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126	Self-consistent reaction field computation of the reactive characteristics of DNA bases in water. 1993 , 33, 1851-1869		32
125	Comparison of 6-31G*-based MST/SCRF and FEP evaluations of the free energies of hydration for small neutral molecules. 1993 , 14, 1498-1503		59
124	Transition structures for carbon dioxide and formaldehyde hydroxylation reactions in the coordinate sphere of zinc. 1993 , 85, 217-230		12
123	Solvent effects on the electronic spectrum of Reichardt's dye. <i>International Journal of Quantum Chemistry</i> , 1994 , 52, 361-377	2.1	32
122	Computer assisted simulations and molecular graphics methods in molecular design. 1. Theory and applications to enzyme active-site directed drug design. 1994 , 3, 377-414		24
121	Computer assisted simulations and molecular graphics methods in molecular design. 1994 , 4, 415-430		
120	Optimization of solute cavities and van der Waals parameters in ab initio MST-SCRF calculations of neutral molecules. 1994 , 15, 446-454		131
119	Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions. 1994 , 182, 237-248		63
118	On the evaluation of the solvent polarization apparent charges in the polarizable continuum model: A new formulation. 1995 , 16, 20-30		40
117	Theoretical studies on nonsteroidal anti-inflammatory drugs. Benoxaprofen, chlorpromazine, and piroxicam. <i>International Journal of Quantum Chemistry</i> , 1995 , 56, 123-136	2.1	1
116	Theoretical studies of electrode potentials in aqueous solution. Investigation of individual contributions from electrostatic, cavity and dispersion interactions to redox potentials. 1995 , 385, 1-8		19
115	On a quantum theory of chemical reactions and the role of in vacuum transition structures. Primary and secondary sources of enzyme catalysis. 1995 , 335, 267-286		19
114	Perturbation-Relaxation Molecular Dynamics Simulations as a Tool to Explore Conformational Space. Reversible Response of the L3 Loop in Porin Towards Charge Screening Effects. 1995 , 15, 35-46		3
113	Current Status of Transition-State Theory. 1996 , 100, 12771-12800		1546
112	Solvent Effects. 5. Influence of Cavity Shape, Truncation of Electrostatics, and Electron Correlation on ab Initio Reaction Field Calculations. 1996 , 100, 16098-16104		1127
111	The Lorentz-Debye-Sack theory and dielectric screening of electrostatic effects in proteins and nucleic acids. 1996 , 371-405		21

110	Optimization of the cavity size for AM1-SCRF calculations of electrode potentials in aqueous solution. 1997 , 425, 139-146		16
109	Perturbation-response theory as a basis for the continuum models of solvation Inclusion of the polarization. 1998 , 428, 9-25		1
108	A theoretical study of the unimolecular decomposition of N-chloro- α -amino acids in aqueous solution. 1998 , 229, 125-136		9
107	omnisol: Fast Prediction of Free Energies of Solvation and Partition Coefficients. <i>Journal of Organic Chemistry</i> , 1998 , 63, 4305-4313	4.2	66
106	Implicit Solvation Models: Equilibria, Structure, Spectra, and Dynamics. 1999 , 99, 2161-2200		1976
105	Two-response-time model based on CM2/INDO/S2 electrostatic potentials for the dielectric polarization component of solvatochromic shifts on vertical excitation energies. <i>International Journal of Quantum Chemistry</i> , 2000 , 77, 264-280	2.1	68
104	A generalized Langevin dynamics approach to model solvent dynamics effects on proteins via a solvent-accessible surface. The carboxypeptidase A inhibitor protein as a model. <i>Theoretical Chemistry Accounts</i> , 2000 , 105, 101-109	1.9	10
