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Nicholas A. Besley

J. Phys. Chem. A, **2004**, *108* (49), pp 10794-10800
Publication Date (Web): November 12, 2004 (Article)
DOI: 10.1021/jp046073c

Nicholas A. **Besley*** ...

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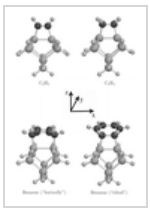
Time-Dependent Density Functional Theory Study of the X-ray Absorption Spectroscopy of Acetylene, Ethylene, and Benzene on Si(100)

Nicholas A. Besley and Adam Noble

J. Phys. Chem. C, **2007**, *111* (8), pp 3333-3340
Publication Date (Web): February 07, 2007 (Article)
DOI: 10.1021/jp065160x

Nicholas A. **Besley*** and Adam Noble ...



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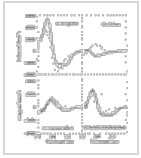
Theoretical Studies toward Quantitative Protein Circular Dichroism Calculations

Nicholas A. Besley and Jonathan D. Hirst

J. Am. Chem. Soc., **1999**, *121* (41), pp 9636-9644
Publication Date (Web): October 01, 1999 (Article)
DOI: 10.1021/ja990627l

Nicholas A. **Besley**† and Jonathan D. Hirst*† ...



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Ab Initio Study of the Electronic Spectrum of Formamide with Explicit Solvent

Nicholas A. Besley and Jonathan D. Hirst

J. Am. Chem. Soc., **1999**, *121* (37), pp 8559-8566
Publication Date (Web): August 31, 1999 (Article)
DOI: 10.1021/ja990064d

Nicholas A. **Besley** and Jonathan D. Hirst* ...

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Figure 1 of 3

Ab Initio Finite-Temperature Electronic Absorption Spectrum of Formamide

Nicholas A. Besley and Nikos L. Doltsinis

J. Chem. Theory Comput., **2006**, *2* (6), pp 1598-1604
Publication Date (Web): September 28, 2006 (Article)
DOI: 10.1021/ct600244z

Nicholas A. **Besley**† and Nikos L. Doltsinis*‡ ...

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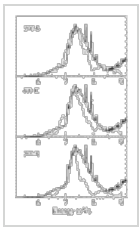

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Electronic Excited States of Si(100) and Organic Molecules Adsorbed on Si(100)

Nicholas A. Besley and Adam J. Blundy

J. Phys. Chem. B, **2006**, *110* (4), pp 1701-1710
Publication Date (Web): January 7, 2006 (Article)
DOI: 10.1021/jp055191c

Nicholas A. **Besley*** and Adam J. Blundy ...

Abstract

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Partial Hessian Vibrational Analysis of Organic Molecules Adsorbed on Si(100)

Nicholas A. Besley and James A. Bryan

J. Phys. Chem. C, **2008**, *112* (11), pp 4308-4314
Publication Date (Web): February 23, 2008 (Article)
DOI: 10.1021/jp076167x

Nicholas A. **Besley*** and James A. Bryan ...

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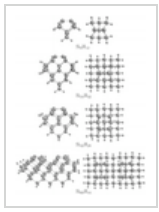

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Ab Initio Study of the Effect of Solvation on the Electronic Spectra of Formamide and *N*-Methylacetamide

Abstract

Nicholas A. Besley and Jonathan D. Hirst

J. Phys. Chem. A, **1998**, *102* (52), pp 10791-10797
Publication Date (Web): December 8, 1998 (Article)
DOI: 10.1021/jp982645f

Nicholas A. **Besley** and Jonathan D. Hirst* ... Nicholas A. **Besley** and Nikos L. Doltsinis ... Nicholas A. **Besley** and Nikos L. Doltsinis ...

