

Rainer E Glaser

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41
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130
ext. papers

2,692
ext. citations

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avg, IF

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L-index

#	Paper	IF	Citations
127	¹³ C NMR study of halogen bonding of haloarenes: measurements of solvent effects and theoretical analysis. <i>Journal of the American Chemical Society</i> , 2004 , 126, 4412-9	16.4	115
126	Planarity of para Hexaphenyl. <i>Physical Review Letters</i> , 1999 , 82, 3625-3628	7.4	93
125	2,6-Dibenzhydryl-N-(2-phenyliminoacenaphthylidene)-4-chloro-aniline nickel dihalides: Synthesis, characterization and ethylene polymerization for polyethylenes with high molecular weights. <i>Journal of Organometallic Chemistry</i> , 2013 , 725, 37-45	2.3	80
124	The effects of the first- and second-row substituents on the structures and energies of PH4X phosphoranes. An ab initio study. <i>Journal of the American Chemical Society</i> , 1991 , 113, 55-64	16.4	70
123	Semipolar phosphorus-oxygen and phosphorus-carbon bonds. A theoretical study of hypophosphite and related methylenephosphoranes. <i>Journal of the American Chemical Society</i> , 1987 , 109, 4184-4188	16.4	70
122	Adenine synthesis in interstellar space: mechanisms of prebiotic pyrimidine-ring formation of monocyclic HCN-pentamers. <i>Astrobiology</i> , 2007 , 7, 455-70	3.7	59
121	Benzenediazonium Ion. Generality, Consistency, and Preferability of the Electron Density Based Dative Bonding Model. <i>Journal of Organic Chemistry</i> , 1995 , 60, 7518-7528	4.2	57
120	Push/pull substitution versus intrinsic or packing related N-N gauche preferences in azines. Synthesis, crystal structures and packing of asymmetrical acetophenone azines. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1995 , 2311-2317		56
119	Stereochemistry and Stereoelectronics of Azines. A Solid State Study of Symmetrical, (E,E)-Configured, Para-Substituted (H, F, Cl, Br, CN) Acetophenone Azines. <i>Journal of Organic Chemistry</i> , 1994 , 59, 4336-4340	4.2	55
118	Charge transfers and polarizations in bonds to silicon. Organosilanes and the SN2(Si) reaction of silane with fluoride. An ab initio study. <i>Journal of the American Chemical Society</i> , 1989 , 111, 3111-3117	16.4	52
117	Aspirin. An ab initio quantum-mechanical study of conformational preferences and of neighboring group interactions. <i>Journal of Organic Chemistry</i> , 2001 , 66, 771-9	4.2	50
116	Ab initio study of the SN1Ar and SN2Ar reactions of benzenediazonium ion with water. On the conception of "unimolecular dediazonation" in solvolysis reactions. <i>Journal of the American Chemical Society</i> , 2004 , 126, 10632-9	16.4	48
115	Synergism of Catalysis and Reaction Center Rehybridization. A Novel Mode of Catalysis in the Hydrolysis of Carbon Dioxide. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 6814-6818	2.8	46
114	The azine bridge as a conjugation stopper: an NMR spectroscopic study of electron delocalization in acetophenone azines. <i>Journal of Organic Chemistry</i> , 2002 , 67, 1441-7	4.2	45
113	Tuning Intermolecular Interactions: A Study of the Structural and Vibrational Properties of p-Hexaphenyl under Pressure. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 6203-6211	2.8	42
112	Theoretical Studies of DNA Base Deamination. 2. Ab Initio Study of DNA Base Diazonium Ions and of Their Linear, Unimolecular Dediazonation Paths. <i>Journal of the American Chemical Society</i> , 1999 , 121, 6108-6119	16.4	39
111	Conjugation in azines. Stereochemical analysis of benzoylformate azines in the solid state, in solution, and in the gas phase. <i>Journal of Organic Chemistry</i> , 1993 , 58, 7446-7455	4.2	39

