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ON THE COVER: Control of steric and electronic properties of both the gold catalyst and 1,6-diyne ester substrate dictating chemoselectivity in a divergent reaction pathway. See Chan and co-workers, p 11301.

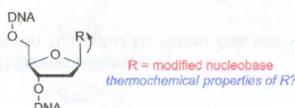
JOC Synopsis

11295

Computational Studies of the Gas-Phase Thermochemical Properties of Modified Nucleobases

Mu Chen and Jeehiun K. Lee*

DOI: 10.1021/jo502058w



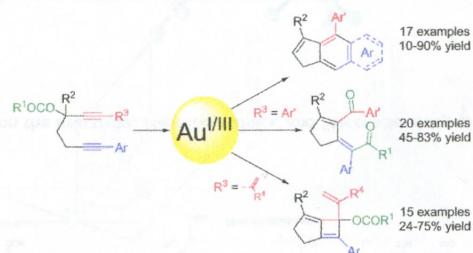
Featured Articles

11301

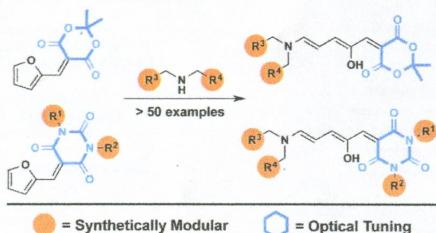
DOI: 10.1021/jo5020195

Gold-Catalyzed Cycloisomerization of 1,6-Diyne Esters to 1*H*-Cyclopenta[*b*]naphthalenes, *cis*-Cyclopenten-2-yl δ-Diketones, and Bicyclo[3.2.0]hepta-1,5-dienes

Dan Li, Weidong Rao, Guan Liang Tay, Benjamin James Ayers, and Philip Wai Hong Chan*



Design and Synthesis of Donor–Acceptor Stenhouse Adducts: A Visible Light Photoswitch Derived from Furfural
Sameh Helmy, Saemi Oh, Frank A. Leibfarth, Craig J. Hawker, and Javier Read de Alaniz*



Palladium-Catalyzed *peri*-Selective Chalcogenation of Naphthylamines with Diaryl Disulfides and Diselenides via C–H Bond Cleavage

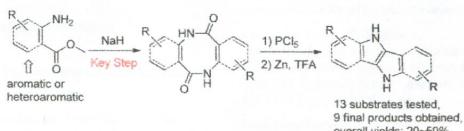
Masayuki Iwasaki, Wataru Kaneshika, Yuta Tsuchiya, Kiyohiko Nakajima, and Yasushi Nishihara*



Articles

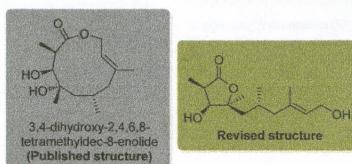
Reductive Ring Closure Methodology toward Heteroacenes Bearing a Dihydropyrrolo[3,2-*b*]pyrrole Core: Scope and Limitation

Li Qiu, Xiao Wang, Na Zhao, Shiliang Xu, Zengjian An, Xuhui Zhuang, Zhenggang Lan, Lirong Wen, and Xiaobo Wan*



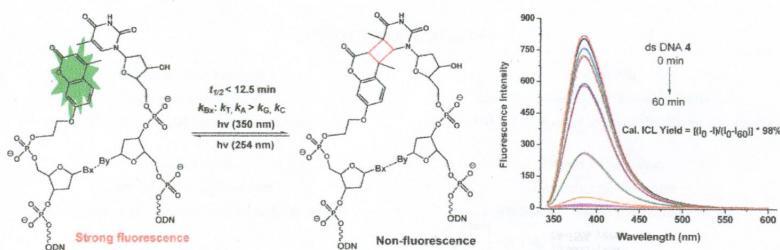
The Asymmetric Total Synthesis of Cinbotolide: A Revision of the Original Structure

José Manuel Botubol, María Jesús Durán-Peña, Antonio J. Macías-Sánchez, James R. Hanson, Isidro G. Collado, and Rosario Hernández-Galán*