103	Theoretical Methods for the Description of the Solvent Effect in Biomolecular Systems. 2000 , 100, 4187-4226		538
102	Semiempirical INDO/S study on the solvatochromism of merocyanine dyes. <i>International Journal of Quantum Chemistry</i> , 2001 , 85, 529-538	2.1	3
101	Using theozymes for designing transition-state analogs for the intramolecular aldol reaction of Ediketones. <i>International Journal of Quantum Chemistry</i> , 2001 , 83, 338-347	2.1	5
100	A general screened Coulomb potential based implicit solvent model: Calculation of secondary structure of small peptides. <i>International Journal of Quantum Chemistry</i> , 2001 , 83, 193-202	2.1	28
99	Solvent Effects and Chemical Reactivity. 2002 ,		5
98	Density functional theory study of the Lewis acid-catalyzed Diels-Alder reaction of nitroalkenes with vinyl ethers using aluminum derivatives. <i>Journal of Physical Organic Chemistry</i> , 2002 , 15, 660-666	2.1	46
97	Origin of the synchronicity on the transition structures of polar Diels-Alder reactions. Are these reactions [4 + 2] processes?. <i>Journal of Organic Chemistry</i> , 2003 , 68, 3884-90	4.2	109
96	Experimental and theoretical investigations for the regio and stereoselective transformation of trans 1,2,3-trisubstituted aziridines into trans oxazolidin-2-ones. 2003 , 59, 677-683		23
95	Continuum solvation models: Dissecting the free energy of solvation. 2003 , 5, 3827-3836		81
94	Experimental and theoretical DFT study of the reaction of 3-amino-1,2-diols with dichloromethane and paraformaldehyde. 2004 , 60, 10353-10358		7
93	The nucleophilic addition of nitrones to carbonyl compounds: insights on the nature of the mechanism of the l-proline induced asymmetric reaction from a DFT analysis. 2004 , 15, 1541-1549		17

92	A DFT study of the Huisgen 1,3-dipolar cycloaddition between hindered thiocarbonyl ylides and tetracyanoethylene. 2004 , 60, 5053-5058		56
91	From quantum chemistry and the classical theory of polar liquids to continuum approximations in molecular mechanics calculations. <i>International Journal of Quantum Chemistry</i> , 2005 , 102, 986-1001	2.1	22
90	Electronic excitation energies of molecules in solution within continuum solvation models: investigating the discrepancy between state-specific and linear-response methods. 2005 , 123, 1345-12		172
89	Electronic excitation energies of molecules in solution: state specific and linear response methods for nonequilibrium continuum solvation models. 2005 , 122, 1045-13		240
88	Theoretical calculations on the cycloreversion of oxetane radical cations. 2005 , 109, 2602-7		15
87	A density functional theory study of the 5-exo cyclization reactions of alpha-substituted 6,6-diphenyl-5-hexenyl radicals. <i>Journal of Organic Chemistry</i> , 2006 , 71, 1984-8	4.2	10
86	Understanding the role of the Lewis acid catalyst on the 1,3-dipolar cycloaddition of N-benzylideneaniline N-oxide with acrolein: a DFT study. 2007 , 63, 4464-4471		36
85	Theoretical study on the enantioselective α -amination reaction of 1,3-dicarbonyl compounds catalyzed by a bifunctional-urea. 2007 , 18, 1655-1662		24
84	A DFT study on the mechanism and regioselectivity of the tandem O-nitroso aldol/Michael reaction of nitrosobenzene and cyclohexenone. 2007 , 815, 105-109		8
83	Theoretical evidence on O \rightarrow N type smiles rearrangement mechanism: a computational study on the intramolecular cyclization of N-methyl-2-(2-chloropyridin-3-yloxy)-acetamide anion. <i>Journal of Physical Organic Chemistry</i> , 2008 , 21, 215-218	2.1	15
