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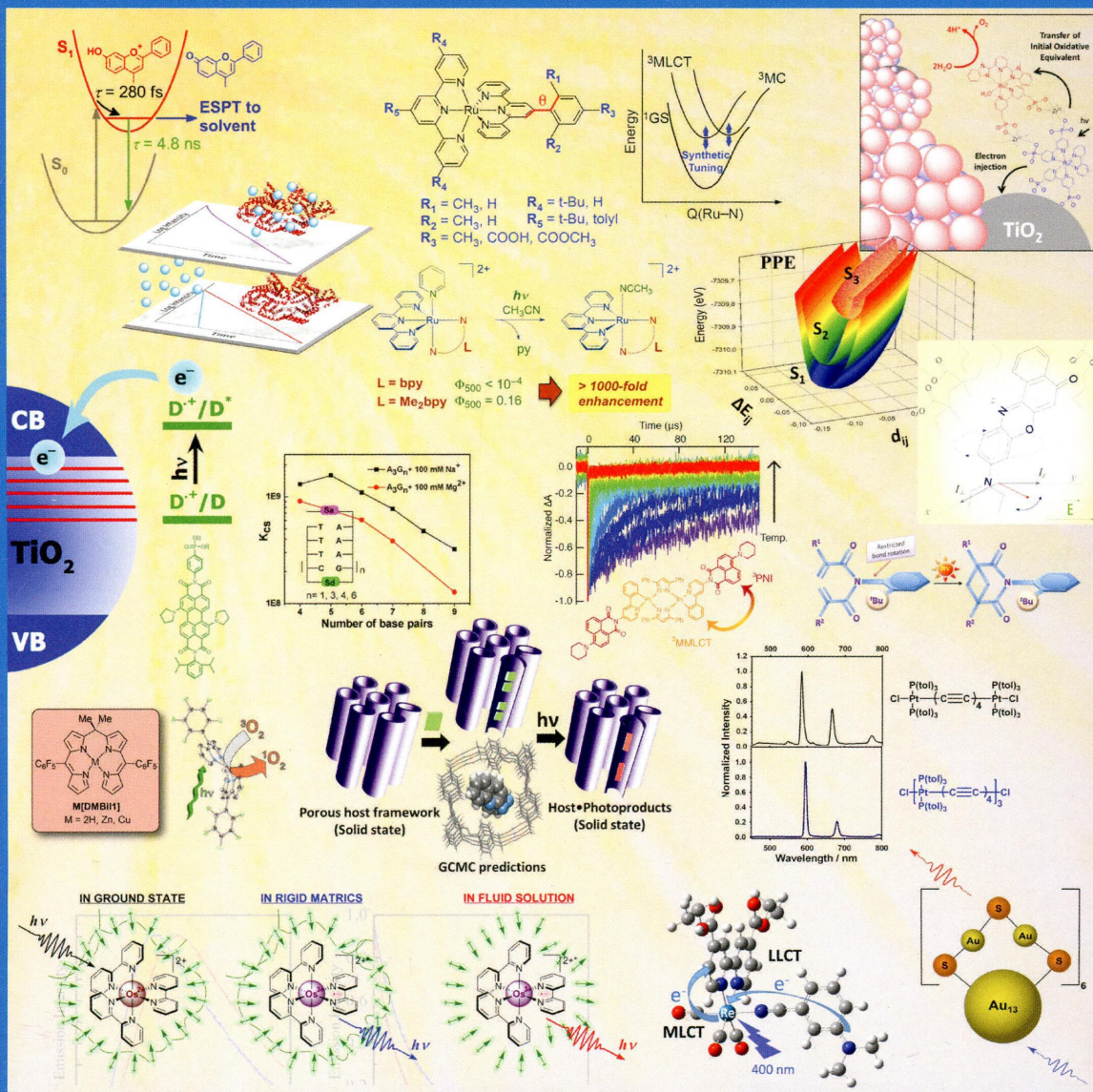
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THE JOURNAL OF PHYSICAL CHEMISTRY

A

CURRENT TOPICS IN PHOTOCHEMISTRY

Use of Photochemistry
and Photophysics of
Molecules and
Materials for
Numerous Applications
(see page 5A)



