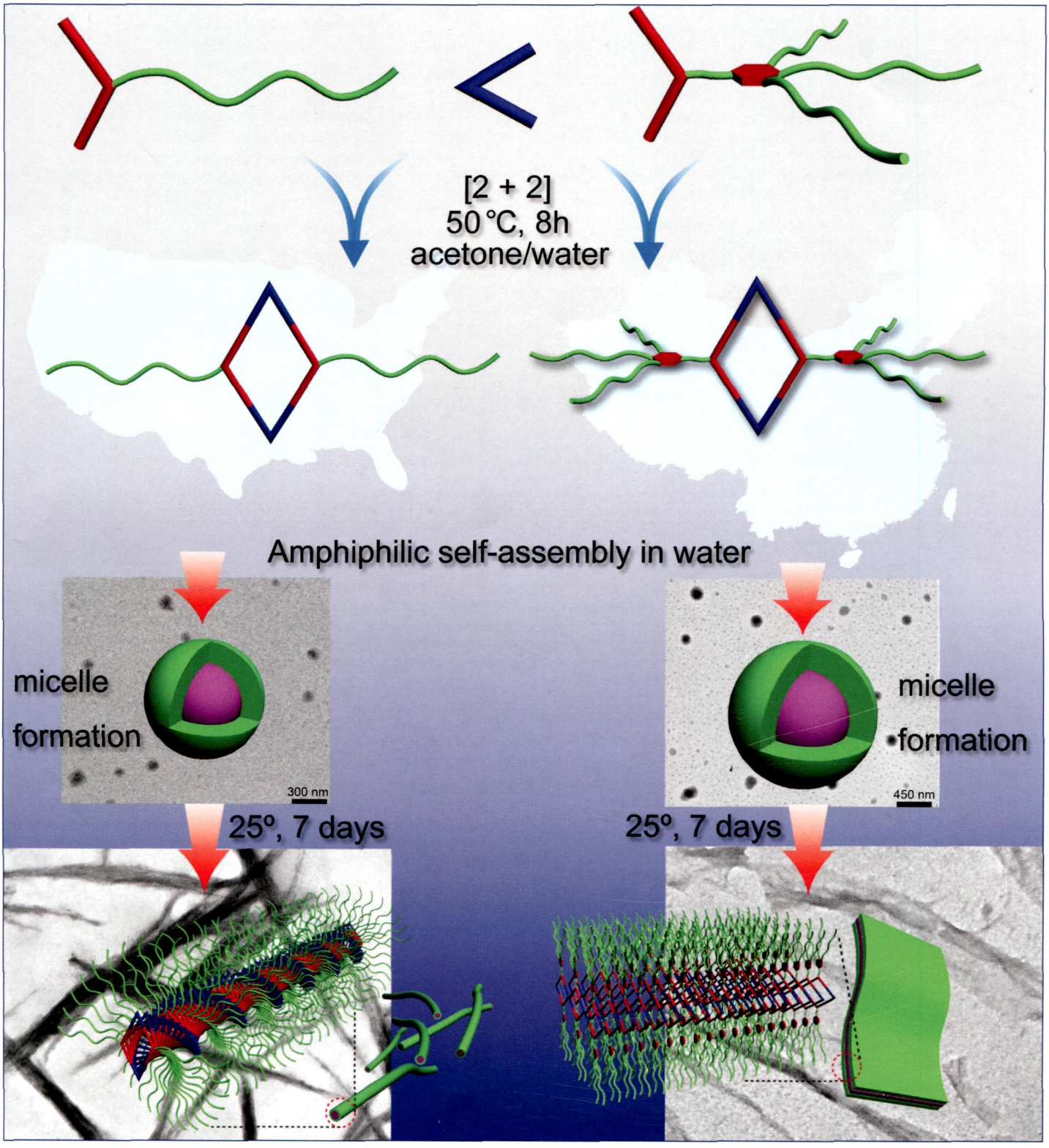
September 25, 2013
Volume 135
Number 38
pubs.acs.org/JACS

JACS

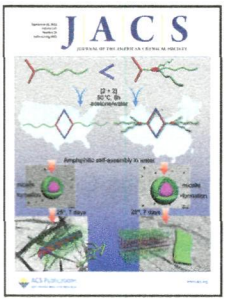
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY



JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

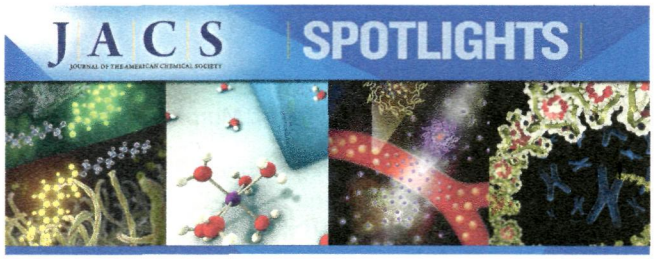
SEPTEMBER 25, 2013
VOLUME 135 ISSUE 38

JACSAT 135(38) 13999–14460 (2013)
ISSN 0002-7863

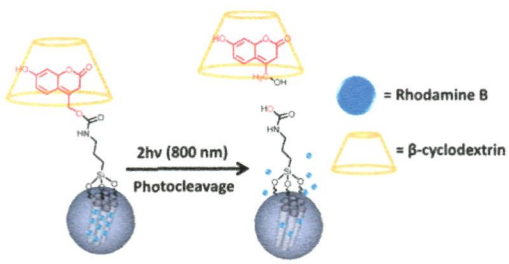


ON THE COVER: Hierarchical self-assembly organizes molecular precursors into complex supramolecular ensembles with multiple, orthogonal interactions acting in concert. Here, coordination-driven self-assembly furnishes polyethylene glycol (PEG) decorated rhomboids. These rhomboids undergo further ordering in water due to their hydrophobic metallacyclic cores and hydrophilic PEG peripheries, resulting in nanoscopic micelles, fibers, and ribbons. See Stang and co-workers, p 14036.

Spotlights



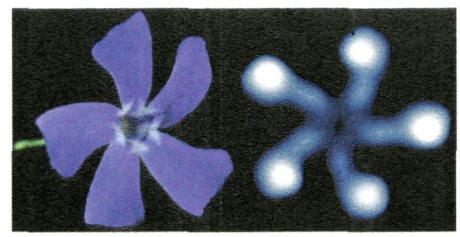
Communications



14004 (S) dx.doi.org/10.1021/ja405456k

Surface-Supported Supramolecular Pentamers

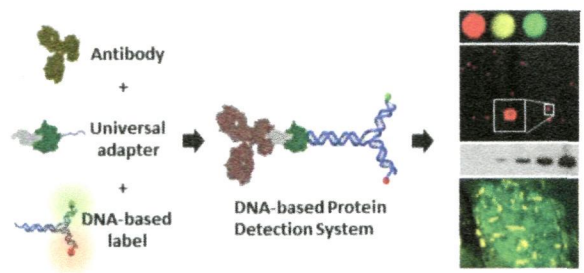
Sujoy Karan,* Yongfeng Wang,* Roberto Robles, Nicolás Lorente, and Richard Berndt



14008 (S) dx.doi.org/10.1021/ja405872g

A Universal DNA-Based Protein Detection System

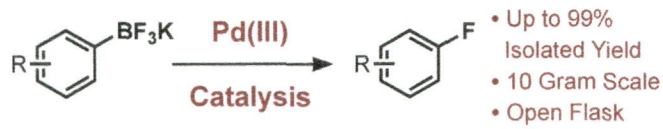
Thua N. N. Tran, Jinhui Cui, Mark R. Hartman, Songming Peng, Hisakage Funabashi, Faping Duan, Dayong Yang, John C. March, John T. Lis, Haixin Cui, and Dan Luo*



