# JosÃ© M Lluch

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6001765/publications.pdf

Version: 2024-02-01

| 282 | 6,274 | 81434 | 150775 |
| --- | --- | --- | --- |
| papers | citations | 41 h-index | 59 g-index |

| 289 | 289 | 289 | 5572 |
| --- | --- | --- | --- |
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | N-Substituted 5-(1H-Indol-2-yl)-2-methoxyanilines Are Allosteric Inhibitors of the Linoleate Oxygenase Activity of Selected Mammalian ALOX15 Orthologs: Mechanism of Action. Journal of Medicinal Chemistry, 2022, 65, 1979-1995. | 2.9 | 4 |
| 2 | The role of acetylated cyclooxygenase-2 in the biosynthesis of resolvin precursors derived from eicosapentaenoic acid. Organic and Biomolecular Chemistry, 2022, 20, 1260-1274. | 1.5 | 3 |
| 3 | Theoretical Characterization of the Step-by-Step Mechanism of Conversion of Leukotriene A4 to Leukotriene B4 Catalysed by the Enzyme Leukotriene A4 Hydrolase. International Journal of Molecular Sciences, 2022, 23, 3140. | 1.8 | 3 |
| 4 | Molecular Insights into the Regulation of 3-Phosphoinositide-Dependent Protein Kinase 1: Modeling the Interaction between the Kinase and the Pleckstrin Homology Domains. ACS Omega, 2022, 7, 25186-25199. | 1.6 | 4 |
| 5 | Conformational Heterogeneity and Cooperative Effects of Mammalian ALOX15. International Journal of Molecular Sciences, 2021, 22, 3285. | 1.8 | 5 |
| 6 | Accounting for the instantaneous disorder in the enzymeâ€“substrate Michaelis complex to calculate the Gibbs free energy barrier of an enzyme reaction. Physical Chemistry Chemical Physics, 2021, 23, 13042-13054. | 1.3 | 5 |
| 7 | Understanding the Molecular Details of the Mechanism That Governs the Oxidation of Arachidonic Acid Catalyzed by Aspirin-Acetylated Cyclooxygenase-2. ACS Catalysis, 2020, 10, 138-153. | 5.5 | 6 |
| 8 | A protocol to obtain multidimensional quantum tunneling corrections derived from QM(DFT)/MM calculations for an enzyme reaction. Physical Chemistry Chemical Physics, 2020, 22, 27385-27393. | 1.3 | 2 |
| 9 | Deciphering the Molecular Details of the Lipoxin Formation Mechanism in the 5(S),15(S)-DiHpETE Biosynthetic Pathway Catalyzed by Reticulocyte 15-Lipoxygenase-1. Journal of Physical Chemistry B, 2020, 124, 11406-11418. | 1.2 | 1 |
| 10 | A role of Gln596 in fine-tuning mammalian ALOX15 specificity, protein stability and allosteric properties. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2020, 1865, 158680. | 1.2 | 6 |
| 11 | Unraveling how the Gly526Ser mutation arrests prostaglandin formation from arachidonic acid catalyzed by cyclooxygenase-2: a combined molecular dynamics and QM/MM study. RSC Advances, 2020, 10, 986-997. | 1.7 | 4 |
| 12 | Deciphering the grounds of the suitability of acylhydrazones as efficient photoswitches. Physical Chemistry Chemical Physics, 2019, 21, 16075-16082. | 1.3 | 5 |
| 13 | Mutations of Triad Determinants Changes the Substrate Alignment at the Catalytic Center of Human ALOX5. ACS Chemical Biology, 2019, 14, 2768-2782. | 1.6 | 13 |
| 14 | Unraveling the Molecular Details of the Complete Mechanism That Governs the Synthesis of Prostaglandin G2 Catalyzed by Cyclooxygenase-2. ACS Omega, 2019, 4, 2063-2074. | 1.6 | 6 |
| 15 | Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. Nature Communications, 2019, 10, 2222. | 5.8 | 20 |
| 16 | Synthetic Photoswitchable Neurotransmitters Based on Bridged Azobenzenes. Organic Letters, 2019, 21, 3780-3784. | 2.4 | 42 |
| 17 | Comparing Hydrolysis and Transglycosylation Reactions Catalyzed by Thermus thermophilus Î²-Glycosidase. A Combined MD and QM/MM Study. Frontiers in Chemistry, 2019, 7, 200. | 1.8 | 18 |
| 18 | Rationally designed azobenzene photoswitches for efficient two-photon neuronal excitation. Nature Communications, 2019, 10, 907. | 5.8 | 86 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Ultrafast action chemistry in slow motion: atomistic description of the excitation and fluorescence processes in an archetypal fluorescent protein. Physical Chemistry Chemical Physics, 2018, 20, 11067-11080. | 1.3 | 4 |
| 20 | Mutagenesis of Sequence Determinants of Truncated Porcine ALOX15 Induces Changes in the Reaction Specificity by Altering the Catalytic Mechanism of Initial Hydrogen Abstraction. Chemistry - A European Journal, 2018, 24, 962-973. | 1.7 | 13 |
| 21 | Understanding the Molecular Mechanism of the Ala-versus-Gly Concept Controlling the Product Specificity in Reactions Catalyzed by Lipoxygenases: A Combined Molecular Dynamics and QM/MM Study of Coral 8R-Lipoxygenase. ACS Catalysis, 2017, 7, 4854-4866. | 5.5 | 17 |
| 22 | Understanding how cAMP-dependent protein kinase can catalyze phosphoryl transfer in the presence of Ca2+and Sr2+: a QM/MM study. Physical Chemistry Chemical Physics, 2017, 19, 10377-10394. | 1.3 | 6 |
| 23 | Computational insights into active site shaping for substrate specificity and reaction regioselectivity in the EXTL2 retaining glycosyltransferase. Organic and Biomolecular Chemistry, 2017, 15, 9095-9107. | 1.5 | 13 |
| 24 | Inhibition of Mammalian 15-Lipoxygenase by Three Ebselen-like Drugs. A QM/MM and MM/PBSA Comparative Study. Journal of Physical Chemistry A, 2017, 121, 9752-9763. | 1.1 | 19 |
| 25 | Kinetic isotope effects in chemical and biochemical reactions: physical basis and theoretical methods of calculation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 584-603. | 6.2 | 21 |
| 26 | The Quest for Photoswitches Activated by Nearâ€Infrared Light: A Theoretical Study of the Photochemistry of BF<sub>2</sub>â€Coordinated Azo Derivatives. ChemPhysChem, 2016, 17, 2824-2838. | 1.0 | 6 |
| 27 | Understanding the Mechanism of the Hydrogen Abstraction from Arachidonic Acid Catalyzed by the Human Enzyme 15-Lipoxygenase-2. A Quantum Mechanics/Molecular Mechanics Free Energy Simulation. Journal of Chemical Theory and Computation, 2016, 12, 2079-2090. | 2.3 | 33 |
| 28 | Î±1,4-N-Acetylhexosaminyltransferase EXTL2: The Missing Link for Understanding Glycosidic Bond Biosynthesis with Retention of Configuration. ACS Catalysis, 2016, 6, 2577-2589. | 5.5 | 13 |
| 29 | Computational insight into the catalytic implication of head/tail-first orientation of arachidonic acid in human 5-lipoxygenase: consequences for the positional specificity of oxygenation. Physical Chemistry Chemical Physics, 2016, 18, 23017-23035. | 1.3 | 22 |
| 30 | Is Regioselectivity in the Enzymeâ€Catalyzed Hydroperoxidation of Arachidonic Acid Necessarily Determined by Hydrogen Abstraction? The Case of Rabbit Leu597Ala/Ile663Ala ALOX15 Mutant. ChemPhysChem, 2016, 17, 3321-3332. | 1.0 | 4 |
| 31 | Evolutionary alteration of ALOX15 specificity optimizes the biosynthesis of antiinflammatory and proresolving lipoxins. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4266-75. | 3.3 | 54 |