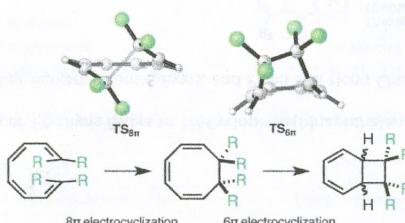
Quantitative DNA Interstrand Cross-Link Formation by Coumarin and Thymine: Structure Determination, Sequence Effect, and Fluorescence Detection

Huabing Sun, Heli Fan, and Xiaohua Peng*



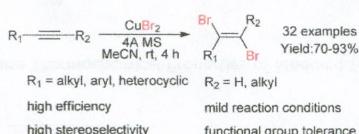
Terminal Substituent Effects on the Reactivity, Thermodynamics, and Stereoselectivity of the $8\pi-6\pi$ Electrocyclization Cascades of 1,3,5,7-Tetraenes

Ashay Patel and K. N. Houk*



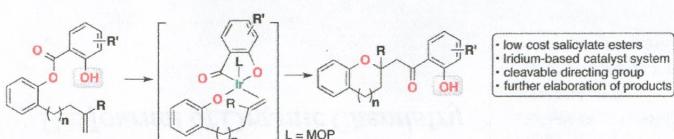
Method for Transforming Alkynes into (*E*)-Dibromoalkenes

Jiannan Xiang, Rui Yuan, Ruijia Wang, Niannian Yi, Linghui Lu, Huaxu Zou, and Weimin He*



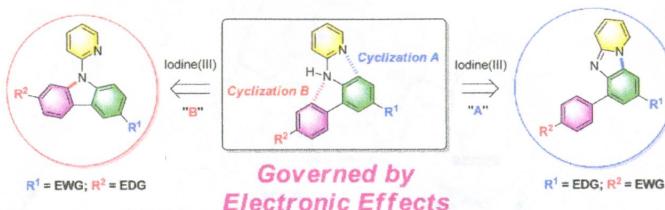
Intramolecular Oxyacylation of Alkenes Using a Hydroxyl Directing Group

Giang T. Hoang, Zhongda Pan, Jason T. Brethorst, and Christopher J. Douglas*



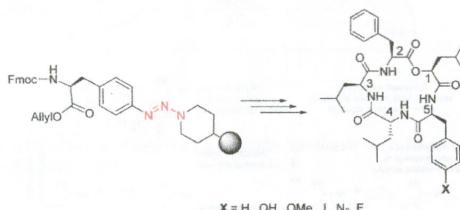
Substituent Electronic Effects Govern Direct Intramolecular C–N Cyclization of *N*-(Biphenyl)pyridin-2-amines Induced by Hypervalent Iodine(III) Reagents

Jean-Ho Chu,* Wen-Ting Hsu, Yi-Hua Wu, Meng-Fan Chiang, Nan-Hai Hsu, Hao-Ping Huang, and Ming-Jung Wu*



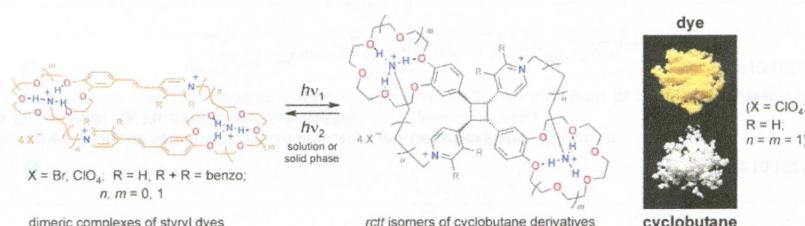
Triazene as a Powerful Tool for Solid-Phase Derivatization of Phenylalanine Containing Peptides: Zygosporamide Analogues as a Proof of Concept

Carolina Torres-García, Daniel Pulido, Fernando Albericio, Miriam Royo,* and Ernesto Nicolás*

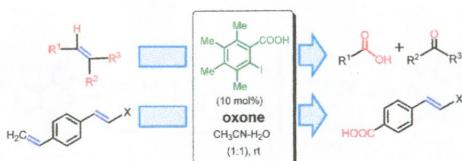


Synthesis, Structure, and Properties of Supramolecular Photoswitches Based on Ammonioalkyl Derivatives of Crown Ether Styryl Dyes

Sergey P. Gromov,* Artem I. Vedernikov, Natalia A. Lobova, Lyudmila G. Kuz'mina, Svetlana N. Dmitrieva, Yuri A. Strelenko, and Judith A. K. Howard