14012 (S) dx.doi.org/10.1021/ja405919z

Palladium(III)-Catalyzed Fluorination of Arylboronic Acid Derivatives

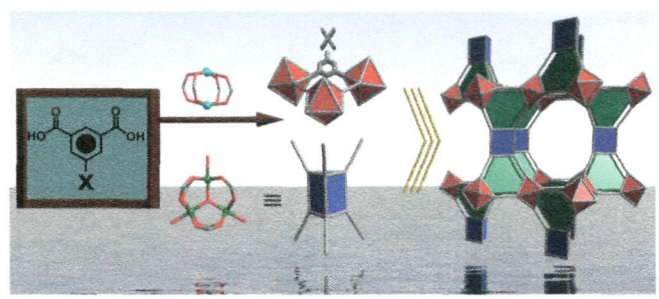
Anthony R. Mazzotti, Michael G. Campbell, Pingping Tang, Jennifer M. Murphy, and Tobias Ritter*



14016 (S) dx.doi.org/10.1021/ja406030p

A Family of Porous Lonsdaleite-e Networks Obtained through Pillaring of Decorated Kagomé Lattice Sheets

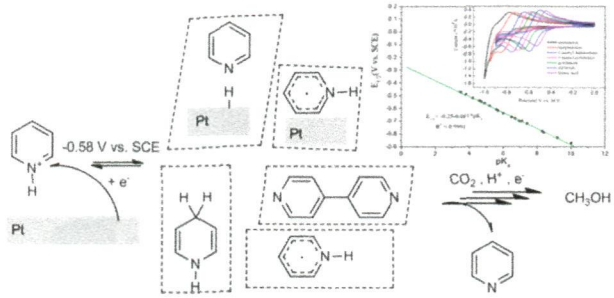
Alexander Schoedel, Wesley Boyette, Lukasz Wojtas, Mohamed Eddaoudi, and Michael J. Zaworotko*



14020 (S) dx.doi.org/10.1021/ja4064052

Electrochemistry of Aqueous Pyridinium: Exploration of a Key Aspect of Electrocatalytic Reduction of CO_2 to Methanol

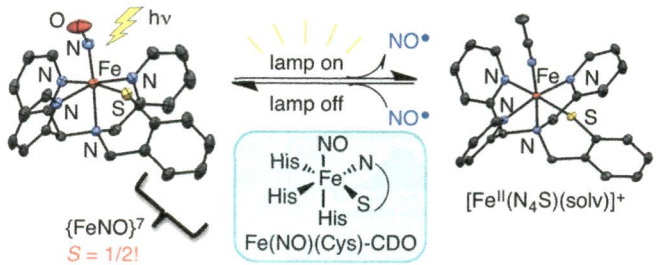
Yong Yan, Elizabeth L. Zeitler, Jing Gu, Yuan Hu, and Andrew B. Bocarsly*



14024 (S) dx.doi.org/10.1021/ja4064487

Preparation of Non-heme {FeNO}^{7} Models of Cysteine Dioxygenase: Sulfur versus Nitrogen Ligation and Photorelease of Nitric Oxide

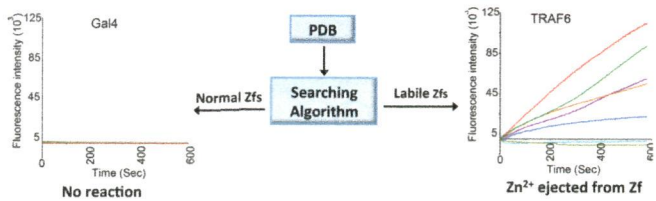
Alison C. McQuilken, Yang Ha, Kyle D. Sutherlin, Maxime A. Siegler, Keith O. Hodgson, Britt Hedman, Edward I. Solomon,* Guy N. L. Jameson,* and David P. Goldberg*



14028 (S) dx.doi.org/10.1021/ja406300c

Identification of Labile Zn Sites in Drug-Target Proteins

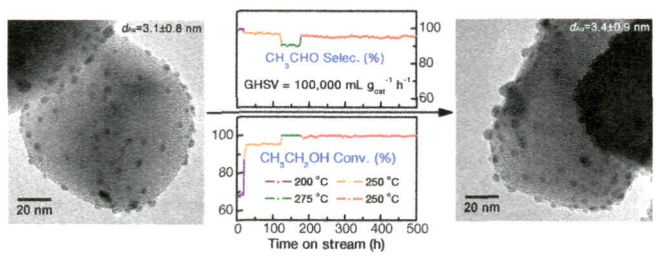
Yu-Ming Lee, Yi-Ting Wang, Yulander Duh, Hanna S. Yuan,* and Carmay Lim*



14032 (S) dx.doi.org/10.1021/ja406820f

Highly Efficient and Robust Au/$MgCuCr_2O_4$ Catalyst for Gas-Phase Oxidation of Ethanol to Acetaldehyde

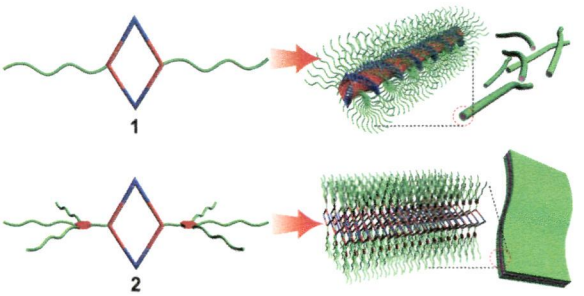
Peng Liu* and Emiel J. M. Hensen*



14036 Ⓢ dx.doi.org/10.1021/ja406877b

Hierarchical Self-Assembly: Well-Defined Supramolecular Nanostructures and Metallohydrogels via Amphiphilic Discrete Organoplatinum(II) Metallacycles

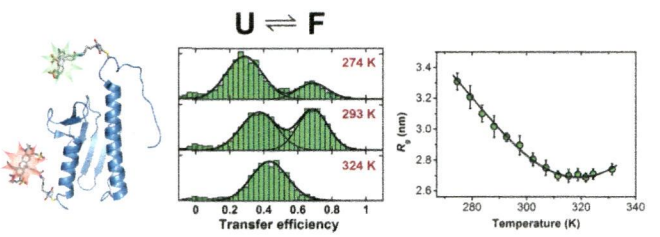
Xuzhou Yan, Shijun Li, Timothy R. Cook, Xiaofan Ji, Yong Yao, J. Bryant Pollock, Yanhui Shi, Guocan Yu, Jinying Li, Feihe Huang,* and Peter J. Stang*



14040 Ⓢ dx.doi.org/10.1021/ja407009w

Single-Molecule Spectroscopy of Cold Denaturation and the Temperature-Induced Collapse of Unfolded Proteins

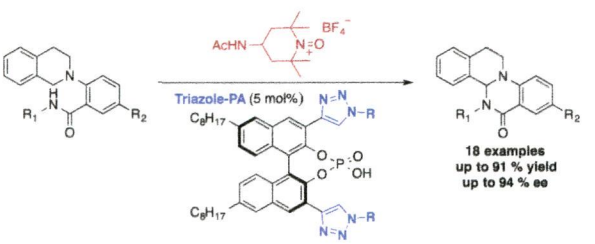
Mikayel Aznauryan, Daniel Nettels, Andrea Holla, Hagen Hofmann, and Benjamin Schuler*



14044 Ⓢ dx.doi.org/10.1021/ja407410b

Asymmetric Cross-Dehydrogenative Coupling Enabled by the Design and Application of Chiral Triazole-Containing Phosphoric Acids

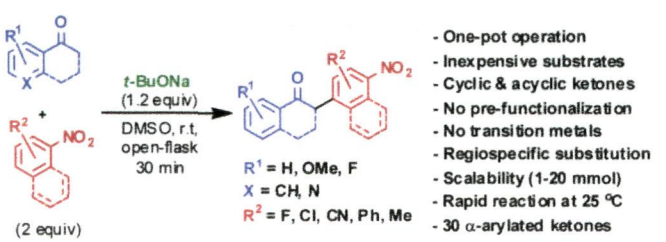
Andrew J. Neel, Jörg P. Hehn, Pascal F. Tripet, and F. Dean Toste*



