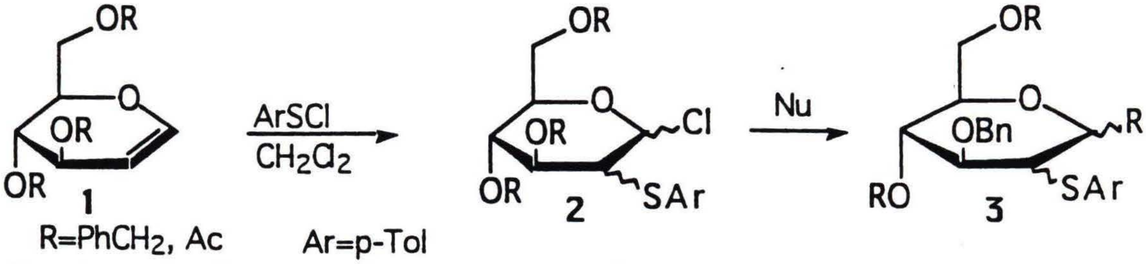
RESEARCH ABSTRACT

1994 SUMMER RESEARCH PROGRAM   UMD CHEMISTRY DEPARTMENT

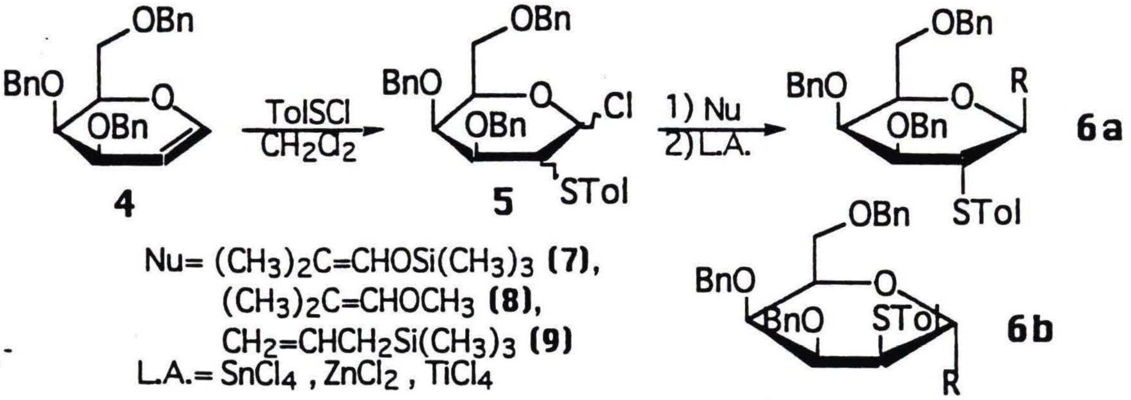
Ruslan M. Arbit
Higher College of Chemistry, Russian Academy Of Sciences.
Faculty advisor – **Prof. Ronald Caple**

REACTION OF C-NUCLEOPHILES WITH ArSCl ADDUCT OF PROTECTED GALACTAL.

Recently it was shown that ArSCl adduct (2) of protected glucal (1) is capable of reacting with different types of *C*-nucleophiles in presence of Lewis acid leading to stereoselective formation of *C-C* glycosidic bond.



Based on these facts another unsuturated sugar (tri-*O*-benzil-D-galactal) was involved to study the possibility of being used in such reaction and stereoselectivity depending on different Lewis acids and solvents.



Nu= $(CH_3)_2C{=}CHOSi(CH_3)_3$ **(7)**,
$(CH_3)_2C{=}CHOCH_3$ **(8)**,
$CH_2{=}CHCH_2Si(CH_3)_3$ **(9)**
L.A.= $SnCl_4$, $ZnCl_2$, $TiCl_4$

The starting substance (4) was synthesized in four steps with yield 36 %.

It was found that ArSCl adduct of (4) reacts with silyl enol ether (7), vinyl ether (8), and allylsilane (9) in presence of $SnCl_4$ as a Lewis acid. In case of silyl enol ether the reaction was studied using $ZnCl_2$, $TiCl_4$, and different solvent. The yield and ratio between isomers are shown below.

