

[RECOMMENDED YOU ARRIVE 5-10 MIN BEFORE THE TIME OF ANY GIVEN TALK. IF YOU ARRIVE LATE TO A SESSION, PLEASE ENTER FROM THE 2ND FLOOR TO AVOID INTERFERING WITH THE SPEAKER]

WEDNESDAY 23 JUNE 2010

- 7:10 PM Nancy Goroff, *Stony Brook University*
T-1. Bare Carbon Wires: Polyynes and Polydiacetylenes
- 8:05 PM David Lemal, *Dartmouth College*
P-1. Novel Chemistry of Hexafluorobicyclo[1.1.0]butane
- 8:25 PM Malcolm Forbes, *University of North Carolina*
T-2. Fun Facts About Triplet States: Photochemistry and Reactive Intermediates in Organic Nanocrystals

THURSDAY 24 JUNE 2010

- 8:35 AM Frank Mallory, *Bryn Mawr College*
T-3. Deep-Seated Rearrangements in the Photocyclizations of Some Stilbene Derivatives
- 9:30 AM Zhi-Xiang Yu, *Beijing University*
T-4. Water Catalysis in [1,n]-Hydrogen Shifts
- 10:45 AM Eric Masson, *Ohio University*
P-2. Self-organizing properties of Cucurbituril Cavitands: A Mechanistic Adventure into the Chemistry of Interlocked Structures
- 11:05 AM Elizabeth Harbron, *The College of William and Mary*
T-5. Fluorescence Modulation in Photochromic Conjugated Polymer Systems
- 12:00 N Peter Chen, *Eidgenössische Technische Hochschule (ETH), Switzerland*
T-6. Ruthenium, Rhenium and Gold Carbenes
- 3:30 PM Poster Session I (Odd numbered posters)
- 7:00 PM Veronica Vaida, *University of Colorado Boulder*
T-7. Water and Photon Mediated Chemistry in the Earth's Atmosphere
- 7:55 PM Donald Aue, *University of California Santa Barbara*
P-3. Bifurcation on Reaction Pathways for Pinacol-type Rearrangements
- 8:15 PM Weston T. Borden, *University of North Texas*
T-8. Tunneling by Hydrogen and By Carbon in Organic Reactions -- Calculations Tell Experimentalists Where to Look and What to Look For

FRIDAY 25 JUNE 2010

- 8:30 AM Ricardo Metz, *University of Massachusetts Amherst*
T-9. Methane Activation by M⁺ and MO⁺: Electronic and Vibrational Spectroscopy of Reaction Intermediates
- 9:25 AM Mark A. Murcko, *Vertex Pharmaceuticals Inc.*
T-10. Clawing Our Way Back from the Abyss
- 10:40 AM Ivan Aprahamian, *Dartmouth College*

P-5. E/Z Isomerization in a Hydrazone-Based Molecular Switch11:00 AM Barry Carpenter, *Cardiff University***T-11. Design of Renewable Amines for Photochemical Reduction of CO₂**7:30 PM Joseph Lambert, *Northwestern University***Introduction for *Journal of Physical Organic Chemistry* Award for Early Excellence in the Field of Physical Organic Chemistry, 2010**7:40 PM Michael Bendikov, *Weizmann Institute***2010 JPOC Award Lecture****T-12. Novel Types of Organic Electronic Materials. Polyselenophenes and Oligofurans**8:40 PM Scott Silverman, *University of Illinois Urbana-Champaign***T-13. DNA as a Catalyst: New Reactions and Mechanistic Questions****SATURDAY 26 JUNE 2010**8:30 AM Christopher Hadad, *The Ohio State University***T-14. Computational Investigations into Organometallic and Macromolecular Catalysts: Conformational and Mechanistic Analyses**9:25 AM Bern Kohler, *Montana State University***T-15. Base Sequence Effects on DNA Photophysics and Photochemistry**10:40 AM Allan Pinhas, *University of Cincinnati***P-6. Chemistry in Water: Coupling Reactions Using Fenton's Reagent**11:00 AM Alison Frontier, *University of Rochester***T-16. Reactions of Pentadienyl and Oxyallyl cations: Rearrangements and the Nazarov Cyclization**1:30 PM Zhibin Guan, *University of California Irvine***T-17. Catalytic Covalent Assembly toward Functional Soft Nanomaterials**3:30 PM Poster Session II (Even numbered posters) (*ISB foyer and hallways*)
(Evening Session Honoring Jerome A. Berson)6:55 PM Marc Greenberg, *Johns Hopkins University*7:00 PM Barry Carpenter, *Cardiff University***Jerome Berson: History, Science and Philosophy**7:30 PM Robert Bergman, *University of California Berkeley***T-18. Selective Stoichiometric and Catalytic Reactions in Water-Soluble Host-Guest Supramolecular Systems**8:15 PM Peter B. Dervan, *California Institute of Technology***T-19. Regulation of Gene Expression by Synthetic DNA Binding Ligands**9:00 PM Dennis A. Dougherty, *California Institute of Technology***T-20. Physical Organic Chemistry on the Brain: Understanding the Nicotine Receptor**