82	A combined experimental and theoretical study of the alkylation of 3,5-dithioxo-[1,2,4]triazepines. <i>Journal of Physical Organic Chemistry</i> , 2008 , 21, 457-463	2.1	3
81	The effects of conformation and solvation on optical rotation: substituted epoxides. 2008 , 20, 357-69		34
80	Theoretical insight into the influences of alpha-substituents in aliphatic aldehydes on the enantioselectivities of aldol reactions. 2008 , 20, 54-61		4
79	Mechanistic details of the domino reaction of nitronaphthalenes with the electron-rich dienes. A DFT study. 2008 , 853, 68-76		25
78	Correlation of global electrophilicity with the activation energy in single-step concerted reactions. 2008 , 112, 97-105		11
77	Reaction of the 4-biphenylnitrenium ion with 4-biphenyl azide to produce a 4,4'-azobisbiphenyl stable product: a time-resolved resonance Raman and density functional theory study. 2008 , 112, 11582-9		9
76	A Density Functional Theory Study on the Ring-Opening Polymerization of D-Lactide Catalyzed by a Bifunctional-Thiourea Catalyst. 2009 , 62, 157		22
75	Co(III) complexes of the type [(L)Co(O ₂ CO)] ⁺ (L = tripodal tetraamine ligand): Synthesis, structure, DFT calculations and ⁵⁹ Co NMR. 2009 , 28, 1459-1468		7

74	Mechanism study of the gold-catalyzed cycloisomerization of alpha-aminoallenes: oxidation state of active species and influence of counterion. 2010 , 114, 4689-96		58
73	Theoretical investigation on the isomerization reaction of 4-phenyl-hexa-1,5-enyne catalyzed by homogeneous Au catalysts. 2010 , 114, 12893-9		32
72	Retracted article: Enantioselectivity of aza-MBH-type reaction of nitroalkene to N-tosylimine catalyzed by thiourea-tertiary amine: a theoretical study. 2011 , 1, 1113		7
71	Calculation of the solvation free energy of neutral and ionic molecules in diverse solvents. 2011 , 51, 105-14		16
70	New insight into the formation mechanism of imidazolium-based halide salts. 2011 , 17, 2099-102		7
69	Theoretical investigation on enantioselective Biginelli reaction catalyzed by natural tartaric acid. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 2031-2038	2.1	5
68	Theoretical investigation on chiral cinchona alkaloid salts-catalyzed asymmetric epoxidation of cyclic enones. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 2874-2881	2.1	6
67	Theoretical mechanistic study of TangPhos-catalyzed asymmetric addition of thiols to allenates. 2011 , 339, 99-107		20
66	Theoretical elucidation of the mechanism of cleavage of the aromatic C-C bond in quinoxaline by a tungsten-based complex [W(PMe ₃) ₄ (η-CH ₂ PMe ₂)H]. 2012 , 18, 15537-45		7
65	Theoretical Insight into PtCl ₂ -Catalyzed Isomerization of Cyclopropenes to Allenes. 2012 , 31, 4769-4778		13
64	Theoretical Insight into the Mechanism of CO Inserting into the N-H Bond of the Iron(II) Amido Complex (dmpe) ₂ Fe(H)(NH ₂): An Unusual Self-Promoted Reaction. 2012 , 31, 365-371		3
63	State-of-the-art and challenges in theoretical simulations of heterogeneous catalysis at the microscopic level. 2012 , 2, 2405		34
62	Synthesis of Benzoindolines via a Copper-Catalyzed Reaction of 1-Bromoethynyl-2-(cyclopropylidene)methyl)arenes with N-Allylsulfonamide. 2012 , 354, 3087-3094		19
61	Enantioselectivity in organocatalytic cascade double Michael addition reaction: a theoretical study. 2012 , 116, 670-9		21
60	A highly oxidizing and isolable oxoruthenium(V) complex [Ru(V)(N ₄ O)(O)] ²⁺ : electronic structure, redox properties, and oxidation reactions investigated by DFT calculations. 2013 , 8, 2046-56		12