No.	*C*--Nu	Lewis acid	Solvent	Ratio	Yield
1	$(H_3C)_2C{=}CH(OSiMe_3)$	$SnCl_4$	CH_2Cl_2	16:1	56%
2	same	$ZnCl_2$	same	>19:1	40%
3	same	$TiCl_4$	same	-	0%
4	$H_2C{=}CHCH_2SiMe_3$	$SnCl_4$	same	>19:1	65%
5	$(H_3C)_2C{=}CH(OMe)$	$SnCl_4$	same	>19:1	79%
6	$(H_3C)_2C{=}CH(OSiMe_3)$	$SnCl_4$	CH_3NO_2		

RESEARCH ABSTRACT
1994 SUMMER UNDERGRADUATE RESEARCH PROGRAM
UMD CHEMISTRY DEPARTMENT

Participant:	Steven Berry University of Minnesota - Duluth
Faculty Advisor:	Dr. Larry Thompson
Title of Project:	Preparation and Investigation of Europium Complexes

ABSTRACT:

Over the past weeks I have prepared a number of Europium complexes using varying ligands. These ligands being any one of a number of neutral ligands in coordination with a trisBeta-diketone complex. The neutral ligands I used were 1,10-phenanthroline, 2,9-dimethyl-1,10-phenanthroline, 2,2'-dipyridyl, or 2,2':6',2"-terpyridine. The Beta-diketones being 1,1,1,5,5,5-hexaflouro-2,4-pentanedione, 1,1,1-triflouro-2.4-pentanedione, 3,5-heptanedione, and 6-methyl-2,4-heptanedione.

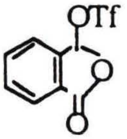
Of the dozen or so complexes that I made, I am able to consistently grow crystals out of five of them. These crystals are then investigated by observing their emission spectra and looking for evidence of possible structural isomers. If the spectra and melting points of the crystals look good then a sample is sent away for elemental analysis. So far, we have sent away four samples to be analyzed. Only two have returned with somewhat discouraging results as the Carbon percentages were a little off.

Research Abstract
1994 Summer Undergraduate Research Program
UMD Chemistry Department

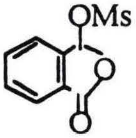
Faculty Advisor: Dr. Viktor V. Zhdankin
Participants: Jason Bolz and Mark Formaneck

Preparation and Chemistry of 1-Organosulfonyloxy-1,2-benziodoxol-3-(1H)-ones: First Example of a Stable Adduct of 2-Iodosobenzoic acid with a Strong Acid.

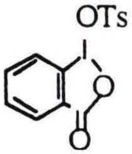
Recently, hypervalent iodine has attracted considerable research interest due to its biological activity. Specific to our research has been trivalent iodine. Many different structures of this type exist, one of which belongs to the general class of compounds called 1-Organosulfonyloxy-1,2-benziodoxol-3-(1*H*)-ones. We wish to report the preparation of many derivatives of the aforementioned class of compounds by the reaction of 2-iodosobenzoic acid with the corresponding sulfonic acids or Me_3SiOTf. Reactions of these compounds with various substituted acetylenes or cyanothimethylsilane afford the respective alkynyl, vinyl, or cyano iodonium salts.



Triflate



Mesylate



Tosylate

References:

1. Zhdankin*, V. V., Kuehl, C. J., Bolz, J. T., Formaneck, M. S., Simonsen, A. J., *Tetrahedron Letters* (Accepted for publication).

2. (a) Varvoglis, A. *The Organic Chemistry of Polycoordinated Iodine;* VCH Publishers, Inc.: New York, 1992. (b) For recent review on synthetic applications of [hydroxy(organosulfonyloxy)iodo]arenes see: Moriarty, R. M.; Vaid, R. K.; Koser, G. F. *Synlett* 1990, 365.

RESEARCH ABSTRACT
1994 SUMMER UNDERGRADUATE RESEARCH PROGRAM
UMD CHEMISTRY DEPARTMENT

"HUMAN GENES REGULATING IRON TRANSPORT"

Craig Byersdorfer, UMD
Sara Duesterhoeft, UMD

Faculty Advisor: Dr. Dave Eide

Living organisms are coded for by a universal genetic sequence. This allows DNA to be taken from one organism and expressed, or overexpressed, in another. Overexpression of human heart DNA in iron sensitive yeast provides a simple test to select genes responsible for iron transport.