110	THE CARRIERS OF THE INTERSTELLAR UNIDENTIFIED INFRARED EMISSION FEATURES: CONSTRAINTS FROM THE INTERSTELLAR C-H STRETCHING FEATURES AT 3.2-3.5 μ m. <i>Astrophysical Journal</i> , 2013 , 776, 110	4.7	38
109	Configurational and conformational preferences in oximes and oxime carbanions. Ab initio study of the syn effect in reactions of oxyimine enolate equivalents. <i>Journal of the American Chemical Society</i> , 1989 , 111, 7340-7348	16.4	38
108	sigma-Dative and pi-Backdative Phenyl Cation-Dinitrogen Interactions and Opposing Sign Reaction Constants in Dual Substituent Parameter Relations. <i>Journal of Organic Chemistry</i> , 1999 , 64, 902-913	4.2	37
107	Chloroyttrium 2-(1-(Arylimino)alkyl)quinolin-8-olate Complexes: Synthesis, Characterization, and Catalysis of the Ring-Opening Polymerization of ϵ -Caprolactone. <i>Organometallics</i> , 2012 , 31, 8178-8188	3.8	36
106	Synergism of Catalysis and Reaction Center Rehybridization. An ab Initio Study of the Hydrolysis of the Parent Carbodiimide. <i>Journal of the American Chemical Society</i> , 1998 , 120, 8541-8542	16.4	35
105	Single- and double-proton-transfer in the aggregate between cytosine and guaninediazonium ion. <i>Organic Letters</i> , 1999 , 1, 273-6	6.2	34
104	Asymmetrization effects on structures and populations of the ground state of dipolar donor-acceptor-substituted molecular organic NLO materials. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1130-1140	3.5	33
103	Pyrimidine Ring Opening in the Unimolecular Dediazonation of Guanine Diazonium Ion. An Ab Initio Theoretical Study of the Mechanism of Nitrosative Guanosine Deamination. <i>Journal of the American Chemical Society</i> , 1996 , 118, 10942-10943	16.4	33
102	Thermochemistry of the initial steps of methylaluminumoxane formation. Aluminoxanes and cycloaluminoxanes by methane elimination from dimethylaluminum hydroxide and its dimeric aggregates. <i>Journal of the American Chemical Society</i> , 2011 , 133, 13323-36	16.4	32
101	Ab Initio and Crystal Structures of (E,E)-1,4-Diphenylbutadiene: A New Type of Arene-Arene Double T-Contact and an Interesting Interlayer Cooperation Involving Diastereoisomeric Contacts. <i>Crystal Growth and Design</i> , 2003 , 3, 291-300	3.5	32
100	Organic Chemistry Online: Building Collaborative Learning Communities through Electronic Communication Tools. <i>Journal of Chemical Education</i> , 1999 , 76, 699	2.4	32
99	Polymorphism and C \equiv N \rightarrow N \rightarrow C Conformational Isomers of Azines: X-ray Crystal and Ab Initio Structures of Two Rotational Isomers of Methyl (para-Tolyl) Ketone Azine. <i>Angewandte Chemie International Edition in English</i> , 1994 , 33, 1081-1084		32
98	Incipient nucleophilic attack as a probe for the electronic structure of diazonium ions. An analysis of neighboring-group interactions in .beta.-(carboxyvinyl)diazonium ions. <i>Journal of Organic Chemistry</i> , 1992 , 57, 215-228	4.2	32
97	Comparative analysis of crystal structures of E,E-configured para-substituted acetophenone azines with halogen, oxygen, nitrogen and carbon functional groups. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1995 , 1449		29
96	Importance of the anisotropy of atoms in molecules for the representation of electron density distributions with Lewis structures. A case study of aliphatic diazonium ions. <i>Journal of the American Chemical Society</i> , 1993 , 115, 2340-2347	16.4	28
95	Crystal Potential Formula for the Calculation of Crystal Lattice Sums ¹ . <i>Journal of Physical Chemistry B</i> , 1998 , 102, 4257-4260	3.4	25
94	Analysis of the remarkable difference in the stabilities of methyl- and ethyldiazonium ions. <i>Journal of the American Chemical Society</i> , 1991 , 113, 1109-1120	16.4	25
93	Electron-Density Relaxation and Oppositely Signed Reaction Constants in Dual Substituent Parameter Relationships in Dediazonation Reactions. <i>Angewandte Chemie International Edition in English</i> , 1997 , 36, 2210-2213		24

