

## Content

### 1. Photoinduced Proton Transfer in Chemistry and Biology

Pi-Tai Chou and Kyril M. Solntsev

*The Journal of Physical Chemistry B* 2015 119 (6), 2089-2089

DOI: 10.1021/jp510024r

### 2. Stepwise Unfolding of Bovine and Human Serum Albumin by an Anionic Surfactant: An Investigation Using the Proton Transfer Probe Norharmane

Saptarshi Ghosh, Satrajit Chakrabarty, Debipreeta Bhowmik, Gopinatha Suresh Kumar, and Nitin Chattopadhyay

*The Journal of Physical Chemistry B* 2015 119 (6), 2090-2102

DOI: 10.1021/jp501150p

### 3. Effect of Ca<sup>2+</sup> on the Steady-State and Time-Resolved Emission Properties of the Genetically Encoded Fluorescent Sensor CatchER

You Zhuo, Kyril M. Solntsev, Florence Reddish, Shen Tang, and Jenny J. Yang

*The Journal of Physical Chemistry B* 2015 119 (6), 2103-2111

DOI: 10.1021/jp501707n

### 4. Mechanisms of Photostability in Kynurenines: A Joint Electronic-Structure and Dynamics Study

Deniz Tuna, Nađa Došlić, Momir Mališ, Andrzej L. Sobolewski, and Wolfgang Domcke

*The Journal of Physical Chemistry B* 2015 119 (6), 2112-2124

DOI: 10.1021/jp501782v

### 5. New Insights into the Dual Fluorescence of Methyl Salicylate: Effects of Intermolecular Hydrogen Bonding and Solvation

Panwang Zhou, Mark R. Hoffmann, Keli Han, and Guozhong He

*The Journal of Physical Chemistry B* 2015 119 (6), 2125-2131

DOI: 10.1021/jp501881j

### 6. Effects of Charge Transfer on the ESIPT Process in Methyl 5-R-Salicylates

J. Catalán

*The Journal of Physical Chemistry B* 2015 119 (6), 2132-2139

DOI: 10.1021/jp502691y

### 7. Chemiexcitation Induced Proton Transfer: Enolate Oxyluciferin as the Firefly Bioluminophore

Luís Pinto da Silva and Joaquim C. G. Esteves da Silva

*The Journal of Physical Chemistry B* 2015 119 (6), 2140-2148

DOI: 10.1021/jp5036458

### 8. Excited State Proton Transfer in the Lysosome of Live Lung Cells: Normal and Cancer Cells

Rajdeep Chowdhury, Abhijit Saha, Amit Kumar Mandal, Batakrishna Jana, Surajit Ghosh, and Kankan Bhattacharyya

*The Journal of Physical Chemistry B* 2015 119 (6), 2149-2156

DOI: 10.1021/jp503804y

### 9. Probing Water Environment of Trp59 in Ribonuclease T1: Insight of the Structure–Water Network Relationship

Wei-Chih Chao, Jiun-Yi Shen, Jyh-Feng Lu, Jinn-Shyan Wang, Hsiao-Ching Yang, Kevin Wee, Li-Ju Lin, Yi-Ching Kuo, Cheng-Han Yang, Shih-Hui Weng, Huai-Ching Huang, You-Hua Chen, and Pi-Tai Chou

*The Journal of Physical Chemistry B* 2015 119 (6), 2157-2167

DOI: 10.1021/jp503914s

**10. Exploring the Interaction of a Micelle Entrapped Biologically Important Proton Transfer Probe with the Model Transport Protein Bovine Serum Albumin**

Debarati Ray, Ashis Kundu, Animesh Pramanik, and Nikhil Guchhait

*The Journal of Physical Chemistry B* **2015** 119 (6), 2168-2179

DOI: 10.1021/jp504037y

**11. TD-DFT Assessment of the Excited State Intramolecular Proton Transfer in Hydroxyphenylbenzimidazole (HBI) Dyes**

Ymène Houari, Siwar Chibani, Denis Jacquemin, and Adèle D. Laurent

*The Journal of Physical Chemistry B* **2015** 119 (6), 2180-2192

DOI: 10.1021/jp505036d

**12. Spectroscopic Study of Jet-Cooled Deuterated Porphycenes: Unusual Isotopic Effects on Proton Tunneling**

Ephriem T. Mengesha, Anne Zehnacker-Rentien, J. Sepioł, M. Kijak, and J. Waluk

*The Journal of Physical Chemistry B* **2015** 119 (6), 2193-2203

DOI: 10.1021/jp505553z

**13. Excited State Structural Events of a Dual-Emission Fluorescent Protein Biosensor for Ca<sup>2+</sup> Imaging Studied by Femtosecond Stimulated Raman Spectroscopy**