POSTER TITLES (* = also presented as a short talk in oral program)

- P-1* Novel Chemistry of Hexafluorobicyclo[1.1.0]butane
- P-2* Self-organizing properties of Cucurbituril Cavitands: A Mechanistic Adventure into the Chemistry of Interlocked Structures
- P-3* Bifurcation on Reaction Pathways for Pinacol-type Rearrangements
- P-4 Evaluation of Computational Errors in DFT and Ab Initio Energies for Carbocations and Hydrocarbons. A Practical Guideline
- P-5* *E/Z* Isomerization in a Hydrazone-Based Molecular Switch
- P-6* Chemistry in Water: Coupling Reactions Using Fenton's Reagent
- P-7 Do Substituents Affect the Shielding Induced by Aromatic Ring Currents? An Experimental and Computational Study
- P-8 Generation of Quinone Alkylating Agents: Factors Governing the Reactivation of Acetylcholinesterase Activity after Prolonged Exposure to Nerve Agents
- P-9 The Use of the CPC Radical Clock Reaction as a Potential Diradical Probe to Study Thermal Rearrangements of Vinylcyclobutanes
- P-10 A New Look at Bimolecular Nucleophilic Substitution in Chlorinated Aromatic Systems
- P-11 Soft UV Photochemical Reactions in Self-Assembled Monolayers (SAMs)
- P-12 An Iterative Method for the Synthesis of Polyynes
- P-13 Gas Phase Studies of Xanthine
- P-14 Analytical Detection of Nitroxyl (HNO) Using Membrane Inlet Mass Spectrometry
- P-15 The Synthesis of a [12]Cyclophenacene Using a Benzene Scaffold
- P-16 Statistical and Nonstatistical Dynamics in a Thermal Rearrangement with Competing 1,3 and 3,3 Shifts — mBLYP/6-31G* Trajectory Results
- P-17 Exploration of Iridium Catalyzed Borylation via C-H Bond Activation of Polycyclic Aromatic Hydrocarbons
- P-18 Implications of Length and Diameter of Short Hydrocarbon Templates for the Metal-free Growth of Carbon Nanotubes
- P-19 Quiazolinespirohexadienones and Oxazinoquinolinespirohexadienones – quinoline analogs of perimidinespirohexadienone photochromes as potential "Photochromic Photooxidants"
- P-20 A Robust and Flexible Route toward three Carbonyl-Substituted Perimidinespirohexadienone Photochromes
- P-21 Incorporation of Solubility Enhancing Groups Via Diels-Alder Additions to Carbon Nanotube Precursors
- P-22 The Mechanism of the Hydride Transfer Reaction between 1-benzyl-3-cyanoquinolinium ion with N-methyl-9, 10-dihydroacridine in acetonitrile
- P-23 Theoretical Investigation of an Unusual Gold(I) Catalyzed Imino-Nazarov Cyclization
- P-24 Diels-Alder Expansion of Polycyclic Aromatic Hydrocarbons
- P-25 Beyond FMO Theory: A Radical Ion Projection Model for Bimolecular Reactions
- P-26 Dehydro[12]annulenes: Comparison of Computed and Experimental Results
- P-27 The First Example of a Persistent Nonacene Derivative
- P-28 Synthesis of Graphene Nanoribbons
- P-29 Investigation of Solvent Effects on the Rate and Stereoselectivity of the Henry Reaction
- P-30 Hydrogen Bridges in the Interactions of Human α -Thrombin with Inhibitors.
- P-31 Thermal Reactions of Tricyclic Vinylcyclobutanes
- P-32 Extra-Terrestrial Transamination Reactions
- P-33 The Mechanism of the Proton Transfer Reactions between Hydroxide Ion and the Simple Nitro Alkanes in Aqueous Solution
- P-34 Computational study of C₆₀-tetraphenylpentacene (C₆₀-TPP) mono and bis adducts and shape control of the monoadduct microparticles
- P-35 Incorporation of Solubility Enhancing t-butyl Groups on Carbon Nanotube Precursors