92	Cytosine catalysis of nitrosative guanine deamination and interstrand cross-link formation. <i>Journal of the American Chemical Society</i> , 2005 , 127, 7346-58	16.4	23
91	Theoretical study of structures and relative energies of isomeric metalated acetaldoximes, models for metalated oxime ethers. <i>Journal of the American Chemical Society</i> , 1987 , 109, 1258-1260	16.4	23
90	Polar order by rational design: crystal engineering with parallel belowamphiphile monolayers. <i>Accounts of Chemical Research</i> , 2007 , 40, 9-17	24.3	22
89	Interpretation of neighboring group interactions in crystal structures. A solid state and quantum-chemical study of "incipient nucleophilic attack" in 2-diazonium benzoic acid and its benzoate. <i>Canadian Journal of Chemistry</i> , 1996 , 74, 1200-1214	0.9	22
88	Origin of the Stabilization of Vinyl Diazonium Ions by π -Substitution; First Crystal Structure of an Aliphatic Diazonium Ion: π -Diethoxyethene-diazonium Hexachloroantimonate. <i>Angewandte Chemie International Edition in English</i> , 1992 , 31, 740-743		22
87	Electronic excitations in homopolyatomic bismuth cations: spectroscopic measurements in molten salts and an ab initio CI-singles study. <i>Chemistry - A European Journal</i> , 2000 , 6, 1078-86	4.8	21
86	A higher level ab initio quantum-mechanical study of the quadrupole moment tensor components of carbon dioxide. <i>Journal of Molecular Structure</i> , 2000 , 556, 131-141	3.4	21
85	The carriers of the unidentified infrared emission features: Clues from polycyclic aromatic hydrocarbons with aliphatic sidegroups. <i>New Astronomy Reviews</i> , 2017 , 77, 1-22	7.9	20
84	5-cyanoimino-4-oxomethylene-4,5-dihydroimidazole and nitrosative guanine deamination. A theoretical study of geometries, electronic structures, and N-protonation. <i>Journal of Organic Chemistry</i> , 2003 , 68, 9882-92	4.2	20
83	On the reaction mechanism of tirapazamine reduction chemistry: unimolecular N-OH homolysis, stepwise dehydration, or triazene ring-opening. <i>Chemical Research in Toxicology</i> , 2012 , 25, 634-45	4	19
82	The supramolecular architecture of 4-aminoacetophenone (1-(4-fluorophenyl)ethylidene)hydrazone hydrate. Double T-contacts and extremely low-density water layers in a mixed azine. <i>Canadian Journal of Chemistry</i> , 1998 , 76, 1371-1378	0.9	19
81	Nitrosation chemistry of pyrroline, 2-imidazoline, and 2-oxazoline: theoretical Curtin-Hammett analysis of retro-ene and solvent-assisted C-X cleavage reactions of alpha-hydroxy-N-nitrosamines. <i>Journal of Organic Chemistry</i> , 2005 , 70, 6790-801	4.2	19
80	5-Cyanoimino-4-oxomethylene-4,5-dihydroimidazole and 5-cyanoamino-4-imidazolecarboxylic acid intermediates in nitrosative guanosine deamination: evidence from 18O-labeling experiments. <i>Journal of the American Chemical Society</i> , 2004 , 126, 9960-9	16.4	19
79	Synergism of catalysis and reaction center rehybridization in nucleophilic additions to cumulenes: the one-, two-, three-water hydrolyses of carbodiimide and methyleneimine. <i>Chemistry - A European Journal</i> , 2002 , 8, 1934-44	4.8	19
78	Structures of nitroso- and nitroguanidine X-ray crystallography and computational analysis. <i>Journal of Chemical Crystallography</i> , 2005 , 35, 317-325	0.5	19
77	Demonstration of an alternative mechanism for G-to-G cross-link formation. <i>Journal of the American Chemical Society</i> , 2005 , 127, 880-7	16.4	18
76	Coordinate covalent C \rightarrow B bonding in phenylborates and latent formation of phenyl anions from phenylboronic Acid. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 1295-304	2.8	18
75	Nitrosative adenine deamination: facile pyrimidine ring-opening in the dediazonation of adeninediazonium ion. <i>Organic Letters</i> , 2003 , 5, 4077-80	6.2	18

