Rainer E Glaser

List of Publications by Year in Descending Order

127 papers	2,532 citations	30 h-index	41 g-index
130 ext. papers	2,692 ext. citations	5.8 avg, IF	4.89 L-index

#	Paper	IF	Citations
127	Transition Metal-Catalyzed and MAO-Assisted Olefin Polymerization; Cyclic Isomers of Sinn Dimer Are Excellent Ligands in Iron Complexes and Great Methylating Reagents. *Catalysts*, **2022**, 12, 312	4	0
126	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. *Journal of Physical Chemistry A*, **2021**, 125, 9578-9593	2.8	1
125	Deuterated Polycyclic Aromatic Hydrocarbons in the Interstellar Medium: The CD Band Strengths of Multideuterated Species. *Astrophysical Journal, Supplement Series*, **2021**, 255, 23	8	0
124	Superhydrogenated Polycyclic Aromatic Hydrocarbon Molecules: Vibrational Spectra in the Infrared. *Astrophysical Journal, Supplement Series*, **2020**, 247, 1	8	6
123	Deuterated Polycyclic Aromatic Hydrocarbons in the Interstellar Medium: The CD Band Strengths of Monodeuterated Species. *Astrophysical Journal, Supplement Series*, **2020**, 251, 12	8	2
122	Video colorimetry of single-chromophore systems based on vector analysis in the 3D color space: Unexpected hysteresis loops in oscillating chemical reactions. *Talanta*, **2020**, 220, 121303	6.2	0
121	Video-Based Kinetic Analysis of Period Variations and Oscillation Patterns in the Ce/Fe-Catalyzed Four-Color Belousov Zhabotinsky Oscillating Reaction. *ACS Symposium Series*, **2019**, 251-270	0.4	0
120	Aluminum alkoxy-catalyzed biomass conversion of glucose to 5-hydroxymethylfurfural: Mechanistic study of the cooperative bifunctional catalysis. *Journal of Computational Chemistry*, **2019**, 40, 1599-1608	3.5	7
119	Enhanced piezoresponse and nonlinear optical properties of fluorinated self-assembled peptide nanotubes. *AIP Advances*, **2019**, 9, 115202	1.5	1
118	Learning To Read Spectra: Teaching Decomposition with Excel in a Scientific Writing Course. *Journal of Chemical Education*, **2018**, 95, 476-481	2.4	7
117	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. *Journal of Physical Chemistry A*, **2018**, 122, 6183-6195	2.8	3
116	Challenges of Globalization and Successful Adaptation Strategies in Implementing a Scientific Writing and Authoring Course in China. *Journal of Chemical Education*, **2018**, 95, 2155-2163	2.4	4
115	Simultaneous Determination of All Species Concentrations in Multiequilibria for Aqueous Solutions of Dihydrogen Phosphate Considering Debye Hckel Theory. *Journal of Chemical & Engineering Data*, **2018**, 63, 2151-2161	2.8	8
114	The carriers of the unidentified infrared emission features: Clues from polycyclic aromatic hydrocarbons with aliphatic sidegroups. *New Astronomy Reviews*, **2017**, 77, 1-22	7.9	20
113	Dynamical Approach to Multi-Equilibria Problems Considering the Debye Hckel Theory of Electrolyte Solutions: Concentration Quotients as a Function of Ionic Strength. *Journal of Solution Chemistry*, **2017**, 46, 643-662	1.8	7
112	THE CH STRETCHING FEATURES AT 3.2 3.5 m OF POLYCYCLIC AROMATIC HYDROCARBONS WITH ALIPHATIC SIDEGROUPS. *Astrophysical Journal*, **2016**, 825, 22	4.7	14
111	Thermochemistry of a Biomimetic and Rubisco-Inspired CO2 Capture System from Air. *Journal of Carbon Research*, **2016**, 2, 18	3.3	2

110	Near-silence of isothiocyanate carbon in (13)C NMR spectra: a case study of allyl isothiocyanate. *Journal of Organic Chemistry*, **2015**, 80, 4360-9	4.2	10
109	RuBisCO-Inspired Biomimetic Approaches to Reversible CO2 Capture from Air. *ACS Symposium Series*, **2015**, 265-293	0.4	3