- P-36 B3LYP and CASPT2 Calculations of the Effect of Relay Orbitals on the Through- Bond Interactions between Mutually Perpendicular Pairs of Allyl Radicals
- P-37 Acyclic CB[n] Congeners Are High Affinity Hosts
- P-38 A Density Functional Study on the Effect of Substituents on the Photochemistry of 3(2H)-Furanones: Factors Influencing Two Novel Photo-induced Rearrangements
- P-39 Photogeneration of O(³P) in Aqueous Media and Subsequent Reaction Mechanisms
- P-40 Dihalocarbene Additions to Strained C-C Bonds
- P-41 Spectroscopy of Free-Base N-Confused Tetraphenylporphyrin Radical Anion and Radical Cation
- P-42 Lewis Acid Catalysis of the Cope Rearrangement
- P-43 Diverse Origins of Conformational Kinetic Isotope Effects
- P-44 Is the single transition state model appropriate for the fundamental reactions of organic chemistry?
- P-45 Intra- and Intermolecular Interactions in Bi- and Terthiophenes: Structural Implications
- P-46 Metal–Metal Redox Synergy in Palladium Catalyzed C–H Oxidations
- P-47 Probing the Efficacy of a Cyclodehydrogenation Approach to Synthesizing a [10,10] Carbon Nanotube End-cap
- P-48 *[Unable to attend conference, poster not available, abstract published in program]*
- P-49 Photoinduced Decomposition of Tetrazolethiones: Intermediacy of a Triplet Biradical
- P-50 Progress in the Synthesis of 1,5-Methanosemibullvalene
- P-51 Oxidative Carbon-Carbon Coupling Induced by Potassium
- P-52 Thiophene Derivatives for Device Applications
- P-53 Regioselectivity in Pd-Catalyzed Cross Coupling Reactions
- P-54 Improvement of Tandem Mass Spectra of Heparan Sulfate by Chemical Modification and Charge State Manipulation
- P-55 Diels-Alder Addition of Masked Acetylenes to Vinylcorannulenes
- P-56 Ortho Substitution Effects in Aryl(trifluoromethyl)carbenes
- P-57 An Ultrafast Spectroscopic and Computational Study On the Photochemistry of Phosphoryl Azides: Singlet and Triplet Manifolds
- P-58 Computational Investigation of the Photochemistry of Naphthalimides
- P-59 Theoretical Hydration Energies of Biologically Relevant alpha-Keto Amides
- P-60 Negative Ion Photoelectron Spectroscopy Studies of Substituted Aromatic Nitrenes
- P-61 Photochemical S_N1 Reactions: Are Substituent Effects in the Excited State Orthogonal to the Ground State?
- P-62 Leaving Group Ability in Gas Phase S_N2 Reactions
- P-63 DFT Studies of the Isomerization of Diphosphine Ligands Attached to Triosmiumdecacarbonyl Clusters
- P-64 Mechanisms of the Schmidt Reaction with Various Azides and Solvent Effects
- P-65 Towards understanding the limits of substrate tolerance in Paraoxonase-1: A physical-organic chemistry approach
- P-66 Comparison of Anticodon Regions of tRNAs and iRNAs and Methylation Reactions
- P-67 Engineering an Orbital Forbidden [3s,5s] Sigmatropic Shift through Palladium(II) Promoted Transition State Complexation
- P-68 Preparation of Switchable Open-Cage Fullerene Derivatives
- P-69 Mechanistic Studies on Irradiation of Ice Mixture of Carbon Dioxide (CO₂), Ammonia (NH₃), and/or Six Hydrocarbons (C_nH_{2n+2}; n = 1–6)