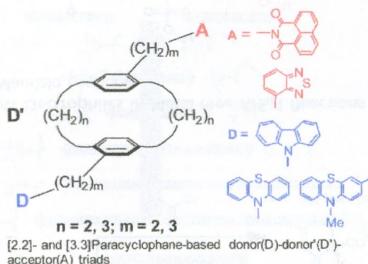


Oxidative Cleavage of Olefins by In Situ-Generated Catalytic 3,4,5,6-Tetramethyl-2-iodoxybenzoic Acid/Oxone
Jarugu Narasimha Moorthy* and Keshaba Nanda Parida



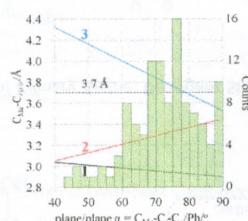
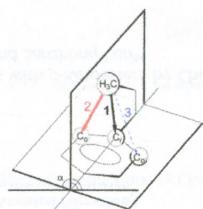
Synthesis and Electronic and Photophysical Properties of [2.2]- and [3.3]Paracyclophane-Based Donor–Donor'–Acceptor Triads

Takaaki Miyazaki, Masahiko Shibahara, Jun-ichi Fujishige, Motonori Watanabe, Kenta Goto, and Teruo Shinmyozu*



Methyl/Phenyl Attraction by CH/π Interaction in 1,2-Substitution Patterns

Henri Brunner,* Takashi Tsuno,* Gábor Balázs, and Michael Bodensteiner

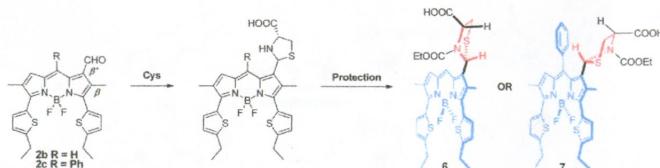


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Thiazolidine Derivatives from Fluorescent Dithienyl-BODIPY-carboxaldehydes and Cysteine
Arnaud Poirel, Antoinette De Nicola,* and Raymond Ziesel*

DOI: 10.1021/jo502068u

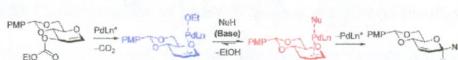


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Stereocontrolled O-Glycosylation with Palladium-Catalyzed Decarboxylative Allylation
Shaohua Xiang, Jingxi He, Yu Jia Tan, and Xue-Wei Liu*

DOI: 10.1021/jo502078c

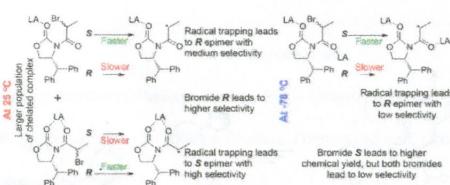


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A Computational Study on Lewis Acid-Catalyzed Diastereoselective Acyclic Radical Allylation Reactions with Unusual Selectivity Dependence on Temperature and Epimer Precursor
Miglena K. Georgieva and A. Gil Santos*

DOI: 10.1021/jo502102s

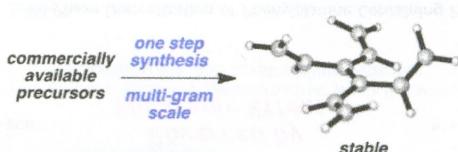


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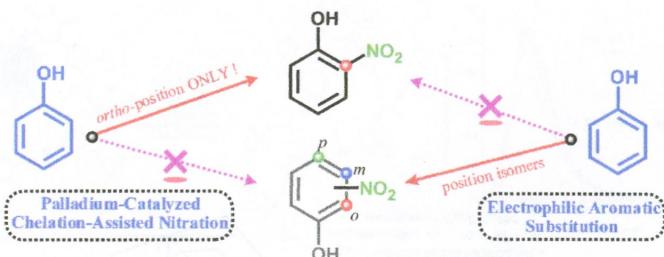
Computational and Synthetic Studies with Tetrvinylenethylenes
Erik J. Lindeboom, Anthony C. Willis, Michael N. Paddon-Row,* and Michael S. Sherburn*