59	Theoretical mechanism studies on the competitive CO-induced N-N bond cleavage of N ₂ O with N-O bond cleavage mediated by (β-C ₅ Me ₅)Mo[N((i)Pr)C(Me)N((i)Pr)](CO) ₂ . 2013 , 42, 13931-9		9
58	A comparison between state-specific and linear-response formalisms for the calculation of vertical electronic transition energy in solution with the CCSD-PCM method. 2013 , 139, 044116		56
57	Theoretical study of enantiomeric and geometric control in chiral guanidine-catalyzed asymmetric 1,4-addition of 5H-oxazol-4-ones. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 2267-2276	2.1	13

56	Theoretical study on the mechanism of the reaction for alkene hydroaminations catalyzed by chiral aldehyde. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 2457-2463	2.1	3
55	Theoretical investigation on Pt(II)- and Au(I)-mediated cycloisomerizations of propargylic 3-indoleacetate: [3 + 2]- versus [2 + 2]-cycloaddition products. 2013 , 11, 336-43		17
54	Theoretical insight into the mechanism of Pt(II)-catalyzed [3+2] cycloaddition reactions of propadienyl silyl ethers with alkenyl ethers. 2013 , 724, 192-199		2
53	Aromaticity effects on the profiles of the lowest triplet-state potential-energy surfaces for rotation about the C=C bonds of olefins with five-membered ring substituents: an example of the impact of Baird's rule. 2013 , 19, 10698-707		23
52	Theoretical mechanism studies on the electrocatalytic reduction of CO ₂ to formate by water-stable iridium dihydride pincer complex. 2013 , 42, 5755-63		34
51	Theoretical investigation on the Pt(II)-catalyzed tandem migration reactions of propargylic carboxylates. 2013 , 1019, 11-17		2
50	Theoretical study of N-heterocyclic carbenes-catalyzed cascade annulation of benzodienones and enals. 2013 , 25, 521-8		5
49	Ketimido metallophthalocyanines: an approach to phthalocyanine-supported mononuclear high-valent ruthenium complexes. 2014 , 9, 338-50		6
48	QM/MM through the 1990s: The First Twenty Years of Method Development and Applications. 2014 , 54, 1250-1263		33
47	Transition metal-free one-pot synthesis of fused 1,4-thiazepin-5(4H)-ones and theoretical study of the S-N type smiles rearrangement process. <i>Journal of Organic Chemistry</i> , 2014 , 79, 8040-8	4.2	22
46	Phosphorescent cyclometalated iridium(III) complexes that contain substituted 2-acetylbenzo[b]thiophen-3-olate ligand for red organic light-emitting devices. 2014 , 9, 3572-85		18
45	Theoretical Investigation of the Controlled Metathesis Reactions of Methylruthenium(II) Complexes with Terminal Acetylenes. 2014 , 2014, 2502-2511		7
44	Mechanism and diastereoselectivity of the prebiotic synthesis of deoxyribonucleotide precursors C5-thiazoline: A DFT study. 2014 , 1033, 1-5		2
43	A theoretical investigation on palladium-catalyzed one-pot coupling of aryl iodides, alkynes, and amines through C-N bond cleavage for the synthesis of indole derivatives. <i>International Journal of Quantum Chemistry</i> , 2015 , 115, 361-368	2.1	2
42	Insight into the activity of efficient acid-base bifunctional catalysts for the coupling reaction of CO ₂ . 2015 , 113, 3524-3530		6
41	Mechanistic insight into water-modulated cycloisomerization of enynyl esters using an Au(I) catalyst. 2015 , 44, 5354-63		37
40	Long-lived excited states of zwitterionic copper(I) complexes for photoinduced cross-dehydrogenative coupling reactions. 2015 , 21, 1184-90		89
39	A simple method for estimating the absolute solvation free energy of monovalent ions in different solvents. 2015 , 119, 160-71		4

38	A theoretical investigation on the N-N bond cleavage in Ta(IV) hydrazidium and Ta(V) hydrazido complexes. 2016 , 57, 47-53		1