ISOLATED MOLECULES, CLUSTERS, RADICALS, AND IONS; ENVIRONMENTAL CHEMISTRY,
GEOCHEMISTRY, AND ASTROCHEMISTRY; THEORY

ON THE COVER: A collage of images from articles in this Special Issue (starting in the top left, from left to right and top to bottom): Quina et al. (DOI: 10.1021/jp504189m); Damrauer et al. (DOI: 10.1021/jp508145w); Papanikolas et al. (DOI: 10.1021/jp411139j); Martí et al. (DOI: 10.1021/jp502837a); Turro et al. (DOI: 10.1021/jp5057732); Tretiak et al. (DOI: 10.1021/jp503350k); Aramendia et al. (DOI: 10.1021/jp500272y); Moore et al. (DOI: 10.1021/jp506284q); Wasielewski, Lewis et al. (DOI: 10.1021/jp502974s); Castellano et al. (DOI: 10.1021/jp503827e); Sivaguru et al. (DOI: 10.1021/jp505678b); Rosenthal et al. (DOI: 10.1021/jp506412r); Shimizu et al. (DOI: 10.1021/jp505304n); Schanze et al. (DOI: 10.1021/jp5021388); Meyer et al. (DOI: 10.1021/jp5019873); Schmehl, Beratan, Rubtsov et al. (DOI: 10.1021/jp5039877); and Knappenberger et al. (DOI: 10.1021/jp505913j). This special issue was organized by Guest Editor Claudia Turro.

SPECIAL SECTION: CURRENT TOPICS IN PHOTOCHEMISTRY

Guest Editor: Claudia Turro

Special Issue Preface

10299

DOI: 10.1021/jp510537x

Preface to Special Issue on Current Topics in Photochemistry

Claudia Turro*

Articles

10301

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DOI: 10.1021/jp411139j

Photophysical Characterization of a Chromophore/Water Oxidation Catalyst Containing a Layer-by-Layer Assembly on Nanocrystalline TiO₂ Using Ultrafast Spectroscopy

Stephanie E. Bettis, Kenneth Hanson, Li Wang, Melissa K. Gish, Javier J. Concepcion, Zhen Fang, Thomas J. Meyer, and John M. Papanikolas*

10309

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DOI: 10.1021/jp500272y

Influence of the Glass Transition on Rotational Dynamics of Dyes in Thin Polymer Films: Single-Molecule and Ensemble Experiments

Beatriz Araoz, Aquiles Carattino, Daniela Täuber, Christian von Borczyskowski,* and Pedro F. Aramendia*


10318

S

DOI: 10.1021/jp500397g

Synthesis, Photophysics, and Reverse Saturable Absorption of Bipyridyl Platinum(II) Bis(acetylide) Complexes Bearing Aromatic Electron-Withdrawing Substituents on the Acetylide Ligands

Xu-Guang Liu and Wenfang Sun*

10326  DOI: 10.1021/jp5019873

Rigid Medium Effects on Photophysical Properties of MLCT Excited States of Polypyridyl Os(II) Complexes in Polymerized Poly(ethylene glycol)dimethacrylate Monoliths

Akitaka Ito, Troy E. Knight, David J. Stewart, M. Kyle Brennaman, and Thomas J. Meyer*

10333  DOI: 10.1021/jp5021388

Photophysics of Platinum Tetrayne Oligomers: Delocalization of Triplet Exciton

Yongjun Li, Russell W. Winkel, Nancy Weisbach, John A. Gladysz,* and Kirk S. Schanze*

10340  DOI: 10.1021/jp502243c

Optoelectronic Properties and Structural Effects of the Incremental Addition of Pyridyl Moieties on a Rhodium Dimer

Daniel Chartrand and Garry S. Hanan*

10353  DOI: 10.1021/jp502837a

Ascertaining Free Histidine from Mixtures with Histidine-Containing Proteins Using Time-Resolved Photoluminescence Spectroscopy