14048 Ⓢ dx.doi.org/10.1021/ja4074563

Aerobic, Transition-Metal-Free, Direct, and Regiospecific Mono-α-arylation of Ketones: Synthesis and Mechanism by DFT Calculations

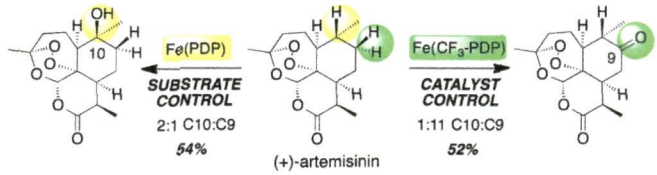
Qing-Long Xu, Hongyin Gao, Muhammed Yousufuddin, Daniel H. Ess,* and László Kürti*



14052 Ⓢ dx.doi.org/10.1021/ja407388y

Catalyst-Controlled Aliphatic C–H Oxidations with a Predictive Model for Site-Selectivity

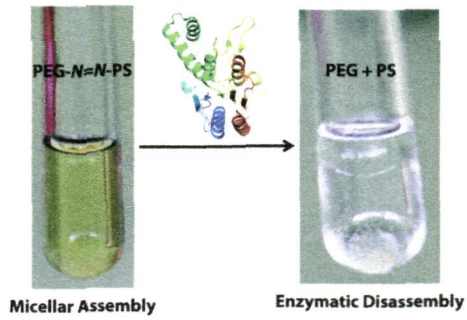
Paul E. Gormisky and M. Christina White*



14056 Ⓢ dx.doi.org/10.1021/ja407514z

Enzyme Sensitive Synthetic Polymer Micelles Based on the Azobenzene Motif

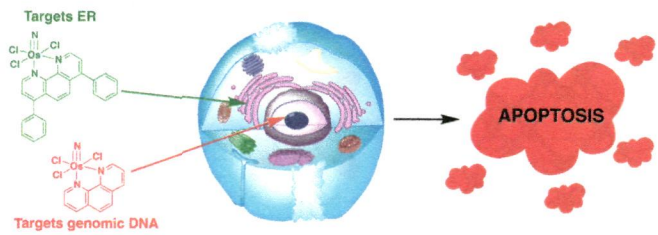
Jingyi Rao and Anzar Khan*



14060 Ⓢ dx.doi.org/10.1021/ja4075375

Bidentate Ligands on Osmium(VI) Nitrido Complexes Control Intracellular Targeting and Cell Death Pathways

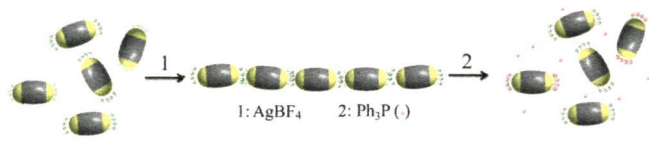
Kogularamanan Suntharalingam, Timothy C. Johnstone, Peter M. Bruno, Wei Lin, Michael T. Hemann, and Stephen J. Lippard*



14064 Ⓢ dx.doi.org/10.1021/ja4075979

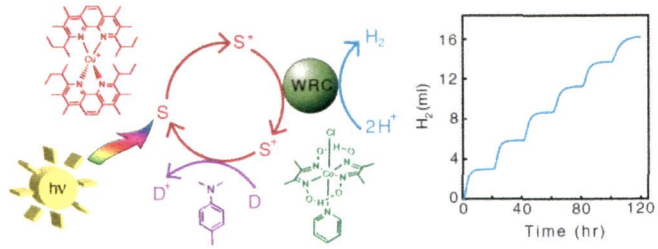
Patchy Particle Self-Assembly via Metal Coordination

Yufeng Wang, Andrew D. Hollingsworth, Si Kyung Yang, Sonal Patel, David J. Pine,* and Marcus Weck*



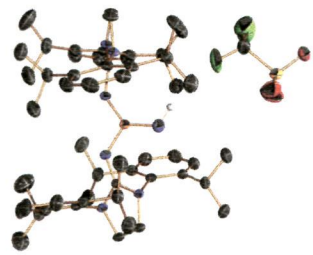
14068 S dx.doi.org/10.1021/ja407816f

Robust Cuprous Phenanthroline Sensitizer for Solar Hydrogen Photocatalysis
Rony S. Khnayzer, Catherine E. McCusker, Babatunde S. Olaiya, and Felix N. Castellano*



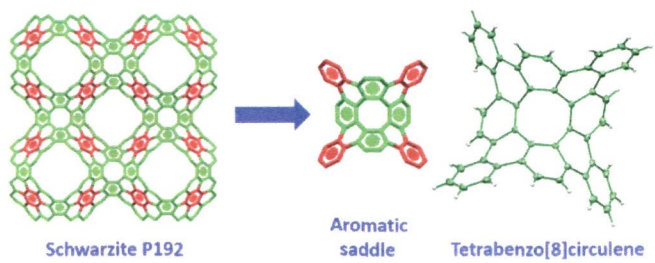
14071 S dx.doi.org/10.1021/ja4080979

Crystalline, Lewis Base-Free, Cationic Phosphoranimines (Iminophosphonium Salts)
Fabian Dielmann, Curtis E. Moore, Arnold L. Rheingold, and Guy Bertrand*



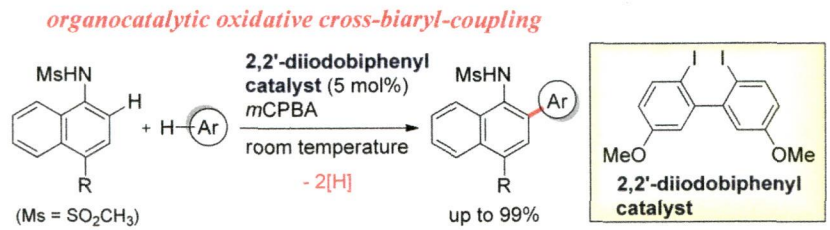
14074 S dx.doi.org/10.1021/ja407842z

Tetrabenzo[8]circulene: Aromatic Saddles from Negatively Curved Graphene
Youichi Sakamoto and Toshiyasu Suzuki*



14078 S dx.doi.org/10.1021/ja407944p

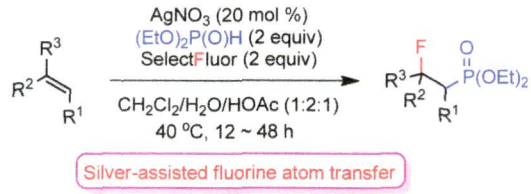
Organocatalytic C–H/C–H′ Cross-Biaryl Coupling: C-Selective Arylation of Sulfonanilides with Aromatic Hydrocarbons
Motoki Ito, Hiroko Kubo, Itsuki Itani, Koji Morimoto, Toshifumi Dohi, and Yasuyuki Kita*



14082 (S) dx.doi.org/10.1021/ja408031s

Silver-Catalyzed Radical Phosphonofluorination of Unactivated Alkenes

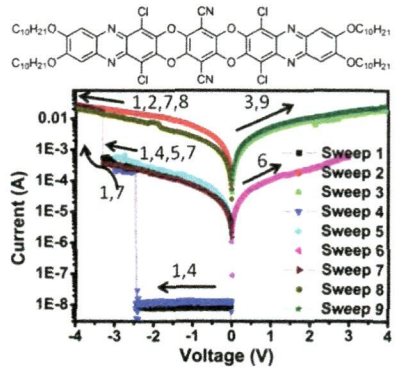
Chengwei Zhang, Zhaodong Li, Lin Zhu, Limei Yu, Zhentao Wang, and Chaozhong Li*



14086 (S) dx.doi.org/10.1021/ja408208c

Synthesis, Characterization, and Nonvolatile Ternary Memory Behavior of a Larger Heteroacene with Nine Linearly Fused Rings and Two Different Heteroatoms

