

Full Publication List

Papers Published (79) or in-press (1)

(H-Index = 12.0 with 320 NON Self-Citations for search string:

chass ga OR chass g OR chasse g* (searched on 2009/12/15)

80. Richard Andrew Davies, Shaghayegh Ardalan, Wei-Hua Mu, Kun Tian, Fariborz Farsaikiya, Brian W. Darvell, **Gregory A. Chass***, Geometric, Electronic and Elastic Properties of Dental Silver Amalgam γ -(Ag₃Sn), γ_1 -(Ag₂Hg₃), γ_2 -(Sn₈Hg) Phases, Comparison of Experiment and Theory, *Intermetallics (in press)*
79. Gregory A. Chass,* Eric Assen B. Kantchev,* De-Cai Fang*, The fine balance between one cross-coupling and two beta-hydride, elimination pathways: A DFT mechanistic study of Ni(pi-allyl)2-catalyzed cross-coupling of alkyl halides and alkyl, Grignard reagents, *Chem. Commun.* (2010), doi: 10.1039/B922326F
78. Mu W-H., **G. A. Chasse**, D-C. Fang*, A Synergy Between Experiment and Theory for the Formation of Pyridine and Pyrrole Derivatives from Selected Butadienes and Organolithium Reagents: Mechanism, Solvent and Substituent Effect, *Organometallics*, **28** (2009), 2848-2856
77. (c) C. J. O'Brien*, J. L. Tellez, Z. S. Nixon, L. J. Kang, K. C. Przeworski, **G. A. Chass***, Catalytic coupling: Wittig without waste, *Nature Chemistry* (2009), doi:10.1038/nchem.395
- 77 (b) C. J. O'Brien*, J. L. Tellez, Z. S. Nixon, L. J. Kang, K. C. Przeworski, **G. A. Chass***, Recycling Wittig Waste: A cyclic catalyst precursor facilitates reuse of the by-product in an olefination reaction *Chemical & Engineering News*, **37** (2009), September 2, 2009
- 77(a) C. J. O'Brien*, J. L. Tellez, Z. S. Nixon, L. J. Kang, K. C. Przeworski, **G. A. Chass*** (2009), Recycling the Waste: The Development of a Catalytic Wittig Reaction *Angew. Chem. Int. Ed.*, **48** (37) (2009) 6836-6839
76. Zoltán Mucsi*, **Gregory A. Chass***, Imre G. Csizmadia (2009), Systemic energy management by strategically located functional components within molecular frameworks, determined by systems chemistry, *Phys. Chem. B.*, **113** (30), 10308-10314
75. Hui Wang, Imre G. Csizmadia, Istvan Marsi, Gregory A. Chasse, DeCai. Fang and Bela Viskolcz* (2009), Network of Hydrogen bonds in Pro-Ala-Pro and Pro-Phe-Pro Diamides A First Principle Study of Ala → Phe Point Mutation in Proline Environment, *J. Chem. Phys.*, **131** (3), 035105
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73. **Gregory A. Chass***, Christopher J. O'Brien, Eric Assen B. Kantchev, Wei-Hua Mu, De-Cai Fang*, Alan C. Hopkinson, Imre G. Csizmadia, Michael G. Organ* (2009), Density Functional Theory (DFT) Investigation of the Alkyl-Alkyl Negishi Cross-Coupling Reaction Catalyzed by N-heterocyclic Carbene (NHC)-Pd Complexes, *Chem. Eur. J.*, **15**(17), 4281-4288
72. Hui Wang, Zoltan Mucsi, Imre G. Csizmadia, **Gregory A. Chass**, De C. Fang, Bela Viskolcz* (2009), A Prelude to Design Biofriendly Nanostructural Arms using Biological Hinges as Models. First Principle Conformational Analysis on the Ala→Phe Point Mutation in Proline Environment, *Phil. Nat.*, **1**(1), 77-98
71. Pablo Echenique*, **Gregory A. Chass** (2009), Efficient model chemistries for peptides. II. Basis set convergence in the B3LYP method, *Phil. Nat.*, **1**(1), 1-18
70. Zoltán Mucsi*, **Gregory A. Chass***, Imre G. Csizmadia (2008), A quantitative scale for the extent of conjugation of carbonyl groups. Carbonylicity percentage as a chemical driving force, *J. Phys. Chem. A.*, **112** (38), 9153-9165
69. Michael G. Organ*, **Gregory A. Chass**, De-Cai Fang, Alan C. Hopkinson, Cory Valente (2008), Pd-NHC (PEPPSI) Complexes: Synthetic Utility and Computational Studies into their Reactivity, *Synthesis*, **17**, 2776–2797
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59. Wutharath Chin*, Michel Mons, Jean-Pierre Dognon, Reinard Mirasol, **Gregory Chass**, Iliana Dimicoli, François Piuzzi, Patrick Butz, Benjamin Tardivel, Isabelle Compagnon, Gert von Helden and Gerard Meijer (2005), The gas phase dipeptide analogue CH₃CO-Phe-NH₂: a model for the study of side-chain/backbone interactions in proteins, *J. Phys. Chem. A*, 109(24), 5281-5288
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54. C. N. J. Marai, **G. A. Chass**, A. B. Doust, G. D. Scholes* (2004) An ab initio conformational study on 2,3-dihydrobilin-1,19(21H,24H)-dione, a model compound for open-chain tetrapyrroles. *J. Mol. Struct. (THEOCHEM)*, 680, 219-225
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