Kewei Huang, Chengmin Jiang, and Angel A. Marti*

10359  DOI: 10.1021/jp502974s

Effect of Mg²⁺ Cations on the Dynamics and Efficiency of Hole Transport in DNA

Arun Kalliat Thazhathveetil, Anton Trifonov, Michael R. Wasielewski,* and Frederick D. Lewis*

10364  DOI: 10.1021/jp503149x

Singlet Oxygen Generation on Porous Superhydrophobic Surfaces: Effect of Gas Flow and Sensitizer Wetting on Trapping Efficiency

Yuanyuan Zhao, Yang Liu, Qianfeng Xu, Mark Barahman, Dorota Bartusik, Alexander Greer,* and Alan M. Lyons*

10372 DOI: 10.1021/jp503350k

Signature of Nonadiabatic Coupling in Excited-State Vibrational Modes

Miguel A. Soler, Tammie Nelson, Adrian E. Roitberg, Sergei Tretiak,* and Sebastian Fernandez-Alberti*

10380  DOI: 10.1021/jp503819u

Tuning Emission Colors from Blue to Green in Polymeric Light-Emitting Diodes Fabricated using Polyfluorene Blends

Fernando Júnior Quites, Gregório Couto Faria, José Carlos Germino, and Teresa Dib Zambon Atvars*

10391  DOI: 10.1021/jp503827e

Excited State Equilibrium Induced Lifetime Extension in a Dinuclear Platinum(II) Complex

Catherine E. McCusker, Arnab Chakraborty, and Felix N. Castellano*

10400  DOI: 10.1021/jp503901v

Photochemical Generation of Strong One-Electron Reductants via Light-Induced Electron Transfer with Reversible Donors Followed by Cross Reaction with Sacrificial Donors
Bing Shan and Russell Schmehl*

10407  DOI: 10.1021/jp5039877

Full-Electron Ligand-to-Ligand Charge Transfer in a Compact Re(I) Complex
Yuankai Yue, Tod Grusenmeyer, Zheng Ma, Peng Zhang, Russell H. Schmehl, David N. Beratan, and Igor V. Rubtsov*

10416  DOI: 10.1021/jp504030f

Fluorescent Ligands and Energy Transfer in Photoactive Ruthenium–Bipyridine Complexes
Guillermo Carrone, Federico Gantov, Leonardo D. Slep, and Roberto Etchenique*

10425  DOI: 10.1021/jp504078g

Investigating the Effects of Solvent on the Ultrafast Dynamics of a Photoreversible Ruthenium Sulfoxide Complex
Albert W. King, Beth Anne McClure, Yuhuan Jin, and Jeffrey J. Rack*

10433  DOI: 10.1021/jp504174t

Trans–Cis Isomerization of Vinylketones through Triplet 1,2-Biradicals
R. A. A. Upul Ranaweera, Tianeka Scott, Qian Li, Sridhar Rajam, Alexander Duncan, Rui Li, Anthony Evans, Cornelia Bohne, John P. Toscano, Bruce S. Ault, and Anna D. Gudmundsdottir*

10448  DOI: 10.1021/jp504189m

Femtosecond and Temperature-Dependent Picosecond Dynamics of Ultrafast Excited-State Proton Transfer in Water–Dioxane Mixtures
Adilson A. Freitas,* Frank H. Quina,* and António A. L. Maçanita

10456 DOI: 10.1021/jp504237p


Repopulation of Nitrogen Excited Triplet State Following Laser-Induced Filamentation
Bradley R. Arnold,* Stephen D. Roberson, and Paul M. Pellegrino


10464  DOI: 10.1021/jp504254a

The Effects of Side-Chain-Induced Disorder on the Emission Spectra and Quantum Yields of Oligothiophene Nanoaggregates: A Combined Experimental and MD-TDDFT Study
Jiyun Hong, SuKyung Jeon, Janice J. Kim, Diane Devi, Kelly Chacon-Madrid, Wynnee Lee, Seung Moh Koo, Jurjen Wildeman, Matthew Y. Sfeir, Linda A. Peteanu,* Jin Wen, and Jing Ma*


10474  DOI: 10.1021/jp504249a

Mechanistic Study on the Photochemical “Light Switch” Behavior of [Ru(bpy)₂dmdppz]²⁺
Erin Wachter and Edith C. Glazer*


