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The Journal of Organic Chemistry

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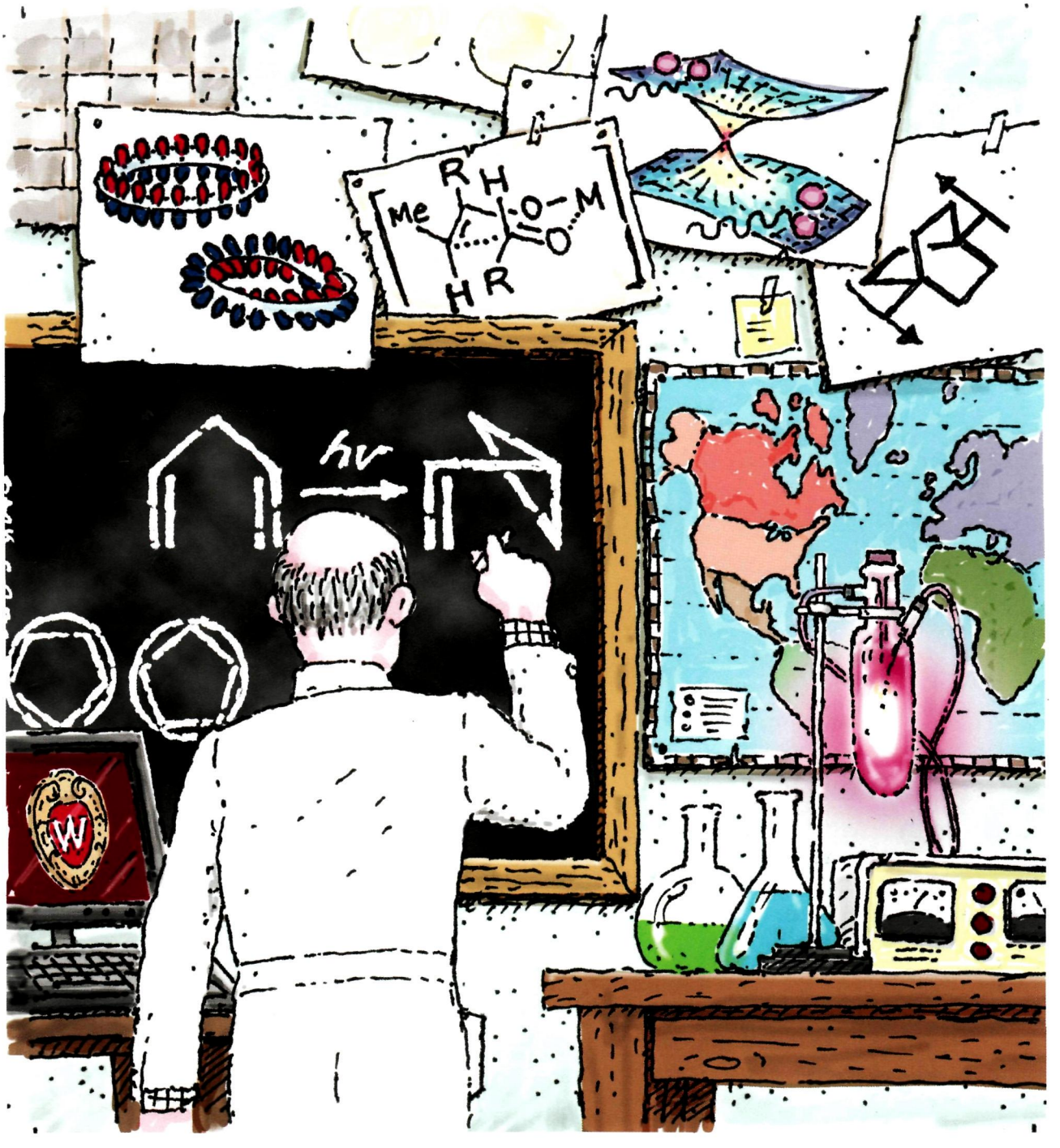

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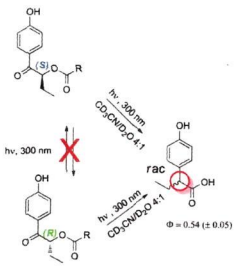
ON THE COVER: Imagery associated with Howard Zimmerman's contributions to organic chemistry during a career spanning 65 years. All of the Articles and Notes in this issue of*The Journal of Organic Chemistry* are authored by some of the many chemists impacted by Howard's distinguished career.