Yanli Wang, Longteng Tang, Weimin Liu, Yongxin Zhao, Breland G. Oscar, Robert E. Campbell, and Chong Fang

*The Journal of Physical Chemistry B* **2015** 119 (6), 2204-2218

DOI: 10.1021/jp505698z

**14. Excited States of Proton-Bound DNA/RNA Base Homodimers: Pyrimidines**

Géraldine Féraud, Matias Berdakin, Claude Dedonder, Christophe Jovet, and Gustavo A. Pino

*The Journal of Physical Chemistry B* **2015** 119 (6), 2219-2228

DOI: 10.1021/jp505756a

**15. Mechanism by which Untwisting of Retinal Leads to Productive Bacteriorhodopsin Photocycle States**

Tino Wolter, Marcus Elstner, Stefan Fischer, Jeremy C. Smith, and Ana-Nicoleta Bondar

*The Journal of Physical Chemistry B* **2015** 119 (6), 2229-2240

DOI: 10.1021/jp505818r

**16. Investigation of the Role of Protonation of Benzophenone and Its Derivatives in Acidic Aqueous Solutions Using Time-Resolved Resonance Raman Spectroscopy: How Are Ketyl Radicals Formed in Aqueous Solutions?**

Ming-De Li, Jinqing Huang, Mingyue Liu, Songbo Li, Jiani Ma, and David Lee Phillips

*The Journal of Physical Chemistry B* **2015** 119 (6), 2241-2252

DOI: 10.1021/jp505954d

**17. How Fast Can a Proton-Transfer Reaction Be beyond the Solvent-Control Limit?**

Ron Simkovitch, Shay Shomer, Rinat Gepshtein, and Dan Huppert

*The Journal of Physical Chemistry B* **2015** 119 (6), 2253-2262

DOI: 10.1021/jp506011e

**18. Dependence of Reaction Rates for Bidirectional PCET on the Electron Donor–Electron Acceptor Distance in Phenol–Ru(2,2'-Bipyridine)<sub>3</sub><sup>2+</sup> Dyads**

Jing Chen, Martin Kuss-Petermann, and Oliver S. Wenger

*The Journal of Physical Chemistry B* **2015** 119 (6), 2263-2273

DOI: 10.1021/jp506087t

**19. Unveiling How an Archetypal Fluorescent Protein Operates: Theoretical Perspective on the Ultrafast Excited State Dynamics of GFP Variant S65T/H148D**

Pau Armengol, Ricard Gelabert, Miquel Moreno, and José M. Lluch

*The Journal of Physical Chemistry B* **2015** 119 (6), 2274-2291

DOI: 10.1021/jp506113g

## **20. Tautomerism in Porphycenes: Analysis of Rate-Affecting Factors**

Piotr Ciałka, Piotr Fita, Arkadiusz Listkowski, Michał Kijak, Santi Nonell, Daiki Kuzuhara, Hiroko Yamada, Czesław Radzewicz, and Jacek Waluk

*The Journal of Physical Chemistry B* **2015** 119 (6), 2292-2301

DOI: 10.1021/jp506150r

## **21. Water-Catalyzed Excited-State Proton-Transfer Reactions in 7-Azaindole and Its Analogues**

Yu-Sin Wu, Huai-Ching Huang, Jiun-Yi Shen, Huan-Wei Tseng, Jr-Wei Ho, You-Hua Chen, and Pi-Tai Chou

*The Journal of Physical Chemistry B* **2015** 119 (6), 2302-2309

DOI: 10.1021/jp506136v

## **22. Stimuli-Sensitive Breathing of Cucurbit[7]uril Cavity: Monitoring through the Environment Responsive Fluorescence of 1'-Hydroxy-2'-acetonaphthone (HAN)**