10487  DOI: 10.1021/jp504281y
Intramolecular Cycloadditions of Photogenerated Azaxylylenes: An Experimental and Theoretical Study
Olga A. Mukhina, W. Cole Cronk, N. N. Bhuvan Kumar, M. Chandra Sekhar, Anunay Samanta, and Andrei G. Kutateladze*


10497  DOI: 10.1021/jp504294j
Ultrafast Structural Dynamics of Cu(I)-Bicinchoninic Acid and Their Implications for Solar Energy Applications
Kelly A. Fransted, Nicholas E. Jackson, Ruifa Zong, Michael W. Mara, Jier Huang, Michael R. Harpham, Megan L. Shelby, Randolph P. Thummel,* and Lin X. Chen*


10507  DOI: 10.1021/jp504330s
Ru(II) Dyads Derived from 2-(1-Pyrenyl)-1*H*-imidazo[4,5-*f*][1,10]phenanthroline: Versatile Photosensitizers for Photodynamic Applications
Mat Stephenson, Christian Reichardt, Mitch Pinto, Maria Wächter, Tariq Sainuddin, Ge Shi, Huimin Yin, Susan Monro, Eric Sampson, Benjamin Dietzek,* and Sherri A. McFarland*

10522  DOI: 10.1021/jp504349b
Direct Determination of Resonance Energy Transfer in Photolyase: Structural Alignment for the Functional State
Chuang Tan, Lijun Guo, Yuejie Ai, Jiang Li, Lijuan Wang, Aziz Sançar, Yi Luo, and Dongping Zhong*

10531 DOI: 10.1021/jp504509s
Effect of Concentration on the Formation of Rose Bengal Triplet State on Microcrystalline Cellulose: A Combined Laser-Induced Optoacoustic Spectroscopy, Diffuse Reflectance Flash Photolysis, and Luminescence Study
Yair Litman, Matthew G. Voss, Hernán B. Rodríguez, and Enrique San Román*

10538  DOI: 10.1021/jp504805y
From Ordinary to Blue Emission in Peralkylated *n*-Oligosilanes: The Calculated Structure of Delocalized and Localized Singlet Excitons
Matthew K. MacLeod and Josef Michl*

10554  DOI: 10.1021/jp505196v
Photoisomerization and Photooxygenation of 1,4-Diaryl-1,3-dienes in a Confined Space
Shampa R. Samanta, Rajib Choudhury, and V. Ramamurthy*

10563  DOI: 10.1021/jp505304n
Applications of a Bis-Urea Phenylethynylene Self-Assembled Nanoreactor for [2 + 2] Photodimerizations
Sandipan Dawn, Sahan R. Salpage, Brent A. Koscher, Andreas Bick, Arief C. Wibowo, Perry J. Pellechia, and Linda S. Shimizu*

