# Minh Tho Nguyen

List of Publications by Year
in descending order



| 670 | 15,693 | 28274 | 66911 |
|---|---|---|---|
| papers | citations | 55 h-index | 78 g-index |

| 694 | 694 | 694 | 8805 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Carboxyl-Functionalized Task-Specific Ionic Liquids for Solubilizing Metal Oxides. Inorganic Chemistry, 2008, 47, 9987-9999. | 4.0 | 232 |
| 2 | Polynitrogen compounds. Coordination Chemistry Reviews, 2003, 244, 93-113. | 18.8 | 173 |
| 3 | Molecular Mechanism for H2Release from BH3NH3, Including the Catalytic Role of the Lewis Acid BH3. Journal of Physical Chemistry A, 2007, 111, 679-690. | 2.5 | 161 |
| 4 | How Many Water Molecules Are Actively Involved in the Neutral Hydration of Carbon Dioxide?. Journal of Physical Chemistry A, 1997, 101, 7379-7388. | 2.5 | 136 |
| 5 | A Unified Perspective on the Hydrogen Atom Transfer and Proton-Coupled Electron Transfer Mechanisms in Terms of Topographic Features of the Ground and Excited Potential Energy Surfaces As Exemplified by the Reaction between Phenol and Radicals. Journal of the American Chemical Society, 2008, 130, 7000-7010. | 13.7 | 135 |
| 6 | Origin of the bright photoluminescence of few-atom silver clusters confined in LTA zeolites. Science, 2018, 361, 686-690. | 12.6 | 134 |
| 7 | Theoretical Study of the Interaction between Thymine and Water. Protonation and Deprotonation Enthalpies and Comparison with Uracil. Journal of Physical Chemistry A, 1998, 102, 6010-6016. | 2.5 | 125 |
| 8 | Computational Study of the Release of H2from Ammonia Borane Dimer (BH3NH3)2and Its Ion Pair Isomers. Journal of Physical Chemistry A, 2007, 111, 8844-8856. | 2.5 | 124 |
| 9 | Unimolecular rearrangements connecting hydroxyethylidene (CH3-C-OH), acetaldehyde (CH3-CH:O), and vinyl alcohol (CH2:CH-OH). Journal of the American Chemical Society, 1991, 113, 6452-6458. | 13.7 | 121 |
| 10 | Thermochemistry and Electronic Structure of Small Boron Clusters (B<sub>n</sub>, n =) Tj ETQq0 0 0 rgBT /Overlock 10 T | 2.5 | 121 |
| 11 | Protonation and Deprotonation Enthalpies of Guanine and Adenine and Implications for the Structure and Energy of Their Complexes with Water:Â Comparison with Uracil, Thymine, and Cytosine. Journal of Physical Chemistry A, 1999, 103, 8853-8860. | 2.5 | 119 |
| 12 | Theoretical Study of Tautomeric Forms of Uracil. 1. Relative Order of Stabilities and Their Relation to Proton Affinities and Deprotonation Enthalpies. Journal of Physical Chemistry A, 2001, 105, 1288-1295. | 2.5 | 111 |
| 13 | Mechanism of [2 + 1] Cycloadditions of Hydrogen Isocyanide to Alkynes:Â Molecular Orbital and Density Functional Theory Study. Journal of the American Chemical Society, 1999, 121, 5992-6001. | 13.7 | 110 |
| 14 | Mechanism of the Hydration of Carbon Dioxide: Direct Participation of H<sub>2</sub>O versus Microsolvation. Journal of Physical Chemistry A, 2008, 112, 10386-10398. | 2.5 | 108 |
| 15 | Structure of boron clusters revisited, Bn with n=14â€“20. Chemical Physics Letters, 2012, 530, 71-76. | 2.6 | 103 |
| 16 | Theoretical Study of Uracil Tautomers. 2. Interaction with Water. Journal of Physical Chemistry A, 2001, 105, 1934-1943. | 2.5 | 100 |