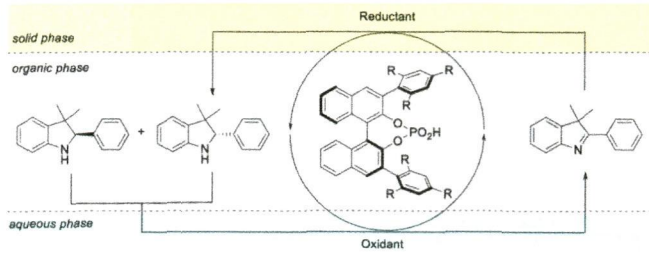
Pei-Yang Gu, Feng Zhou, Junkuo Gao, Gang Li, Chengyuan Wang, Qing-Feng Xu, Qichun Zhang,* and Jian-Mei Lu*



14090 (S) dx.doi.org/10.1021/ja4082827

Single-Operation Deracemization of 3H-Indolines and Tetrahydroquinolines Enabled by Phase Separation

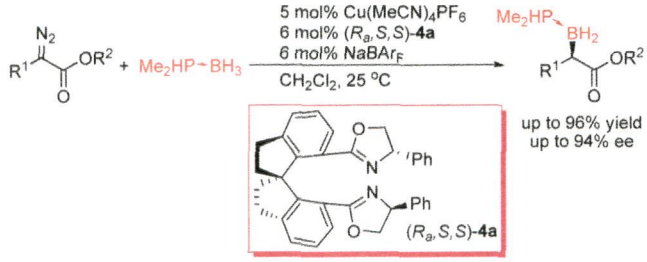
Aaron D. Lackner, Andrew V. Samant, and F. Dean Toste*



14094 (S) dx.doi.org/10.1021/ja408306a

Copper-Catalyzed B–H Bond Insertion Reaction: A Highly Efficient and Enantioselective C–B Bond-Forming Reaction with Amine–Borane and Phosphine–Borane Adducts

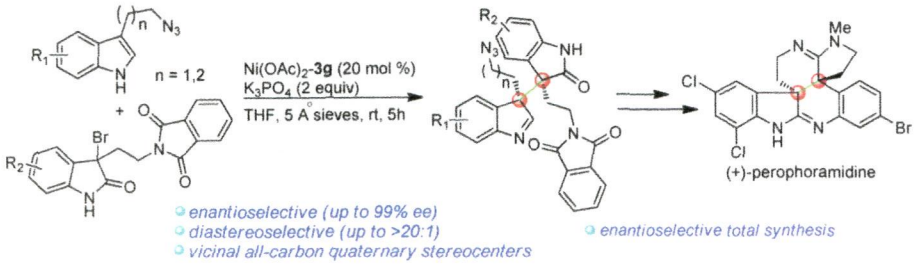
Qing-Qing Cheng, Shou-Fei Zhu,* Yong-Zhen Zhang, Xiu-Lan Xie, and Qi-Lin Zhou*



14098 (S) dx.doi.org/10.1021/ja408336v

Construction of Vicinal All-Carbon Quaternary Stereocenters by Catalytic Asymmetric Alkylation Reaction of 3-Bromooxindoles with 3-Substituted Indoles: Total Synthesis of (+)-Perophoramidine

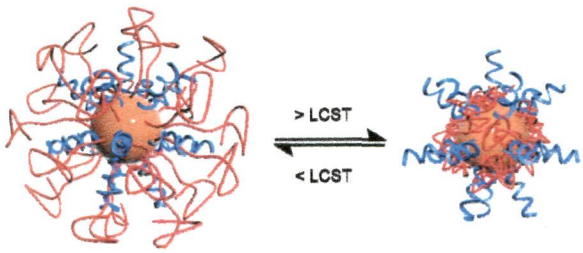
Hailong Zhang, Liang Hong, Hong Kang, and Rui Wang*

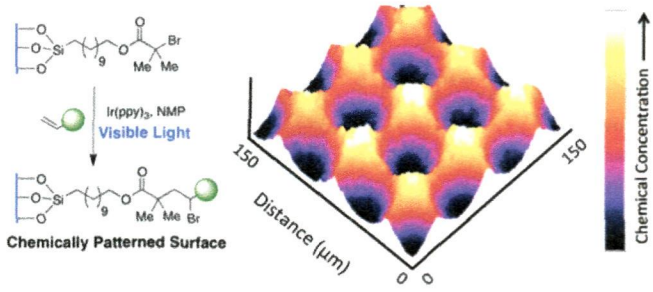


14102 (S) dx.doi.org/10.1021/ja408465t

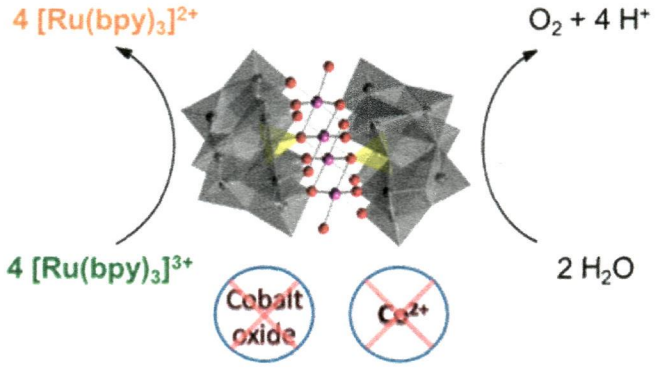
Temperature-Activated Nucleic Acid Nanostructures

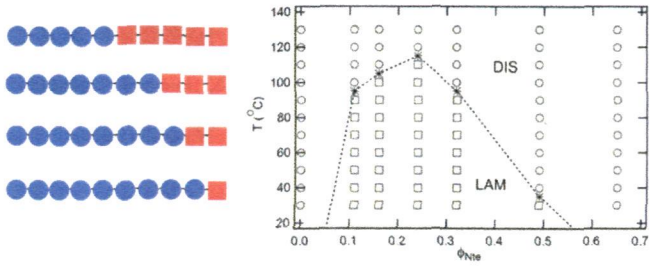
Ke Zhang,* Xiao Zhu, Fei Jia, Evelyn Auyeung, and Chad A. Mirkin*





Articles

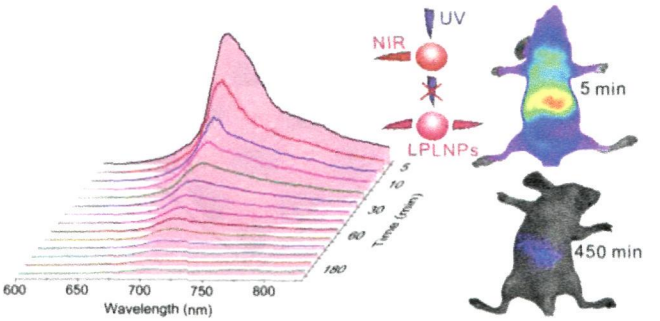




14125 Ⓢ dx.doi.org/10.1021/ja404243v

Functional Near Infrared-Emitting Cr^{3+}/Pr^{3+} Co-Doped Zinc Gallogermanate Persistent Luminescent Nanoparticles with Superlong Afterglow for *in Vivo* Targeted Bioimaging

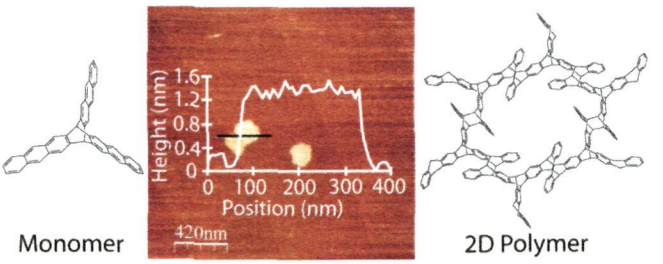
Abdukader Abdukayum, Jia-Tong Chen, Qiang Zhao, and Xiu-Ping Yan*