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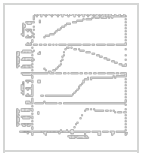

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Electronic Structure of a Rigid Cyclic Diamide

Nicholas A. Besley, Marie-Josèphe Brienne, and Jonathan D. Hirst

J. Phys. Chem. B, **2000**, *104* (51), pp 12371-12377
Publication Date (Web): November 23, 2000 (Article)
DOI: 10.1021/jp0024524

Nicholas A. **Besley**,† Marie-Josèphe Brienne,‡ and Jonathan D. Hirst*† ...

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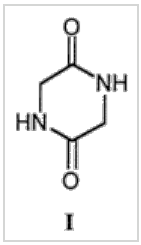

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Figure 1 of 5

Theoretical Study of the ^{13}C NMR Spectroscopy of Single-Walled Carbon Nanotubes

Nicholas A. Besley, Jeremy J. Titman, and Matthew D. Wright

J. Am. Chem. Soc., **2005**, *127* (50), pp 17948-17953
Publication Date (Web): November 24, 2005 (Article)
DOI: 10.1021/ja055888b

Nicholas A. **Besley**,* Jeremy J. Titman, and Matthew D. Wright ...

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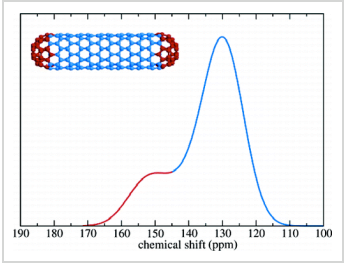

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A Sequential Molecular Mechanics/Quantum Mechanics Study of the Electronic Spectra of Amides

Nicholas A. Besley, Mark T. Oakley, Alexander J. Cowan, and Jonathan D. Hirst

J. Am. Chem. Soc., **2004**, *126* (41), pp 13502-13511
Publication Date (Web): September 21, 2004 (Article)
DOI: 10.1021/ja047603l

Nicholas A. **Besley**,* Mark T. Oakley, Alexander J. Cowan, and Jonathan D. Hirst ...

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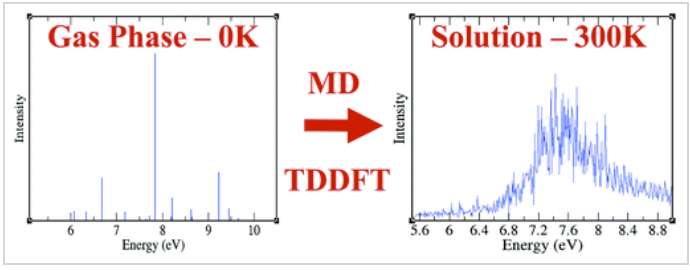

Figure 1 of 10

Calculating the Fluorescence of 5-Hydroxytryptophan in Proteins

David Robinson, Nicholas A. Besley, Paul O'Shea and Jonathan D. Hirst

J. Phys. Chem. B, **2009**, *113* (43), pp 14521-14528
Publication Date (Web): October 1, 2009 (Article)
DOI: 10.1021/jp9071108

David Robinson†, Nicholas A. **Besley**†, Paul O'Shea‡ and Jonathan D. Hirst*† ... Rogers, D. M.; **Besley**, N. A.; O'Shea, P.; Hirst, J. D. ... *Robinson, D.*; ***Besley***, *N. A.; Lunt, E. A. M.; O'Shea, P.; Hirst, J. D. ...*

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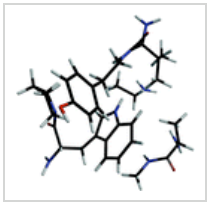

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Modeling the Absorption Spectrum of Tryptophan in Proteins

David M. Rogers, Nicholas A. Besley, Paul O'Shea, and Jonathan D. Hirst

J. Phys. Chem. B, **2005**, *109* (48), pp 23061-23069
Publication Date (Web): November 12, 2005 (Article)
DOI: 10.1021/jp053309j

David M. Rogers,† Nicholas A. **Besley**,† Paul O'Shea,‡ and Jonathan D. Hirst*† ...