DOI: 10.1021/jo5021294



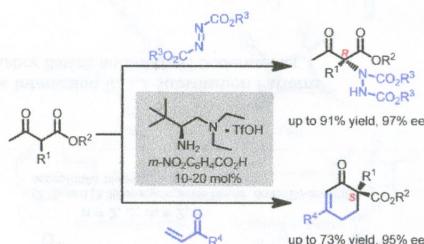
Palladium-Catalyzed Aromatic C–H Bond Nitration Using Removable Directing Groups: Regiospecific Synthesis of Substituted *o*-Nitrophenols from Related Phenols

Wei Zhang, Jian Zhang, Shaobo Ren, and Yunkui Liu*



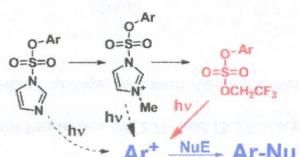
Asymmetric Enamine Catalysis with β -Ketoesters by Chiral Primary Amine: Divergent Stereocontrol Modes

Changming Xu, Long Zhang, and Sanzhong Luo*

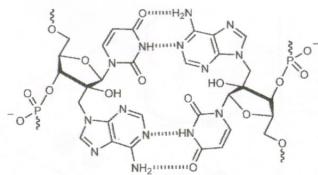


Aryl Imidazylates and Aryl Sulfates As Electrophiles in Metal-Free ArS_N1 Reactions

Hisham Qrareya, Stefano Protti, and Maurizio Fagnoni*

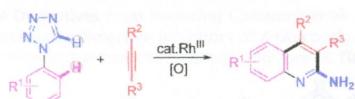


Double-Headed Nucleotides with Arabino Configuration: Synthesis and Hybridization Properties
Pawan Kumar, Pawan K. Sharma, and Pouli Nielsen*

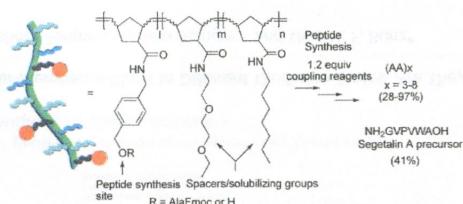


One-Pot Synthesis of Multisubstituted 2-Aminoquinolines from Annulation of 1-Aryl Tetrazoles with Internal Alkynes via Double C–H Activation and Denitrogenation

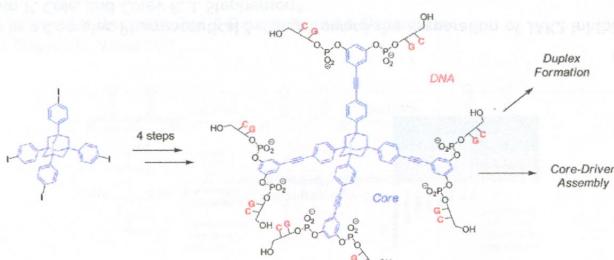
Lei Zhang, Liyao Zheng, Biao Guo, and Ruimao Hu*



Soluble Non-Cross-Linked Poly(norbornene) Supports for Peptide Synthesis with Minimal Reagents
Nimmashetti Naganna and Nandita Madhavan*

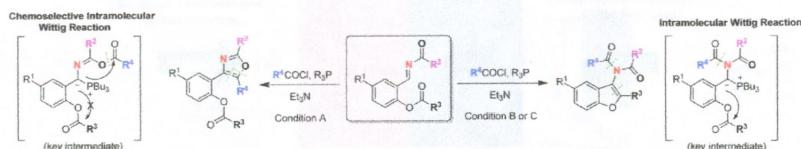


Synthesis of Eight-Arm, Branched Oligonucleotide Hybrids and Studies on the Limits of DNA-Driven Assembly
Alexander Schwenger, Claudia Gerlach, Helmut Griesser, and Clemens Richert*

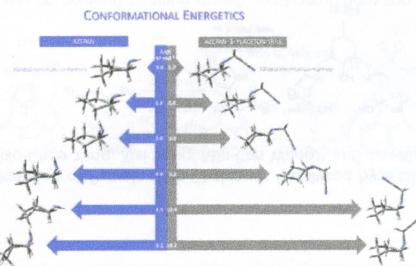


Chemoselective Intramolecular Wittig Reactions for the Synthesis of Oxazoles and Benzofurans