Iron is a vital mineral, used in numerous reactions and functions inside the body. However, the exact method and genetic regulation of iron uptake remains a mystery. By cloning the gene(s) responsible for regulation, the exact method of iron uptake can be determined. This would lead to medical advances in understanding, preventing, and treating iron transport diseases.

Eide, D. et al. (1994) The *Fet3* gene of S. *cerevisiae* encodes a multicopper oxidase required for ferrous iron uptake. Cell. **76**, 403-410

Eide, D., et al. (awaiting publication) The *Fet4* gene of S. *cerevisiae* encodes a Fe(II) transport protein.

Thorstensen, K., & Romslo, I. (1990) The role of transferrin in the mechanism of cellular iron uptake. Biochem. J. **271**, 1-10

Weintraub, L. R., Edwards, C. Q., Krikker, M. (1988) Hemochromatosis: proceedings of the first international conference. New York Academy of Sciences. New York

RESEARCH ABSTRACT
1994 SUMMER UNDERGRADUATE RESEARCH PROGRAM
UMD CHEMISTRY DEPARTMENT

Participant: Bradley E. Enerson, UMD

Faculty Advisor: Dr. Drewes

Immunocytochemistry of system y+ (CAT-1) basic amino acid transporter of the rat blood brain barrier.

ABSTRACT

Cationic amino acid transport across the blood brain barrier (BBB) is required for brain metabolism. The gene responsible for this transport process has recently been cloned and sequenced. It was originally identified as a murine (mouse) ecotropic retrovirus receptor and was subsequently shown to possess the properties of a system y^+ cationic amino transporter, now called CAT-1. Studies have shown the presence of similar genes in rat and human species. The conservation of the CAT-1 protein at the amino acid level among these species is about 90%. Further studies have shown that CAT-1 is the basic amino acid transporter in the rat BBB. To study brain regions that contain this transporter, it's distribution, and role in transport across the BBB, we have designed a peptide to be used in the formation of an antibody to CAT-1. Studies of CAT-1 in the brain will proceed via immunocytochemistry.

REFERENCES

Albritton L. M., Tseng L., Scadden D., and Cunningham J. M. (1989) A putative murine ecotropic retrovirus receptor gene encodes a multiple membrane-spanning protein and confers susceptibility to virus infection. *Cell* **57**, 659-666.

Wang, H., Kavanaugh M. P., North R. A., and Kabat D. (1991) Cell-surface receptor for ecotropic murine retroviruses is a basic amino acid transporter. *Nature* **352**, 729-731.

Yoshimoto T., Yoshimoto E., and Meruelo D. (1991) Molecular cloning and characterization of a novel human gene homologous to the murine ecotropic retroviral receptor. *Virology* **185**, 10-17.

Stoll J., Wadhwani K. C., and Smith Q. (1993) Identification of the cationic amino acid transporter (system y^+) of the rat blood brain barrier. *J. of Neurochemistry* **60**, 1956-1959.

Woodard, M., Dunn W. A., Laine R.O., Malandro M., McMahon R., Simell O., Block E. R., and Kilberg M. S. (1994) Plasma membrane clustering of y^+ (CAT-1) amino acid transporter as detected by immunohistochemistry. *Am. J. of Physiology* **266**, E817-E824.

RESEARCH ABSTRACT

1994 SUMMER RESEARCH PROGRAM UMD CHEMISTRY DEPARTMENT

Kryschenko Yury Konstantinovitch,
Higher College of Chemistry, Russian Academy Of Sciences.

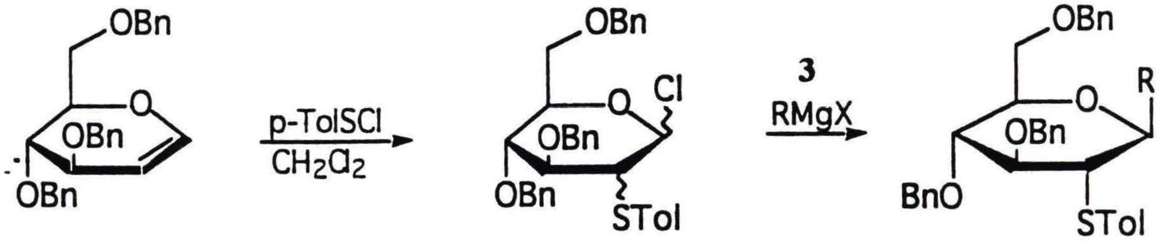
Faculty advisor – **Dr. Ronald Caple**

REACTION OF GRIGNARD REAGENTS WITH ArSCl ADDUCT OF PROTECTED GLUCAL.