14134 Ⓢ dx.doi.org/10.1021/ja404351p

A *Two-Dimensional Polymer from the Anthracene Dimer and Triptycene Motifs*

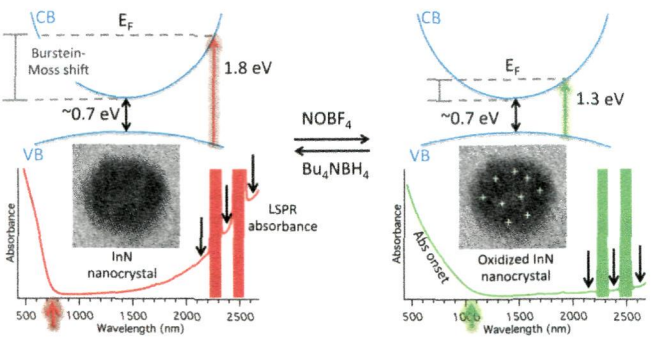
Radha Bhola, Payam Payamyar, Daniel J. Murray, Bharat Kumar, Aaron J. Teator, Martin U. Schmidt, Sonja M. Hammer, Animesh Saha, Junji Sakamoto, A. Dieter Schlüter, and Benjamin T. King*



14142 Ⓢ dx.doi.org/10.1021/ja404599g

Control of Plasmonic and Interband Transitions in Colloidal Indium Nitride Nanocrystals

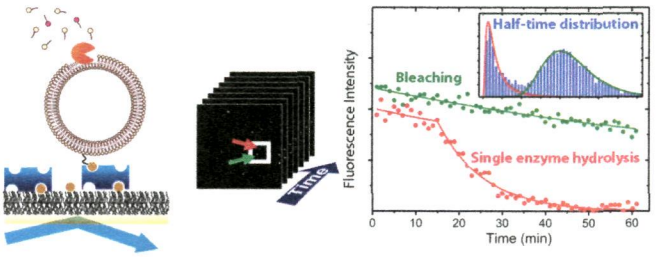
Peter K. B. Palomaki, Elisa M. Miller, and Nathan R. Neale*



14151 Ⓢ dx.doi.org/10.1021/ja4046313

Single Lipid Vesicle Assay for Characterizing Single-Enzyme Kinetics of Phospholipid Hydrolysis in a Complex Biological Fluid

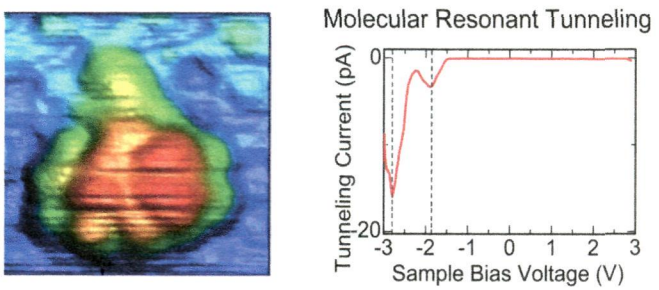
Seyed R. Tabaei, Michael Rabe, Henrik Zetterberg, Vladimir P. Zhdanov, and Fredrik Höök*



14159 Ⓢ dx.doi.org/10.1021/ja404512w

Negative Differential Resistance by Molecular Resonant Tunneling between Neutral Tribenzosubporphine Anchored to a Au(111) Surface and Tribenzosubporphine Cation Adsorbed on to a Tungsten Tip

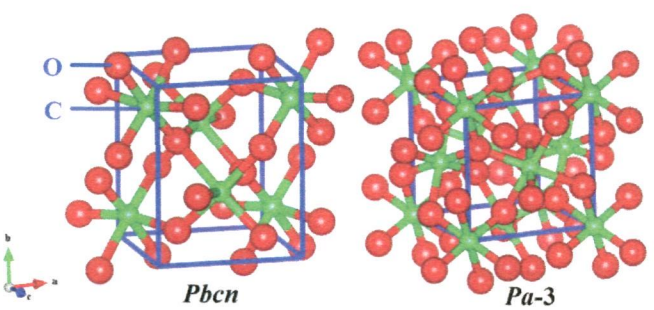
Yutaka Majima,* Daisuke Ogawa, Masachika Iwamoto, Yasuo Azuma, Eiji Tsurumaki, and Atsuhiro Osuka*



14167 Ⓢ dx.doi.org/10.1021/ja404854x

Structural Evolution of Carbon Dioxide under High Pressure

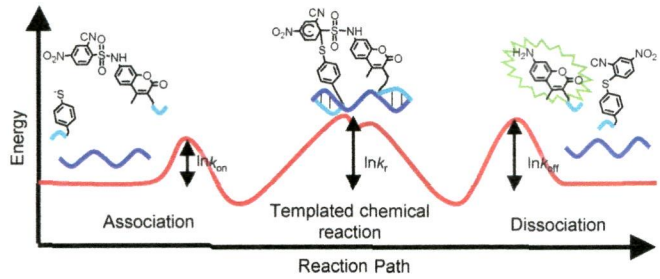
Cheng Lu, Maosheng Miao,* and Yanming Ma*



14172 Ⓢ dx.doi.org/10.1021/ja404743m

Very Rapid DNA-Templated Reaction for Efficient Signal Amplification and Its Steady-State Kinetic Analysis of the Turnover Cycle

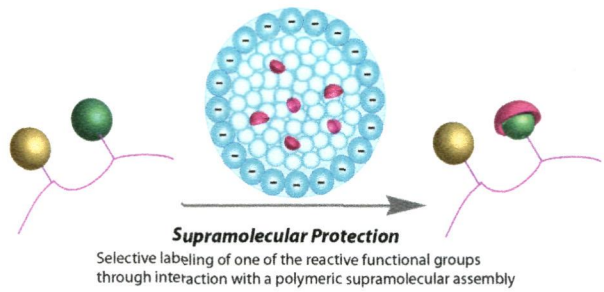
Aya Shibata, Takanori Uzawa, Yuko Nakashima, Mika Ito, Yukiko Nakano, Satoshi Shuto, Yoshihiro Ito,* and Hiroshi Abe*



14179 Ⓢ dx.doi.org/10.1021/ja404940s

Electrostatic Control of Peptide Side-Chain Reactivity Using Amphiphilic Homopolymer-Based Supramolecular Assemblies

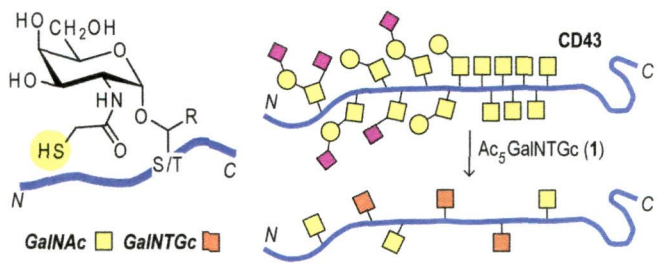
Feng Wang, Andrea Gomez-Escudero, Rajasekhar R. Ramireddy, Gladys Murage, S. Thayumanavan,* and Richard W. Vachet*



14189 Ⓢ dx.doi.org/10.1021/ja405189k

Inhibition of Mucin-Type *O*-Glycosylation through Metabolic Processing and Incorporation of *N*-Thioglycolyl-D-galactosamine Peracetate (Ac_5GalNTGc)

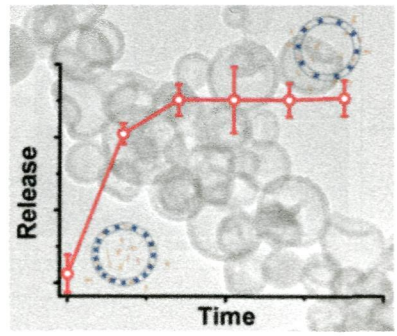
Kavita Agarwal, Rachna Kaul, Monika Garg, Asif Shajahan, Saroj Kumar Jha, and Srinivasa-Gopalan Sampathkumar*