| 17 | Protonation and deprotonation energies of uracil Implications for the uracilâ€“water complex. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 1277-1280. | 1.7 | 99 |
| 18 | Another Look at the Mechanism of the Concerted 1,3-Dipolar Cycloaddition of Fulminic Acid to Acetylene. Journal of Organic Chemistry, 1999, 64, 65-69. | 3.2 | 99 |

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| 19 | A New Look at the Classical Beckmann Rearrangement:â€‰ A Strong Case of Active Solvent Effect. Journal of the American Chemical Society, 1997, 119, 2552-2562. | 13.7 | 97 |
| 20 | Theoretical Study of the Thermal Decomposition of Acetic Acid: Decarboxylation Versus Dehydration. The Journal of Physical Chemistry, 1995, 99, 11883-11888. | 2.9 | 93 |
| 21 | A Stochastic Search for the Structures of Small Germanium Clusters and Their Anions: Enhanced Stability by Spherical Aromaticity of the Ge<sub>10</sub> and Ge<sub>12</sub><sup>2â^'</sup> Systems. Journal of Chemical Theory and Computation, 2011, 7, 1119-1130. | 5.3 | 92 |
| 22 | Potential Energy Surfaces, Product Distributions and Thermal Rate Coefficients of the Reaction of O(3P) with C2H4(X1Ag):Â A Comprehensive Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 7489-7499. | 2.5 | 91 |
| 23 | Disk Aromaticity of the Planar and Fluxional Anionic Boron Clusters B<sub>20</sub><sup>â^'/2â^'</sup>. Chemistry - A European Journal, 2012, 18, 4510-4512. | 3.3 | 90 |
| 24 | The Alcoholysis Reaction of Isocyanates Giving Urethanes:Â Evidence for a Multimolecular Mechanism. Journal of Organic Chemistry, 1998, 63, 6878-6885. | 3.2 | 88 |
| 25 | In Search of Singlet Phosphinidenes. Journal of Organic Chemistry, 1996, 61, 7077-7084. | 3.2 | 87 |
| 26 | Decomposition mechanism of the polynitrogen N5 and N6 clusters and their ions. Chemical Physics Letters, 2001, 335, 311-320. | 2.6 | 87 |
| 27 | Density Functional Approach to Regiochemistry, Activation Energy, and Hardness Profile in 1,3-Dipolar Cycloadditions. Journal of Physical Chemistry A, 1998, 102, 6181-6185. | 2.5 | 85 |
| 28 | Theoretical Study of Formamide Decomposition Pathways. Journal of Physical Chemistry A, 2011, 115, 841-851. | 2.5 | 82 |
| 29 | The 2D-to-3D geometry hopping in small boron clusters: The charge effect. Chemical Physics Letters, 2013, 577, 32-37. | 2.6 | 81 |
| 30 | Thermochemistry and Electronic Structure of Small Boron and Boron Oxide Clusters and Their Anions. Journal of Physical Chemistry A, 2009, 113, 4895-4909. | 2.5 | 80 |
| 31 | The boron buckyball has an unexpected Th symmetry. Chemical Physics Letters, 2008, 450, 175-177. | 2.6 | 75 |
| 32 | The Sâ^'H Bond Dissociation Enthalpies and Acidities of Para and Meta Substituted Thiophenols:Â A Quantum Chemical Study. Journal of Physical Chemistry A, 2003, 107, 9182-9188. | 2.5 | 74 |
| 33 | Heats of formation of the Criegee formaldehyde oxide and dioxirane. Chemical Physics Letters, 2007, 448, 183-188. | 2.6 | 73 |
| 34 | Nitromethaneâ^'Methyl Nitrite Rearrangement:Â A Persistent Discrepancy between Theory and Experiment. Journal of Physical Chemistry A, 2003, 107, 4286-4291. | 2.5 | 70 |