74	Stereochemistry and Stereoelectronics of Azines. 13. Conformational Effects on the Quadrupolarity of Azines. An Ab Initio Quantum-Mechanical Study of a Lateral Synthon. <i>Journal of Molecular Modeling</i> , 2000 , 6, 86-98	2	17
73	Spin Polarization versus Spin Delocalization. Topological Electron and Spin Density Analysis of the Rotational Automerization of Allyl Radical Including Electron Correlation Effects ¹ . <i>The Journal of Physical Chemistry</i> , 1994 , 98, 11379-11393		17
72	Stereochemistry of metalated aldimines. 1. An ab initio study of the potential energy surfaces of isolated acetalimine anions, their monomeric lithium and sodium ion pairs, and mechanistic consequences. <i>Journal of Organic Chemistry</i> , 1991 , 56, 6612-6624	4.2	16
71	Stabilities and Spin Distributions of Benzannulated Benzyl Radicals. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1091-9	6.4	15
70	Chemistry Is in the News: Assessment of Student Attitudes toward Authentic News Media-Based Learning Activities. <i>Journal of Chemical Education</i> , 2006 , 83, 662	2.4	15
69	5-Cyanoamino-4-imidazolecarboxamide and nitrosative guanine deamination: experimental evidence for pyrimidine ring-opening during deamination. <i>Journal of the American Chemical Society</i> , 2004 , 126, 2274-5	16.4	15
68	Chemistry Is in the News: Taxonomy of authentic news media-based learning activities ¹ 1. This paper was presented at the symposium Organic Chemistry Teaching in the New Century ¹ 21st ACS National Meeting, San Diego, California, 18 April 2001, and at the 28th Improving University Teaching 2003 Conference, Växjö University, Växjö, Sweden, 16-19 June 2003. View all notes.	2.2	15
67	4-chloroacetophenone. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2000 , 56 (Pt 3), 393-6		15
66	Polarizabilities of Carbon Dioxide and Carbodiimide. Assessment of Theoretical Model Dependencies on Dipole Polarizabilities and Dipole Polarizability Anisotropies ¹ <i>Journal of Physical Chemistry A</i> , 2000 , 104, 11355-11361	2.8	15
65	THE C-H STRETCHING FEATURES AT 3.2-5.5 μm OF POLYCYCLIC AROMATIC HYDROCARBONS WITH ALIPHATIC SIDEGROUPS. <i>Astrophysical Journal</i> , 2016 , 825, 22	4.7	14
64	Dynamical Approach to Multiequilibria Problems for Mixtures of Acids and Their Conjugated Bases. <i>Journal of Chemical Education</i> , 2014 , 91, 1009-1016	2.4	14
63	Multifurcated halogen bonding involving PhI ⁺ ⋯H ⁺ ⋯PhNR ⁻ interactions and its relation to idioteloamphiphile layer architecture. <i>CrystEngComm</i> , 2006 , 8, 372-376	3.3	14
62	Nitrosative guanine deamination: ab initio study of deglycation of N-protonated 5-cyanoimino-4-oxomethylene-4,5-dihydroimidazoles. <i>Chemical Research in Toxicology</i> , 2004 , 17, 1157-69 ⁴		14
61	Theoretical Study of the Quadrupolarity of Carbodiimide ¹ <i>Journal of Physical Chemistry A</i> , 2002 , 106, 7950-7957	2.8	14
60	Electron and spin density analysis of spin-projected unrestricted Hartree-Fock density matrixes of radicals. <i>The Journal of Physical Chemistry</i> , 1993 , 97, 3188-3198		14
59	Heterosubstituted diazonium ions FNN ⁺ , HONN ⁺ , and H ₂ NNN ⁺ . Automerization, dediazonation, and deprotonation. <i>The Journal of Physical Chemistry</i> , 1991 , 95, 7682-7693		14
58	Ammonia elimination from protonated nucleobases and related synthetic substrates. <i>Journal of the American Society for Mass Spectrometry</i> , 2007 , 18, 2040-57	3.5	13
57	Near-perfect dipole parallel-alignment in the highly anisotropic crystal structure of 4-iodoacetophenone-(4-methoxyphenylethylidene) hydrazone. <i>Journal of Chemical Crystallography</i> , 2000 , 30, 489-496	0.5	13