This work is the part of the research, the general goal of which is to apply previously elaborated protocol of stepwise electrophilic additions involving *S*-containing electrophiles to the synthesis of *C*-glycosides. The purpose of this very part is to study the reaction using Grignard reagents and to modify the conditions of it towards better yields. The other goal was to find out the dependance of this reaction on various conditions like solvent (THF or ether), concentration, and the nature of a halogene (chlorine, bromine or iodine) in Grignard reagent.

The general reaction sequence is shown on Scheme 1.

Scheme 1



1 2 4

Various Grignard reagents were tested as nucleophiles in this reaction. The results of this work can be summarized as following:

- The proper reaction conditions have been found for the reaction
- Grignard reagents with different halogenes were shown to undergo this reaction with good yields.
- Neither nature of halogene nor one of solvent showed to have strong effect on the reaction yields.
- The possibility of making crystals of the product for further X-ray analysis was shown.

RESEARCH ABSTRACT
1994 SUMMER UNDERGRADUATE RESEARCH PROGRAM
UMD CHEMISTRY DEPARTMENT

Participant: Wade Daniel Kubat-University of Minnesota Duluth

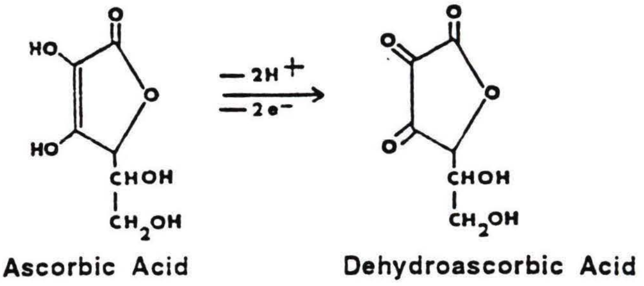
Faculty Advisor: Dr. Joseph Prohaska

Title of Project: Ascorbic Acid Concentration in Organs of Copper-Deficient Rats Determined By HPLC with Electrochemical Detection

ABSTRACT

In Dr. Prohaska's published papers, "Ascorbic Acid Synthesis and Concentrations in Organs of Copper-Deficient and Brindled Mice" (1983) and "Decreased Brain Ascorbate Levels in Copper-Deficient Mice and in Brindled Mice"(1984), it was found that copper-deficient mice showed different levels of ascorbic acid in several organs. For unknown reasons, copper deficiency was also shown to affect the ascorbic acid levels in certain organs and not others.

In my experiments, I measured ascorbic acid concentrations in rat tissues by high performance liquid chromatography (HPLC) with electrochemical detection. When an applied voltage of .7V is used, the oxidation of ascorbic acid to dehydroascorbic acid proceeds (Figure below).



The two electrons released create a current that is measured and recorded. A fresh standard (of known concentration) is used to find the concentration of the sample.

The applied voltage, mobile phase, and extraction process were optimized to give a coefficient of variation of 3.75%. Kidney, spleen, and several brain regions were assayed and found to agree with Dr. Prohaska's findings. Currently, ascorbic acid analysis is in progress on other rat tissues.

RESEARCH ABSTRACT
1994 SUMMER UNDERGRADUATE RESEARCH PROGRAM
UMD CHEMISTRY DEPARTMENT

Participant: Hung Pham
Concordia College, Moorhead, Minnesota

Faculty Advisor: Dr. Vincent Magnuson

Title of Project: Synthesis and Characterization of Lead and Gallium Complexes

ABSTRACT:

We attempted the synthesis of lead and gallium complexes using a number of lead and gallium salts such as $Pb(NO_3)_2$, $PbCl_2$, $PbBr_2$, and $Ga(NO_3)_3$. We used the ligands bis(diphenylphosphino)-methane (dppm) and amino acid derivatives containing glycine such as sodium glycinate hydrate, N-acetylglycine, glycine-L-leucine, and glycine-alanine. The solvents used were dimethyl formamide (DMF), methylsulfoxide (DMSO), DMF/H_2O, and DMSO/H_2O. A variety of ratios of ligands and types of solvents were used.