Debasis Banik, Jagannath Kuchlyan, Arpita Roy, Niloy Kundu, and Nilmoni Sarkar

*The Journal of Physical Chemistry B* **2015** 119 (6), 2310-2322

DOI: 10.1021/jp5064879

## **23. Spatiotemporal Control of Synergistic Gel Disintegration Consisting of Boroxole- and Glyco-Based Polymers via Photoinduced Proton Transfer**

Yohei Kotsuchibashi, Mitsuhiro Ebara, Takeshi Sato, Yinan Wang, Rajender Rajender, Dennis G. Hall, Ravin Narain, and Takao Aoyagi

*The Journal of Physical Chemistry B* **2015** 119 (6), 2323-2329

DOI: 10.1021/jp506478p

## **24. Photophysics of 2-(4'-Amino-2'-hydroxyphenyl)-1H-imidazo-[4,5-c]pyridine and Its Analogues: Intramolecular Proton Transfer versus Intramolecular Charge Transfer**

Santosh Kumar Behera, Ananda Karak, and G. Krishnamoorthy

*The Journal of Physical Chemistry B* **2015** 119 (6), 2330-2344

DOI: 10.1021/jp5064808

## **25. Efficient Femtosecond Energy Transfer from Carotenoid to Retinal in Gloeobacter Rhodopsin–Salinixanthin Complex**

E. Siva Subramaniam Iyer, Itay Gdor, Tamar Eliash, Mordechai Sheves, and Sanford Ruhman

*The Journal of Physical Chemistry B* **2015** 119 (6), 2345-2349

DOI: 10.1021/jp506639w

## **26. Photoisomerization and Proton Transfer in the Forward and Reverse Photoswitching of the Fast-Switching M159T Mutant of the Dronpa Fluorescent Protein**

Marius Kaucikas, Martijn Tros, and Jasper J. van Thor

*The Journal of Physical Chemistry B* **2015** 119 (6), 2350-2362

DOI: 10.1021/jp506640q

## **27. Excited State Proton Transfer Dynamics of Topotecan Inside Biomimicking Nanocavity**

Raj Kumar Koninti, Krishna Gavvala, Abhigyan Sengupta, and Partha Hazra

*The Journal of Physical Chemistry B* **2015** 119 (6), 2363-2371

DOI: 10.1021/jp5066902

## **28. Short Hydrogen Bonds and Negative Charge in Photoactive Yellow Protein Promote Fast Isomerization but not High Quantum Yield**

Jingyi Zhu, Jocelyne Vreede, Marijke Hospes, Jos Arents, John T. M. Kennis, Ivo H. M. van Stokkum, Klaas J. Hellingwerf, and Marie Louise Groot

*The Journal of Physical Chemistry B* **2015** 119 (6), 2372-2383

DOI: 10.1021/jp506785q

**29. 2-(2-Hydroxyphenyl)-benzothiazole (HBT)-Rhodamine Dyad: Acid-Switchable Absorption and Fluorescence of Excited-State Intramolecular Proton Transfer (ESIPT)**

Poulomi Majumdar and Jianzhang Zhao

*The Journal of Physical Chemistry B* **2015** 119 (6), 2384-2394

DOI: 10.1021/jp5068507

**30. Reversible Tuning of Chemical Structure of Nafion Cast Film by Heat and Acid Treatment**

Nancy Singhal and Anindya Datta

*The Journal of Physical Chemistry B* **2015** 119 (6), 2395-2403

DOI: 10.1021/jp506911w

**31. Real-Time Monitoring of Chromophore Isomerization and Deprotonation during the Photoactivation of the Fluorescent Protein Dronpa**

Dheerendra Yadav, Fabien Lacombat, Nadia Dozova, Fabrice Rappaport, Pascal Plaza, and Agathe Espagne

*The Journal of Physical Chemistry B* **2015** 119 (6), 2404-2414

DOI: 10.1021/jp507094f

**32. Theoretical Study on the Size Dependence of Excited State Proton Transfer in 1-Naphthol–Ammonia Clusters**

Toshihiko Shimizu, Shunpei Yoshikawa, Kenro Hashimoto, Mitsuhiko Miyazaki, and Masaaki Fujii

*The Journal of Physical Chemistry B* **2015** 119 (6), 2415-2424

DOI: 10.1021/jp507222n

**33. Femtosecond Transient Absorption Spectroscopy of the Medicinal Agent Curcumin in Diamide Linked  $\gamma$ -Cyclodextrin Dimers**