108	Dynamical Approach to Multiequilibria Problems for Mixtures of Acids and Their Conjugated Bases. *Journal of Chemical Education*, **2014**, 91, 1009-1016	2.4	14
107	Biomimetic Approaches to Reversible CO2 Capture from Air. N-Methylcarbaminic Acid Formation in Rubisco-Inspired Models **2013**, 501-534		4
106	2,6-Dibenzhydryl-N-(2-phenyliminoacenaphthylenylidene)-4-chloro-aniline nickel dihalides: Synthesis, characterization and ethylene polymerization for polyethylenes with high molecular weights. *Journal of Organometallic Chemistry*, **2013**, 725, 37-45	2.3	80
105	Electronic structures and spin density distributions of BrO2 and (HO)2BrO radicals. Mechanisms for avoidance of hypervalency and for spin delocalization and spin polarization. *Inorganic Chemistry*, **2013**, 52, 11806-20	5.1	1
104	Mechanistic models for LAH reductions of acetonitrile and malononitrile. Aggregation effects of Li+ and AlH3 on imide-enamide equilibria. *Journal of Organic Chemistry*, **2013**, 78, 1113-26	4.2	5
103	THE CARRIERS OF THE INTERSTELLAR UNIDENTIFIED INFRARED EMISSION FEATURES: CONSTRAINTS FROM THE INTERSTELLAR C-H STRETCHING FEATURES AT 3.2-3.5 □m. *Astrophysical Journal*, **2013**, 776, 110	4.7	38
102	Iodine bonding stabilizes iodomethane in MIDAS pesticide. Theoretical study of intermolecular interactions between iodomethane and chloropicrin. *Journal of Agricultural and Food Chemistry*, **2012**, 60, 1776-87	5.7	3
101	On the reaction mechanism of tirapazamine reduction chemistry: unimolecular N-OH homolysis, stepwise dehydration, or triazene ring-opening. *Chemical Research in Toxicology*, **2012**, 25, 634-45	4	19
100	Chloroyttrium 2-(1-(Arylimino)alkyl)quinolin-8-olate Complexes: Synthesis, Characterization, and Catalysis of the Ring-Opening Polymerization of □Caprolactone. *Organometallics*, **2012**, 31, 8178-8188	3.8	36
99	Electron and spin-density analysis of tirapazamine reduction chemistry. *Chemical Research in Toxicology*, **2012**, 25, 620-33	4	10
98	Disproportionation of bromous acid HOBrO by direct O-transfer and via anhydrides O(BrO)2 and BrO-BrO2. An ab initio study of the mechanism of a key step of the Belousov-Zhabotinsky oscillating reaction. *Journal of Physical Chemistry A*, **2012**, 116, 8352-65	2.8	8
97	Thermochemistry of the initial steps of methylaluminoxane formation. Aluminoxanes and cycloaluminoxanes by methane elimination from dimethylaluminum hydroxide and its dimeric aggregates. *Journal of the American Chemical Society*, **2011**, 133, 13323-36	16.4	32
96	Asymmetric imine N-inversion in 3-methyl-4-pyrimidinimine. Molecular dipole analysis of solvation effects. *Journal of Organic Chemistry*, **2011**, 76, 3987-96	4.2	5
95	Chemistry Is in the News: assessing intra-group peer review. *Assessment and Evaluation in Higher Education*, **2010**, 35, 381-402	3.1	6
94	Asymmetry in the N-inversion of heteroarene imines: pyrimidin-4(3H)-imine, pyridin-2(1H)-imine, and 1H-purine-6(9H)-imine. *Journal of Organic Chemistry*, **2010**, 75, 1132-42	4.2	6
93	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. *Journal of Physical Chemistry A*, **2008**, 112, 4800-14	2.8	5

92	Polar order by rational design: crystal engineering with parallel beloamphiphile monolayers. *Accounts of Chemical Research*, **2007**, 40, 9-17	24.3	22
91	Stabilities and Spin Distributions of Benzannulated Benzyl Radicals. *Journal of Chemical Theory and Computation*, **2007**, 3, 1091-9	6.4	15
90	Ammonia elimination from protonated nucleobases and related synthetic substrates. *Journal of the American Society for Mass Spectrometry*, **2007**, 18, 2040-57	3.5	13