SPECIAL ISSUE: HOWARD ZIMMERMAN MEMORIAL ISSUE

Editorial

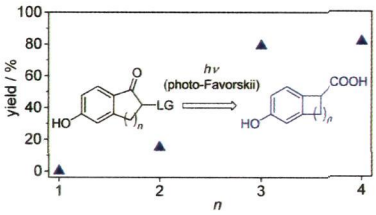
Articles



1718 S dx.doi.org/10.1021/jo300850a

A Photo-Favorskii Ring Contraction Reaction: The Effect of Ring Size

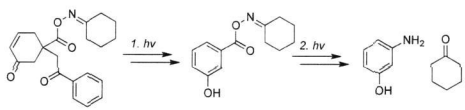
Viju Balachandran Kammath, Tomáš Šolomek, Bokolombe Pitchou Ngoy, Dominik Heger, Petr Klán,* Marina Rubina, and Richard S. Givens*



1730 S dx.doi.org/10.1021/jo3021488

Design and Synthesis of a Photoaromatization-Based Two-Stage Photobase Generator for Pitch Division Lithography

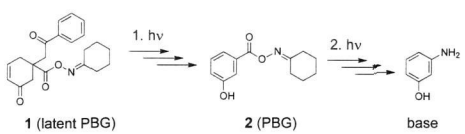
Yuji Hagiwara, Ryan A. Mesch, Takanori Kawakami, Masahiro Okazaki, Steffen Jockusch, Yongjun Li, Nicholas J. Turro, and C. Grant Willson*



1735 S dx.doi.org/10.1021/jo302149u

Study of a Two-Stage Photobase Generator for Photolithography in Microelectronics

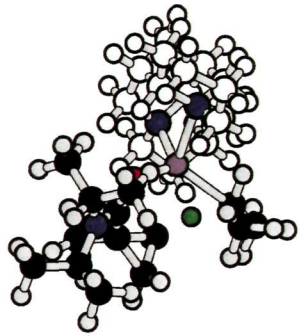
Nicholas J. Turro,* Yongjun Li, Steffen Jockusch, Yuji Hagiwara, Masahiro Okazaki, Ryan A. Mesch, David I. Schuster, and C. Grant Willson*



1742 S dx.doi.org/10.1021/jo300786v

Computational Study of the Enantioselective Deprotonation of a Cyclopropanecarboxamide with an Alkyllithium in the Presence of Sparteine

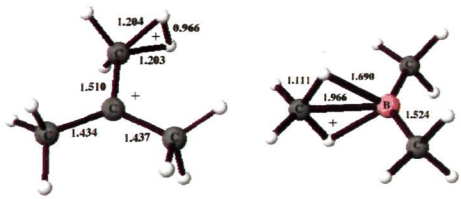
Kenneth B. Wiberg* and William F. Bailey



1747 S dx.doi.org/10.1021/jo300845a

Comparative Study of Alkane Dications (Protonated Alkyl Cations, $C_nH_{2n+2}^{2+}$) and Their Isoelectronic Boron Cation Analogues

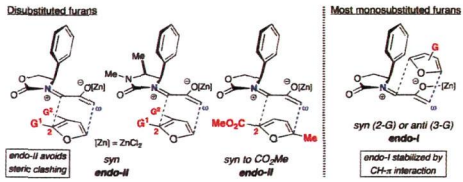
Golam Rasul,* G. K. Surya Prakash, and George A. Olah*



1753 S dx.doi.org/10.1021/jo3011792

Control of Regioselectivity and Stereoselectivity in (4 + 3) Cycloadditions of Chiral Oxyallyls with Unsymmetrically Disubstituted Furans

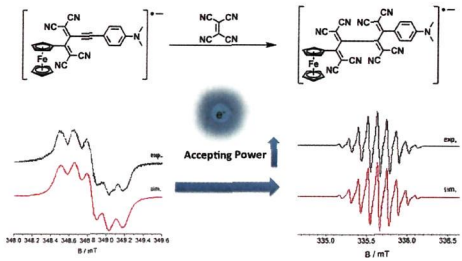
Yunfei Du, Elizabeth H. Krenske,* Jennifer E. Antoline, Andrew G. Lohse, K. N. Houk,* and Richard P. Hsung*