| 35 | Chromium-Doped Germanium Clusters CrGe<sub>n</sub> (n = 1â^'5):â€‰ Geometry, Electronic Structure, and Topology of Chemical Bonding. Journal of Physical Chemistry A, 2007, 111, 13544-13553. | 2.5 | 70 |
| 36 | Fullerene-like boron clusters stabilized by an endohedrally doped iron atom: B<sub>n</sub>Fe with n = 14, 16, 18 and 20. Physical Chemistry Chemical Physics, 2015, 17, 3000-3003. | 2.8 | 70 |

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| 37 | Fast and accurate determination of the relative binding affinities of small compounds to HIV-1 protease using non-equilibrium work. Journal of Computational Chemistry, 2016, 37, 2734-2742. | 3.3 | 70 |
| 38 | Theoretical Study of the Structureâ^'Property Relationship in Phosphole Monomers. Journal of Organic Chemistry, 2000, 65, 2631-2636. | 3.2 | 68 |
| 39 | Influence of building block aromaticity in the determination of electronic properties of five-membered heterocyclic oligomers. Physical Chemistry Chemical Physics, 2002, 4, 1522-1530. | 2.8 | 68 |
| 40 | A disk-aromatic bowl cluster B<sub>30</sub>: toward formation of boron buckyballs. Chemical Communications, 2014, 50, 1558-1560. | 4.1 | 67 |
| 41 | High Magnetic Moments in Manganeseâ€Doped Silicon Clusters. Chemistry - A European Journal, 2012, 18, 15788-15793. | 3.3 | 66 |
| 42 | Electronic structure and photoelectron spectra of B<sub>n</sub>with n = 26â€“29: an overview of structural characteristics and growth mechanism of boron clusters. Physical Chemistry Chemical Physics, 2015, 17, 13672-13679. | 2.8 | 66 |
| 43 | Disparate Effects of Cu and V on Structures of Exohedral Transition Metal-Doped Silicon Clusters: A Combined Far-Infrared Spectroscopic and Computational Study. Journal of the American Chemical Society, 2010, 132, 15589-15602. | 13.7 | 65 |
| 44 | Experimental and Theoretical Evidence for a Concerted Catalysis by Water Clusters in the Hydrolysis of Isocyanates. Journal of Organic Chemistry, 1998, 63, 6867-6877. | 3.2 | 64 |
| 45 | The boron conundrum: Bonding in the bowl B30 and B36, fullerene B40 and triple ring B42 clusters. Chemical Physics Letters, 2014, 608, 295-302. | 2.6 | 63 |
| 46 | Another Look at the Decomposition of Methyl Azide and Methanimine:Â How Is HCN Formed?. The Journal of Physical Chemistry, 1996, 100, 6499-6503. | 2.9 | 62 |
| 47 | On the Asynchronism of Isocyanide Addition to Dipolarophiles:Â Application of Local Softness. Journal of Organic Chemistry, 1997, 62, 6417-6419. | 3.2 | 62 |
| 48 | Heats of Formation of Boron Hydride Anions and Dianions and Their Ammonium Salts [BnHmy-][NH4+]y with y = 1â^'2. Inorganic Chemistry, 2007, 46, 7561-7570. | 4.0 | 62 |
| 49 | The Boron conundrum: the case of cationic clusters B n + with nÂ=Â2â€“20. Theoretical Chemistry Accounts, 2012, 131, 1. | 1.4 | 61 |
| 50 | Approach to regiochemistry using local softness in 1,3-dipolar cycloadditions. Journal of Computational Chemistry, 1998, 19, 195-202. | 3.3 | 60 |
| 51 | A particle on a hollow cylinder: the triple ring tubular cluster B<sub>27</sub><sup>+</sup>. Physical Chemistry Chemical Physics, 2014, 16, 19470-19478. | 2.8 | 60 |