89	Adenine synthesis in interstellar space: mechanisms of prebiotic pyrimidine-ring formation of monocyclic HCN-pentamers. *Astrobiology*, **2007**, 7, 455-70	3.7	59
88	Coordinate covalent C --> B bonding in phenylborates and latent formation of phenyl anions from phenylboronic Acid. *Journal of Physical Chemistry A*, **2006**, 110, 1295-304	2.8	18
87	Perfect polar stacking of parallel beloamphiphile layers. Synthesis, structure and solid-state optical properties of the unsymmetrical acetophenone azine DCA. *Dalton Transactions*, **2006**, 2891-9	4.3	11
86	What's in a name? Noncovalent Ar□□?(H□Ar?)n interactions and terminology based on structure and nature of the bonding. *CrystEngComm*, **2006**, 8, 948-951	3.3	12
85	Multifurcated halogen bonding involving Ph□□?H□□PhN□? interactions and its relation to idioteloamphiphile layer architecture. *CrystEngComm*, **2006**, 8, 372-376	3.3	14
84	Dipole Parallel-Alignment in the Crystal Structure of a Polar Biphenyl: 4'-Acetyl-4-Methoxybiphenyl (AMB). *Crystal Growth and Design*, **2006**, 6, 235-240	3.5	5
83	Embedding 1,6-Diphenyl-1,2-Dihydronaphthalene (DHN) in 1,4-Distyrylbenzene (DSB): Arene□Arene Interactions in a □Crossed Bis-Diarene□ *Crystal Growth and Design*, **2006**, 6, 1014-1021	3.5	3
82	Chemistry Is in the News: Assessment of Student Attitudes toward Authentic News Media-Based Learning Activities. *Journal of Chemical Education*, **2006**, 83, 662	2.4	15
81	Chemical carcinogens in non-enzymatic cytosine deamination: 3-isocyanatoacrylonitrile. *Journal of Molecular Modeling*, **2006**, 12, 731-7	2	4
80	Chemical carcinogens in non-enzymatic cytosine deamination: 3-isocyanatoacrylonitrile **2006**, 731-737		
79	Demonstration of an alternative mechanism for G-to-G cross-link formation. *Journal of the American Chemical Society*, **2005**, 127, 880-7	16.4	18
78	Cytosine catalysis of nitrosative guanine deamination and interstrand cross-link formation. *Journal of the American Chemical Society*, **2005**, 127, 7346-58	16.4	23
77	Amino effect on the protonation of beta-aminoacrylonitrile. *Chemical Research in Toxicology*, **2005**, 18, 111-4	4	10
76	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. *Journal of Organic Chemistry*, **2005**, 70, 6790-801	4.2	19
75	Nitrosative cytosine deamination. An exploration of the chemistry emanating from deamination with pyrimidine ring-opening. *Chemical Research in Toxicology*, **2005**, 18, 1211-8	4	12

74	Structures of nitroso- and nitroguanidine X-ray crystallography and computational analysis. *Journal of Chemical Crystallography*, **2005**, 35, 317-325	0.5	19
73	Chemistry Is in the News: Taxonomy of authentic news media-based learning activities1 1. This paper was presented at the symposium Organic Chemistry Teaching in the New Century, 221st ACS National Meeting, San Diego, California, 15 April 2001, and at the 28th Improving University Teaching 2003 Conference, V University, V Sweden, 16 19 June 2003. View all notes.	2.2	15
72	ADDITIVITY SCHEMES IN CONFORMATIONAL ANALYSIS: CONCEPT AND DEMONSTRATION. *Journal of Theoretical and Computational Chemistry*, **2005**, 04, 373-381	1.8	2
71	5-Cyanoimino-4-oxomethylene-4,5-dihydroimidazole and 5-cyanoamino-4-imidazolecarboxylic acid intermediates in nitrosative guanosine deamination: evidence from 18O-labeling experiments. *Journal of the American Chemical Society*, **2004**, 126, 9960-9	16.4	19
70	5-Cyanoamino-4-imidazolecarboxamide and nitrosative guanine deamination: experimental evidence for pyrimidine ring-opening during deamination. *Journal of the American Chemical Society*, **2004**, 126, 2274-5	16.4	15