Takaaki Harada, Hamish L. McTernan, Duc-Truc Pham, Stephen F. Lincoln, and Tak W. Kee

*The Journal of Physical Chemistry B* **2015** 119 (6), 2425-2433

DOI: 10.1021/jp507272f

**34. Excited-State Dynamics of 3-Hydroxyflavone Anion in Alcohols**

Bogdan Dereka, Romain Letrun, Denis Svechkarov, Arnulf Rosspeintner, and Eric Vauthey

*The Journal of Physical Chemistry B* **2015** 119 (6), 2434-2443

DOI: 10.1021/jp507311n

**35. Competition and Interplay of Various Intermolecular Interactions in Ultrafast Excited-State Proton and Electron Transfer Reactions**

Michael G. Kuzmin, Irina V. Soboleva, Vladimir L. Ivanov, Elizabeth-Ann Gould, Dan Huppert, and Kyril M. Solntsev

*The Journal of Physical Chemistry B* **2015** 119 (6), 2444-2453

DOI: 10.1021/jp507390r

**36. Photoinduced Electron Detachment and Proton Transfer: The Proposal for Alternative Path of Formation of Triplet States of Guanine (G) and Cytosine (C) Pair**

Jiande Gu, Jing Wang, and Jerzy Leszczynski

*The Journal of Physical Chemistry B* **2015** 119 (6), 2454-2458

DOI: 10.1021/jp507385r

**37. Describing Excited State Intramolecular Proton Transfer in Dual Emissive Systems: A Density Functional Theory Based Analysis**

Liam Wilbraham, Marika Savarese, Nadia Rega, Carlo Adamo, and Ilaria Ciofini

*The Journal of Physical Chemistry B* **2015** 119 (6), 2459-2466

DOI: 10.1021/jp507425x

**38. Role of Zwitterions in Kindling Fluorescent Protein Photochemistry**

Vladimir A. Mironov, Ksenia B. Bravaya, and Alexander V. Nemukhin

*The Journal of Physical Chemistry B* **2015** 119 (6), 2467-2474

DOI: 10.1021/jp5075219

**39. Excited-State Proton and Charge Transfer in Protonated Amino and Methylated Derivatives of 2-(2'-Hydroxyphenyl)benzimidazole**

Sonia Ríos Vázquez, J. Luis Pérez Lustres, Flor Rodríguez-Prieto, Manuel Mosquera, and M. Carmen Ríos Rodríguez

*The Journal of Physical Chemistry B* **2015** 119 (6), 2475-2489

DOI: 10.1021/jp507917u

**40. Stepwise versus Concerted Mechanism of Photoinduced Proton Transfer in sec-1,2-Dihydroquinolines: Effect of Excitation Wavelength and Solvent Composition**

Tatiana D. Nekipelova, Ivan S. Shelaev, Fedor E. Gostev, Victor A. Nadochenko, and Vladimir A. Kuzmin

*The Journal of Physical Chemistry B* **2015** 119 (6), 2490-2497

DOI: 10.1021/jp507954h

**41. Excited-State Hydroxide Ion Transfer from a Model Xanthenol Photobase**

Yun Xie, Hoi Ling Luk, Xin Yang, and Ksenija D. Glusac

*The Journal of Physical Chemistry B* **2015** 119 (6), 2498-2506

DOI: 10.1021/jp5080169

**42. Optical Behavior of Substituted 4-(2'-Hydroxyphenyl)imidazoles**

Artur Jeżewski, Tommy Hammann, Piotr J. Cywiński, and Daniel T. Gryko

*The Journal of Physical Chemistry B* **2015** 119 (6), 2507-2514

DOI: 10.1021/jp507992x

**43. Synthesis and Spectroscopic Characterization of 1,8-Naphthalimide Derived "Super" Photoacids**

Tatu Kumpulainen, Bert H. Bakker, Michiel Hilbers, and Albert M. Brouwer

*The Journal of Physical Chemistry B* **2015** 119 (6), 2515-2524

DOI: 10.1021/jp508334s

**44. Correlation between Excited-State Intramolecular Proton-Transfer and Singlet-Oxygen Quenching Activities in 1-(Acylamino)anthraquinones**