56	Diazonium ions. Topological electron density analysis of cyclopropenyldiazonium dications and of their stability toward dediazonation. <i>Journal of Computational Chemistry</i> , 1990 , 11, 663-679	3.5	13
55	What's in a name? Noncovalent $\text{Ar}^{\oplus}(\text{H}\text{Ar}^{\ominus})_n$ interactions and terminology based on structure and nature of the bonding. <i>CrystEngComm</i> , 2006 , 8, 948-951	3.3	12
54	Nitrosative cytosine deamination. An exploration of the chemistry emanating from deamination with pyrimidine ring-opening. <i>Chemical Research in Toxicology</i> , 2005 , 18, 1211-8	4	12
53	Perfect polar stacking of parallel beloamphiphile layers. Synthesis, structure and solid-state optical properties of the unsymmetrical acetophenone azine DCA. <i>Dalton Transactions</i> , 2006 , 2891-9	4.3	11
52	Conformational Preferences and Pathways for Enantiomerization and Diastereomerization of Benzyl Alcohol. Data Mining and ab Initio Quantum-Mechanical Study. <i>Journal of Organic Chemistry</i> , 2000 , 65, 755-766	4.2	11
51	Tris(chalkogeno)carbenium-Ionen $[\text{C}(\text{XR})_3]^+$ (X = O, S, Se, Te): ein experimenteller und quantenchemischer Vergleich. <i>Angewandte Chemie</i> , 1996 , 108, 317-320	3.6	11
50	Ursache der Stabilisierung von Vinyldiazonium-Ionen durch π -Substitution; erste Kristallstrukturanalyse einer aliphatischen Diazoniumverbindung: π -Diethoxy-ethendiazonium-hexachloroantimonat. <i>Angewandte Chemie</i> , 1992 , 104, 749-752	3.6	11
49	3-Methylcarboxy-1H-indazole. Theoretical study of its formation via intramolecular aliphatic diazonium coupling and x-ray crystal structure. <i>Journal of Physical Organic Chemistry</i> , 1993 , 6, 201-214	2.1	11
48	Near-silence of isothiocyanate carbon in $(13)\text{C}$ NMR spectra: a case study of allyl isothiocyanate. <i>Journal of Organic Chemistry</i> , 2015 , 80, 4360-9	4.2	10
47	Electron and spin-density analysis of tirapazamine reduction chemistry. <i>Chemical Research in Toxicology</i> , 2012 , 25, 620-33	4	10
46	The Cation-Dinitrogen Interaction in the Benzylidiazonium ion-Preferential Electrostatic Complex Formation and Dinitrogen Catalysis of Benzyl Cation Rotational Automerization. <i>Chemistry - A European Journal</i> , 1997 , 3, 1244-1253	4.8	10
45	Amino effect on the protonation of beta-aminoacrylonitrile. <i>Chemical Research in Toxicology</i> , 2005 , 18, 111-4	4	10
44	Stereochemistry of metalated aldimines. 2. A theoretical study of dimeric ion-pair aggregates of isomeric lithioacetaldimines and of their kinetically controlled reaction with formaldehyde. <i>Journal of Organic Chemistry</i> , 1991 , 56, 6625-6637	4.2	10
43	The crystal structure of 4-iodoacetophenone azine. <i>Journal of Chemical Crystallography</i> , 1999 , 29, 1043-1048	4.8	9
42	Crystal Structure of the Explosive Parent Benzyne Precursor: 2-Diazoniobenzenecarboxylate Hydrate. <i>Chemische Berichte</i> , 1993 , 126, 243-249		9
41	Disproportionation of bromous acid HOBrO by direct O-transfer and via anhydrides $\text{O}(\text{BrO})_2$ and $\text{BrO}-\text{BrO}_2$. An ab initio study of the mechanism of a key step of the Belousov-Zhabotinsky oscillating reaction. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 8352-65	2.8	8
40	Inductive and Conjugative S->C Polarizations in π -Rithiocarbenium Ions $[\text{C}(\text{SH})_3]^+$ and $[\text{C}(\text{SH})_3]_2^+$. Potential Energy Surface Analysis, Electronic Structure Motif, and Spin Density Distribution. <i>Journal of the American Chemical Society</i> , 1996 , 118, 11617-11628	16.4	8
39	Simultaneous Determination of All Species Concentrations in Multiequilibria for Aqueous Solutions of Dihydrogen Phosphate Considering Debye-Hückel Theory. <i>Journal of Chemical & Engineering Data</i> , 2018 , 63, 2151-2161	2.8	8