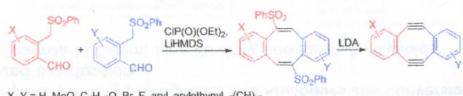
Yu-Shiou Fan, Utpal Das, Ming-Yu Hsiao, Meng-Hsien Liu, and Wenwei Lin*

**Thermochemical Insights on the Conformational Energies of Azepan and Azepan-1-ylacetonitrile**

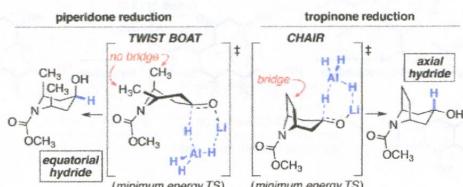
Vera L. S. Freitas, Sara Leirosa, Rafael Notario, and Maria D. M. C. Ribeiro da Silva*

**Substituted 5,6,11,12-Tetrahydrodibenz[b,e]cyclooctenes: Syntheses, Properties, and DFT Studies of Substituted Sondheimer-Wong Diynes**

Feng Xu, Lifen Peng, Kenta Shinohara, Takamoto Morita, Suguru Yoshida, Takamitsu Hosoya, Akihiro Orita,* and Junzo Otera

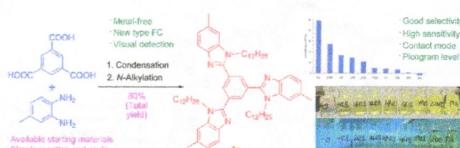
**A Twist on Facial Selectivity of Hydride Reductions of Cyclic Ketones: Twist-Boat Conformers in Cyclohexanone, Piperidone, and Tropinone Reactions**

Sharon R. Neufeldt, Gonzalo Jiménez-Osés,* Daniel L. Comins,* and K. N. Houk*

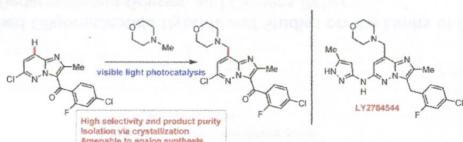


Benzimidazole Derivatives: Selective Fluorescent Chemosensors for the Picogram Detection of Picric Acid

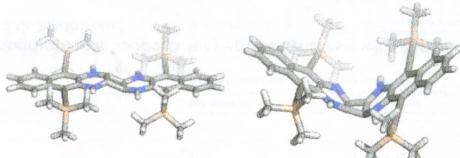
Jin-Feng Xiong, Jian-Xiao Li, Guang-Zhen Mo, Jing-Pei Huo, Jin-Yan Liu, Xiao-Yun Chen,* and Zhao-Yang Wang*

**Photoredox Catalysis in a Complex Pharmaceutical Setting: Toward the Preparation of JAK2 Inhibitor LY2784544**

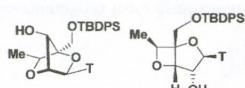
James J. Douglas, Kevin P. Cole, and Corey R. J. Stephenson*

**Tetraazaacenes Containing Four-Membered Rings in Different Oxidation States. Are They Aromatic? A Computational Study**

Manuel Schaffroth, Renana Gershoni-Poranne, Amnon Stanger,* and Uwe H. F. Bunz*

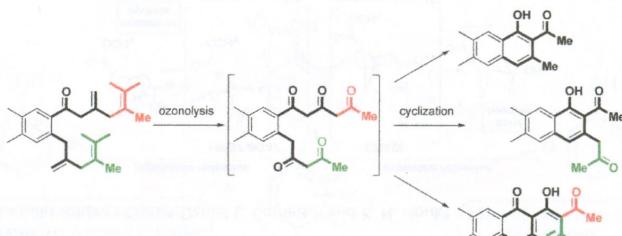
**Alternative Syntheses of (S)-cEt-BNA: A Key Constrained Nucleoside Component of Bioactive Antisense Gapmer Sequences**

Juan C. Salinas, Michael T. Migawa, Bradley L. Merner, and Stephen Hanessian*



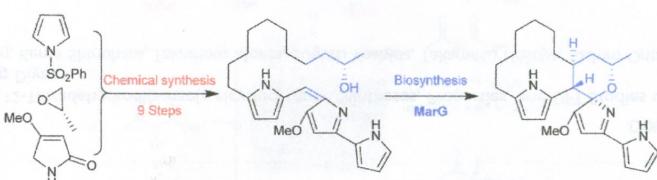
Synthesis of Tri-, Tetra-, and Pentacarbonyl Derivatives via Ozonolysis of 1,4-Dienes and Cyclization to Polyaromatic Systems