| 32 | Chromophore interactions leading to different absorption spectra in mNeptune1 and mCardinal red fluorescent proteins. Physical Chemistry Chemical Physics, 2016, 18, 16964-16976. | 1.3 | 9 |
| 33 | How Can Linoleic Acid Be the Preferential Substrate of the Enzyme 15-Lipoxygenase-1? A QM/MM Approach. Journal of Physical Chemistry B, 2016, 120, 1950-1960. | 1.2 | 18 |
| 34 | Theoretical Computerâ€Aided Mutagenic Study on the Triple Green Fluorescent Protein Mutant S65T/H148D/Y145F. ChemPhysChem, 2015, 16, 2134-2139. | 1.0 | 3 |
| 35 | A Native Ternary Complex Trapped in a Crystal Reveals the Catalytic Mechanism of a Retaining Glycosyltransferase. Angewandte Chemie - International Edition, 2015, 54, 9898-9902. | 7.2 | 35 |
| 36 | A QM/MM study of Kemptide phosphorylation catalyzed by protein kinase A. The role of Asp166 as a general acid/base catalyst. Physical Chemistry Chemical Physics, 2015, 17, 3497-3511. | 1.3 | 18 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | QM/MM Studies Reveal How Substrateâ€“Substrate and Enzymeâ€“Substrate Interactions Modulate Retaining Glycosyltransferases Catalysis and Mechanism. Advances in Protein Chemistry and Structural Biology, 2015, 100, 225-254. | 1.0 | 14 |
| 38 | SP20 Phosphorylation Reaction Catalyzed by Protein Kinase A: QM/MM Calculations Based on Recently Determined Crystallographic Structures. ACS Catalysis, 2015, 5, 4897-4912. | 5.5 | 19 |
| 39 | Transient low-barrier hydrogen bond in the photoactive state of green fluorescent protein. Physical Chemistry Chemical Physics, 2015, 17, 30876-30888. | 1.3 | 14 |
| 40 | Molecular modelling of the pH influence in the geometry and the absorbance spectrum of near-infrared TagRFP675 fluorescent protein. Physical Chemistry Chemical Physics, 2015, 17, 29363-29373. | 1.3 | 2 |
| 41 | Unveiling How an Archetypal Fluorescent Protein Operates: Theoretical Perspective on the Ultrafast Excited State Dynamics of GFP Variant S65T/H148D. Journal of Physical Chemistry B, 2015, 119, 2274-2291. | 1.2 | 16 |
| 42 | Regioâ€•and Stereospecificity in the Oxygenation of Arachidonic Acid Catalyzed by Leu597 Mutants of Rabbit 15â€Lipoxygenase: A QM/MM Study. ChemPhysChem, 2014, 15, 2303-2310. | 1.0 | 11 |
| 43 | Unraveling How Enzymes Can Use Bulky Residues To Drive Site-Selective Câ€“H Activation: The Case of Mammalian Lipoxygenases Catalyzing Arachidonic Acid Oxidation. ACS Catalysis, 2014, 4, 4351-4363. | 5.5 | 39 |
| 44 | Introducing Mutations to Modify the C13/C9 Ratio in Linoleic Acid Oxygenations Catalyzed by Rabbit 15â€Lipoxygenase: A QM/MM and MD Study. ChemPhysChem, 2014, 15, 4049-4054. | 1.0 | 7 |
| 45 | A QM/MM study of the associative mechanism for the phosphorylation reaction catalyzed by protein kinase A and its D166A mutant. Journal of Computer-Aided Molecular Design, 2014, 28, 1077-1091. | 1.3 | 11 |
| 46 | New insights into the structureâ€“spectrum relationship in S65T/H148D and E222Q/H148D green fluorescent protein mutants: a theoretical assessment. Organic and Biomolecular Chemistry, 2014, 12, 9845-9852. | 1.5 | 5 |
| 47 | Are There Really Low-Barrier Hydrogen Bonds in Proteins? The Case of Photoactive Yellow Protein. Journal of the American Chemical Society, 2014, 136, 3542-3552. | 6.6 | 51 |
| 48 | A computational and experimental study of O-glycosylation. Catalysis by human UDP-GalNAc polypeptide:GalNAc transferase-T2. Organic and Biomolecular Chemistry, 2014, 12, 2645-2655. | 1.5 | 39 |
| 49 | A time-dependent DFT/molecular dynamics study of the proton-wire responsible for the red fluorescence in the LSSmKate2 protein. Highlights in Theoretical Chemistry, 2014, , 133-141. | 0.0 | 0 |
| 50 | A time-dependent DFT/molecular dynamics study of the proton-wire responsible for the red fluorescence in the LSSmKate2 protein. Theoretical Chemistry Accounts, 2013, 132, 1. | 0.5 | 10 |
| 51 | An Insight into the Regiospecificity of Linoleic Acid Peroxidation Catalyzed by Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2013, 117, 3747-3754. | 1.2 | 17 |
| 52 | On the Regioâ€•and Stereospecificity of Arachidonic Acid Peroxidation Catalyzed by Mammalian 15â€Lypoxygenases: A Combined Molecular Dynamics and QM/MM Study. ChemPhysChem, 2013, 14, 3777-3787. | 1.0 | 11 |
| 53 | Substrate-Assisted and Nucleophilically Assisted Catalysis in Bovine Î±1,3-Galactosyltransferase. Mechanistic Implications for Retaining Glycosyltransferases. Journal of the American Chemical Society, 2013, 135, 7053-7063. | 6.6 | 42 |
| 54 | A theoretical study of the photochemistry of indigo in its neutral and dianionic (leucoindigo) forms. Physical Chemistry Chemical Physics, 2013, 15, 20236. | 1.3 | 37 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | How Does the Environment Affect the Absorption Spectrum of the Fluorescent Protein mKeima?. Journal of Chemical Theory and Computation, 2013, 9, 1731-1742. | 2.3 | 24 |
| 56 | Retaining Glycosyltransferase Mechanism Studied by QM/MM Methods: Lipopolysaccharyl-Î±-1,4-galactosyltransferase C Transfers Î±-Galactose via an Oxocarbenium Ion-like Transition State. Journal of the American Chemical Society, 2012, 134, 4743-4752. | 6.6 | 89 |
| 57 | Peek at the Potential Energy Surfaces of the LSSmKate1 and LSSmKate2 Proteins. Journal of Physical Chemistry B, 2012, 116, 14302-14310. | 1.2 | 16 |
| 58 | Theoretical Analysis of the Catalytic Mechanism of Helicobacter pylori Glutamate Racemase. Journal of Physical Chemistry B, 2012, 116, 12406-12414. | 1.2 | 12 |
| 59 | Theoretical Study of the Mechanism of the Hydride Transfer between Ferredoxinâ€“NADP<sup>+</sup> Reductase and NADP<sup>+</sup>: The Role of Tyr303. Journal of the American Chemical Society, 2012, 134, 20544-20553. | 6.6 | 40 |
| 60 | Ligandâ€induced formation of transient dimers of mammalian 12/15â€lipoxygenase: A key to allosteric behavior of this class of enzymes?. Proteins: Structure, Function and Bioinformatics, 2012, 80, 703-712. | 1.5 | 33 |
| 61 | Essential role of glutamate 317 in galactosyl transfer by Î±3GalT: a computational study. Carbohydrate Research, 2012, 356, 204-208. | 1.1 | 17 |
| 62 | Influence of the enzyme phosphorylation state and the substrate on PKA enzyme dynamics. Biophysical Chemistry, 2012, 161, 17-28. | 1.5 | 9 |
| 63 | A QM/MM study of the phosphoryl transfer to the Kemptide substrate catalyzed by protein kinase A. The effect of the phosphorylation state of the protein on the mechanism. Physical Chemistry Chemical Physics, 2011, 13, 530-539. | 1.3 | 25 |
| 64 | Photo-deactivation pathways of a double H-bonded photochromic Schiff base investigated by combined theoretical calculations and experimental time-resolved studies. Physical Chemistry Chemical Physics, 2011, 13, 14960. | 1.3 | 51 |
| 65 | Substrate binding to mammalian 15-lipoxygenase. Journal of Computer-Aided Molecular Design, 2011, 25, 825-835. | 1.3 | 15 |