| 52 | Experimental Investigation of the Reaction between Nitric Oxide and Ketenyl Radicals (HCCO + NO): Rate Coefficient at T = 290-670 K and Product Distribution at 700 K. The Journal of Physical Chemistry, 1994, 98, 8036-8043. | 2.9 | 59 |
| 53 | Theoretical Characterization of the Reaction between Nitric Oxide and Ketenyl Radicals (HCCO + NO): CO versus CO2 Loss. The Journal of Physical Chemistry, 1994, 98, 8030-8035. | 2.9 | 58 |
| 54 | Azidopentazole is Probably the Lowestâ€Energy N<sub>8</sub> Species â€“ A Theoretical Study. Chemische Berichte, 1996, 129, 1157-1159. | 0.2 | 58 |

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| 55 | Hydrogen Bonding between Phenol and Acetonitrile. Journal of Physical Chemistry A, 2002, 106, 4267-4271. | 2.5 | 58 |
| 56 | Difficulties of Density Functional Theory in Investigating Addition Reactions of the Hydrogen Atom. The Journal of Physical Chemistry, 1996, 100, 18422-18425. | 2.9 | 57 |
| 57 | Theoretical Study of the H2+ NO and Related Reactions of [H2NO] Isomers. Journal of Physical Chemistry A, 1998, 102, 3175-3183. | 2.5 | 57 |
| 58 | A density functional study of weakly bound hydrogen bonded complexes. Chemical Physics, 1998, 232, 299-306. | 1.9 | 55 |
| 59 | Nitrous Oxide as a 1,3-Dipole:Â A Theoretical Study of Its Cycloaddition Mechanism. Journal of Organic Chemistry, 2001, 66, 6096-6103. | 3.2 | 55 |
| 60 | An ab initio study of the electronic spectrum of dichlorocarbene CCl2. Chemical Physics Letters, 1985, 117, 295-300. | 2.6 | 54 |
| 61 | Chemical bonding in the boron buckyball. Chemical Physics Letters, 2008, 461, 226-228. | 2.6 | 53 |
| 62 | Structureâ^'Property Relationships in Phosphole-Containing Ï€-Conjugated Systems:Â A Quantum Chemical Study. Journal of Physical Chemistry A, 2003, 107, 838-846. | 2.5 | 52 |
| 63 | Singletâ^'Triplet Energy Gaps of Gas-Phase RNA and DNA Bases. A Quantum Chemical Study. Journal of Physical Chemistry A, 2004, 108, 6554-6561. | 2.5 | 52 |
| 64 | A Theoretical Study of the CH2N System:â€‰ Reactions in both Lowest Lying Doublet and Quartet States. Journal of Physical Chemistry A, 1998, 102, 8013-8020. | 2.5 | 51 |
| 65 | Ionized Phenol and Its Isomers in the Gas Phase. Journal of Physical Chemistry A, 2001, 105, 11582-11592. | 2.5 | 51 |
| 66 | Tuning the Geometric Structure by Doping Silicon Clusters. ChemPhysChem, 2008, 9, 703-706. | 2.1 | 51 |
| 67 | Theoretical study of the vinyl azide-.upsilon.-triazole isomerization. Journal of the American Chemical Society, 1978, 100, 3668-3674. | 13.7 | 50 |
| 68 | The Cu<sub>7</sub>Sc Cluster is a Stable Ïƒâ€Aromatic Sevenâ€Membered Ring. ChemPhysChem, 2008, 9, 833-838. | 2.1 | 50 |
| 69 | Ï€-Conjugated Molecules Containing Naphtho[2,3-b]thiophene and Their Derivatives: Theoretical Design for Organic Semiconductors. Journal of Physical Chemistry C, 2013, 117, 10175-10184. | 3.1 | 50 |
| 70 | A quantum chemical study of three isomers of N20. Chemical Physics Letters, 1999, 315, 327-334. | 2.6 | 49 |
| 71 | The triplet state of cytosine and its derivatives: Electron impact and quantum chemical study. Journal of Chemical Physics, 2004, 121, 11668-11674. | 3.0 | 47 |