1760 dx.doi.org/10.1021/jo301194y

Donor-Substituted Octacyano[4]dendralenes: Investigation of π-Electron Delocalization in Their Radical Ions

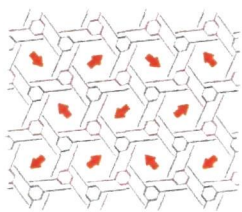
Benjamin Breiten, Markus Jordan, Daisuke Taura, Michal Zalibera, Markus Griesser, Daria Confortin, Corinne Boudon, Jean-Paul Gisselbrecht, W. Bernd Schweizer, Georg Gescheidt,* and François Diederich*



1768 dx.doi.org/10.1021/jo3009897

Inclusion Compound Based Approach to Arrays of Artificial Dipolar Molecular Rotors: Bulk Inclusions

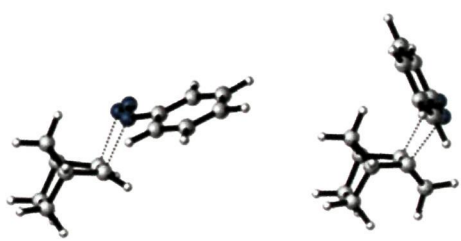
Lukáš Kobr, Ke Zhao, Yongqiang Shen, Kateřina Polívková, Richard K. Shoemaker, Noel A. Clark, John C. Price, Charles T. Rogers, and Josef Michl*



1778 dx.doi.org/10.1021/jo301267b

Alkene Distortion Energies and Torsional Effects Control Reactivities, and Stereoselectivities of Azide Cycloadditions to Norbornene and Substituted Norbornenes

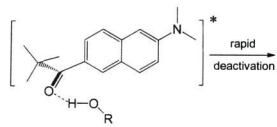
Steven A. Lopez and K. N. Houk*



1784 S dx.doi.org/10.1021/jo301263g

Carbonyl-Twisted 6-Acyl-2-dialkylaminonaphthalenes as Solvent Acidity Sensors

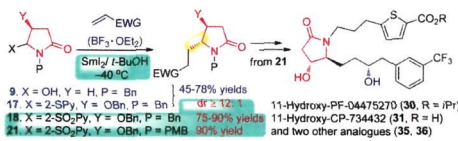
Amy M. Green, Hannah R. Naughton, Zachariah B. Nealy, Robert D. Pike, and Christopher J. Abelt*



1790 S dx.doi.org/10.1021/jo301277n

SmI_2-Mediated Intermolecular Coupling of γ-Lactam *N*-α-Radicals with Activated Alkenes: Asymmetric Synthesis of 11-Hydroxylated Analogues of the Lead Compounds CP-734432 and PF-04475270

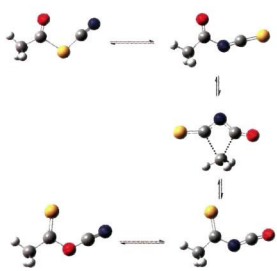
Kong-Zhen Hu, Jie Ma, Shi Qiu, Xiao Zheng, and Pei-Qiang Huang*



1802 S dx.doi.org/10.1021/jo3013786

Rearrangements of Acyl, Thioacyl, and Imidoyl (Thio)cyanates to Iso(thio)cyanates, Acyl Iso(thio)cyanates to (Thio)acyl Isocyanates, and Imidoyl Iso(thio)cyanates to (Thio)acyl Carbodiimides, RCX-YCN ⇌ RCX-NCY ⇌ RCY-NCX ⇌ RCY-XCN (X and Y = O, S, NR′)

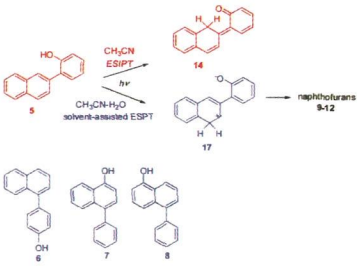
Rainer Koch* and Curt Wentrup*



1811 S dx.doi.org/10.1021/jo301456y

Excited State Intramolecular Proton Transfer (ESIPT) from Phenol to Carbon in Selected Phenylnaphthols and Naphthylphenols