| 66 | A variational transition state theory description of periselectivity effects on cycloadditions of ketenes with cyclopentadiene. Theoretical Chemistry Accounts, 2011, 128, 569-577. | 0.5 | 7 |
| 67 | Variational transitionâ€state theory study of the rate constant of the DMSÂ·OH scavenging reaction by O<sub>2</sub>. Journal of Computational Chemistry, 2011, 32, 2104-2118. | 1.5 | 2 |
| 68 | A theoretical study of the DMSÂ·OH scavenging reaction by OH. Its relevance in DMSO formation. Computational and Theoretical Chemistry, 2011, 965, 249-258. | 1.1 | 5 |
| 69 | A method to compute probability current in generic coordinates. Journal of Chemical Physics, 2011, 134, 074115. | 1.2 | 0 |
| 70 | Modulating the Photochemistry of Bipyridylic Compounds by Symmetric Substitutions. ChemPhysChem, 2010, 11, 3696-3703. | 1.0 | 5 |
| 71 | Bipyridyl Derivatives as Photomemory Devices: A Comparative Electronicâ€Structure Study. Chemistry - A European Journal, 2010, 16, 6693-6703. | 1.7 | 20 |
| 72 | Insights into the Mechanism of Binding of Arachidonic Acid to Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2010, 114, 7037-7046. | 1.2 | 30 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Mechanism of the Hydride Transfer between Anabaena Tyr303Ser FNR<sub>rd</sub>/FNR<sub>ox</sub> and NADP<sup>+</sup>/H. A Combined Pre-Steady-State Kinetic/Ensemble-Averaged Transition-State Theory with Multidimensional Tunneling Study. Journal of Physical Chemistry B, 2010, 114, 3368-3379. | 1.2 | 27 |
| 74 | Canonical Variational Transition-State Theory Study of the CF3CHFCH2F + OH Reaction. Journal of Physical Chemistry A, 2010, 114, 2768-2777. | 1.1 | 2 |
| 75 | Formation pathways of DMSO from DMSâ€OH in the presence of O<sub>2</sub> and NO<sub>x</sub>: A theoretical study. Journal of Computational Chemistry, 2009, 30, 173-182. | 1.5 | 9 |
| 76 | Formation pathways of DMSO<sub>2</sub> in the addition channel of the OHâ€initiated DMS oxidation: A theoretical study. Journal of Computational Chemistry, 2009, 30, 1477-1489. | 1.5 | 5 |
| 77 | The 65th birthday of Professor Santiago Olivella Nello. Theoretical Chemistry Accounts, 2009, 123, 1-2. | 0.5 | 0 |
| 78 | Formation pathways of CH3SOH from CH3S(OH)CH3 in the presence of O2: a theoretical study. Theoretical Chemistry Accounts, 2009, 123, 93-103. | 0.5 | 6 |
| 79 | Benchmark calculations on models of the phosphoryl transfer reaction catalyzed by protein kinase A. Theoretical Chemistry Accounts, 2009, 124, 197-215. | 0.5 | 4 |
| 80 | The effect of electron-withdrawing groups in the fragmentation of the radical anions of benzyl phenyl ethers. Computational and Theoretical Chemistry, 2009, 913, 228-235. | 1.5 | 3 |
| 81 | A Theoretical Assessment of Factors Causing Different Molecular Volumes in Isotopologues. Journal of Physical Chemistry A, 2009, 113, 14161-14169. | 1.1 | 3 |
| 82 | How the Substrate d-Glutamate Drives the Catalytic Action of Bacillus subtilis Glutamate Racemase. Journal of the American Chemical Society, 2009, 131, 3509-3521. | 6.6 | 23 |
| 83 | Study of the Photochemical Properties and Conical Intersections of [2,2â€²â€Bipyridyl]â€³â€amineâ€³â€²â€ol. ChemPhysChem, 2008, 9, 2068-2076. | 1.0 | 10 |
| 84 | A Potential Energy Function for Heterogeneous Proton-Wires. Ground and Photoactive States of the Proton-Wire in the Green Fluorescent Protein. Journal of Chemical Theory and Computation, 2008, 4, 1138-1150. | 2.3 | 40 |
| 85 | Operation of the Proton Wire in Green Fluorescent Protein. A Quantum Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 5500-5511. | 1.2 | 63 |
| 86 | Canonical Variational Transition-State Theory Study of the CF3CH2CH3 + OH Reaction. Journal of Physical Chemistry B, 2008, 112, 328-335. | 1.2 | 16 |
| 87 | Exploring the Effects of Intramolecular Vibrational Energy Redistribution on the Operation of the Proton Wire in Green Fluorescent Protein. Journal of Physical Chemistry B, 2008, 112, 13443-13452. | 1.2 | 16 |
| 88 | Electronic-structure and quantum dynamical study of the photochromism of the aromatic Schiff base salicylideneaniline. Journal of Chemical Physics, 2008, 129, 214308. | 1.2 | 92 |
| 89 | Electronic and quantum dynamical insight into the ultrafast proton transfer of 1-hydroxy-2-acetonaphthone. Journal of Chemical Physics, 2007, 127, 084318. | 1.2 | 22 |
| 90 | Tunneling in Green Tea:Â Understanding the Antioxidant Activity of Catechol-Containing Compounds. A Variational Transition-State Theory Study. Journal of the American Chemical Society, 2007, 129, 5846-5854. | 6.6 | 96 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Secondary Kinetic Isotope Effect on the Photoenolization of Triplet O-Methylanthrones. A Microcanonical Transition State Theory Calculation. Journal of Physical Chemistry A, 2007, 111, 10090-10097. | 1.1 | 1 |
| 92 | Methanesulfinic Acid Reaction with OH:â€‰ Mechanism, Rate Constants, and Atmospheric Implications. Journal of Physical Chemistry A, 2007, 111, 7825-7832. | 1.1 | 9 |
| 93 | Theoretical Modeling of Hydroxyl-Radical-Induced Lipid Peroxidation Reactions. Journal of Physical Chemistry B, 2007, 111, 5684-5693. | 1.2 | 46 |
| 94 | New Insights into the Reaction Mechanism Catalyzed by the Glutamate Racemase Enzyme:Â pH Titration Curves and Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 2385-2397. | 1.2 | 13 |
| 95 | Methyl Vinyl Ketone+OH and Methacrolein+OH Oxidation Reactions: A Master Equation Analysis of the Pressure- and Temperature-Dependent Rate Constants. Chemistry - A European Journal, 2007, 13, 1180-1190. | 1.7 | 8 |
| 96 | A PM3/d specific reaction parameterization for iron atom in the hydrogen abstraction catalyzed by soybean lipoxygenase-1. Journal of Computational Chemistry, 2007, 28, 997-1005. | 1.5 | 15 |
| 97 | Kinetic Study on the Reaction of OH Radical with Dimethyl Sulfide in the Absence of Oxygen. ChemPhysChem, 2007, 8, 255-263. | 1.0 | 11 |
| 98 | A Comparative Study on the Photochemistry of Two Bipyridyl Derivatives: [2,2â€²-Bipyridyl]-3,3â€²-diamine and [2,2â€²-Bipyridyl]-3,3â€²-diol. ChemPhysChem, 2007, 8, 1199-1206. | 1.0 | 15 |
| 99 | Comparative study of the prereactive protein kinase A Michaelis complex with Kemptide substrate. Journal of Computer-Aided Molecular Design, 2007, 21, 603-615. | 1.3 | 7 |
| 100 | Enzyme Dynamics and Tunneling Enhanced by Compression in the Hydrogen Abstraction Catalyzed by Soybean Lipoxygenase-1. Journal of Physical Chemistry B, 2006, 110, 24708-24719. | 1.2 | 51 |
| 101 | Variational Transition-State Theory Study of the Dimethyl Sulfoxide (DMSO) and OH Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 798-808. | 1.1 | 23 |
| 102 | On the Ionization State of the Substrate in the Active Site of Glutamate Racemase. A QM/MM Study about the Importance of Being Zwitterionicâ€. Journal of Physical Chemistry A, 2006, 110, 717-725. | 1.1 | 33 |