| 72 | Distonic Isomers and Tautomers of the Adenine Cation Radical in the Gas Phase and Aqueous Solution. Journal of Physical Chemistry A, 2004, 108, 9283-9293. | 2.5 | 46 |

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| 73 | Isocyanogen (NCNC) and diisocyanogen (CNNC): Structures and some spectroscopic properties. Chemical Physics Letters, 1989, 157, 430-435. | 2.6 | 45 |
| 74 | New look at free radical addition to olefins using local reactivity indices. Journal of the Chemical Society Perkin Transactions II, 1997, , 1415-1418. | 0.9 | 45 |
| 75 | Low Energy Barrier Proton Transfer in Protonated Benzeneâ˜Water Complex. Journal of Physical Chemistry A, 2001, 105, 153-155. | 2.5 | 45 |
| 76 | The Câ˜H and Î±(Câ˜X) Bond Dissociation Enthalpies of Toluene, C6H5-CH2X (X = F, Cl), and Their Substituted Derivatives:â€‰ A DFT Study. Journal of Physical Chemistry A, 2005, 109, 10342-10347. | 2.5 | 45 |
| 77 | Theoretical study of the pentanitrogen cation (N5+). Chemical Physics Letters, 2000, 317, 135-141. | 2.6 | 44 |
| 78 | Theoretical Prediction of the Heats of Formation of C2H5Oâ€¢Radicals Derived from Ethanol and of the Kinetics of Î²-Câ˜C Scission in the Ethoxy Radical. Journal of Physical Chemistry A, 2007, 111, 113-126. | 2.5 | 44 |
| 79 | The leapfrog principle for boron fullerenes: a theoretical study of structure and stability of B112. Physical Chemistry Chemical Physics, 2011, 13, 7524. | 2.8 | 44 |
| 80 | Particle on a Boron Disk: Ring Currents and Disk Aromaticity in B<sub>20</sub><sup>2â€“</sup>. Inorganic Chemistry, 2013, 52, 10595-10600. | 4.0 | 44 |
| 81 | A new chiral boron cluster B44containing nonagonal holes. Chemical Communications, 2016, 52, 1653-1656. | 4.1 | 44 |
| 82 | Efficient Calculation of Isotropic Hyperfine Constants of Phosphorus Radicals Using Density Functional Theory. Journal of Physical Chemistry A, 1997, 101, 3174-3181. | 2.5 | 43 |
| 83 | Regiochemistry of 1,3-dipolar cycloadditions between azides and substituted ethylenes: a theoretical study. Journal of the Chemical Society Perkin Transactions II, 1999, , 2117-2121. | 0.9 | 43 |
| 84 | Electronic Structure and Chemical Bonding in the Double Ring Tubular Boron Clusters. Journal of Physical Chemistry C, 2014, 118, 24181-24187. | 3.1 | 43 |
| 85 | Reaction of Isocyanic Acid and Hydrogen Atom (H + HNCO):Â Theoretical Characterization. The Journal of Physical Chemistry, 1996, 100, 1615-1621. | 2.9 | 42 |
| 86 | Experimental and theoretical study of the reaction of the ethynyl radical with acetylene (HCĩ†C+HCĩ†CH). Chemical Physics, 2000, 262, 243-252. | 1.9 | 42 |
| 87 | A concerted mechanism of proton transfer in green fluorescent protein. A theoretical study. Chemical Physics Letters, 2005, 404, 250-256. | 2.6 | 42 |
| 88 | Use of DFT-based reactivity descriptors for rationalizing radical addition reactions: applicability and difficulties. Faraday Discussions, 2007, 135, 191-201. | 3.2 | 42 |
| 89 | The effect of the NH2 substituent on NH3: hydrazine as an alternative for ammonia in hydrogen release in the presence of boranes and alanes. Physical Chemistry Chemical Physics, 2009, 11, 6339. | 2.8 | 42 |