69	Nitrosative guanine deamination: ab initio study of deglycation of N-protonated 5-cyanoimino-4-oxomethylene-4,5-dihydroimidazoles. *Chemical Research in Toxicology*, **2004**, 17, 1157-69	4	14
68	Ab initio study of the SN1Ar and SN2Ar reactions of benzenediazonium ion with water. On the conception of "unimolecular dediazoniation" in solvolysis reactions. *Journal of the American Chemical Society*, **2004**, 126, 10632-9	16.4	48
67	13C NMR study of halogen bonding of haloarenes: measurements of solvent effects and theoretical analysis. *Journal of the American Chemical Society*, **2004**, 126, 4412-9	16.4	115
66	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 *Crystal Growth and Design*, **2003**, 3, 291-300	3.5	32
65	Synergism of Catalysis and Reaction Center Rehybridization. A Novel Mode of Catalysis in the Hydrolysis of Carbon Dioxide. *Journal of Physical Chemistry A*, **2003**, 107, 6814-6818	2.8	46
64	The Heterolytic Dissociation of Neutral and Protonated Nitrous Acid. *Journal of Physical Chemistry A*, **2003**, 107, 11112-11119	2.8	5
63	5-cyanoimino-4-oxomethylene-4,5-dihydroimidazole and nitrosative guanine deamination. A theoretical study of geometries, electronic structures, and N-protonation. *Journal of Organic Chemistry*, **2003**, 68, 9882-92	4.2	20
62	Nitrosative adenine deamination: facile pyrimidine ring-opening in the dediazoniation of adeninediazonium ion. *Organic Letters*, **2003**, 5, 4077-80	6.2	18
61	Synergism of catalysis and reaction center rehybridization in nucleophilic additions to cumulenes: the one-, two-, three-water hydrolyses of carbodiimide and methyleneimine. *Chemistry - A European Journal*, **2002**, 8, 1934-44	4.8	19
60	Theoretical Study of the Quadrupolarity of Carbodiimide *Journal of Physical Chemistry A*, **2002**, 106, 7950-7957	2.8	14
59	The azine bridge as a conjugation stopper: an NMR spectroscopic study of electron delocalization in acetophenone azines. *Journal of Organic Chemistry*, **2002**, 67, 1441-7	4.2	45
58	Lattice sum calculations for 1/rp interactions via multipole expansions and Euler summation. *Journal of Computational Chemistry*, **2001**, 22, 208-215	3.5	5
57	Aspirin. An ab initio quantum-mechanical study of conformational preferences and of neighboring group interactions. *Journal of Organic Chemistry*, **2001**, 66, 771-9	4.2	50

56	Arene-Arene Double T-Contacts: Lateral Synthons in the Engineering of Highly Anisotropic Organic Molecular Crystals. *ACS Symposium Series*, **2001**, 97-111	0.4	0
55	Tuning Intermolecular Interactions: A Study of the Structural and Vibrational Properties of p-Hexaphenyl under Pressure. *Journal of Physical Chemistry A*, **2001**, 105, 6203-6211	2.8	42
54	Electronic excitations in homopolyatomic bismuth cations: spectroscopic measurements in molten salts and an ab initio CI-singles study. *Chemistry - A European Journal*, **2000**, 6, 1078-86	4.8	21
53	4-chloroacetophenone. *Acta Crystallographica Section C: Crystal Structure Communications*, **2000**, 56 (Pt 3), 393-6		15
52	A higher level ab initio quantum-mechanical study of the quadrupole moment tensor components of carbon dioxide. *Journal of Molecular Structure*, **2000**, 556, 131-141	3.4	21
51	Near-perfect dipole parallel-alignment in the highly anisotropic crystal structure of 4-iodoacetophenone-(4-methoxyphenylethylidene) hydrazone. *Journal of Chemical Crystallography*, **2000**, 30, 489-496	0.5	13