14198 Ⓢ dx.doi.org/10.1021/ja405279t

Redox Responsive Release of Hydrophobic Self-Healing Agents from Polyaniline Capsules

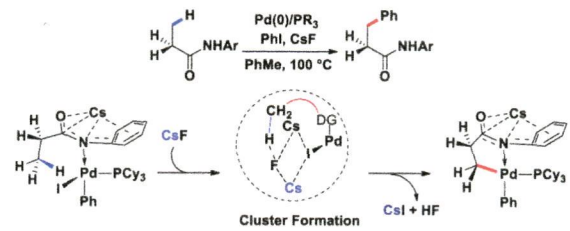
Li-Ping Lv, Yi Zhao, Nicole Vilbrandt, Markus Gallei, Ashokanand Vimalanandan, Michael Rohwerder, Katharina Landfester, and Daniel Crespy*



14206 Ⓢ dx.doi.org/10.1021/ja4053416

Understanding the Reactivity of Pd^0/PR_3-Catalyzed Intermolecular $C(sp^3)$–H Bond Arylation

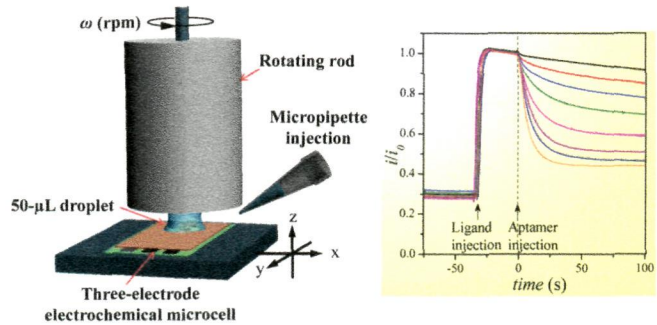
Travis M. Figg, Masayuki Wasa, Jin-Quan Yu,* and Djamaladdin G. Musaev*



14215 Ⓢ dx.doi.org/10.1021/ja405415q

Kinetic Rotating Droplet Electrochemistry: A Simple and Versatile Method for Reaction Progress Kinetic Analysis in Microliter Volumes

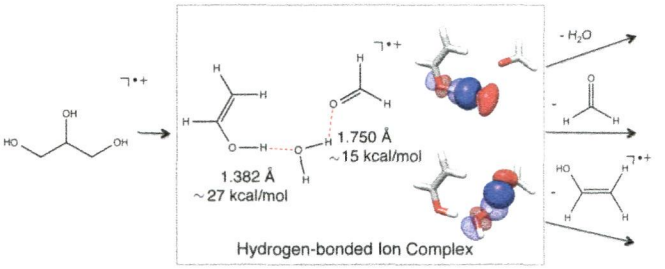
Lylian Challier, Rebeca Miranda-Castro, Damien Marchal, Vincent Noël, François Mavré,* and Benoît Limoges*



14229 (S) dx.doi.org/10.1021/ja405511v

Dissociative Photoionization of Glycerol and its Dimer Occurs Predominantly via a Ternary Hydrogen-Bridged Ion–Molecule Complex

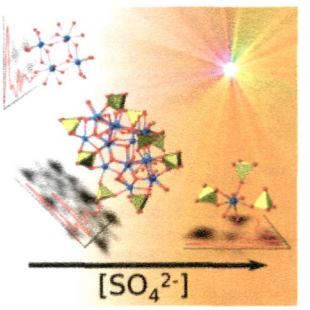
Franziska Bell, Qiao N. Ruan, Amir Golan, Paul R. Horn, Musahid Ahmed, Stephen R. Leone, and Martin Head-Gordon*



14240 (S) dx.doi.org/10.1021/ja405555h

Understanding the Role of Aqueous Solution Speciation and Its Application to the Directed Syntheses of Complex Oxidic Zr Chlorides and Sulfates

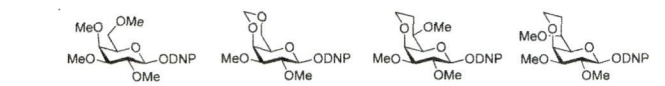
Yung-Jin Hu, Karah E. Knope, S. Skanthakumar, Mercouri G. Kanatzidis, John F. Mitchell, and L. Soderholm*



14249 (S) dx.doi.org/10.1021/ja405588x

Probing the Influence of a 4,6-*O*-Acetal on the Reactivity of Galactopyranosyl Donors: Verification of the Disarming Influence of the *trans–gauche* Conformation of C5–C6 Bonds

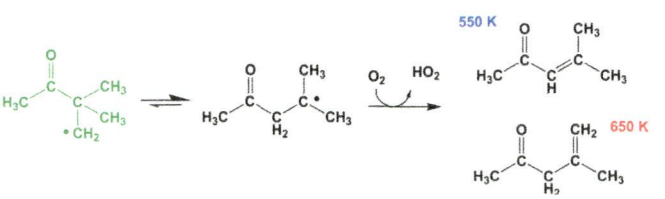
Myriame Moumé-Pymbock, Takayuki Furukawa, Sujit Mondal, and David Crich*



14256 (S) dx.doi.org/10.1021/ja405892y

Facile Rearrangement of 3-Oxoalkyl Radicals is Evident in Low-Temperature Gas-Phase Oxidation of Ketones

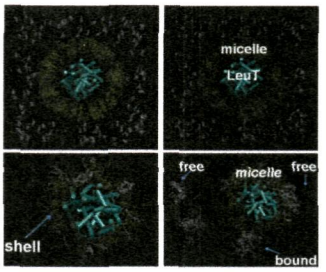
Adam M. Scheer,* Oliver Welz, Darryl Y. Sasaki, David L. Osborn, and Craig A. Taatjes*



14266 Ⓢ dx.doi.org/10.1021/ja405984v

The Membrane Protein LeuT in Micellar Systems: Aggregation Dynamics and Detergent Binding to the S2 Site

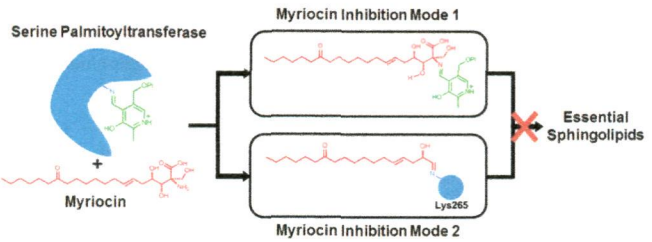
George Khelashvili,* Michael V. LeVine, Lei Shi, Matthias Quick, Jonathan A. Javitch, and Harel Weinstein



14276 Ⓢ dx.doi.org/10.1021/ja4059876

The Chemical Basis of Serine Palmitoyltransferase Inhibition by Myriocin

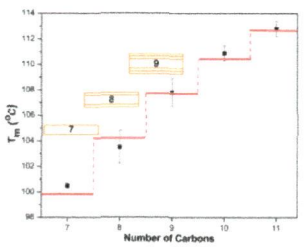
John M. Wadsworth, David J. Clarke, Stephen A. McMahon, Jonathan P. Lowther, Ashley E. Beattie, Pat R. R. Langridge-Smith, Howard B. Broughton, Teresa M. Dunn, James H. Naismith, and Dominic J. Campopiano*



14286 Ⓢ dx.doi.org/10.1021/ja4059958

Size Effect and Odd–Even Alternation in the Melting of Single and Stacked AgSC*n* Layers: Synthesis and Nanocalorimetry Measurements

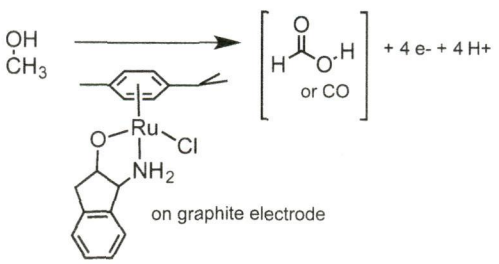
Lito P. de la Rama, Liang Hu, Zichao Ye, Mikhail Y. Efremov, and Leslie H. Allen*