| 90 | The Aromatic 8-Electron Cubic Silicon Clusters Be@Si<sub>8</sub>, B@Si<sub>8</sub><sup>+</sup>, and C@Si<sub>8</sub><sup>2+</sup>. Journal of Physical Chemistry A, 2010, 114, 7609-7615. | 2.5 | 42 |

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| 91 | From Formamide to Purine: A Self-Catalyzed Reaction Pathway Provides a Feasible Mechanism for the Entire Process. Journal of Physical Chemistry B, 2013, 117, 9333-9342. | 2.6 | 42 |
| 92 | The B<sub>32</sub>cluster has the most stable bowl structure with a remarkable heptagonal hole. Chemical Communications, 2015, 51, 7677-7680. | 4.1 | 42 |
| 93 | Can hexazine (N6) be stable?. Chemical Physics Letters, 1981, 83, 317-319. | 2.6 | 41 |
| 94 | A theoretical study of the phosphinonitrene (H2P:N)-iminophosphane (HP:NH) rearrangement. Journal of the American Chemical Society, 1985, 107, 8029-8033. | 13.7 | 41 |
| 95 | Tripletâ€“singlet energy gaps in iodo-carbenes (Iâ€“Câ€“X): Remarkable discrepancy between theory and experiment. Physical Chemistry Chemical Physics, 2000, 2, 5041-5045. | 2.8 | 41 |
| 96 | Theoretical Study of the Decomposition of Formamide in the Presence of Water Molecules. Journal of Physical Chemistry A, 2013, 117, 2543-2555. | 2.5 | 41 |
| 97 | Ab initio study of the hydration of carbon dioxide: Additional comments based on refined calculations. Computational and Theoretical Chemistry, 1987, 150, 319-325. | 1.5 | 40 |
| 98 | Molecular structure and spectroscopic properties of carbodiimide (HNî—»Cî—»NH). Chemical Physics, 1988, 122, 305-315. | 1.9 | 40 |
| 99 | Heats of Formation and Singletâ^'Triplet Separations of Hydroxymethylene and 1-Hydroxyethylidene. Journal of Physical Chemistry A, 2006, 110, 8864-8871. | 2.5 | 40 |
| 100 | Heats of Formation of Diphosphene, Phosphinophosphinidene, Diphosphine, and Their Methyl Derivatives, and Mechanism of the Borane-Assisted Hydrogen Release. Journal of Physical Chemistry A, 2007, 111, 1726-1736. | 2.5 | 40 |
| 101 | Existence of both blue-shifting hydrogen bond and Lewis acidâ€“base interaction in the complexes of carbonyls and thiocarbonyls with carbon dioxide. Physical Chemistry Chemical Physics, 2011, 13, 14033. | 2.8 | 40 |
| 102 | Enhanced Stability by Three-Dimensional Aromaticity of Endohedrally Doped Clusters X<sub>10</sub>M<sup>0/â€“</sup> with X = Ge, Sn, Pb and M = Cu, Ag, Au. Journal of Physical Chemistry A, 2011, 115, 9993-9999. | 2.5 | 40 |
| 103 | Electronic Structures and Thermochemical Properties of the Small Siliconâ€Doped Boron Clusters B<sub>n</sub>Si (n=1â€“7) and Their Anions. ChemPhysChem, 2011, 12, 2948-2958. | 2.1 | 40 |
| 104 | A three-dimensional aromatic B<sub>6</sub>Li<sub>8</sub>complex as a high capacity hydrogen storage material. Chemical Communications, 2013, 49, 913-915. | 4.1 | 40 |
| 105 | The structures of neutral transition metal doped silicon clusters, Sin X (n = 6â^'9;) Tj ETQq1 1 0.784314 rgBT /Ov | 3.0 | 40 |