Laura Kersten, Klaus Harms, and Gerhard Hilt*



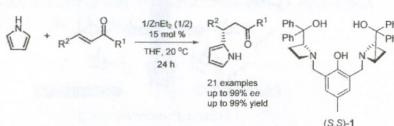
Stereospecific Synthesis of 23-Hydroxyundecylprodiginines and Analogues and Conversion to Antimalarial Premarineosins via a Rieske Oxygenase Catalyzed Bicyclization

Papireddy Kancharla, Wanli Lu, Shaimaa M. Salem, Jane Xu Kelly, and Kevin A. Reynolds*



Enantioselective Friedel-Crafts Alkylation of Pyrrole with Chalcones Catalyzed by a Dinuclear Zinc Catalyst

Yuan-Zhao Hua, Xing-Wang Han, Xiao-Chao Yang, Xixi Song, Min-Can Wang,* and Jun-Biao Chang*



Synthesis of β - and γ -Hydroxy α -Amino Acids via Enzymatic Kinetic Resolution and Cyanate-to-Isocyanate Rearrangement

Piotr Szczęśniak, Agnieszka Październik-Holewa, Urszula Klimczak, and Sebastian Stecko*

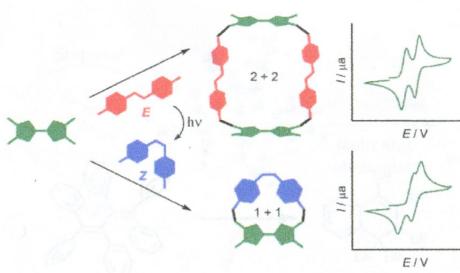


11714 S

DOI: 10.1021/jo502469z

Light-Controlled Macrocyclization of Tetrathiafulvalene with Azobenzene: Designing an Optoelectronic Molecular Switch

Vladimir A. Azov,* Jens Cordes, Dirk Schlüter, Thomas Dülcks, Marcus Böckmann,* and Nikos L. Doltsinis

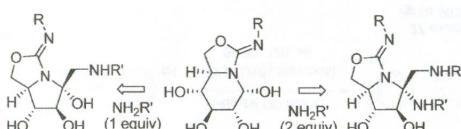


11722 S

DOI: 10.1021/jo5025283

Synthesis of Multibranched Australine Derivatives from Reducing Castanospermine Analogues through the Amadori Rearrangement of *gem*-Diamine Intermediates: Selective Inhibitors of β -Glucosidase

Elena M. Sánchez-Fernández, Eleuterio Álvarez, Carmen Ortiz Mellet,* and José M. García Fernández*



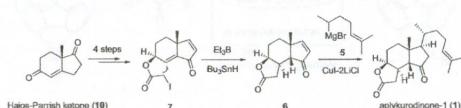
Notes

11729 S

DOI: 10.1021/jo501684k

Protecting-Group-Free Total Synthesis of Aplykuroidinone-1

Yu Tang,* Ji-tian Liu, Ping Chen, Ming-can Lv, Zhen-zhen Wang, and Yi-kun Huang

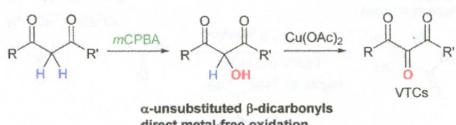


11735 S

DOI: 10.1021/jo501985u

Metal-Free α -Hydroxylation of α -Unsubstituted β -Oxoesters and β -Oxoamides

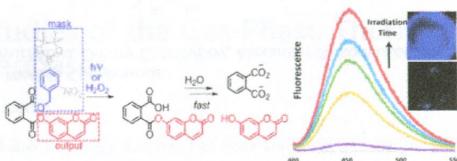
Haruyasu Asahara and Nagatoshi Nishiwaki*



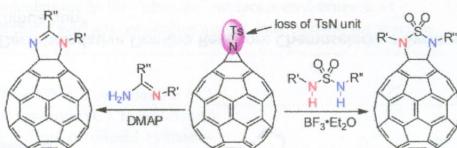
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Self-Immolative Phthalate Esters Sensitive to Hydrogen Peroxide and Light