14299 Ⓢ dx.doi.org/10.1021/ja4055564

Electrooxidation of Alcohols Catalyzed by Amino Alcohol Ligated Ruthenium Complexes

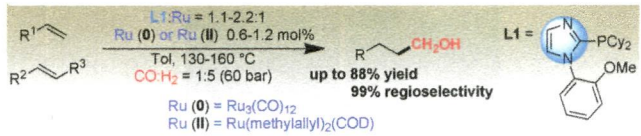
Kristen R. Brownell, Charles C. L. McCrory, Christopher E. D. Chidsey, Richard H. Perry, Richard N. Zare, and Robert M. Waymouth*



14306 (S) dx.doi.org/10.1021/ja4060977

Ruthenium-Catalyzed Hydroformylation/Reduction of Olefins to Alcohols: Extending the Scope to Internal Alkenes

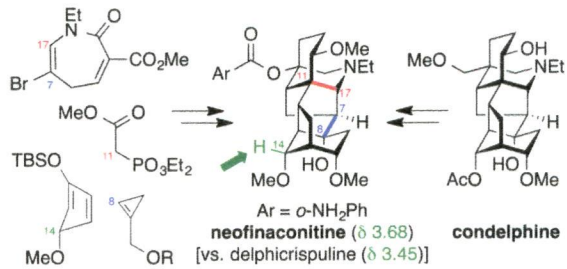
Lipeng Wu, Ivana Fleischer, Ralf Jackstell, Irina Profir, Robert Franke, and Matthias Beller*



14313 (S) dx.doi.org/10.1021/ja4064958

Total Synthesis, Relay Synthesis, and Structural Confirmation of the C18-Norditerpenoid Alkaloid Neofinaconitine

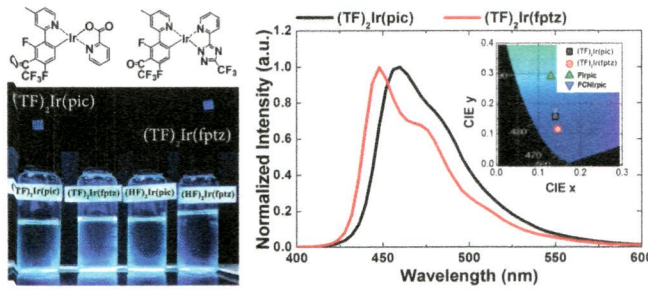
Yuan Shi,* Jeremy T. Wilmot, Lars Ulrik Nordstrøm, Derek S. Tan,* and David Y. Gin



14321 (S) dx.doi.org/10.1021/ja4065188

Deep-Blue Phosphorescence from Perfluoro Carbonyl-Substituted Iridium Complexes

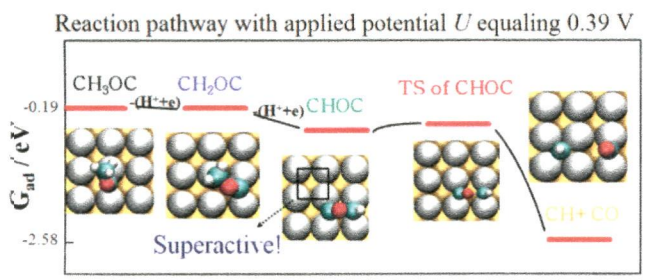
Sunghun Lee, Seul-Ong Kim, Hyun Shin, Hui-Jun Yun, Kiyull Yang, Soon-Ki Kwon,* Jang-Joo Kim,* and Yun-Hi Kim*



14329 (S) dx.doi.org/10.1021/ja406655q

Why (1 0 0) Terraces Break and Make Bonds: Oxidation of Dimethyl Ether on Platinum Single-Crystal Electrodes

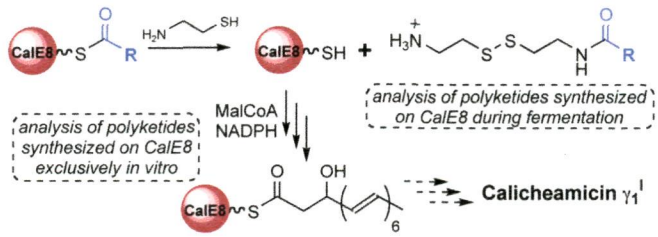
Hongjiao Li, Federico Calle-Vallejo, Manuel J. Kolb, Youngkook Kwon, Yongdan Li, and Marc T.M. Koper*



14339 Ⓢ dx.doi.org/10.1021/ja406697t

Biochemical Determination of Enzyme-Bound Metabolites: Preferential Accumulation of a Programmed Octaketide on the Enediyne Polyketide Synthase CalE8

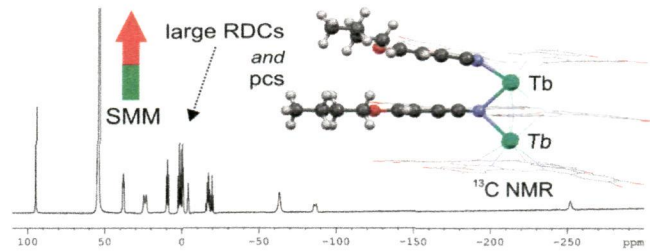
Katherine Belecki and Craig A. Townsend*



14349 Ⓢ dx.doi.org/10.1021/ja4069485

Combined NMR Analysis of Huge Residual Dipolar Couplings and Pseudocontact Shifts in Terbium(III)-Phthalocyaninato Single Molecule Magnets

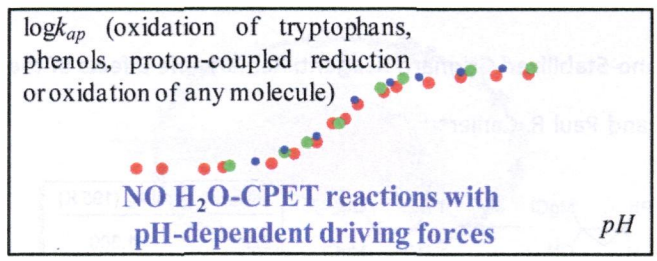
Marko Damjanovic, Keiichi Katoh, Masahiro Yamashita, and Markus Enders*



14359 Ⓢ dx.doi.org/10.1021/ja406712c

Proton-Coupled Electron Transfers: pH-Dependent Driving Forces? Fundamentals and Artifacts

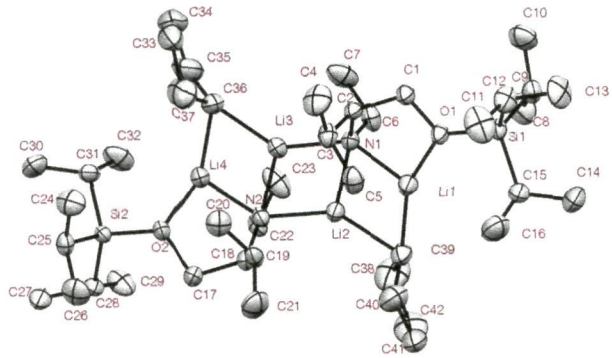
Julien Bonin, Cyrille Costentin, Marc Robert, Mathilde Routier, and Jean-Michel Savéant*



14367 Ⓢ dx.doi.org/10.1021/ja406912h

Mixed Aggregates of an Alkyl Lithium Reagent and a Chiral Lithium Amide Derived from *N*-Ethyl-*O*-triisopropylsilyl Valinol