| 106 | Structure Assignment, Electronic Properties, and Magnetism Quenching of Endohedrally Doped Neutral Silicon Clusters, Si<sub>n</sub>Co (n = 10â€“12). Journal of Physical Chemistry A, 2014, 118, 8198-8203. | 2.5 | 40 |
| 107 | Another look at structure of gold clusters Au n from perspective of phenomenological shell model. Chemical Physics, 2017, 493, 140-148. | 1.9 | 40 |
| 108 | Amination of Ketenes:Â Evidence for a Mechanism Involving Enols of Amides as Intermediates. Journal of Organic Chemistry, 1998, 63, 9669-9677. | 3.2 | 39 |

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| 109 | Thiouracils:Â Acidity, Basicity, and Interaction with Water. Journal of Physical Chemistry A, 2001, 105, 3379-3387. | 2.5 | 39 |
| 110 | Use of DFT-Based Reactivity Descriptors for Rationalizing Radical Reactions:â€‰ A Critical Analysis. Journal of Physical Chemistry A, 2004, 108, 484-489. | 2.5 | 39 |
| 111 | Comment on the accurate theoretical determination of heats of formation. Chemical Physics Letters, 1992, 196, 390-396. | 2.6 | 38 |
| 112 | Phosphinidene Transition Metal Complexes: A Combined Ab Initio MO-DFT Study of Cr(CO)5â€“PR. European Journal of Inorganic Chemistry, 1999, 1999, 107-115. | 2.0 | 38 |
| 113 | Thiolâ^'Thione Tautomerism in Thioformic Acid:â€‰ Importance of Specific Solvent Interactions. Journal of Physical Chemistry A, 1999, 103, 171-177. | 2.5 | 38 |
| 114 | The reaction of C2H with H2: Absolute rate coefficient measurements andab initiostudy. Journal of Chemical Physics, 2002, 116, 3700-3709. | 3.0 | 38 |
| 115 | Fluxionality and Ïƒâ€Aromaticity in Small Yttriumâ€Doped Gold Clusters. ChemPhysChem, 2008, 9, 2471-2474. | 2.1 | 38 |
| 116 | Heats of Formation of Triplet Ethylene, Ethylidene, and Acetylene. Journal of Physical Chemistry A, 2008, 112, 2082-2087. | 2.5 | 38 |
| 117 | Fundamental Thermochemical Properties of Ammonia Borane and Dehydrogenated Derivatives (BNHn,) Tj ETQq1 1 0.784314 rgBT /O | 3.1 | 38 |
| 118 | Thermochemical properties, electronic structure and bonding of mixed lithium boron clusters (BnLi,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 | 1.9 | 38 |
| 119 | Thermodynamic Properties of the XO<sub>2</sub>, X<sub>2</sub>O, XYO, X<sub>2</sub>O<sub>2</sub>, and XYO<sub>2</sub> (X, Y = Cl, Br, and I) Isomers. Journal of Physical Chemistry A, 2010, 114, 4254-4265. | 2.5 | 38 |
| 120 | Free radical routes for prebiotic formation of DNA nucleobases from formamide. Physical Chemistry Chemical Physics, 2013, 15, 21084. | 2.8 | 38 |
| 121 | Replica exchange molecular dynamics study of the amyloid beta (11â€“40) trimer penetrating a membrane. RSC Advances, 2017, 7, 7346-7357. | 3.6 | 38 |
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| 123 | Ab initiocalculations on low-lying electronic states of the PX, PX+and PX-species (X= H, F and Cl). Molecular Physics, 1986, 59, 547-558. | 1.7 | 37 |
| 124 | Regioselectivity of Oxetane Formation in the Photocycloaddition of Lowest3(n,Ï€*) State of Carbonyl Compounds:Â Interpretation Using Local Softness. Journal of Organic Chemistry, 1997, 62, 6404-6406. | 3.2 | 37 |
| 125 | Calculation of the hyperfine constants of phosphorus-containing radicals. Molecular Physics, 1997, 91, 537-550. | 1.7 | 37 |