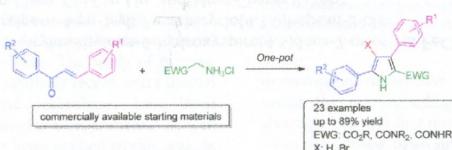
Kaitlyn M. Mahoney, Pratik P. Goswami, Aleem Syed, Patrick Kolker, Brian Shannan, Emily A. Smith, and Arthur H. Winter*

**BF₃·Et₂O- or DMAP-Catalyzed Double Nucleophilic Substitution Reaction of Aziridinofullerenes with Sulfamides or Amidines**

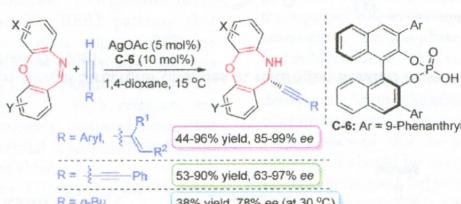
Hai-Tao Yang,* Meng-Lei Xing, Xin-Wei Lu, Jia-Xing Li, Jiang Cheng, Xiao-Qiang Sun, and Chun-Bao Miao

**One-Pot Synthesis of Pyrrole-2-carboxylates and -carboxamides via an Electrocyclization/Oxidation Sequence**

Dennis Imbri, Natalie Netz, Murat Kucukdisli, Lisa Marie Kammer, Philipp Jung, Annika Kretzschmann, and Till Opatz*

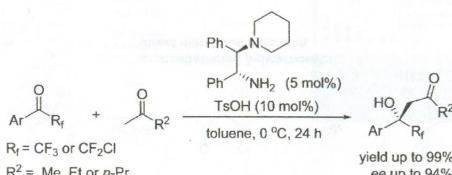
**Asymmetric Alkynylation of Seven-Membered Cyclic Imines by Combining Chiral Phosphoric Acids and Ag(I) Catalysts: Synthesis of 11-Substituted-10,11-dihydrobenzo[b,f][1,4]oxazepine Derivatives**

Yuan-Yuan Ren, You-Qing Wang,* and Shuang Liu



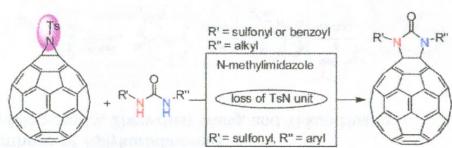
Fine-Tuning the Structures of Chiral Diamine Ligands in the Catalytic Asymmetric Aldol Reactions of Trifluoromethyl Aromatic Ketones with Linear Aliphatic Ketones

Hua Zong, Huayin Huang, Guangling Bian, and Ling Song*



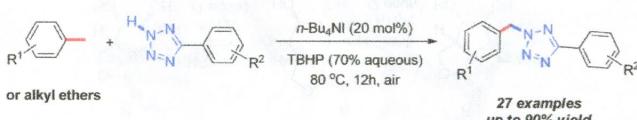
Lewis Base-Catalyzed Reaction of Aziridinofullerene with Ureas for the Preparation of Fulleroimidazolidinones

Meng-Lei Xing, Xin-Wei Lu, Chun-Bao Miao, Jia-Xing Li, Xiao-Qiang Sun, and Hai-Tao Yang*



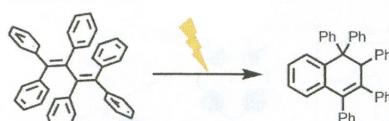
Transition-Metal-Free Direct Alkylation of Aryl Tetrazoles via Intermolecular Oxidative C–N Formation

Liang Wang,* Kaiqiang Zhu, Qun Chen, and Mingyang He*

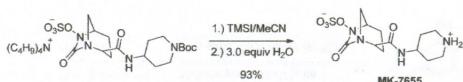


Photolability of Per-Arylated Butadienes: En Route to Dihydronaphthalenes

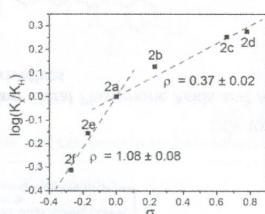
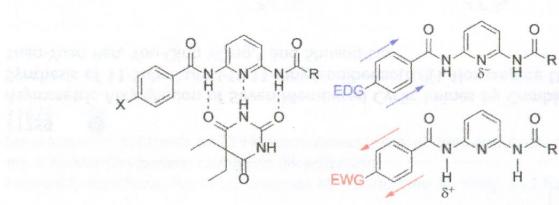
Jan Freudenberg, Andrea C. Uptmoor, Frank Rominger, and Uwe H. F. Bunz*