| 103 | Searching for Saddle Points by Using the Nudged Elastic Band Method:â€‰ An Implementation for Gas-Phase Systems. Journal of Chemical Theory and Computation, 2006, 2, 895-904. | 2.3 | 33 |
| 104 | Charge-Transfer Ï€Ï€* Excited State in the 7-Azaindole Dimer. A Hybrid Configuration Interactions Singles/Time-Dependent Density Functional Theory Description. Journal of Physical Chemistry A, 2006, 110, 1145-1151. | 1.1 | 30 |
| 105 | Potential Energy Landscape of the Photoinduced Multiple Proton-Transfer Process in the Green Fluorescent Protein:Â Classical Molecular Dynamics and Multiconfigurational Electronic Structure Calculations. Journal of the American Chemical Society, 2006, 128, 3564-3574. | 6.6 | 80 |
| 106 | Theoretical Study on the Excited-State Intramolecular Proton Transfer in the Aromatic Schiff Base Salicylidene Methylamine:Â an Electronic Structure and Quantum Dynamical Approach. Journal of Physical Chemistry A, 2006, 110, 4649-4656. | 1.1 | 57 |
| 107 | A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reactant Valleys in Lactate Dehydrogenase. Journal of the American Chemical Society, 2006, 128, 16851-16863. | 6.6 | 52 |
| 108 | Molecular modeling of the kinetic isotope effect on the intramolecular hydrogen atom transfer in triplet 6,9-dimethylbenzosuberone. Chemical Physics, 2006, 328, 410-420. | 0.9 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | On the intramolecular proton transfer of 3-hydroxyflavone in the first singlet excited state: A theoretical study. Chemical Physics, 2006, 325, 243-250. | 0.9 | 38 |
| 110 | Theoretical study of the photoinduced intramolecular proton transfer and rotational processes in 2-(2â€²hydroxyphenyl)-4-methyloxazole in gas phase and embedded in Î²-cyclodextrin. Journal of Photochemistry and Photobiology A: Chemistry, 2005, 173, 365-374. | 2.0 | 17 |
| 111 | overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" | 1.2 | 10 |
| 112 | Enthalpies of formation of isopreneâ€™s major oxidation byproducts. Chemical Physics Letters, 2005, 409, 255-259. | 1.2 | 1 |
| 113 | Electronic structure study of the initiation routes of the dimethyl sulfide oxidation by OH. Journal of Computational Chemistry, 2005, 26, 569-583. | 1.5 | 27 |
| 114 | Pressure Dependence in the Methyl Vinyl Ketone+OH and Methacrolein+OH Oxidation Reactions: An Electronic Structure Study. ChemPhysChem, 2005, 6, 1567-1573. | 1.0 | 7 |
| 115 | Elongated Dihydrogen Versus Compressed Dihydride Complexes: The Temperature Dependence of the H-D Spin-Spin Coupling Constant as a Criterion To Distinguish between Them. Chemistry - A European Journal, 2005, 11, 6315-6325. | 1.7 | 20 |
| 116 | Determination of the Temperature Dependence of the Hâ‹¯D Spinâ‹¯Spin Coupling Constant and the Isotope Effect on the Proton Chemical Shift for the Compressed Dihydride Complex [Cp*Ir(Pâ‹¯P)H2]2+. Journal of the American Chemical Society, 2005, 127, 5632-5640. | 6.6 | 37 |
| 117 | A Molecular Dynamics Simulation of the Binding Modes of d-Glutamate and d-Glutamine to Glutamate Racemase. Journal of Chemical Theory and Computation, 2005, 1, 737-749. | 2.3 | 9 |
| 118 | Reaction Mechanism of the Mandelate Anion Racemization Catalyzed by Mandelate Racemase Enzyme:Â A QM/MM Molecular Dynamics Free Energy Study. Journal of Physical Chemistry B, 2005, 109, 21089-21101. | 1.2 | 10 |
| 119 | A Theoretical Study of the Competitive Homolytic/Heterolytic Aniomesolytic Cleavages of Câ‹¯O Alkyl Ether Bonds. Journal of Organic Chemistry, 2005, 70, 540-548. | 1.7 | 10 |
| 120 | A Fast Radical Chain Mechanism in the Polyfluoroalkoxylation of Aromatics through NO2 Group Displacement. Mechanistic and Theoretical Studies. Journal of Organic Chemistry, 2005, 70, 1718-1727. | 1.7 | 29 |
| 121 | A QM/MM Exploration of the Potential Energy Surface of Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions. Journal of Chemical Theory and Computation, 2005, 1, 750-761. | 2.3 | 22 |
| 122 | Hydrogen Abstraction by Soybean Lipoxygenase-1. Density Functional Theory Study on Active Site Models in Terms of Gibbs Free Energies. Journal of Physical Chemistry B, 2004, 108, 13831-13838. | 1.2 | 20 |
| 123 | Fast hydrogen elimination from the [Ru(PH3)3(CO)(H)2] and [Ru(PH3)4(H)2] complexes in the first singlet excited states: A diabatic quantum dynamics study. Journal of Chemical Physics, 2004, 121, 6258-6267. | 1.2 | 4 |
| 124 | Geometry optimization and transition state search in enzymes: Different options in the microiterative method. International Journal of Quantum Chemistry, 2004, 98, 367-377. | 1.0 | 26 |
| 125 | Quantum Dynamics Study of the Excited-State Double-Proton Transfer in 2,2â€²-Bipyridyl-3,3â€²-diol. ChemPhysChem, 2004, 5, 1372-1378. | 1.0 | 37 |
| 126 | Testing electronic structure methods for describing intermolecular H Â· Â· Â· H interactions in supramolecular chemistry. Journal of Computational Chemistry, 2004, 25, 99-105. | 1.5 | 35 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Elongated Dihydrogen Complexes: What Remains of the Hâ€"H Bond?. ChemInform, 2004, 35, no. | 0.1 | 0 |
| 128 | Rate constants of gas-phase hydrogen abstraction reactions: a balance between the association and the abstraction dynamical bottlenecks. Computational and Theoretical Chemistry, 2004, 709, 35-43. | 1.5 | 12 |
| 129 | Photoinduced proton transfer from the green fluorescent protein chromophore to a water molecule: analysis of the transfer coordinate. Chemical Physics Letters, 2004, 396, 202-207. | 1.2 | 34 |
| 130 | Photo-oxidation of lipids by singlet oxygen: a theoretical study. Chemical Physics Letters, 2004, 398, 336-342. | 1.2 | 23 |
| 131 | Variational Transition State Theory as a Tool To Determine Kinetic Selectivity in Reactions Involving a Valley-Ridge Inflection Point. Journal of the American Chemical Society, 2004, 126, 13089-13094. | 6.6 | 40 |
| 132 | Kinetic Isotope Effect on the Photoenolization ofo-Methylanthrone. A Microcanonical Transition State Theory Calculation. Journal of Physical Chemistry A, 2004, 108, 4536-4541. | 1.1 | 6 |
| 133 | Molecular Dynamics of Excited State Intramolecular Proton Transfer:â€‰ 2-(2â€˜-Hydroxyphenyl)-4-methyloxazole in Gas Phase, Solution, and Protein Environments. Journal of Physical Chemistry B, 2004, 108, 6616-6623. | 1.2 | 22 |
| 134 | Synthesis and Properties of Compressed Dihydride Complexes of Iridium:Â Theoretical and Spectroscopic Investigations. Journal of the American Chemical Society, 2004, 126, 8813-8822. | 6.6 | 79 |
| 135 | Rate Constants for the Hydrogen Abstractions in the OH-Initiated Oxidation of Glycolaldehyde. A Variational Transition-state Theory Calculation. Journal of Physical Chemistry A, 2004, 108, 5117-5125. | 1.1 | 12 |