- 10575  DOI: 10.1021/jp5056478
Four-Component Fluorescence of *trans*-1,2-Di(1-methyl-2-naphthyl)ethene at 77 K in Glassy Media. Conformational Subtleties Revealed
Christopher Redwood, V. K. Ratheesh Kumar, Stuart Hutchinson, Frank B. Mallory, Clelia W. Mallory, Olga Dmitrenko, and Jack Saltiel*
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- 10587  DOI: 10.1021/jp505656e
NIR Photocleavage of the Si–C Bond in Axial Si-Phthalocyanines
Tennyson Doane, Yu Cheng, Nipun Sodhi, and Clemens Burda*
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- 10596  DOI: 10.1021/jp505678b
Dictating Photoreactivity through Restricted Bond Rotations: Cross-Photoaddition of Atropisomeric Acrylimide Derivatives under UV/Visible-Light Irradiation
Akila Iyer, Steffen Jockusch,* and J. Sivaguru*
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- 10603  DOI: 10.1021/jp5057732
Unusually Efficient Pyridine Photodissociation from Ru(II) Complexes with Sterically Bulky Bidentate Ancillary Ligands
Jessica D. Knoll, Bryan A. Albani, Christopher B. Durr, and Claudia Turro*
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- 10611  DOI: 10.1021/jp505913j
Temperature-Dependent Photoluminescence of Structurally-Precise Quantum-Confined Au₂₅(SC₈H₉)₁₈ and Au₃₈(SC₁₂H₂₅)₂₄ Metal Nanoparticles
Thomas D. Green, Chongyue Yi, Chenjie Zeng, Rongchao Jin, Stephen McGill, and Kenneth L. Knappenberger Jr.*
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- 10622  DOI: 10.1021/jp5059148
Electronic Excited State Redox Properties for BODIPY Dyes Predicted from Hammett Constants: Estimating the Driving Force of Photoinduced Electron Transfer
Richard Lincoln, Lana E. Greene, Katerina Krumova, Zhutian Ding, and Gonzalo Cosa*
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- 10631  DOI: 10.1021/jp506284q
Controlling Surface Defects and Photophysics in TiO₂ Nanoparticles
Manuel J. Llansola-Portoles,* Jesse J. Bergkamp, Daniel Finkelstein-Shapiro, Benjamin D. Sherman, Gerdenis Kodis, Nada M. Dimitrijevic, Devens Gust, Thomas A. Moore, and Ana L. Moore
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- 10639  DOI: 10.1021/jp506412r
Electrochemical, Spectroscopic, and ¹O₂ Sensitization Characteristics of 10,10-Dimethylbiladiene Complexes of Zinc and Copper
Allen J. Pistner, Rachel C. Pupillo, Glenn P. A. Yap, Daniel A. Lutterman, Ying-Zhong Ma, and Joel Rosenthal*

10649 

DOI: 10.1021/jp508145w

Synthesis, Electrochemical Characterization, and Photophysical Studies of Structurally Tuned Aryl-Substituted Terpyridyl Ruthenium(II) Complexes

Karen E. Spettel and Niels H. Damrauer*

10663 

DOI: 10.1021/jp508283d

Deactivating Unproductive Pathways in Multichromophoric Sensitizers

Randy Pat Sabatini, Bo Zheng, Wen-Fu Fu, Daniel J. Mark, Michael F. Mark, Emily Anne Hillenbrand, Richard Eisenberg,* and David W. McCamant*

Articles

Kinetics and Dynamics

10673 

DOI: 10.1021/jp507596b

Extensive Study of Shape and Surface Structure Formation in the Mercury Beating Heart System

E. Ramirez-Álvarez,* J. L. Ocampo-Espindola, Fernando Montoya, F. Yousif, F. Vázquez, and M. Rivera

10679 

DOI: 10.1021/jp508059j

Collision-Induced Dissociation of Monolayer Protected Clusters Au₁₄₄ and Au₁₃₀ in an Electrospray Time-of-Flight Mass Spectrometer

David M. Black, Nabraj Bhattarai, Robert L. Whetten,* and Stephan B. H. Bach*

10688

DOI: 10.1021/jp5085247

Reaction of Iodine Atoms with Submicrometer Squalane and Squalene Droplets: Mechanistic Insights into Heterogeneous Reactions

Denisia M. Popolan-Vaida, Kevin R. Wilson, and Stephen R. Leone*

10699

DOI: 10.1021/jp508836p

Spatiotemporal Behavior Induced by Differential Diffusion in Landolt Systems

István Szalai*

10706

DOI: 10.1021/jp509158p

Kinetics of the Oxidation of Iodide Ion by Persulfate Ion in the Critical Water/Bis(2-ethylhexyl) Sodium Sulfosuccinate/*n*-Decane Microemulsions

Handi Yin, Zhongyu Du, Jihua Zhao, and Weiguo Shen*






10713 

DOI: 10.1021/jp509164e

Kinetics and Mechanism of the Oxidation of Bromide by Periodate in Aqueous Acidic Solution