Index of Authors for Presentations

Abdelrahman, Y.	P-2	Dong, H.	P-36
Achalkumar, A. S.	P-11	Doubleday, C.	P-16
Alawode, O.	P-49	Dougherty, D. A.	T-20
Alemán, E. A.	P-40	Eisenberg, R.	T-16
Anson, C. W.	T-7	Eliseeva, M. N.	P-17
Aprahamian, I.	P-5	Ellis, J. A.	P-42
Arvnites, A.	P-10	Evans, S. D.	P-11
Aue, D.H.	P-3, P-4	Forbes, M. D. E.	T-2
Baldwin, J. E.	P-9, P-31	Fort, E. H.	P-18, P-24
Baykal, Ah.	P-30	Frontier, A. J.	T-16
Beck, J. M.	P-8	Gan, L.	P-68
Belanger, A. P.	P-51	Garcia-Garibay, M.	T-2
Bell, R. M.	P-9	Gillmore, J. G.	P-19, P-20
Bendikov, M.	T-12	Gleiter, R.	P-36
Bensinger, A. S.	P-9	Glusac, K. D.	P-58
Bergman, R.	T-18	Gorge, M. S.	T-11
Black, A.	P-12	Goroff, N. S.	T-1, P-12, P-15
Boerth, D. W.	P-10	Greene, A. K.	P-21, P-35
Bohnen, M.	P-16	Grither, W. R.	P-39
Borden, W. T.	T-8, P-36, P-63	Guan, Zhibin	T-17
Border, S.	P-50	Gutierrez, O.	P-67
Breslow, R.	P-32	Hadad, C. M.	T-14, P-8, P-57, P-58, P-65
Brown, J.	P-8	Hamman, C. S.	P-59
Brown, K. L.	P-52	Hancock-Cerutti, W.	P-31
Bushby, R. J.	P-11	Hao, W.	P-22
Cahill, K. J.	P-25	Harbron, E. J.	T-5
Calladine, J.	T-11	Harrison, J. G.	P-23
Campo, R.	P-12	Hawken, S. R.	P-19
Carpenter, B. K.	T-11	Holland, E.	T-11
Castro, C.	P-26	Hotz, R. P.	P-6
Chen, J.	T-15	Hou, X. S.	P-52
Chen, M.	P-13	Houston, K.	P-50
Chen, P.	T-6	Hrovat, D. A.	T-8, P-36, P-63
Cheng, J-P.	P-33	Huang, J.	T-16
Chiesl, T. N.	P-69	Huang, Y.	P-54
Cline, M. R.	P-14	Huynh, V.	P-26
Connors, D. M.	P-15	Isaacs, L.	P-37
Critchley, K.	P-11	Jeffreys, M. S.	P-24
Critser, D. A.	P-8	Johnson, R. P.	P-25
Cui, L.	P-15	Jordan, F.	P-30
Datta, A.	T-8	Jorgensen, W. L.	P-29
Davis, K. B.	P-42	Kaiser, R. I.	P-69
de La Harpe, K.	T-15	Karney, W. L.	P-26
Dervan, P. B.	T-19	Katsamanis, Z. E.	P-15