| 136 | Ground and Excited State Hydrogen Atom Transfer Reactions and Cyclization of 2-Acetylbenzoic Acid. Journal of Physical Chemistry A, 2004, 108, 9331-9341. | 1.1 | 12 |
| 137 | Elongated dihydrogen complexes: what remains of the Hâ€"H Bond?. Chemical Society Reviews, 2004, 33, 175-182. | 18.7 | 178 |
| 138 | The curvature of the Arrhenius plots predicted by conventional canonical transition-state theory in the absence of tunneling. Theoretical Chemistry Accounts, 2003, 110, 352-357. | 0.5 | 25 |
| 139 | Dependence of the rate constants on the treatment of internal rotation modes: The reaction OH + CH3SH â†' CH3S + H2O as an example. Journal of Computational Chemistry, 2003, 24, 701-706. | 1.5 | 9 |
| 140 | How important is the refinement of transition state structures in enzymatic reactions?. Computational and Theoretical Chemistry, 2003, 632, 297-307. | 1.5 | 14 |
| 141 | A theoretical study of the ground and first excited singlet state proton transfer reaction in isolated 7-azaindoleâ€"water complexes. Chemical Physics, 2003, 290, 319-336. | 0.9 | 51 |
| 142 | Determination of enzymatic reaction pathways using QM/MM methods. International Journal of Quantum Chemistry, 2003, 93, 229-244. | 1.0 | 52 |
| 143 | Fast hydrogen elimination from the [Ru(PH3)3(CO)(H)2] complex in the first singlet excited states. A quantum dynamics study. Chemical Physics, 2003, 286, 149-163. | 0.9 | 2 |
| 144 | Variational Transition-State Theory Rate Constant Calculations of the OH + CH3SH Reaction and Several Isotopic Variants. Journal of Physical Chemistry A, 2003, 107, 4490-4496. | 1.1 | 30 |

| # | Article | IF | Citations |
|---|---|---|---|
| 145 | Semiclassical initial value representation description of molecular structure problems: An elongated dihydrogen ruthenium complex. Journal of Chemical Physics, 2002, 117, 7094-7101. | 1.2 | 5 |
| 146 | A combined nuclear dynamics and electronic study of the coupling between the internal rotation of the methyl group and the intramolecular proton transfer in 5-methyltropolone. Journal of Chemical Physics, 2002, 117, 7525-7533. | 1.2 | 21 |
| 147 | Variational Transition-State Theory Rate Constant Calculations with Multidimensional Tunneling Corrections of the Reaction of Acetone with OH. Journal of Physical Chemistry A, 2002, 106, 11760-11770. | 1.1 | 40 |
| 148 | Thermodynamics, Kinetics, and Dynamics of the Two Alternative Aniomesolytic Fragmentations of Câ^'O Bonds:â€‰ An Electrochemical and Theoretical Study. Journal of the American Chemical Society, 2002, 124, 4708-4715. | 6.6 | 28 |
| 149 | On the modulation of the substrate activity for the racemization catalyzed by mandelate racemase enzyme. A QM/MM study. Physical Chemistry Chemical Physics, 2002, 4, 5365-5371. | 1.3 | 9 |
| 150 | The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. Theoretical Chemistry Accounts, 2002, 107, 147-153. | 0.5 | 16 |
| 151 | Test of variational transition state theory with multidimensional tunneling contributions against experimental kinetic isotope effects for the CH n D 4â^'n + OHâ†'P (n=0, 4) reactions. Theoretical Chemistry Accounts, 2002, 108, 38-40. | 0.5 | 11 |
| 152 | On the evaluation of quasi-thermodynamic magnitudes from rate constant values. Influence of the variational and tunnelling contributions. Chemical Physics Letters, 2002, 353, 154-162. | 1.2 | 8 |
| 153 | The photoinduced intramolecular proton transfer in 2-(2â€²-hydroxyphenyl)-4-methyloxazole embedded in Î²-cyclodextrin. Chemical Physics Letters, 2002, 356, 423-430. | 1.2 | 15 |
| 154 | TUNNELING IN 5-METHYLTROPOLONE: COUPLING BETWEEN INTERNAL ROTATION OF METHYL GROUP AND PROTON TRANSFER. , 2002, , . | | 0 |
| 155 | THE 7-AZAINDOLE BASE PAIR PHOTOTAUTOMERIZATION REVISITED: AN AB INITIO STUDY OF THE POTENTIAL ENERGY SURFACE. , 2002, , . | | 0 |
| 156 | Monte Carlo Simulations of Chemical Reactions in Solution. , 2002, , 125-177. | | 0 |
| 157 | Ab Initio Based Exploration of the Potential Energy Surface for the Double Proton Transfer in the First Excited Singlet Electronic State of the 7-Azaindole Dimer. Journal of Physical Chemistry A, 2001, 105, 3887-3893. | 1.1 | 70 |
| 158 | The1H NMR Chemical Shift for the Hydroxy Proton of 4-(Dimethylamino)-2â€˜-hydroxychalcone in Chloroform:â€‰ A Theoretical Approach to Its Inverse Dependence on the Temperature. Organic Letters, 2001, 3, 589-592. | 2.4 | 11 |
| 159 | A QM/MM Study of the Racemization of Vinylglycolate Catalyzed by Mandelate Racemase Enzyme. Journal of the American Chemical Society, 2001, 123, 709-721. | 6.6 | 38 |
| 160 | Variational Transition State Calculations of the CH2F2 + OH Hydrogen Abstraction Reaction. Journal of Physical Chemistry A, 2001, 105, 10553-10561. | 1.1 | 21 |
| 161 | Equilibrium Isotope Effect for the W(CO)3(PCy3)2(H)2/W(Co)3(PCy3)2(Î·2-H2) Tautomeric Equilibrium:Â A Nuclear Dynamics Variable Representation Study. Journal of Physical Chemistry A, 2001, 105, 4676-4681. | 1.1 | 11 |
| 162 | A discrete variable representation study of the dynamics of the double proton transfer in bicyclic oxalamidines. Chemical Physics Letters, 2001, 340, 591-596. | 1.2 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 163 | Quantum mechanical phenomena in dihydrogen and polyhydride transition metal systems. , 2001, , 419-461. | | 0 |
| 164 | The reactions CHnD4â^'n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics computational methods to determine variational transition-state rate constants. I.. Journal of Chemical Physics, 2001, 114, 2154-2165. | 1.2 | 44 |
| 165 | The reactions CHnD4â^'n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics multicoefficient methods to determine variational transition state rate constants. II. Journal of Chemical Physics, 2001, 115, 4515-4526. | 1.2 | 29 |
| 166 | Effective way of modeling chemical catalysis: Empirical valence bond picture of role of solvent and catalyst in alkylation reactions. Journal of Computational Chemistry, 2000, 21, 607-625. | 1.5 | 17 |
| 167 | On the theoretical reports on 7-azaindole base-pair phototautomerization. Chemical Physics Letters, 2000, 324, 75-80. | 1.2 | 27 |
| 168 | A theoretical insight into the internal H-bond and related rotational motion and proton transfer processes of 1-hydroxy-2-acetonaphthone in the S0 state. Chemical Physics Letters, 2000, 328, 83-89. | 1.2 | 28 |
| 169 | On the experimental evidences for 7-azaindole base-pair model ultrafast phototautomerization. Chemical Physics Letters, 2000, 324, 81-87. | 1.2 | 31 |
| 170 | Perspective on "On the theory of oxidation-reduction reactions involving electron transfer. I". Theoretical Chemistry Accounts, 2000, 103, 231-233. | 0.5 | 7 |
| 171 | Structure and Dynamics of [Nb(Î·5-C5H4SiMe3)2(Î·2-H2BR2)] (R2 = O2C6H4, C8H14, H2) Complexes. A Combined Experimental and Theoretical Study. Organometallics, 2000, 19, 3654-3663. | 1.1 | 26 |