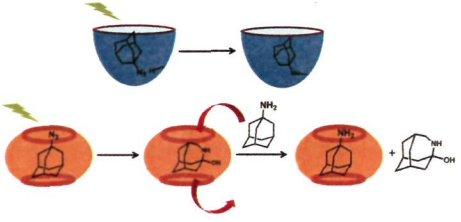
Nikola Basarić,* Nađa Došlić, Jakov Ivković, Yu-Hsuan Wang, Jelena Veljković, Kata Mlinarić-Majerski, and Peter Wan



1824 S dx.doi.org/10.1021/jo301499t

Deep-Cavity Cavitand Octa Acid as a Hydrogen Donor: Photofunctionalization with Nitrenes Generated from Azidoadamantanes

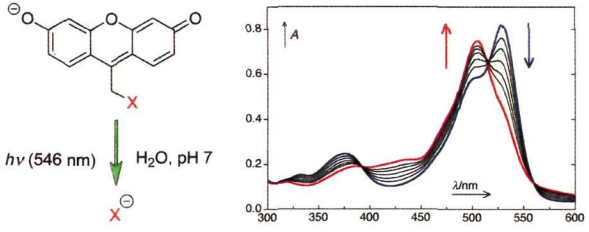
Rajib Choudhury, Shipra Gupta, José P. Da Silva,* and V. Ramamurthy*

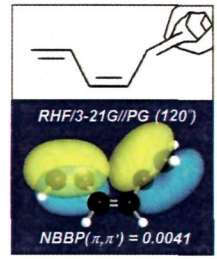


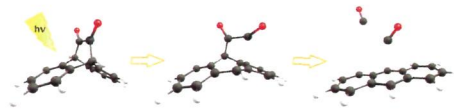
1833 S dx.doi.org/10.1021/jo301455n

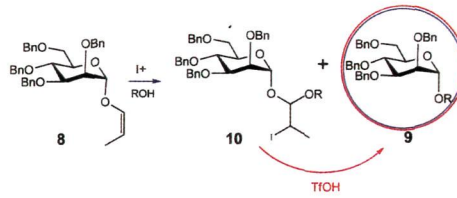
Fluorescein Analogues as Photoremovable Protecting Groups Absorbing at ~520 nm

Peter Šebej, Jürgen Wintner, Pavel Müller, Tomáš Slanina, Jamaludin Al Anshori, Lovely Angel Panamparambil Antony, Petr Klán,* and Jakob Wirz*





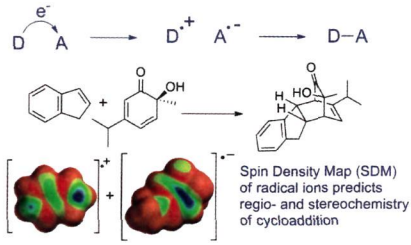




1864 S dx.doi.org/10.1021/jo301731v

Beyond Frontier Molecular Orbital Theory: A Systematic Electron Transfer Model (ETM) for Polar Bimolecular Organic Reactions

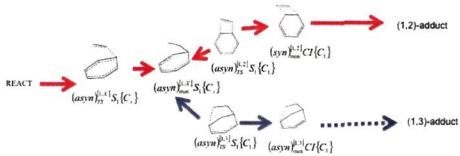
Katharine J. Cahill and Richard P. Johnson*



1874 S dx.doi.org/10.1021/jo3017549

How the Conical Intersection Seam Controls Chemical Selectivity in the Photocycloaddition of Ethylene and Benzene

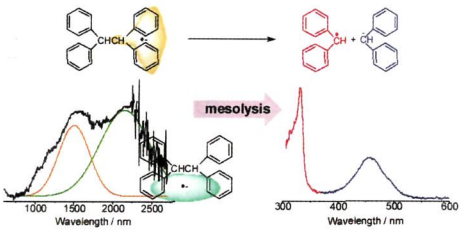
Juan J. Serrano-Pérez, Freija de Vleeschouwer, Frank de Proft, David Mendive-Tapia, Michael J. Bearpark, and Michael A. Robb*



1887 S dx.doi.org/10.1021/jo301853g

Mesolysis of Radical Anions of Tetra-, Penta-, and Hexaphenylethanes

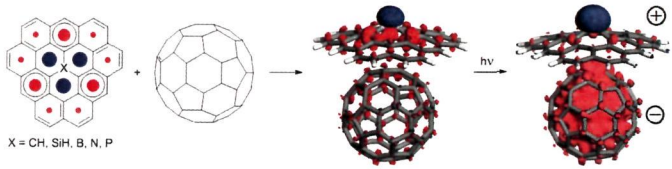
Sachiko Tojo, Mamoru Fujitsuka, and Tetsuro Majima*