Kaur, I.	P-27	Morgan, K. M.	P-42
Ketchum, A. R.	P-52	Murcko, M.	T-10
Kim, S. Y.	P-69	Muthukrishnan, S.	P-8, P-57, P-65
Kintigh, J.	P-28	Naber, M. D.	P-6
Kohler, B.	T-15	Nocket, A. J.	P-9
Korang, J.	P-39	O'Leary, D. J.	P-43
Kostal, J.	P-29	Orman, M.	P-40
Kovach, I. M.	P-30	Parker, V. D.	P-22
Kubicki, J.	P-57	Parker, V. D.	P-33, P-44
Kyeremeh-Mensah, L.	P-2	Patchell, D. L.	P-2
Lacoske, M.	P-15	Peterson, L. J.	P-20
Landage, S. M.	P-5	Petronico, A.	P-62
Lauzon, E. P.	P-52	Pinhas, A. R.	P-6
Law, Y. K.	T-15	Platz, M. S.	P-57
Lawrence, S.	P-66	Pollock, B. J.	P-19
Lebedeva, N. V.	T-2	Pomerantz, M.	P-45
Leber, P. A.	P-9, P-31	Porter, L. M.	P-65
LeBoeuf, D.	T-16	Poutsuma, J. L.	P-64
Lee, J. K.	P-13, P-62	Powers, D.	P-46
Lemal, D. M.	P-1	Promnit, P.	P-11
Levine, M.	P-32	Quimby, J. M.	P-47
Li, Lei	P-12	Rablen, P. R.	P-43
Li, Yushi	P-34	Rajeev, R.	P-48
Li, Zhao	P-33	Rayat, S.	P-49
Li, Zhuoran	P-35	Reingold, L. D.	P-50
Lindberg, K. A.	P-20	Resendiz, M.	T-2
Ling, X.	P-2	Richardson, R. D.	T-11
Liquido, F.	P-35	Richmod, M. G.	P-63
Lovitt, C. F.	P-36	Rickhaus, M.	P-51
Lu, X.	P-2	Ritter, T.	P-46
Luk, H. L.	P-8, P-57	Robinson, C.	P-49
Ma, D.	P-37	Rocha, J. M.	P-41
Magliery, T. J.	P-65	Samuel, E. L.	P-2
Mallory, F. B.	T-3	Sanford, E. M.	P-52
Mann, G. R., III	P-31	Schoenenbeck, F.	P-53
Martin, C. B.	P-38	Scott, L. T.	P-17, P-18, P-21, P-24, P-35, P-47, P-51, P-55
Martin, C. P.	P-38	Sears-Dundes, C.	P-6
Masson, E.	P-2	Shelton, G. R.	T-8
Mathies, R. A.	P.69	Sheridan, M.	P-40
McCulla, R. D.	P-39	Sheridan, R. S.	P-56
Merrer, D. C.	P-40	Shete, V. S.	P-65
Metz, R. B.	T-9	Shi, X.	P-54
Meyer, J. L.	P-6	Silverman, S.	T-13
Miller, G. P.	P-27, P-28, P-34	Singh, P. N. D.	P-11
Modarelli, D. A.	P-41	Smith, N. J.	P-55
Mora-Tovar, L. A. G.	P-41		

Song, M-G.	P-56
Soniat, M.	P-38
Stuart-Cole, S.	P-11
Su, C.	T-15
Su, X.	P-5
Suen, L.	P-40
Sunoj, R. B.	P-48
Tantillo, D. J.	P-23, P-59, P-67
Tarasov, V. F.	T-2
Thamattoor, D. M.	P-7
Tolentino, J.	P-40
Toscano, J. P.	P-14
Turkman, N.	P-45
Vaida, V.	T-7
Vaidya, T.	T-16
Voutchkova, A. M.	P-29
Vyas, S.	P-57, P-58
Walti, C. P.	P-11
Wedler, H. B.	P-59
Weena, U.	P-40
Wei, H.	P-63
Wenthold, P. G.	P-60
White, R. C.	T-2
Wijeratne, N.	P-60
Winter, A. H.	P-61
Wipperman, M. F.	P-31
Wongwitwichote, W.	P-41
Wood, T. S.	P-26
Xie-Zhong, S.	T-11
Yu, Z-X.	T-4
Yuwono, C.	P-2
Zachkina, A.	P-62
Zaia, J.	P-54
Zhang, Q.	P-68
Zhang, X.	T-8, P-63
Zhou, Lei	P-28
Zhou, Lu	P-15
Zohrabian, S.	P-31