Viktor Szél, György Csekő, and Attila K. Horváth*

Spectroscopy, Photochemistry, and Excited States

- 10720  DOI: 10.1021/jp5053858
Infrared Spectroscopy and Density Functional Theory Investigation of Calcite, Chalk, and Coccoliths—Do We Observe the Mineral Surface?
M. P. Andersson,* C. P. Hem, L. N. Schultz, J. W. Nielsen, C. S. Pedersen, K. K. Sand, D. V. Okhrimenko, A. Johansson, and S. L. S. Stipp
- 10730  DOI: 10.1021/jp506530g
Gas Phase UV Spectrum of a Cu(II)–Bis(benzene) Sandwich Complex: Experiment and Theory
Lifu Ma, Joseph Koka, Anthony J. Stace,* and Hazel Cox*
- 10738  DOI: 10.1021/jp506600p
Interactions between Carboxylic Acids and Aldehydes: A Rotational Study of HCOOH–CH₂O
Qian Gou, Laura B. Favero, Somana S. Bahamyirou, Zhining Xia, and Walther Caminati*
- 10742 DOI: 10.1021/jp504720n
Computational Study of Photoexcited Dynamics in Bichromophoric Cross-Shaped Oligofluorene
D. Ondarse-Alvarez, N. Oldani, S. Tretiak, and S. Fernandez-Alberti*
- 10754 DOI: 10.1021/jp508605c
Shape of the Absorption and Fluorescence Spectra of Condensed Phases and Transition Energies
Miguel Lagos* and Rodrigo Paredes*
- 10763 DOI: 10.1021/jp509512u
Predictable Valence Excited States of Anions
Ryan C. Fortenberry,* W. James Morgan, and Jordan D. Enyard
- Environmental and Atmospheric Chemistry, Aerosol Processes, Geochemistry, and Astrochemistry**
- 10770  DOI: 10.1021/jp506377w
Photochemical Properties of Hydrofluoroethers CH₃OCHF₂, CH₃OCF₃, and CHF₂OCH₂CF₃: Reactivity toward OH, IR Absorption Cross Sections, Atmospheric Lifetimes, and Global Warming Potentials
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- 10778  DOI: 10.1021/jp506815v
Atmospheric Oxidation Mechanism of *m*-Xylene Initiated by OH Radical
Shanshan Pan and Liming Wang*

10788  DOI: 10.1021/jp506206b

Effects of Axial Coordination on Immobilized Mn(salen) Catalysts

Filipe Teixeira,* Ricardo A. Mosquera, André Melo, Cristina Freire, and M. Natália D. S. Cordeiro*

10797  DOI: 10.1021/jp507865h

C_α Hydrogen Atom Transfer in Post-Cleavage Radical-Cation Complexes: Short and Steep versus Long Winding Road

Benjamin J. Bythell*

10804  DOI: 10.1021/jp5082033

How Short is the Strongest Hydrogen Bond in the Proton-Bound Homodimers of Pyridine Derivatives?

Andrey A. Gurinov, Stepan B. Lesnichin, Hans-Heinrich Limbach, and Ilya G. Shenderovich*

10813  DOI: 10.1021/jp508220h

The Role of Charge States in the Atomic Structure of Cu_n and Pt_n (n = 2–14 atoms) Clusters: A DFT Investigation

Anderson S. Chaves,* Gustavo G. Rondina,* Maurício J. Piotrowski,* Polina Tereshchuk,* and Juarez L. F. Da Silva*

10822 DOI: 10.1021/jp5083906

A Quantitative Metric for Conjugation in Polyene Hydrocarbons Having a Single Classical Structure

Jerry Ray Dias*

10837  DOI: 10.1021/jp508657s

Theoretical Study on Diradical Characters and Nonlinear Optical Properties of 1,3-Diradical Compounds

Ryohei Kishi,* Yusuke Murata, Michika Saito, Keisuke Morita, Manabu Abe, and Masayoshi Nakano*

10849  DOI: 10.1021/jp509212t

Chalcogen Bonding between Tetravalent SF₄ and Amines

Vincent de Paul N. Nziko and Steve Scheiner*

10857  DOI: 10.1021/jp509549q

Molecular Design and Property Prediction of High Density Polynitro[3.3.3]-Propellane-Derivatized Frameworks as Potential High Explosives

Qinghua Zhang,* Jiaheng Zhang, Xiujuan Qi, and Jean'ne M. Shreeve*