1894 S dx.doi.org/10.1021/jo3018395

Doped Polycyclic Aromatic Hydrocarbons as Building Blocks for Nanoelectronics: A Theoretical Study

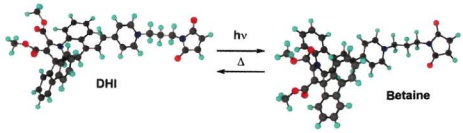
Pavlo O. Dral, Milan Kivala,* and Timothy Clark*



1903 S dx.doi.org/10.1021/jo301894s

Maleimide-Functionalized Photochromic Spirodihydroindolizines

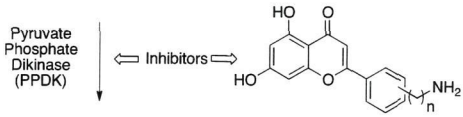
Tej B. Shrestha,* Mausam Kalita, Megh Raj Pokhrel, Yao Liu, Deryl L. Troyer, Claudia Turro, Stefan H. Bossmann,* and Heinz Dürr*



1910 S dx.doi.org/10.1021/jo3018473

Design, Synthesis, and Evaluation of Inhibitors of Pyruvate Phosphate Dikinase

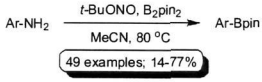
Chun Wu, Debra Dunaway-Mariano, and Patrick S. Mariano*



1923 S dx.doi.org/10.1021/jo3018878

Synthesis of Pinacol Arylboronates from Aromatic Amines: A Metal-Free Transformation

Di Qiu, Liang Jin, Zhitong Zheng, He Meng, Fanyang Mo,* Xi Wang, Yan Zhang, and Jianbo Wang*

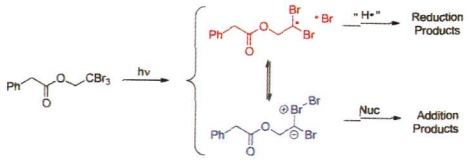


1934 S

dx.doi.org/10.1021/jo301816z

Solvent-Dependent Photochemistry of 2,2,2-Tribromoethyl-(2′-phenylacetate)

Derek M. Denning and Daniel E. Falvey*

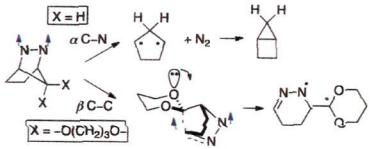


1940 S

dx.doi.org/10.1021/jo3019472

Substituent Effect on Reactivity of Triplet Excited State of 2,3-Diazabicyclo[2.2.1]hept-2-enes, DBH Derivatives: α C−N Bond Cleavage versus β C−C Bond Cleavage

Manabu Abe,* Shinji Watanabe, Hiroshi Tamura, Srikanth Boinapally, Kousei Kanahara, and Yoshihisa Fujiwara

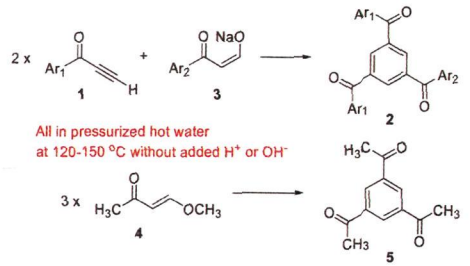


1949 S

dx.doi.org/10.1021/jo301979p

Mechanistic and Exploratory Investigations into the Synthesis of 1,3,5-Triaroylbenzenes from 1-Aryl-2-propyn-1-ones and 1,3,5-Triacetylbenzene from 4-Methoxy-3-buten-2-one by Cyclotrimerization in Hot Water in the Absence of Added Acid or Base

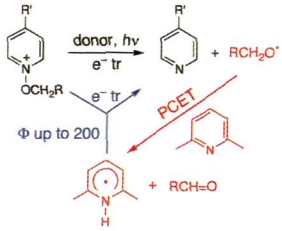
Tatsuya Iwado, Keiya Hasegawa, Toshiyuki Sato, Masaki Okada, Kiwamu Sue, Hiizu Iwamura,* and Toshihiko Hiaki*