| 172 | Nuclear Dynamics Discrete Variable Representation Study of the Equilibrium Isotope Effect on H2Binding in M(Î·2-H2)LnComplexes:Â An Effective Theoretical Way To Account for Anharmonicity. Journal of Physical Chemistry A, 2000, 104, 7898-7905. | 1.1 | 19 |
| 173 | Photoinduced Proton Transfer and Rotational Motion of 1-Hydroxy-2-acetonaphthone in the S1 State:â€‰ A Theoretical Insight into Its Photophysics. Journal of Physical Chemistry A, 2000, 104, 8424-8431. | 1.1 | 56 |
| 174 | A DVR analysis of some vibrational modes in the elongated dihydrogen complex [Ru(Î·2-H2)(C5H5)(H2PCH2PH2)]+. Chemical Physics, 1999, 241, 155-166. | 0.9 | 17 |
| 175 | Effect of deuteration on the fluorescence excitation spectrum of tropolone: a theoretical study. Chemical Physics, 1999, 246, 103-113. | 0.9 | 2 |
| 176 | DNA Mutations Induced by Proton and Charge Transfer in the Low-Lying Excited Singlet Electronic States of the DNA Base Pairs:Â A Theoretical Insight. Journal of Physical Chemistry A, 1999, 103, 6251-6256. | 1.1 | 104 |
| 177 | Effect of a complex formation on the calculated low-pressure rate constant of a bimolecular gas-phase reaction governed by tunneling. Journal of Computational Chemistry, 1999, 20, 1685-1692. | 1.5 | 17 |
| 178 | Theoretical Study of the Effect of Lewis Acids on Dihydrogen Elimination from Niobocene Trihydrides. Chemistry - A European Journal, 1999, 5, 1166-1171. | 1.7 | 15 |
| 179 | Mechanism of the Gas-Phase HO + H2O â†' H2O + OH Reaction and Several Associated Isotope Exchange Reactions:â€‰ A Canonical Variational Transition State Theory Plus Multidimensional Tunneling Calculation. Journal of Physical Chemistry A, 1999, 103, 1044-1053. | 1.1 | 34 |
| 180 | Variational Transition-State Theory with Optimized Orientation of the Dividing Surface and Semiclassical Tunneling Calculations for Deuterium and Muonium Kinetic Isotope Effects in the Free Radical Association Reaction H + C2H4 â†' C2H5. Journal of Physical Chemistry A, 1999, 103, 5061-5074. | 1.1 | 50 |

| # | Article | IF | Citations |
|---|---|---|---|
| 181 | Asymmetry of the Hydrogen Bond of Hydrogen Phthalate Anion in Solution. A QM/MM Study. Journal of the American Chemical Society, 1999, 121, 9198-9207. | 6.6 | 51 |
| 182 | Proton-Transfer Reaction in Isolated and Water-Complexed 8-Hydroxyimidazo[1,2-a]Pyridine in the S0 and S1 Electronic States. A Theoretical Study. Journal of Physical Chemistry A, 1999, 103, 5301-5306. | 1.1 | 11 |
| 183 | On the unexpected isotope effect on the exchange coupling constant in partially deuterated transitionâ€metal trihydride complexes. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 354-358. | 0.9 | 3 |
| 184 | On the localization of the electronic excitation in supramolecules built up by equivalent units linked by hydrogen bonds. Chemical Physics, 1998, 228, 1-7. | 0.9 | 4 |
| 185 | Theoretical study of the role of arginine 127 in the water-promoted mechanism of peptide cleavage by carboxypeptidase A. New Journal of Chemistry, 1998, 22, 319-326. | 1.4 | 21 |
| 186 | Effect of the Spinning Motion of the Dihydrogen Ligand on the Properties of an Elongated Dihydrogen Complex. A Theoretical Study of the trans-[Os(HÂ·Â·Â·H)Cl(H2PCH2CH2PH2)2]+ Complex. Journal of the American Chemical Society, 1998, 120, 8168-8176. | 6.6 | 45 |
| 187 | Temperature Dependence of Proton NMR Chemical Shift As a Criterion To Identify Low-Barrier Hydrogen Bonds. Journal of the American Chemical Society, 1998, 120, 10203-10209. | 6.6 | 53 |
| 188 | Explanation of Deuterium and Muonium Kinetic Isotope Effects for Hydrogen Atom Addition to an Olefin. Journal of the American Chemical Society, 1998, 120, 12141-12142. | 6.6 | 20 |
| 189 | Reaction-Path and Dual-Level Dynamics Calculations of the CH3F + OH Reaction. Journal of Physical Chemistry A, 1998, 102, 10715-10722. | 1.1 | 23 |
| 190 | Variational Transition State Theory and Tunneling Calculations with Reorientation of the Generalized Transition States for Methyl Cation Transfer. Journal of Physical Chemistry A, 1998, 102, 3420-3428. | 1.1 | 48 |
| 191 | Ab Initio Study of Nitromethane Deprotonation by (OH)-Â·nH2O Clusters. Journal of Physical Chemistry A, 1998, 102, 3977-3984. | 1.1 | 14 |
| 192 | Entropic Effects on the Dynamical Bottleneck Location and Tunneling Contributions for C2H4 + H â†' C2H5:â€‰ Variable Scaling of External Correlation Energy for Association Reactions. Journal of the American Chemical Society, 1998, 120, 5559-5567. | 6.6 | 30 |
| 193 | A theoretical study of the isotope effects on the fluorescence excitation spectrum of 5-aminotropolone. Journal of Chemical Physics, 1998, 108, 8114-8122. | 1.2 | 12 |
| 194 | Theoretical Study of the Effect of a Lewis Acid on Hydrogen Exchange Coupling in a Trihydride Metallocene:Â The Cp2NbH3Â·AlH3System. Inorganic Chemistry, 1998, 37, 2334-2339. | 1.9 | 12 |
| 195 | Theoretical study of the unimolecular dissociation of the acetone cation radical. Molecular Physics, 1997, 92, 393-398. | 0.8 | 6 |
| 196 | Is an Extremely Low-Field Proton Signal in the NMR Spectrum Conclusive Evidence for a Low-Barrier Hydrogen Bond?. Journal of Physical Chemistry A, 1997, 101, 8727-8733. | 1.1 | 55 |
| 197 | Isotope effects on the reaction of proton transfer to benzene anions in ethanol. Canadian Journal of Chemistry, 1997, 75, 1229-1233. | 0.6 | 1 |
| 198 | On the photoisomerization of 5-hydroxytropolone: An abâ€‰initio and nuclear wave function study. Journal of Chemical Physics, 1997, 107, 6275-6282. | 1.2 | 18 |

| # | Article | IF | Citations |
|---|---|---|---|
| 199 | Elongated Dihydrogen Complexes:Â A Combined Electronic DFT + Nuclear Dynamics Study of the [Ru(HÂ·Â·Â·H)(C5H5)(H2PCH2PH2)]+Complex. Journal of the American Chemical Society, 1997, 119, 9840-9847. | 6.6 | 64 |
| 200 | On pKaMatching as a Requirement To Form a Low-Barrier Hydrogen Bond. A Theoretical Study in Gas Phase. Journal of Physical Chemistry A, 1997, 101, 3880-3886. | 1.1 | 48 |
| 201 | Structure and Dynamics of LRhâ€œH4â€•(L = Cp, Tp) Systems. A Theoretical Study. Organometallics, 1997, 16, 3805-3814. | 1.1 | 48 |
| 202 | Synthesis and Spectroscopic Properties of Dihydrogen Isocyanide Niobocene [Nb(Î·5-C5H4SiMe3)2(Î·2-H2)(CNR)]+Complexes. Experimental and Theoretical Study of the Blocked Rotation of a Coordinated Dihydrogen. Journal of the American Chemical Society, 1997, 119, 6107-6114. | 6.6 | 57 |
| 203 | Theoretical Study of the Low-Barrier Hydrogen Bond in the Hydrogen Maleate Anion in the Gas Phase. Comparison with Normal Hydrogen Bonds. Journal of the American Chemical Society, 1997, 119, 1081-1086. | 6.6 | 151 |
| 204 | Understanding the activation energy trends for the C2H4+OHâ†'C2H4OH reaction by using canonical variational transition state theory. Journal of Chemical Physics, 1997, 107, 7266-7274. | 1.2 | 50 |