38	Dynamical Approach to Multi-Equilibria Problems Considering the Debye-Hückel Theory of Electrolyte Solutions: Concentration Quotients as a Function of Ionic Strength. <i>Journal of Solution Chemistry</i> , 2017 , 46, 643-662	1.8	7
37	Aluminum alkoxy-catalyzed biomass conversion of glucose to 5-hydroxymethylfurfural: Mechanistic study of the cooperative bifunctional catalysis. <i>Journal of Computational Chemistry</i> , 2019 , 40, 1599-1608	3.5	7
36	Learning To Read Spectra: Teaching Decomposition with Excel in a Scientific Writing Course. <i>Journal of Chemical Education</i> , 2018 , 95, 476-481	2.4	7
35	Elektronendichteverchiebungen und Reaktionskonstanten mit entgegengesetzten Vorzeichen bei der Analyse von Dediazonierungsreaktionen mit Hilfe dualer Substituentenparameter. <i>Angewandte Chemie</i> , 1997 , 109, 2324-2328	3.6	7
34	Dynamic aspects of the stereochemistry of metalated oxime ethers. An ab initio study of the pathways for coordination-isomerization, for syn/anti isomerization, and for racemization of the lithium ion pairs from acetaldoxime. <i>Journal of the American Chemical Society</i> , 1989 , 111, 8799-8809	16.4	7
33	Chemistry Is in the News: assessing intra-group peer review. <i>Assessment and Evaluation in Higher Education</i> , 2010 , 35, 381-402	3.1	6
32	Asymmetry in the N-inversion of heteroarene imines: pyrimidin-4(3H)-imine, pyridin-2(1H)-imine, and 1H-purine-6(9H)-imine. <i>Journal of Organic Chemistry</i> , 2010 , 75, 1132-42	4.2	6
31	Superhydrogenated Polycyclic Aromatic Hydrocarbon Molecules: Vibrational Spectra in the Infrared. <i>Astrophysical Journal, Supplement Series</i> , 2020 , 247, 1	8	6
30	Mechanistic models for LAH reductions of acetonitrile and malononitrile. Aggregation effects of Li ⁺ and AlH ₃ on imide-enamide equilibria. <i>Journal of Organic Chemistry</i> , 2013 , 78, 1113-26	4.2	5
29	Asymmetric imine N-inversion in 3-methyl-4-pyrimidinimine. Molecular dipole analysis of solvation effects. <i>Journal of Organic Chemistry</i> , 2011 , 76, 3987-96	4.2	5
28	Electronic structures and spin topologies of gamma-picoliniumyl radicals. A study of the homolysis of N-methyl-gamma-picolinium and of benzo-, dibenzo-, and naphthoannulated analogs. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 4800-14	2.8	5
27	Dipole Parallel-Alignment in the Crystal Structure of a Polar Biphenyl: 4'-Acetyl-4-Methoxybiphenyl (AMB). <i>Crystal Growth and Design</i> , 2006 , 6, 235-240	3.5	5
26	The Heterolytic Dissociation of Neutral and Protonated Nitrous Acid. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 11112-11119	2.8	5
25	Lattice sum calculations for 1/rp interactions via multipole expansions and Euler summation. <i>Journal of Computational Chemistry</i> , 2001 , 22, 208-215	3.5	5
24	Biomimetic Approaches to Reversible CO ₂ Capture from Air. N-Methylcarbaminic Acid Formation in Rubisco-Inspired Models 2013 , 501-534		4
23	Chemical carcinogens in non-enzymatic cytosine deamination: 3-isocyanatoacrylonitrile. <i>Journal of Molecular Modeling</i> , 2006 , 12, 731-7	2	4
22	Challenges of Globalization and Successful Adaptation Strategies in Implementing a Scientific Writing and Authoring Course in China. <i>Journal of Chemical Education</i> , 2018 , 95, 2155-2163	2.4	4
21	Measurements and Simulations of the Acidity Dependence of the Kinetics of the Iron-Catalyzed Belousov-Zhabotinsky Reaction: Proton-Catalysis in the Electron Transfer Reaction Involving the [Fe(phen)] Species. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 6183-6195	2.8	3