1955 S dx.doi.org/10.1021/jo301975j

Chain-Amplified Photochemical Fragmentation of *N*-Alkoxypyridinium Salts: Proposed Reaction of Alkoxyl Radicals with Pyridine Bases To Give Pyridinyl Radicals

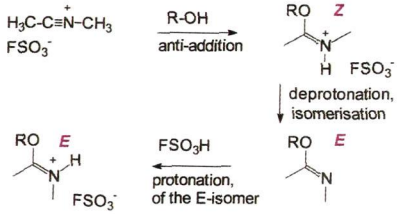
Deepak Shukla,* Shashishekar P. Adiga,* Wendy G. Ahearn, Joseph P. Dinnocenzo,* and Samir Farid*



1965 S dx.doi.org/10.1021/jo301983s

Stereoselectivity of Additions to *N*-Methyl Acetonitrilium Fluorosulfonate

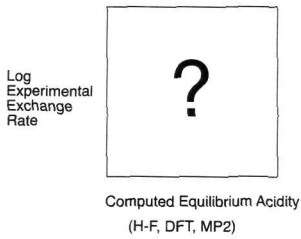
Reinhart Keese,* François Berdat, and Piero Macchi



1971 S dx.doi.org/10.1021/jo3020159

Kinetic and Equilibrium Lithium Acidities of Substituted Toluenes: Semitheoretical Brönsted Correlations

Andrew Streitwieser,* Yew Hung Leong, Eric C. Wu, and Xingyue Zhang

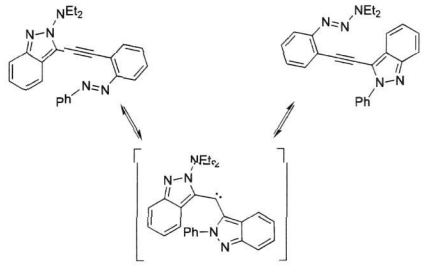


1977 S

dx.doi.org/10.1021/jo3020374

Doubly Coarctate-Stabilized Carbenes: Synthetic and Computational Studies

Brian S. Young, Rainer Herges, and Michael M. Haley*

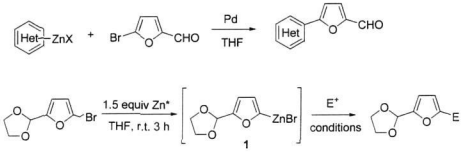


1984 S

dx.doi.org/10.1021/jo301836x

5-Substituted-2-furaldehydes: A Synthetic Protocol Utilizing an Organozinc Route

Seung-Hoi Kim and Reuben D. Rieke*

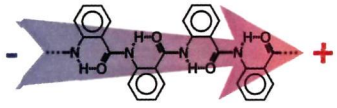


1994 S

dx.doi.org/10.1021/jo301942g

Anthranilamides as Bioinspired Molecular Electrets: Experimental Evidence for a Permanent Ground-State Electric Dipole Moment

Bing Xia, Duoduo Bao, Srigokul Upadhyayula, Guilford Jones II, and Valentine I. Vullev*

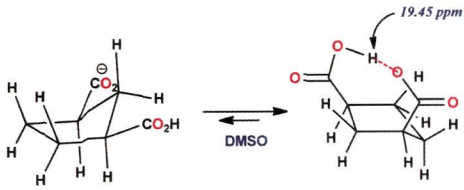


2005 S

dx.doi.org/10.1021/jo302049z

Conformational Preferences of *cis*-1,3-Cyclopentanedicarboxylic Acid and Its Salts by ^{1}H NMR Spectroscopy: Energetics of Intramolecular Hydrogen Bonds in DMSO

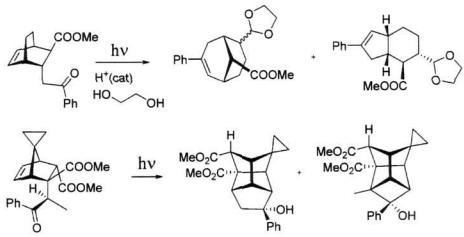
Bright U. Emenike, William R. Carroll, and John D. Roberts*



2012 S dx.doi.org/10.1021/jo301909j

Photoinduced Intramolecular Cyclopentanation vs Photoprotolytic Oxametathesis in Polycyclic Alkenes Outfitted with Conformationally Constrained Aroylmethyl Chromophores