50	Stereochemistry and Stereoelectronics of Azines. 13. Conformational Effects on the Quadrupolarity of Azines. An Ab Initio Quantum-Mechanical Study of a Lateral Synthon. *Journal of Molecular Modeling*, **2000**, 6, 86-98	2	17
49	Polarizabilities of Carbon Dioxide and Carbodiimide. Assessment of Theoretical Model Dependencies on Dipole Polarizabilities and Dipole Polarizability Anisotropies *Journal of Physical Chemistry A*, **2000**, 104, 11355-11361	2.8	15
48	Conformational Preferences and Pathways for Enantiomerization and Diastereomerization of Benzyl Alcohol. Data Mining and ab Initio Quantum-Mechanical Study. *Journal of Organic Chemistry*, **2000**, 65, 755-766	4.2	11
47	Planarity of para Hexaphenyl. *Physical Review Letters*, **1999**, 82, 3625-3628	7.4	93
46	The crystal structure of 4-iodoacetophenone azine. *Journal of Chemical Crystallography*, **1999**, 29, 1043-1048	0.5	9
45	Theoretical Studies of DNA Base Deamination. 2. Ab Initio Study of DNA Base Diazonium Ions and of Their Linear, Unimolecular Dediazoniation Paths. *Journal of the American Chemical Society*, **1999**, 121, 6108-6119	16.4	39
44	Single- and double-proton-transfer in the aggregate between cytosine and guaninediazonium ion. *Organic Letters*, **1999**, 1, 273-6	6.2	34
43	sigma-Dative and pi-Backdative Phenyl Cation-Dinitrogen Interactions and Opposing Sign Reaction Constants in Dual Substituent Parameter Relations. *Journal of Organic Chemistry*, **1999**, 64, 902-913	4.2	37
42	Organic Chemistry Online: Building Collaborative Learning Communities through Electronic Communication Tools. *Journal of Chemical Education*, **1999**, 76, 699	2.4	32
41	Asymmetrization effects on structures and populations of the ground state of dipolar donor–acceptor-substituted molecular organic NLO materials. *Journal of Computational Chemistry*, **1998**, 19, 1130-1140	3.5	33
40	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. *Canadian Journal of Chemistry*, **1998**, 76, 1371-1378	0.9	19
39	Crystal Potential Formula for the Calculation of Crystal Lattice Sums1. *Journal of Physical Chemistry B*, **1998**, 102, 4257-4260	3.4	25

38	Synergism of Catalysis and Reaction Center Rehybridization. An ab Initio Study of the Hydrolysis of the Parent Carbodiimide. *Journal of the American Chemical Society*, **1998**, 120, 8541-8542	16.4	35
37	Electron-Density Relaxation and Oppositely Signed Reaction Constants in Dual Substituent Parameter Relationships in Dediazoniation Reactions. *Angewandte Chemie International Edition in English*, **1997**, 36, 2210-2213		24
36	Elektronendichteverschiebungen und Reaktionskonstanten mit entgegengesetzten Vorzeichen bei der Analyse von Dediazonierungsreaktionen mit Hilfe dualer Substituentenparameter. *Angewandte Chemie*, **1997**, 109, 2324-2328	3.6	7
35	The Cation-Dinitrogen Interaction in the Benzyldiazonium ion. Preferential Electrostatic Complex Formation and Dinitrogen Catalysis of Benzyl Cation Rotational Automerization. *Chemistry - A European Journal*, **1997**, 3, 1244-1253	4.8	10
34	Effects of electron correlation and spin projection on rotational barriers of trithiocarbenium ion [C(SH)3]+ and Radical Dication [C(SH)3]?,2+. *Journal of Computational Chemistry*, **1997**, 18, 1023-1035	3.5	3
33	Inductive and Conjugative S->C Polarizations in Trithiocarbenium Ions [C(SH)3]+ and [C(SH)3]2+. Potential Energy Surface Analysis, Electronic Structure Motif, and Spin Density Distribution. *Journal of the American Chemical Society*, **1996**, 118, 11617-11628	16.4	8