37	Mechanism and Origin of Selectivity in Platinum(II)-Catalyzed Reactions of Acyclic β -Kynones with Alkenes. 2016 , 8, 2771-2780		3
36	Theoretical Studies on the Photochemistry of Pentose Aminooxazoline, a Hypothetical Intermediate Product in the Prebiotic Synthetic Scenario of RNA Nucleotides. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 9329-37	3-4	3
35	Mechanisms and origins of the switchable regioselectivity of FeBr ₃ -catalyzed [1,2]-aryl and [1,2]-alkyl shifts of β -aryl aldehydes. 2016 , 14, 2522-36		8
34	An efficient route to regioselective functionalization of benzo[b]thiophenes via palladium-catalyzed decarboxylative Heck coupling reactions: insights from experiment and computation. 2016 , 14, 895-904		10
33	Luminescent Iridium(III) Complexes Supported by a Tetradentate Trianionic Ligand Scaffold with Mixed O, N, and C Donor Atoms: Synthesis, Structures, Photophysical Properties, and Material Applications. 2017 , 36, 1331-1344		15
32	Alkylation of 2- and 3-alkoxycarbonyl-4-quinolinones. DFT study on the regioselectivity. <i>Journal of Molecular Structure</i> , 2017 , 1128, 142-150	3-4	3
31	Theoretical Studies on the Photophysics and Photochemistry of 5-Formylcytosine and 5-Carboxylcytosine: The Oxidative Products of Epigenetic Modification of Cytosine in DNA. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 2704-2714	3-4	8
30	Theoretical Insight into the Mechanism and Origin of Ligand-Controlled Regioselectivity in Homogenous Gold-Catalyzed Intramolecular Hydroarylation of Alkynes. <i>Journal of Organic Chemistry</i> , 2018 , 83, 2763-2772	4-2	24
29	Incorporation of Hydrogen Bond Angle Dependency into the Generalized Solvation Free Energy Density Model. 2018 , 58, 761-772		2
28	Does a fluorinated Lewis acid catalyst change the molecular mechanism of the decomposition process of nitroethyl carboxylates?. 2018 , 44, 325-337		10
27	Shape, Size, and Internal Dynamics of Loosely Bound Colloidlike Ionic Clusters in Ternary Solvent Systems. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 8154-8165	3-4	1
26	Mechanistic Study on the Decarboxylative C-N Cross-Coupling between Alkyl Carboxylic Acids and Nitrogen Nucleophiles via Dual Copper and Photoredox Catalysis. <i>Inorganic Chemistry</i> , 2019 , 58, 12669-12677	5-1	9
25	Unexpected molecular mechanism of trimethylsilyl bromide elimination from 2-(trimethylsilyloxy)-3-bromo-3-methyl-isoxazolidines. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1-9	11
24	The structural aspects of the transformation of 3-nitroisoxazoline-2-oxide to 1-aza-2,8-dioxabicyclo[3.3.0]octane derivatives: Experimental and MEDT theoretical study. <i>Journal of Molecular Structure</i> , 2019 , 1192, 27-34	3-4	10
23	A molecular electron density theory study of the Lewis acid-catalyzed decomposition reaction of nitroethyl benzoate using aluminum derivatives. <i>Journal of Physical Organic Chemistry</i> , 2019 , 32, e3938	2-1	15
22	Understanding the Molecular Mechanism of the Rearrangement of Internal Nitronic Ester into Nitronorbornene in Light of the MEDT Study. <i>Molecules</i> , 2019 , 24,	4-8	15
21	Theoretical Insight into the Au(I)-Catalyzed Intermolecular Condensation of Homopropargyl Alcohols with Terminal Alkynes: Reactant Stoichiometric Ratio-Controlled Chemodivergence. <i>Journal of Organic Chemistry</i> , 2019 , 84, 579-588	4-2	3

20	Push-pull nitronates in the [3+2] cycloaddition with nitroethylene: Molecular Electron Density Theory study. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 97, 107549	2.8	8