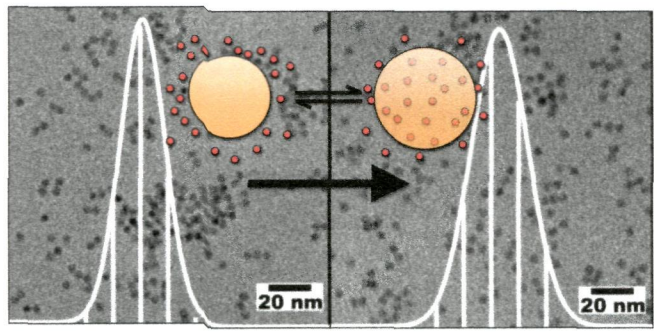
Chicheung Su, Russell Hopson, and Paul G. Williard*



14380 Ⓢ dx.doi.org/10.1021/ja4072207

Nanocrystal Diffusion Doping

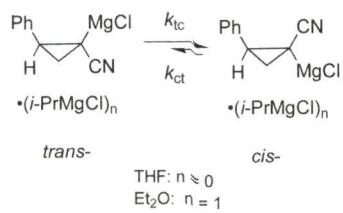
Vladimir A. Vlaskin, Charles J. Barrows, Christian S. Erickson, and Daniel R. Gamelin*



14390 Ⓢ dx.doi.org/10.1021/ja407348s

Stereochemical Inversion of a Cyano-Stabilized Grignard Reagent: Remarkable Effects of the Ethereal Solvent Structure and Concentration

Ming Gao, Neeraj N. Patwardhan, and Paul R. Carlier*

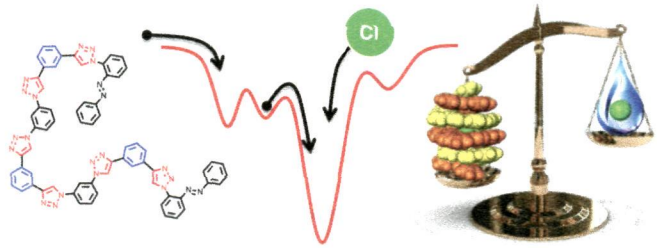


solvent	rel k_{tc} (195 K)
THF	1,300
2-MeTHF	800
Et_2O	26
0.12 M Et_2O in toluene	1.0

14401 S dx.doi.org/10.1021/ja4074744

Hydrophobic Collapse of Foldamer Capsules Drives Picomolar-Level Chloride Binding in Aqueous Acetonitrile Solutions

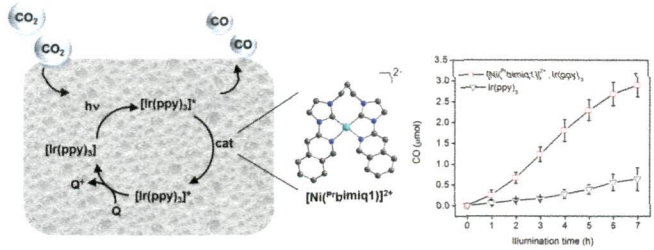
Yuran Hua, Yun Liu, Chun-Hsing Chen, and Amar H. Flood*



14413 S dx.doi.org/10.1021/ja4074003

Visible-Light Photoredox Catalysis: Selective Reduction of Carbon Dioxide to Carbon Monoxide by a Nickel *N*-Heterocyclic Carbene–Isoquinoline Complex

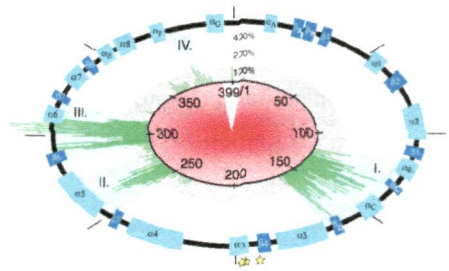
V. Sara Thoi, Nikolay Kornienko, Charles G. Margarit, Peidong Yang, and Christopher J. Chang*



14425 S dx.doi.org/10.1021/ja4074886

Improved Biocatalysts from a Synthetic Circular Permutation Library of the Flavin-Dependent Oxidoreductase Old Yellow Enzyme

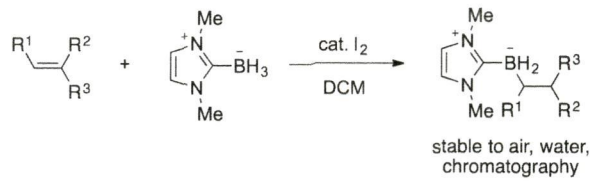
Ashley B. Daugherty, Sridhar Govindarajan, and Stefan Lutz*



14433 S dx.doi.org/10.1021/ja407678e

Molecular Iodine Initiates Hydroborations of Alkenes with N-Heterocyclic Carbene Boranes

Xiangcheng Pan, Anne Boussonnière, and Dennis P. Curran*

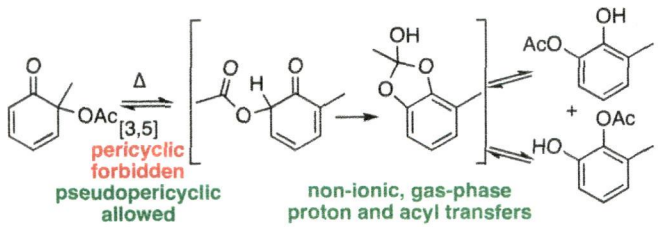


stable to air, water, chromatography

14438 Ⓢ dx.doi.org/10.1021/ja4077364

Experimental and Computational Studies on the [3,3]- and [3,5]-Sigmatropic Rearrangements of Acetoxycyclohexadienones: A Non-ionic Mechanism for Acyl Migration

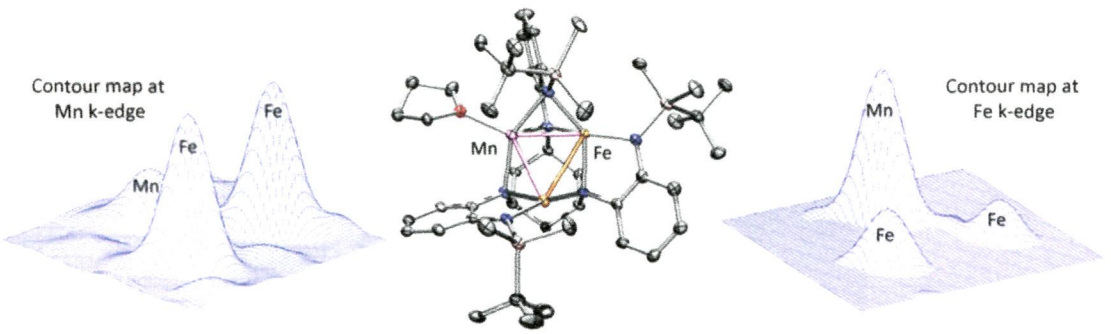
Shikha Sharma, Trideep Rajale, David B. Cordes, Fernando Hung-Low, and David M. Birney*



14448 Ⓢ dx.doi.org/10.1021/ja408003d

Synthesis of Open-Shell, Bimetallic Mn/Fe Trinuclear Clusters

Tamara M. Powers, Nina X. Gu, Alison R. Fout, Anne M. Baldwin, Raúl Hernández Sánchez, Denise M. Alfonso, Yu-Sheng Chen, Shao-Liang Zheng, and Theodore A. Betley*



Additions and Corrections

14459 dx.doi.org/10.1021/ja407418m

Correction to "A Sugar-Functionalized Amphiphilic Pillar[5]arene: Synthesis, Self-Assembly in Water, and Application in Bacterial Cell Agglutination"

Guocan Yu, Yingjie Ma, Chengyou Han, Yong Yao, Guping Tang, Zhengwei Mao, Changyou Gao, and Feihe Huang*

14460 dx.doi.org/10.1021/ja4082217

Correction to "Synthesis, Characterization, and Heterobimetallic Cooperation in a Titanium–Chromium Catalyst for Highly Branched Polyethylenes"

Shaofeng Liu, Alessandro Motta, Massimiliano Delferro,* and Tobin J. Marks*

Ⓢ Supporting Information available via online article