20	RuBisCO-Inspired Biomimetic Approaches to Reversible CO ₂ Capture from Air. <i>ACS Symposium Series</i> , 2015 , 265-293	0.4	3
19	Iodine bonding stabilizes iodomethane in MIDAS pesticide. Theoretical study of intermolecular interactions between iodomethane and chloropicrin. <i>Journal of Agricultural and Food Chemistry</i> , 2012 , 60, 1776-87	5.7	3
18	Effects of electron correlation and spin projection on rotational barriers of trithiocarbenium ion [C(SH) ₃] ⁺ and Radical Dication [C(SH) ₃] ²⁺ . <i>Journal of Computational Chemistry</i> , 1997 , 18, 1023-1035	3.5	3
17	Embedding 1,6-Diphenyl-1,2-Dihydronaphthalene (DHN) in 1,4-Distyrylbenzene (DSB): Arene-Arene Interactions in a Crossed Bis-Diarene <i>Crystal Growth and Design</i> , 2006 , 6, 1014-1021	3.5	3
16	Ab initio study of the regiochemistry of dimetalated oximes. The importance of triple ions in isomeric lithium and sodium ion pairs of the acetaldoxime dianion. <i>Journal of Organic Chemistry</i> , 1989 , 54, 5491-5502	4.2	3
15	Software for the Synergistic Integration of Science with ICT Education. <i>Journal of Information Technology Education: Research</i> , 3 , 325-339		3
14	ADDITIVITY SCHEMES IN CONFORMATIONAL ANALYSIS: CONCEPT AND DEMONSTRATION. <i>Journal of Theoretical and Computational Chemistry</i> , 2005 , 04, 373-381	1.8	2
13	Potential Energy Surface and Electron Density Analysis of Phosphorus Analogues of Aromatic and Aliphatic Diazonium Ions. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 1993 , 77, 73-76	1	2
12	Deuterated Polycyclic Aromatic Hydrocarbons in the Interstellar Medium: The CD Band Strengths of Monodeuterated Species. <i>Astrophysical Journal, Supplement Series</i> , 2020 , 251, 12	8	2
11	Thermochemistry of a Biomimetic and Rubisco-Inspired CO ₂ Capture System from Air. <i>Journal of Carbon Research</i> , 2016 , 2, 18	3.3	2
10	Electronic structures and spin density distributions of BrO ₂ and (HO) ₂ BrO radicals. Mechanisms for avoidance of hypervalency and for spin delocalization and spin polarization. <i>Inorganic Chemistry</i> , 2013 , 52, 11806-20	5.1	1
9	Polymorphie und C?N?N?C-Konformations-isomerie in Azinen: Strukturen zweier Rotationsisomere von Methyl(para-tolyl)ketonazin im Kristall und mit ab-initio-Methoden berechnet. <i>Angewandte Chemie</i> , 1994 , 106, 1150-1152	3.6	1
8	Computational Investigation of the Thermochemistry of the CO Capture Reaction by Ethylamine, Propylamine, and Butylamine in Aqueous Solution Considering the Full Conformational Space via Boltzmann Statistics. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 9578-9593	2.8	1
7	Enhanced piezoresponse and nonlinear optical properties of fluorinated self-assembled peptide nanotubes. <i>AIP Advances</i> , 2019 , 9, 115202	1.5	1
6	Video-Based Kinetic Analysis of Period Variations and Oscillation Patterns in the Ce/Fe-Catalyzed Four-Color Belousov-Zhabotinsky Oscillating Reaction. <i>ACS Symposium Series</i> , 2019 , 251-270	0.4	0
5	Arene-Arene Double T-Contacts: Lateral Synthons in the Engineering of Highly Anisotropic Organic Molecular Crystals. <i>ACS Symposium Series</i> , 2001 , 97-111	0.4	0
4	Video colorimetry of single-chromophore systems based on vector analysis in the 3D color space: Unexpected hysteresis loops in oscillating chemical reactions. <i>Talanta</i> , 2020 , 220, 121303	6.2	0
3	Deuterated Polycyclic Aromatic Hydrocarbons in the Interstellar Medium: The CD Band Strengths of Multideuterated Species. <i>Astrophysical Journal, Supplement Series</i> , 2021 , 255, 23	8	0

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- 1 Chemical carcinogens in non-enzymatic cytosine deamination: 3-isocyanatoacrylonitrile **2006**, 731-737