Shin-ichi Nagaoka, Hikaru Endo, Keishi Ohara, and Umpei Nagashima

*The Journal of Physical Chemistry B* **2015** 119 (6), 2525-2532

DOI: 10.1021/jp508355k

**45. Ground and Excited State Proton Transfer of the Bioactive Plant Flavonol Robinetin in a Protein Environment: Spectroscopic and Molecular Modeling Studies**

Biswa Pathik Pahari, Sudip Chaudhuri, Sandipan Chakraborty, and Pradeep K. Sengupta

*The Journal of Physical Chemistry B* **2015** 119 (6), 2533-2545

DOI: 10.1021/jp508410v

**46. Excited State Proton Transfer of Natural Flavonoids and Their Chromophores in Duplex and Tetraplex DNAs**

Bidisha Sengupta, Samantha M. Reilly, Donald E. Davis, Jr., Kisa Harris, Randy M. Wadkins, Denise Ward, D'Asia Gholar, and Cari Hampton

*The Journal of Physical Chemistry B* **2015** 119 (6), 2546-2556

DOI: 10.1021/jp508599h

**47. Anomalous Cage Effect of the Excited State Dynamics of Catechol in the 18-Crown-6-Catechol Host-Guest Complex**

Fumiya Morishima, Ryoji Kusaka, Yoshiya Inokuchi, Takeharu Haino, and Takayuki Ebata

*The Journal of Physical Chemistry B* **2015** 119 (6), 2557-2565

DOI: 10.1021/jp508619f

**48. Locally-Excited (LE) versus Charge-Transfer (CT) Excited State Competition in a Series of Para-Substituted Neutral Green Fluorescent Protein (GFP) Chromophore Models**

Seth Olsen

*The Journal of Physical Chemistry B* **2015** 119 (6), 2566-2575

DOI: 10.1021/jp508723d

#### **49. Solvatochromism of BODIPY-Schiff Dye**

Aleksander Filarowski, Marina Lopatkova, Paweł Lipkowski, Mark Van der Auweraer, Volker Leen, and Wim Dehaen

*The Journal of Physical Chemistry B* **2015** 119 (6), 2576-2584

DOI: 10.1021/jp508718d

#### **50. Fluorescent Amino Acid Undergoing Excited State Intramolecular Proton Transfer for Site-Specific Probing and Imaging of Peptide Interactions**

Marianna Sholokh, Oleksandr M. Zamotaiev, Ranjan Das, Viktoriia Y. Postupalenko, Ludovic Richert, Denis Dujardin, Olga A. Zaporozhets, Vasyl G. Pivovarenko, Andrey S. Klymchenko, and Yves Mély

*The Journal of Physical Chemistry B* **2015** 119 (6), 2585-2595

DOI: 10.1021/jp508748e

#### **51. Solvent-Dependent Excited-State Hydrogen Transfer and Intersystem Crossing in 2-(2'-Hydroxyphenyl)-Benzothiazole**

Shawkat M. Aly, Anwar Usman, Maytham AlZayer, Ghada A. Hamdi, Erkki Alarousu, and Omar F. Mohammed

*The Journal of Physical Chemistry B* **2015** 119 (6), 2596-2603

DOI: 10.1021/jp508777h

#### **52. Unveiling the Eigen-Weller Ion Pair from the Excited State Proton Transfer Kinetics of 3-Chloro-4-methyl-7-hydroxycoumarin**

J. Sérgio Seixas de Melo and António L. Maçanita

*The Journal of Physical Chemistry B* **2015** 119 (6), 2604-2610

DOI: 10.1021/jp508782h

#### **53. Linear Energy Relationships in Ground State Proton Transfer and Excited State Proton-Coupled Electron Transfer**

Ana P. Gamiz-Hernandez, Artiom Magomedov, Gerhard Hummer, and Ville R. I. Kaila

*The Journal of Physical Chemistry B* **2015** 119 (6), 2611-2619

DOI: 10.1021/jp508790n

#### **54. Excited State Intramolecular Proton Transfer Dynamics of 1-Hydroxy-2-acetonaphthone**

Jinyong Kim, Wooseok Heo, and Taiha Joo

*The Journal of Physical Chemistry B* **2015** 119 (6), 2620-2627

DOI: 10.1021/jp5088306

#### **55. Vibrational Excitation Induced Proton Transfer in Hydrated Nafion Membranes**

Liyuan Liu and Huib J. Bakker

*The Journal of Physical Chemistry B* **2015** 119 (6), 2628-2637

DOI: 10.1021/jp508862t

#### **56. Emission Properties of Oxyluciferin and Its Derivatives in Water: Revealing the Nature of the Emissive Species in Firefly Bioluminescence**