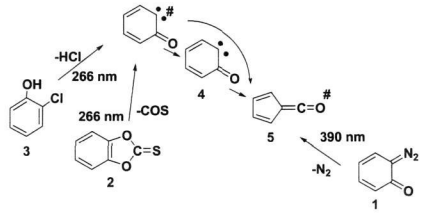
Roman A. Valiulin, Teresa M. Arisco, and Andrei G. Kutateladze*



2026 S dx.doi.org/10.1021/jo302023a

Mechanistic Aspects of Ketene Formation Deduced from Femtosecond Photolysis of Diazocyclohexadienone, *o*-Phenylene *Thioxocarbonate, and 2-Chlorophenol*

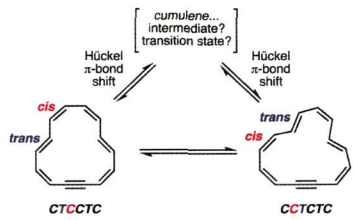
Gotard Burdzinski,* Jacek Kubicki, Michel Sliwa, Julien Réhault, Yunlong Zhang, Shubham Vyas, Hoi Ling Luk, Christopher M. Hadad, and Matthew S. Platz*



2033 S dx.doi.org/10.1021/jo302072p

Hückel and Möbius Bond-Shifting Routes to Configuration Change in Dehydro[*4n*+2]annulenes

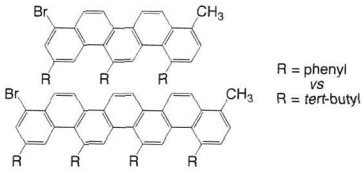
Mitchell V. Santander, Michael B. Pastor, Jordan N. Nelson, Claire Castro,* and William L. Karney*



2040 S dx.doi.org/10.1021/jo3020819

Phenyl Groups versus *tert*-Butyl Groups as Solubilizing Substituents for Some [5]Phenacenes and [7]Phenacenes

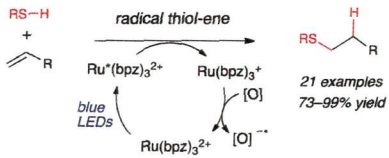
Frank B. Mallory,* Clelia W. Mallory, Colleen K. Regan, Rebecca J. Aspden, Annie Butler Ricks, Joy M. Racowski, Abigail I. Nash, Ahmara V. Gibbons, Patrick J. Carroll, and Joseph M. Bohen



2046 S dx.doi.org/10.1021/jo3020825

Transition Metal Photoredox Catalysis of Radical Thiol-Ene Reactions

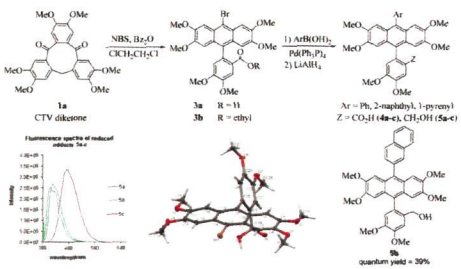
Elizabeth L. Tyson, Michael S. Ament, and Tehshik P. Yoon*



2051 S dx.doi.org/10.1021/jo302139w

Rearrangement of Cyclotriveratrylene (CTV) Diketone: 9,10-Diarylanthracenes with OLED Applications

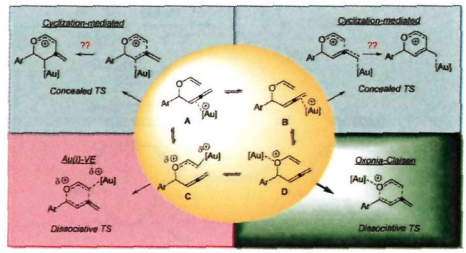
Samuel R. S. Sarsah, Marlon R. Lutz Jr., Matthias Zeller, David S. Crumrine, and Daniel P. Becker*



2059 S dx.doi.org/10.1021/jo302152j

Gold(I)-Catalyzed Claisen Rearrangement of Allenyl Vinyl Ethers: Missing Transition States Revealed through Evolution of Aromaticity, Au(I) as an Oxophilic Lewis Acid, and Lower Energy Barriers from a High Energy Complex