Characterization of these complexes was accomplished by checking density and IR-spectra to determine that crystal products contained both the desired metal and ligand. The resultant products contained lead if these crystal products were heavier than bromoform. Infrared-spectra (IR-spectra) were used as a method to determine if the organic ligands were in the crystal products. This was accomplished by comparing the IR-spectra of the ligands to that of the crystal products to diagnose whether the crystals contained the ligand. We used a microscope to select suitable crystals for X-ray diffraction.

Elemental analysis was used to determine the percentage of lead in the crystal products by ethylenediaminetetraacetic acid (EDTA) titration. We compared the expected percentage of lead in possible molecular formulas with the experimental percentage.

The most two successful types of crystal products that I obtained were from reactions of $PbCl_2$ in DMSO and glycine-L-leucine in H_2O as solvent, and $PbBr_2$ in DMF with N-acetylglycine in H_2O as solvent.

X-ray structure determination is in progress.

Research Abstract
1994 Summer Undergraduate Research Program
UMD Chemistry Department

Dana Reed: UMD
Faculty Advisor: Robert Carlson

Substituted Ring Groups in Y-Aromaticity

The concept of Y-aromaticity was proposed by Gund in 1972 to explain the properties of guanidine.[1] Y-aromaticity can also be used to explain the similar pK_a values for ethyl acetate and the acetate ion.[2]

We have been using Y-aromaticity to generate dicarbanions. These dianions are useful in synthesis due to the ease with which they can form new carbon-carbon bonds through addition to electrophiles. The current research involves the dianion of 2-methylindene. Selective addition to the dianion is possible because the addition of one equivalent of electrophile will leave the more stable carbanion. However, since 2-methylindene is not commercially available, it must first be synthesized from the corresponding indanone.

Future work will involve the production of a large amount of 2-methylindene using the synthetic sequence developed by Smonou and Orfanopoulos.[3] Then it will be possible to test the properties of the dianion using a variety of different electrophiles.

1. P. Gund, J. Chem. Ed., **49**, 100 (1972).

2. J. Li, Effects of Heteroatoms and Geometry on Allylic Carbanions, M.S. Thesis, p. 15 (1988).

3. I. Smonou and M.Orfanopoulos, Syn. Commun., **20** (9), 1387 (1990).

RESEARCH ABSTRACT
1994 SUMMER UNDERGRADUATE RESEARCH PROGRAM

UMD CHEMISTRY DEPARTMENT

Participant: Dan Rutherford
U of M, Morris

Faculty Advisor: R. Carlson, R. Caple, G. Rapp, G. Glass

Title of Project: Collection and Analysis of Precipitation for Mercury Contamination

ABSTRACT:

Mercury contamination of lakes and streams presents serious environmental risks which have only recently begun to be quantified. Mercury's ability to change form and be transported long distances before deposition complicates any risk assessment. Contaminated precipitation serves as the major source of mercury in northern Minnesota lakes. After deposition, mercury can manifest itself in the water column, plankton, vegetation, fish, or sediments of lakes and streams. Various projects are currently underway which generate samples from each of these compartments for analysis. Precipitation is collected by nine samplers strategically located to reveal trends in mercury deposition throughout the Great Lakes area. Once collected, these samples are shipped to our lab for analysis.

This project utilizes cold-vapor atomic absorption spectrometry (CVAAS) for mercury analysis. EPA method 245.1 achieves a detection limit of 200 ng/L, which this project has managed to lower to 2 ng/L through various modifications. The use of a closed circuit bubbler system to maximize volatilization and detection of mercury and the screening of reagents for lowest mercury content are chief among these revisions. Mercury concentrations in precipitation are inversely related to event depth, suggesting that soluble atmospheric mercury washes out quickly in precipitation. Mercury concentrations also vary upon location, with samples from areas more isolated from anthropogenic influences showing lower concentrations than those from urban or agricultural areas.