| 205 | Dihydrogen Formation in a Trihydride Metallocene and Its Elimination, Both Assisted by Lewis Acids: The[Cp2NbH3]+BH3 System. Angewandte Chemie International Edition in English, 1997, 36, 265-266. | 4.4 | 23 |
| 206 | Lewisâ€šÃ„uren begÃ¼nstigen die Umwandlung eines Metallocentrihydrids in einen Diwasserstoffkomplex und die H<sub>2</sub>â€Freisetzung aus ihm: das System [Cp<sub>2</sub>NbH<sub>3</sub>] + BH<sub>3</sub>. Angewandte Chemie, 1997, 109, 259-261. | 1.6 | 2 |
| 207 | H-Atom Transfer and Rotational Processes in the Ground and First Singlet Excited Electronic States of 2-(2â€˜-Hydroxyphenyl)oxazole Derivatives:Â Experimental and Theoretical Studiesâ€. The Journal of Physical Chemistry, 1996, 100, 19789-19794. | 2.9 | 86 |
| 208 | Theoretical Study of the Hydrogen Exchange Coupling in the Metallocene Trihydride Complexes [(C5H5)2MH3]n+(M = Mo, W,n= 1; M = Nb, Ta,n= 0). Journal of the American Chemical Society, 1996, 118, 4617-4621. | 6.6 | 60 |
| 209 | On the interpolation of the frequencies of vibrational modes in variational transition state calculations: an adiabatic or diabatic scheme?. Molecular Physics, 1996, 89, 633-644. | 0.8 | 9 |
| 210 | Î±-Bond cleavage upon electronic excitation of acetyl chloride study of CI single surfaces by full geometry optimization. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 373-375. | 1.7 | 9 |
| 211 | On the deprotonation of the cation radicals of substituted ethylenes. A heterolytic or homolytic process?. Chemical Physics, 1996, 204, 419-427. | 0.9 | 2 |
| 212 | Tunnelling paths for proton transfer reactions in solution. A discussion over a simplified model. Computational and Theoretical Chemistry, 1996, 371, 161-169. | 1.5 | 1 |
| 213 | Theoretical study of molecular dynamics in model base pairs. Chemical Physics Letters, 1996, 256, 370-376. | 1.2 | 90 |
| 214 | Kinetic Isotope Effects as Tools To Reveal Solvation Changes Accompanying a Proton Transfer. A Canonical Unified Statistical Theory Calculation. The Journal of Physical Chemistry, 1996, 100, 19389-19397. | 2.9 | 10 |
| 215 | Solvent fluctuations in electron transfer processes. Journal of Molecular Liquids, 1995, 63, 77-88. | 2.3 | 1 |
| 216 | Transition state structures in solution. AIP Conference Proceedings, 1995, , . | 0.3 | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 217 | Bidimensional tunneling splitting in the Aìƒâ€‰1B2 and Xìƒâ€‰1A1 states of tropolone. Journal of Chemical Physics, 1995, 103, 353-359. | 1.2 | 58 |
| 218 | Topologically Controlled Coulombic Interactions, a New Tool in the Developing of Novel Reactivity. Photochemical and Electrochemical Cleavage of Phenyl Alkyl Ethers. Journal of Organic Chemistry, 1995, 60, 3814-3825. | 1.7 | 29 |
| 219 | Quantum Mechanical Hydrogen Exchange Coupling in [(C5H5)Ir(L)H3]+ Complexes (L = PH3, CO). A Combined ab Initio/Tunneling Dynamics Study. Journal of the American Chemical Society, 1995, 117, 1069-1075. | 6.6 | 46 |
| 220 | Choice of the reaction coordinate in electron-transfer reactions in solution. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 1451-1455. | 1.7 | 1 |
| 221 | The Anomalous Isotope Effect for the Addition of Protium and Muonium to Pyrazine. A Theoretical Study. The Journal of Physical Chemistry, 1994, 98, 7858-7861. | 2.9 | 9 |
| 222 | Applicability of the WKB method in asymmetric double wells with degenerate and nondegenerate minima. Journal of Computational Chemistry, 1994, 15, 125-131. | 1.5 | 6 |
| 223 | On the validity of marcus relationship for dissociative electron transfer reactions in solution. Journal of Molecular Liquids, 1994, 60, 147-160. | 2.3 | 2 |
| 224 | Intramolecular hydrogen bonding in primary hydroxyl of thymine 1-(1-Deoxy-Î²-D-Psicofuranosyl) nucleoside. Tetrahedron, 1994, 50, 6689-6694. | 1.0 | 5 |
| 225 | On the water-promoted mechanism of peptide cleavage by carboxypeptidase A. A theoretical study. Canadian Journal of Chemistry, 1994, 72, 2077-2083. | 0.6 | 18 |
| 226 | A Monte Carlo Simulation of the Electrochemical Reduction of Alkyl Halides in Water. On the Validity of Marcus' Relationship. Journal of the American Chemical Society, 1994, 116, 10117-10123. | 6.6 | 15 |
| 227 | A CI all-single-excitations study of the Norrish type I process in acetyl chloride. The Journal of Physical Chemistry, 1993, 97, 12186-12188. | 2.9 | 12 |
| 228 | Ab initio calculations of the quantum mechanical hydrogen exchange coupling in the [(C5H5)Ir(PH3)H3]+ complex. Journal of the American Chemical Society, 1993, 115, 5861-5862. | 6.6 | 32 |
| 229 | Carbonâ€“oxygen alkyl ether fragmentation in the radical anions of phenyl and nitrophenyl methyl ethers. An AM1 study. Journal of the Chemical Society Perkin Transactions II, 1993, , 87-90. | 0.9 | 8 |
| 230 | The role of coupling in intramolecular proton transfer reactions. The hydrogen oxalate anion as an example. Canadian Journal of Chemistry, 1992, 70, 100-106. | 0.6 | 10 |
| 231 | Ab initio study on the effect of attaching a hydrogen molecule to the (H5O2)+ ion cluster. Journal of Chemical Physics, 1992, 97, 6469-6471. | 1.2 | 10 |
| 232 | The mechanism of exchange of intramolecularly hydrogen-bonded protons in a diamide. Journal of the Chemical Society Perkin Transactions II, 1992, , 1621-1624. | 0.9 | 1 |
| 233 | Preferential solvation of Clâ€“in binary equimolecular waterâ€“methanol mixtures. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 3537-3540. | 1.7 | 13 |
| 234 | Intramolecular hydrogen bonding in ribonucleoside sugar hydroxyls. An abinitio study. Canadian Journal of Chemistry, 1992, 70, 1640-1644. | 0.6 | 8 |

| # | Article | IF | Citations |
|---|---|---|---|
| 235 | Tunneling dynamics in isotopically substituted malonaldehyde. Comparison between symmetric and asymmetric species. Journal of the American Chemical Society, 1992, 114, 2072-2076. | 6.6 | 35 |
| 236 | Ab initio study of the NH3 + OH reaction. Chemical Physics, 1992, 165, 41-46. | 0.9 | 18 |
| 237 | A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion. Chemical Physics, 1992, 159, 99-107. | 0.9 | 26 |
| 238 | The use of optimized tunneling paths within a model based on classical trajectories. Chemical Physics Letters, 1992, 196, 73-78. | 1.2 | 4 |
| 239 | Monte Carlo simulation of the diabatic free energy curves for a dissociative electron transfer reaction in a polar solvent. Journal of Computational Chemistry, 1992, 13, 1057-1065. | 1.5 | 11 |
| 240 | Use of intramolecular coulombic interactions to achieve impossible reactions. Photochemical cleavage of 4-nitrophenyl ethers. Journal of the American Chemical Society, 1991, 113, 8970-8972. | 6.6 | 19 |
| 241 | An ab initio study of the collinear reaction of Fe+ (4F) and Fe+ (6D) with H2. Journal of Chemical Physics, 1991, 94, 4352-4355. | 1.2 | 1 |