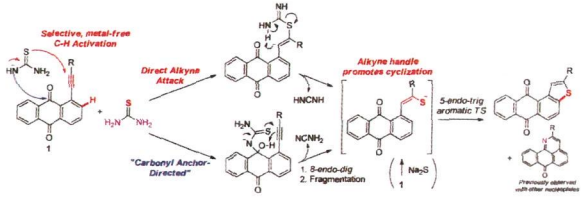
Dinesh V. Vidhani,* John W. Cran, Marie E. Krafft, Mariappan Manoharan, and Igor V. Alabugin*



2074 S dx.doi.org/10.1021/jo302146r

Divergent Cyclizations of 1-R-Ethynyl-9,10-anthraquinones: Use of Thiourea as a "S^{2-}" Equivalent in an "Anchor-Relay" Addition Mediated by Formal C–H Activation

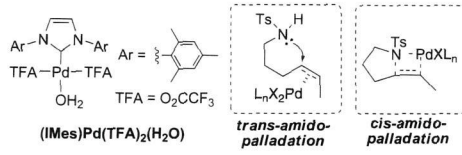
Denis S. Baranov, Brian Gold, Sergei F. Vasilevsky,* and Igor V. Alabugin*



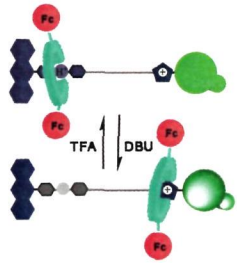
2083 S dx.doi.org/10.1021/jo302266t

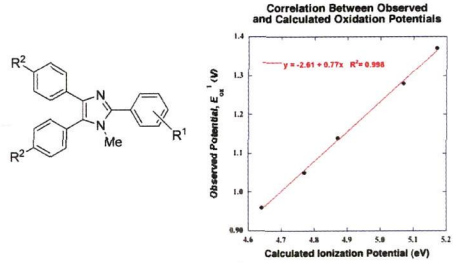
Mechanistic Studies of Wacker-Type Amidocyclization of Alkenes Catalyzed by (IMes)Pd(TFA)$_2$(H$_2$O): Kinetic and Stereochemical Implications of Proton Transfer

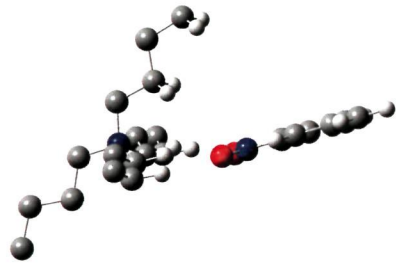
Xuan Ye, Paul B. White, and Shannon S. Stahl*

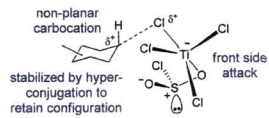


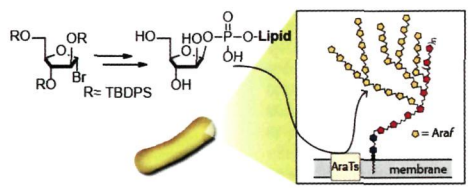
without added base: both *cis*- and *trans*-amidopalladation
with added Na_2CO_3: exclusive *cis*-amidopalladation











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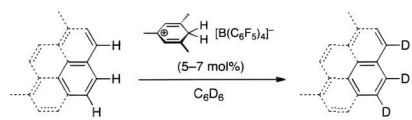
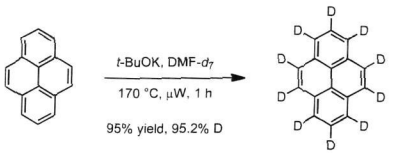


2139 Ⓢ

dx.doi.org/10.1021/jo301903m

Rapid, Microwave-Assisted Perdeuteration of Polycyclic Aromatic Hydrocarbons

Allison K. Greene and Lawrence T. Scott*

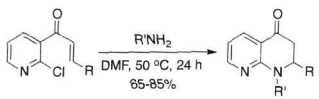


2144 Ⓢ

dx.doi.org/10.1021/jo3018632

1-Alkyl- and (±)-1,2-Dialkyl-2,3-dihydro-1,8-naphthyridin-4(1*H*)-ones by a Tandem Michael–S_NAr Annulation Reaction

Richard A. Bunce,* Scott T. Squires, and Baskar Nammalwar



Ⓢ Supporting Information available via online article