Avisek Ghose, Mateusz Rebarz, Oleg V. Maltsev, Lukas Hintermann, Cyril Ruckebusch, Eduard Fron, Johan Hofkens, Yves Mély, Panče Naumov, Michel Sliwa, and Pascal Didier

*The Journal of Physical Chemistry B* **2015** 119 (6), 2638-2649

DOI: 10.1021/jp508905m

#### **57. Intrinsic and Dynamical Reaction Pathways of an Excited State Proton Transfer**

Umberto Raucci, Marika Savarese, Carlo Adamo, Ilaria Ciofini, and Nadia Rega

*The Journal of Physical Chemistry B* **2015** 119 (6), 2650-2657

DOI: 10.1021/jp508947f

#### **58. Protonated Water Dimer on Benzene: Standing Eigen or Crouching Zundel?**

Huan Wang and Noam Agmon

*The Journal of Physical Chemistry B* **2015** 119 (6), 2658-2667

DOI: 10.1021/jp509004j

**59. Phototautomerization on the Singlet and Triplet Surface in o-Hydroxyacetophenone Derivatives in Polar Solvents**

Sujan K. Sarkar, Geethika K. Weragoda, R. A. A. Upul Ranaweera, and Anna D. Gudmundsdottir  
*The Journal of Physical Chemistry B* **2015** 119 (6), 2668-2676

DOI: 10.1021/jp509062w

**60. Seven Steps of Alternating Electron and Proton Transfer in Photosystem II Water Oxidation Traced by Time-Resolved Photothermal Beam Deflection at Improved Sensitivity**

André Klauss, Michael Haumann, and Holger Dau  
*The Journal of Physical Chemistry B* **2015** 119 (6), 2677-2689

DOI: 10.1021/jp509069p

**61. Bifunctional Photoacids: Remote Protonation Affecting Chemical Reactivity**

Julia Ditkovich, Tzach Mukra, Dina Pines, Dan Huppert, and Ehud Pines  
*The Journal of Physical Chemistry B* **2015** 119 (6), 2690-2701

DOI: 10.1021/jp509104x

**62. Photoswitching of Salicylidene Methylamine: A Theoretical Photodynamics Study**

Lasse Spörkel, Joanna Jankowska, and Walter Thiel  
*The Journal of Physical Chemistry B* **2015** 119 (6), 2702-2710

DOI: 10.1021/jp5095678

**63. Hydrogen Bonding Induced Enhancement of Fermi Resonances: Ultrafast Vibrational Energy Flow Dynamics in Aniline-d5**

Rene Costard, Christian Greve, Henk Fidder, and Erik T. J. Nibbering  
*The Journal of Physical Chemistry B* **2015** 119 (6), 2711-2725

DOI: 10.1021/jp509977r

**64. Proton-Coupled Electron Transfer in Tyrosine and a  $\beta$ -Hairpin Maquette: Reaction Dynamics on the Picosecond Time Scale**

Cynthia V. Pagba, San-Hui Chi, Joseph Perry, and Bridgette A. Barry  
*The Journal of Physical Chemistry B* **2015** 119 (6), 2726-2736

DOI: 10.1021/jp510171z

**65. Ultrafast Hydrolysis of a Lewis Photoacid**

Joseph D. Henrich, Scott Suchyta, and Bern Kohler  
*The Journal of Physical Chemistry B* **2015** 119 (6), 2737-2748

DOI: 10.1021/jp510953e

**66. Excited-State Proton Transfer in Confined Medium. 4-Methyl-7-hydroxyflavylium and  $\beta$ -Naphthol Incorporated in Cucurbit[7]uril**

Nuno Basílio, César A. T. Laia, and Fernando Pina  
*The Journal of Physical Chemistry B* **2015** 119 (6), 2749-2757

DOI: 10.1021/jp511351w

**67. Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer in a Solvated Phenol–Amine Complex**

Puja Goyal, Christine A. Schwerdtfeger, Alexander V. Soudackov, and Sharon Hammes-Schiffer  
*The Journal of Physical Chemistry B* **2015** 119 (6), 2758-2768

DOI: 10.1021/jp5126969