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Self-Consistent Field Calculations of Excited States Using the Maximum Overlap Method (MOM)

Andrew T. B. Gilbert, Nicholas A. Besley and Peter M. W. Gill

J. Phys. Chem. A, **2008**, *112* (50), pp 13164-13171
Publication Date (Web): August 26, 2008 (Article)
DOI: 10.1021/jp801738f

We present a simple algorithm, which we call the maximum overlap method (MOM), for finding excited-state solutions to self-consistent field (SCF) equations. Instead of using the aufbau principle, the algorithm maximizes the overlap between the occupied ...

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Electronic Structure of 5-Hydroxyindole: From Gas Phase to Explicit Solvation

David Robinson, Nicholas A. Besley, Elizabeth A. M. Lunt, Paul O'Shea and Jonathan D. Hirst

J. Phys. Chem. B, **2009**, *113* (8), pp 2535-2541
Publication Date (Web): February 5, 2009 (Article)
DOI: 10.1021/jp808943d

David Robinson†, Nicholas A. **Besley**†, Elizabeth A. M. Lunt‡, Paul O'Shea‡ and Jonathan D. Hirst*† ... Rogers, D. M.; **Besley**, N. A.; O'Shea, P.; Hirst, J. D. ... *Shao, Y.; Molnar, L. F.; Jung, Y.; Kussmann, J.; Ochsenfeld, C.; Brown, S. T.; Gilbert, A. T. B.; Slipchenko, L. V.; Levchenko, S. V.; O'Neill, D. P.; DiStasio, R. A., Jr.; Lochan, R. C.; Wang, T.; Beran, G. J. O.*; ***Besley***, *N. A.; Herbert, J. M.; Lin, C. Y.; Van Voorhis, T.; Chien, S. H.; Sodt, A.; Steele, R. P.; Rassolov, V. A.; Maslen, P. E.; Korambath, P. P.; Adamson, R. D.; Austin, B.; Baker, J.; Byrd, E. F. C.; Dachsel, H.; Doerksen, R. J.; Dreuw, A.; Dunietz, B. D.; Dutoi, A. D.; Furlani, T. R.; Gwaltney, S. R.; Heyden, A.; Hirata, S.; Hsu, C.-P.; Kedziora, G.; Khaliullin, R. Z.; Klunzinger, P.; Lee, A. M.; Lee, M. S.; Liang, W.; Lotan, I.; Nair, N.; Peters, B.; Proynov, E. I.; Pieniazek, P. A.; Rhee, Y. M.; Ritchie, J.; Rosta, E.; Sherrill, C. D.; Simmonett, A. C.; Subotnik, J. E.; Woodcock, H. L., III; Zhang, W.; Bell, A. T.; Chakraborty, A. K.; Chipman, D. M.; Keil, Frerich, J.; Warshel, A.; Hehre, W. J.; Schaefer, H. F., III; Kong, J.; Krylov, A. I.; Gill, P. M. W.; Head-Gordon, M. Phys. ...*

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Probing the Reactivity of Photoinitiators for Free Radical Polymerization: Time-Resolved Infrared Spectroscopic Study of Benzoyl Radicals

Christopher S. Colley, David C. Grills, Nicholas A. Besley, Steffen Jockusch, Pavel Matousek, Anthony W. Parker, Michael Towrie, Nicholas J. Turro, Peter M. W. Gill, and Michael W. George

J. Am. Chem. Soc., **2002**, *124* (50), pp 14952-14958
Publication Date (Web): November 21, 2002 (Article)
DOI: 10.1021/ja026099m

Christopher S. Colley,† David C. Grills,† Nicholas A. **Besley**,† Steffen Jockusch,‡ Pavel Matousek,§ Anthony W. Parker,§ Michael Towrie,§ Nicholas J. Turro,‡ Peter M. W. Gill,† and Michael W. George*† ...

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