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| 127 | Experimental observation and computational identification of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Sc</mml:mi><mml:mi>@</mml:mi><mml:msubsup><mml:mi mathvariant="normal">Cu</mml:mi><mml:mn>16</mml:mn><mml:mo>+</mml:mo></mml:msubsup></mml:mrow></mml:math>, a stable dopant-encapsulated copper cage. Physical Review A, 2007, 76, . | 2.5 | 37 |
| 128 | Reactions of Diborane with Ammonia and Ammonia Borane: Catalytic Effects for Multiple Pathways for Hydrogen Release. Journal of Physical Chemistry A, 2008, 112, 9946-9954. | 2.5 | 37 |
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| 130 | Ring currents in boron and carbon buckyballs, B80 and C60. Physical Chemistry Chemical Physics, 2011, 13, 20855. | 2.8 | 37 |
| 131 | Thermochemical Parameters and Growth Mechanism of the Boron-Doped Silicon Clusters, Si<sub>n</sub>B<sup>q</sup> with n = 1â€“10 and q = â”1, 0, +1. Journal of Physical Chemistry C, 2012, 116, 20086-20098. | 3.1 | 37 |
| 132 | From Formamide to Purine: An Energetically Viable Mechanistic Reaction Pathway. Journal of Physical Chemistry B, 2013, 117, 2314-2320. | 2.6 | 37 |
| 133 | Is N6 an open-chain molecule?. Computational and Theoretical Chemistry, 1983, 105, 351-358. | 1.5 | 36 |
| 134 | Diphosphene (HPPH) and phosphino-phosphinidene (H2PP): An ab initio SCF and CI study of stability and electronic structure. Chemical Physics, 1984, 87, 23-29. | 1.9 | 36 |
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| 145 | Farâ€Infrared Spectra of Yttriumâ€Doped Gold Clusters Au<sub>n</sub>Y (n=1â€“9). ChemPhysChem, 2010, 11, 1932-1943. | 2.1 | 35 |
| 146 | Thermochemical Properties and Electronic Structure of Boron Oxides B<sub>n</sub>O<sub>m</sub> (n = 5â^'10, m = 1â^'2) and Their Anions. Journal of Physical Chemistry A, 2010, 114, 2893-2912. | 2.5 | 35 |
| 147 | Structure and properties of phosphaketene (Hâ€“Pî€†Cî€†O): phosphorus versus oxygen protonation?. Journal of the Chemical Society Perkin Transactions II, 1985, , 1991-1997. | 0.9 | 34 |
| 148 | DFT study of the interaction between guanine and water. Journal of Molecular Structure, 2000, 555, 61-66. | 3.6 | 34 |
| 149 | Condensation Reactions between 1,3-Butadiene Radical Cation and Acetylene in the Gas Phase. Journal of Physical Chemistry A, 2000, 104, 5778-5786. | 2.5 | 34 |
| 150 | Protonation of Gaseous Halogenated Phenols and Anisoles and Its Interpretation Using DFT-Based Local Reactivity Indices. Journal of Physical Chemistry A, 2001, 105, 8709-8717. | 2.5 | 34 |
| 151 | Unified reaction pathways for the prebiotic formation of RNA and DNA nucleobases. Physical Chemistry Chemical Physics, 2016, 18, 20177-20188. | 2.8 | 34 |
| 152 | Unimolecular Chemistry of the Gaseous Cyclopropylamine Radical Cation. Journal of the American Chemical Society, 1998, 120, 152-160. | 13.7 | 33 |
| 153 | Theoretical Study of [2 + 1] Cycloaddition of CO and CS to Acetylenes Forming Cyclopropenones and Cyclopropenethiones. Journal of Organic Chemistry, 2001, 66, 4316-4326. | 3.2 | 33 |
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