19	Theoretical investigation on transformation of Cr(II) to Cr(V) complexes bearing tetra-N-heterocyclic carbene and group transfer reactivity. <i>International Journal of Quantum Chemistry</i> , 2020 , 120, e26340	2.1	2
18	Participation of Phosphorylated Analogues of Nitroethene in Diels-Alder Reactions with Anthracene: A Molecular Electron Density Theory Study and Mechanistic Aspect. <i>Organics</i> , 2020 , 1, 36-48 ⁹		11
17	Molecular mechanism of Hetero Diels-Alder reactions between (E)-1,1,1-trifluoro-3-nitrobut-2-enes and enamine systems in the light of Molecular Electron Density Theory. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 101, 107714	2.8	8
16	Expanded Coumarins: One-Pot Photo Synthesis of 5-Benzo[12,1]tetrapheno[7,6,5]-chromen-5-ones and Photophysical Properties. <i>Journal of Organic Chemistry</i> , 2020 , 85, 3689-3698	4.2	9
15	Theoretical investigation on the mechanism and enantioselectivity of organocatalytic asymmetric Povarov reactions of anilines and aldehydes. <i>International Journal of Quantum Chemistry</i> , 2021 , 121, e26574	2.1	2
14	Understanding the uniqueness of the stepwise [4 + 1] cycloaddition reaction between conjugated nitroalkenes and electrophilic carbene systems with a molecular electron density theory perspective. <i>International Journal of Quantum Chemistry</i> , 2021 , 121, e26440	2.1	5
13	Perfluorobicyclo[2.2.0]hex-1(4)-ene as unique partner for Diels-Alder reactions with benzene: a density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2021 , 140, 1	1.9	2
12	Application of Phosphorylated Nitroethenes in [3+2] Cycloaddition Reactions Involving Benzonitrile N-Oxide in the Light of a DFT Computational Study. <i>Organics</i> , 2021 , 2, 26-37	9	8
11	Experimental and Theoretical Mechanistic Study on the Thermal Decomposition of 3,3-diphenyl-4-(trichloromethyl)-5-nitropyrazoline. <i>Molecules</i> , 2021 , 26,	4.8	5
10	Quantum Theory of Solvent Effects and Chemical Reactions. 2002 , 283-361		1
9	Theoretical Mechanism Studies on the Enantioselectivity of aza-MBH-type Reaction of Nitroalkene to N-tosylimine Catalyzed by Thiourea-tertiary Amine. <i>Bulletin of the Korean Chemical Society</i> , 2013 , 34, 3591-3596	1.2	6
8	Theoretical investigation of the mechanism of DMAP-promoted [4 + 2]-annulation of prop-2-ynylsulfonium with isatoic anhydride. <i>Canadian Journal of Chemistry</i> , 1-9	0.9	
7	Theoretical Investigation on the Mechanism and Selectivity of Catalyst-Free Annulation of Ynediones and (Iso)quinoline N-oxides. <i>Heterocycles</i> , 2022 , 104,	0.8	
6	Catalytic mechanism of the ruthenium-catalyzed benzonitrile hydrogenation: insights from quantum mechanics calculations. <i>Chemical Physics Letters</i> , 2022 , 139803	2.5	
5	Olefin Hydrogenation Mechanism Catalyzed by Ruthenium Complexes Containing N-Heterocyclic Carbene Ligands.		0
4	Theoretical Investigation of the Mechanism of Rh(III)-catalyzed Annulation of 2-Biphenylboronic Acid with Activated Alkene.		0
3	On the Question of the Formation of Nitro-Functionalized 2,4-Pyrazole Analogs on the Basis of Nitylimine Molecular Systems and 3,3,3-Trichloro-1-Nitroprop-1-Ene. 2022 , 27, 8409		0

- 2 Mechanistic Investigation into the Regio-Controllable Hydroallylations of Alkynes with Allylborons under Pd-Based Synergetic Catalyses. **2023**, 88, 4536-4545 ○
- 1 Regio- and stereoselectivity of [3+2] cycloaddition reactions between (Z)-1-(anthracen-9-yl)-N-methyl nitrene and analogs of trans- β -nitrostyrene on the basis of MEDT computational study. ○