| 242 | A Monte Carlo simulation of free energy relationships for the electron transfer reaction between Fe+and Fe2+in water. Journal of Computational Chemistry, 1991, 12, 1165-1171. | 1.5 | 11 |
| 243 | Reaction mechanism of 1,2-hydrogen migration of hydrogen peroxide. Canadian Journal of Chemistry, 1990, 68, 666-673. | 0.6 | 9 |
| 244 | The role of many-body interactions in the stability of hydrated Cu2+ clusters. Chemical Physics, 1990, 141, 379-392. | 0.9 | 23 |
| 245 | Comparison between intramolecular proton transfers involving the carboxylate and alkoxide groups. Chemical Physics, 1990, 148, 77-83. | 0.9 | 13 |
| 246 | Bidimensional tunneling dynamics of malonaldehyde and hydrogenoxalate anion. A comparative study. Journal of Chemical Physics, 1990, 93, 5685-5692. | 1.2 | 85 |
| 247 | Ab initio study of the ground and lowâ€lying states of FeH. Journal of Chemical Physics, 1990, 92, 2478-2480. | 1.2 | 24 |
| 248 | Canonical variational transition-state comparative study for M+(= Li+, Na+and K+)+ H2O â†'[M Â·(H2O)]+association reactions. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 241-245. | 1.7 | 0 |
| 249 | The regioselectivity of 4-nitroanisole photosubstitution with primary amines. A mechanistic and theoretical study. Journal of Organic Chemistry, 1990, 55, 3303-3310. | 1.7 | 33 |
| 250 | Symmetric intramolecular proton transfers between oxygen atoms in anionic systems. An ab initio study. Journal of the American Chemical Society, 1990, 112, 3868-3874. | 6.6 | 21 |
| 251 | Ground and lowâ€lying states of FeH+ as derived from ab initio selfâ€consistent field and configuration interaction calculations. Journal of Chemical Physics, 1989, 90, 6436-6442. | 1.2 | 19 |
| 252 | Intrinsic reaction coordinate calculations for reaction paths possessing branching points. Chemical Physics Letters, 1989, 160, 543-548. | 1.2 | 24 |

| # | Article | IF | Citations |
|---|---|---|---|
| 253 | Theoretical study of the conformational preferences in the Cl4W:CH2 complex. Organometallics, 1989, 8, 1837-1841. | 1.1 | 16 |
| 254 | Theoretical study of solvation effects on chemical reactions. A combined quantum chemical/Monte Carlo study of the Meyer-Schuster reaction mechanism in water. Journal of the American Chemical Society, 1989, 111, 829-835. | 6.6 | 39 |
| 255 | Effect of solvent fluctuations in the electron-transfer process between two Fe+ ions. Journal of the Chemical Society Faraday Transactions I, 1989, 85, 1207. | 1.0 | 2 |
| 256 | On constraining solvent molecule displacements in electron-transfer reactions: a critical discussion. The Journal of Physical Chemistry, 1989, 93, 4677-4682. | 2.9 | 3 |
| 257 | Hydration of Fe+: A Monte Carlo simulation of water clusters and of a dilute aqueous solution. Journal of Computational Chemistry, 1988, 9, 819-826. | 1.5 | 3 |
| 258 | Analytical potential from ab initio calculations for the Fe+-H2O and Feo-H2O systems. International Journal of Quantum Chemistry, 1988, 33, 77-85. | 1.0 | 4 |
| 259 | A theoretical study of hydrogenâ€"atom abstraction by methyl radical. Tetrahedron, 1988, 44, 7621-7625. | 1.0 | 9 |
| 260 | Excited states and electronic spectra of monosubstituted benzenes. An AM1 study. Spectrochimica Acta Part A: Molecular Spectroscopy, 1988, 44, 1427-1434. | 0.1 | 15 |
| 261 | The Cu+â€“H2O interaction potential and its application to the study of [Cu(H2O)n]+clusters at different temperatures. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 693-704. | 1.1 | 9 |
| 262 | The reactivity of triplet carbenes: An ab initio study. Computational and Theoretical Chemistry, 1988, 164, 17-24. | 1.5 | 3 |
| 263 | Reactions of singlet and triplet methylene with a C-H bond of ethylene. An ab initio study. The Journal of Physical Chemistry, 1988, 92, 4180-4184. | 2.9 | 11 |
| 264 | Hydrogen abstraction from methane and its fluoro derivatives by methyl radicals. Journal of the Chemical Society Perkin Transactions II, 1987, , 211-213. | 0.9 | 8 |
| 265 | The effect of electron-pair donor solvents on methylene reactivity. Canadian Journal of Chemistry, 1987, 65, 2774-2778. | 0.6 | 8 |
| 266 | A theoretical insight into the insertion reaction of singlet methylene to the hydrogen molecule. Canadian Journal of Chemistry, 1987, 65, 1995-1999. | 0.6 | 5 |
| 267 | The nucleophilic aromatic photosubstitutions of 4,5-dinitroveratrole with amines. Tetrahedron, 1987, 43, 351-360. | 1.0 | 28 |
| 268 | A Monte Carlo simulation of Fe2+ aqueous solvation. Chemical Physics, 1987, 111, 241-247. | 0.9 | 30 |
| 269 | Theoretical study of the dependence on substrate of the reactivity of carbenes. Journal of the Chemical Society Perkin Transactions II, 1986, , 183. | 0.9 | 4 |
| 270 | Theoretical study of several Fe(H2o)n2+clusters at different temperatures. International Journal of Quantum Chemistry, 1986, 29, 1373-1382. | 1.0 | 14 |

| # | Article | IF | Citations |
|---|---|---|---|
| 271 | An intermolecular potential function for the Fe(II)-H2O system from ab initio calculations. International Journal of Quantum Chemistry, 1986, 30, 663-670. | 1.0 | 9 |
| 272 | The Reactivity Of singlet carbenes. An ab initio study. Chemical Physics, 1985, 100, 33-37. | 0.9 | 6 |
| 273 | Solvent effects on chemical reaction profiles. I. Monte Carlo simulation of hydration effects on quantum chemically calculated stationary structures. Journal of Chemical Physics, 1985, 83, 3970-3982. | 1.2 | 13 |
| 274 | The location of transition states for the addition of singlet methylene to substituted ethylenes. Journal of the Chemical Society Perkin Transactions II, 1985, , 131-134. | 0.9 | 3 |
| 275 | Solvent effect in the Walden inversion reactions. Chemical Physics Letters, 1984, 106, 232-236. | 1.2 | 23 |
| 276 | Nitrophenyl ethers as possible photoaffinity labels. The nucleophilic aromatic photosubstitution revisited.. Tetrahedron Letters, 1984, 25, 4147-4150. | 0.7 | 28 |
| 277 | The use of quantum mechanics calculations for the study of corrosion inhibitors. Corrosion Science, 1984, 24, 929-933. | 3.0 | 127 |
| 278 | The mechanism of the methylene addition to ethylene. Computational and Theoretical Chemistry, 1984, 107, 227-232. | 1.5 | 0 |
| 279 | The effect of the correlation energy on the mechanism of the Dielsâ€"Alder reaction. Chemical Physics Letters, 1983, 102, 317-320. | 1.2 | 23 |
| 280 | Methodological strategy in locating transition states. Cyclization of the carbonyl ylide CH2î€†O+â€“CH2â€“and its cycloaddition to ethylene. Journal of the Chemical Society Perkin Transactions II, 1982, , 1419-1423. | 0.9 | 3 |
| 281 | Theoretical interpretation of experimental data on 1,3-dipolar cycloadditions. Tetrahedron, 1982, 38, 1847-1852. | 1.0 | 10 |
| 282 | Theoretical study of the mechanism of the 1,3-dipolar cycloadditions. Tetrahedron, 1979, 35, 2601-2606. | 1.0 | 9 |