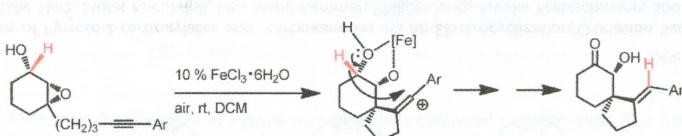
N-Boc Deprotection and Isolation Method for Water-Soluble Zwitterionic Compounds
Zhijian Liu,* Nobuyoshi Yasuda, Michael Simeone, and Robert A. Reamer



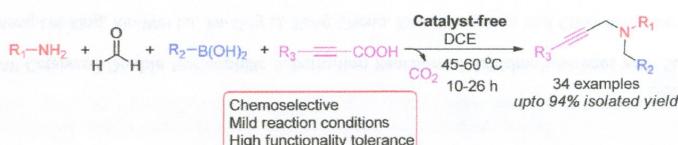
Linear Free Energy Relationships Reveal Structural Changes in Hydrogen-Bonded Host–Guest Interactions
Jacqueline M. McGrath and Michael D. Pluth*



Diastereoselective Synthesis of 2-Arylmethylene-6-hydroxyspiro[4.5]deca-7-ones via $\text{FeCl}_3\cdot 6\text{H}_2\text{O}$ -Catalyzed Spiroannulation/Hydride Transfer of 6-(5-Arylpent-4-yn-1-yl)-7-oxabicyclo[4.1.0]heptan-2-ols
Hsin-Hui Lin, Kuan-Yi Lee, Yin-An Chen, Chi-Fan Liu, and Ming-Chang P. Yeh*

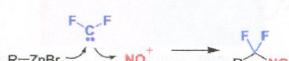


Mild and Catalyst-Free Petasis/Decarboxylative Domino Reaction: Chemoselective Synthesis of *N*-Benzyl Propargylamines
Huangdi Feng, Huihui Jia, and Zhihua Sun*



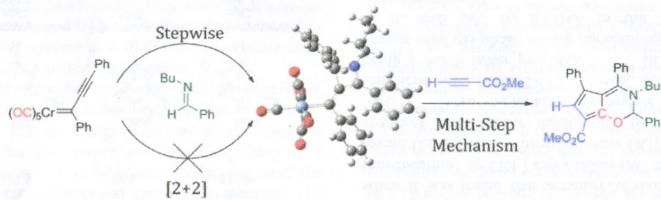
Synthesis of *gem*-Difluorinated Nitroso Compounds

Vladimir O. Smirnov, Marina I. Struchkova, Dmitry E. Arkhipov, Alexander A. Korlyukov, and Alexander D. Dilman*



Computational Assessment of Non-Heteroatom-Stabilized Carbene Complexes Reactivity: Formation of Oxazine Derivatives

Ignacio Funes-Ardoiz and Diego Sampedro*



oxazine derivatives have been reported in the literature, the mechanism of their formation has not been fully elucidated. In this work, we have performed a computational study of the formation of oxazine derivatives from non-heteroatom-stabilized carbene complexes. The results show that the formation of oxazine derivatives can proceed through a multi-step mechanism involving the formation of a dimeric intermediate followed by reaction with methyl isocyanide.

The reaction starts with the formation of a dimeric intermediate from a chromium carbene complex and a substituted imine. The chromium carbene complex is formed by the reaction of a chromium(0) complex with a phenyl isocyanide. The resulting chromium carbene complex then reacts with a substituted imine to form a dimeric intermediate. This intermediate then reacts with methyl isocyanide to form the final oxazine product. The reaction is labeled "Multi-Step Mechanism". The final product is a five-membered ring containing a carbene carbon, two phenyl groups, a methyl group, and an oxygen atom. The reaction is labeled "Multi-Step Mechanism".

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