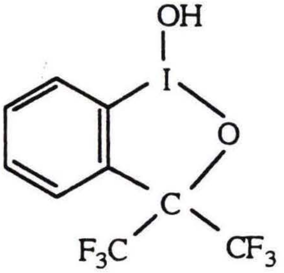
Research Abstract
1994 Summer Undergraduate Research Program
UMD Chemistry Department

Participant: Angela Simonsen

Faculty Advisor: Viktor Zhdankin

New Fluoroalkyliodoso Reagents

Two new structural types of iodine(III) have been prepared, namely, ortho-iodosohexafluorocumyl alcohol and iodosoperfluoroalkanes. Synthesis and application of these compounds will be discussed.



o-iodosohexafluorocumyl alcohol

$C_nF_{2n+1}I = O$

iodosoperfluoroalkane

References:

1. Zhdankin, V., Kuehl, C., Bolz, J., Formaneck, M., Simonsen, A., *Tetrahedron Letters* (in press).

2. Varvoglis, A. *The Organic Chemistry of Polycoordinated Iodine*; VCH Publishers, Inc.: New York, 1992.

RESEARCH ABSTRACT
1994 SUMMER UNDERGRADUATE RESEARCH PROGRAM
UMD CHEMISTRY DEPARTMENT

Participant:	Joe Thorman University of Minnesota - Duluth
Faculty Advisor:	Larry Thompson
Title of Project:	Possible Isomerism in Adducts of Rare Earth Tris(ß-diketonates)

ABSTRACT:

In general, rare earth complexes are very labile and the existence of discrete isomers is precluded. However, in previous work at UMD such isomers have been found in adducts of the rare earth tris(ß-diketonates). In one case (Holz, 1986) the chelate rings span the square antiprism in different ways whereas in the other (Raven, 1991) two solids could be preposed in one of which the coordination sphere was a square antiprism and in the other it was a dodecahedron. It is not at all obvious what factors determine this isomerism and this study was undertaken in an attempt to study the effect of the ß-diketone.

Adducts of five different ß-diketones(1,3-diphenyl-1,3-propanedione, 1,1,1-trifluoro-5, 5-dimethyl-2,4-hexanedione, 2,4-nonanedione, 5,5-dimethyl-2,4-hexanedione, and 1-phenyl-2,4-pentanedione) have been studied using 1,10-phenanthroline, 2,2'-dipyridyl, 2,9-dimethyl-1,10-phenanthroline, and 2,2':6',2"-terpyridine as the adduct ligand.

All the adducts that have been prepared have been studied by luminescence spectroscopy, and for a number of them satisfactory elemental analyses have been obtained. Although x-ray quality crystals have been obtained for five of the adducts, no structures are yet available.

RESEARCH ABSTRACT
1994 SUMMER UNDERGRADUATE RESEARCH PROGRAM
UMD CHEMISTRY DEPARTMENT

Participant:	Tricia Tomlinson University of Minnesota - Duluth
Faculty Advisor:	Dr. Poe
Title of Project:	Effect of Solute Retention on Efficiency in Liquid and Supercritical Fluid

The efficiency of modern packed chromatographic columns is described by the Knox equation :

$$H = Au^{1/3} + B/u + Cu$$

where H = plate height of column
u = linear velocity
A,B,C = coefficients

The plate height of a column is inversely related to its efficiency. At high linear velocities the C term becomes the dominant term in the plate height expression, and it is the magnitude of the C coefficient which in many cases limits the speed at which a separation can be carried out with adequate resolution.

Knox and Scott (1) have described the effect of solute retention on the magnitude of C in High Performance Liquid Chromatography (HPLC). An extension of their work suggests that in SFC the value of C should steadily increase as retention increases. The goal of this project is to examine the effect of solute retention on efficiency in SFC. A series of alkylbenzenes will be used as the model solutes.

The worked performed thus far has focused on confirming Knox and Scott's observations for HPLC. In doing this a system was devised that produced a minimal amount of extra-column band spreading. The components of this system are : an Alltech model 450 UV Detector, a Fisher Strip Chart Recorder, a Beckman model 110A Pump, and a Beckman model 210 Injector.

The elution of 0.05% (v/v) benzene in hexane on porous silica based packed columns, using hexane as the mobile phase, was used to determine the efficiency of an unretained solute. A study of the contribution of the individual components (injector, tubing, column, and detector) to the total band variance resulted in modifications to minimize the extra-column band variance. The resulting system utilizes an injection volume of 5.1 uL, a detector with a 0.8-uL flow cell and 50-ms time constant, 5-cm lengths of 0.007" i.d. connecting tubing. This system yielded approximately 12,000 plates for the elution of benzene on a 150 mm X 3.2 mm column packed with 5-micron C8-silica particles.

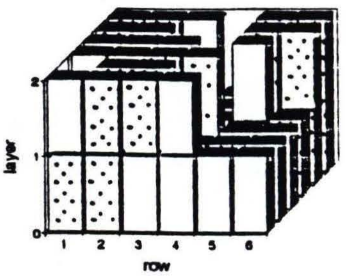
1. J.H. Knox and H.P. Scott, "**B and C Terms in the Van Deemter Equation for Liquid Chromatography**", Elsevier Science Publishers B.V. Chromsymp 191, (1983), 297-313.

RESEARCH ABSTRACT
1994 SUMMER UNDERGRADUATE RESEARCH PROGRAM
UMD CHEMISTRY DEPARTMENT

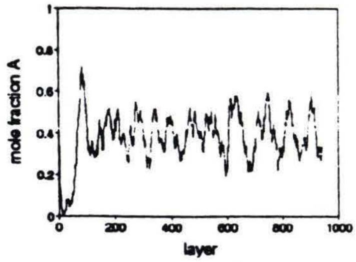
Participant: Tim Zensen
Faculty Advisor: Paul Siders
Title of Project: Monte Carlo study of oscillatory zoning

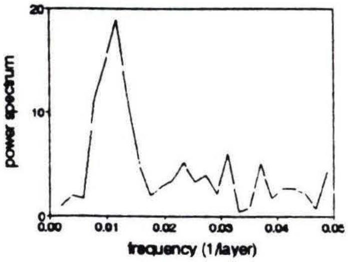
Oscillatory zoning is observed in feldspar and carbonate minerals. This work was a computational kinetic study of the effect of local surface feedback on crystallization of a two-component mineral from its melt, and the resulting zoning.

The growing mineral surface was represented in the computer as gridded layers. Every grid site was a site for potential addition of a unit cell of the mineral. Each layer was completely filled before the next layer started to fill. At right is a picture of a 6X6 section of two layers. Layer 1 is filled, and layer 2 is about half filled. The grid sites can be filled with either component "A" or "B". These are indicated in the picture by different patterns. Consistent with a surface-feedback model, "A" molecules add more readily to sites that have mostly "A" neighbors in the current layer and the layer below. Similarly, "B" addition is favored at sites with "B" neighbors. In this model, the A and B precipitation rate constants are nonlinear functions of local surface composition. This nonlinear surface feedback is expected to cause oscillatory zoning as follows: Fluctuation in surface composition, or an inhomogeneous initial surface, favors growth of either A-rich or B-rich mineral. After the major component is depleted from the melt, the surface switches to a complementary composition, and so on.



Growth kinetics were modeled using a Monte Carlo algorithm coded in Fortran. Open sites on the current layer were selected at random. The probabilities of A and B attachment at that site, based on its neighbors and on A and B mole fractions in the melt, were calculated. These probabilities were then compared to random numbers and either A or B deposited in the site. The random-number comparison allows fluctuations while guaranteeing correct long-time statistics. Melt composition was adjusted for species deposited on the surface, so that rapidly deposited species were gradually depleted in the melt, eventually reducing their deposition probabilities. After each layer was filled, its composition was recorded. At upper right is a graph of crystal composition as a function of the growth layer. The corresponding Fourier power spectrum is at right. An oscillatory pattern is evident, with wavelength approximately 100 layers.





In addition to layer zoning, islands may form within layers and persist through many layers. No results are yet available regarding such patterns.

(Top row, l to r) *Sara Duesterhoeft*, UMD; *Yury Kryschenko*, Moscow State Univ.; *Dana Reed*, UMD; *Tim Zensen*, UMD; *Joe Thorman*, UMD

(Middle row) *Mark Formaneck*, U of M-Morris; *Brad Enerson*, UMD; *Ruslan Arbit*, Moscow State Univ.; *Jason Bolz*, UMD; *Dan Gregory*, SWSU

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