32	Pyrimidine Ring Opening in the Unimolecular Dediazoniation of Guanine Diazonium Ion. An Ab Initio Theoretical Study of the Mechanism of Nitrosative Guanosine Deamination. *Journal of the American Chemical Society*, **1996**, 118, 10942-10943	16.4	33
31	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. *Canadian Journal of Chemistry*, **1996**, 74, 1200-1214	0.9	22
30	Tris(chalkogeno)carbenium-Ionen [C(XR)3]+(X = O, S, Se, Te): ein experimenteller und quantenchemischer Vergleich. *Angewandte Chemie*, **1996**, 108, 317-320	3.6	11
29	Benzenediazonium Ion. Generality, Consistency, and Preferability of the Electron Density Based Dative Bonding Model. *Journal of Organic Chemistry*, **1995**, 60, 7518-7528	4.2	57
28	Push-pull substitution versus intrinsic or packing related N=N gauche preferences in azines. Synthesis, crystal structures and packing of asymmetrical acetophenone azines. *Journal of the Chemical Society Perkin Transactions II*, **1995**, 2311-2317		56
27	Comparative analysis of crystal structures of E,E-configured para-substituted acetophenone azines with halogen, oxygen, nitrogen and carbon functional groups. *Journal of the Chemical Society Perkin Transactions II*, **1995**, 1449		29
26	Spin Polarization versus Spin Delocalization. Topological Electron and Spin Density Analysis of the Rotational Automerization of Allyl Radical Including Electron Correlation Effects1. *The Journal of Physical Chemistry*, **1994**, 98, 11379-11393		17
25	Polymorphism and C?N?N?C Conformational Isomers of Azines: X-ray Crystal and Ab Initio Structures of Two Rotational Isomers of Methyl (para-Tolyl) Ketone Azine. *Angewandte Chemie International Edition in English*, **1994**, 33, 1081-1084		32
24	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. *Angewandte Chemie*, **1994**, 106, 1150-1152	3.6	1
23	Stereochemistry and Stereoelectronics of Azines. A Solid State Study of Symmetrical, (E,E)-Configured, Para-Substituted (H, F, Cl, Br, CN) Acetophenone Azines. *Journal of Organic Chemistry*, **1994**, 59, 4336-4340	4.2	55
22	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. *Journal of the American Chemical Society*, **1993**, 115, 2340-2347	16.4	28
21	Conjugation in azines. Stereochemical analysis of benzoylformate azines in the solid state, in solution, and in the gas phase. *Journal of Organic Chemistry*, **1993**, 58, 7446-7455	4.2	39

20	Electron and spin density analysis of spin-projected unrestricted Hartree-Fock density matrixes of radicals. *The Journal of Physical Chemistry*, **1993**, 97, 3188-3198		14
19	Potential Energy Surface and Electron Density Analysis of Phosphorus Analogues of Aromatic and Aliphatic Diazonium Ions. *Phosphorus, Sulfur and Silicon and the Related Elements*, **1993**, 77, 73-76	1	2
18	Crystal Structure of the Explosive Parent Benzyne Precursor: 2-Diazoniobenzenecarboxylate Hydrate. *Chemische Berichte*, **1993**, 126, 243-249		9
17	3-Methylcarboxy-1H-indazole. Theoretical study of its formation via intramolecular aliphatic diazonium coupling and x-ray crystal structure. *Journal of Physical Organic Chemistry*, **1993**, 6, 201-214	2.1	11
16	Incipient nucleophilic attack as a probe for the electronic structure of diazonium ions. An analysis of neighboring-group interactions in .beta.-(carboxyvinyl)diazonium ions. *Journal of Organic Chemistry*, **1992**, 57, 215-228	4.2	32
15	Origin of the Stabilization of Vinyldiazonium Ions by ß-Substitution; First Crystal Structure of an Aliphatic Diazonium Ion: ß-Diethoxyethene-diazonium Hexachloroantimonate. *Angewandte Chemie International Edition in English*, **1992**, 31, 740-743		22
14	Ursache der Stabilisierung von Vinyldiazonium-Ionen durch ß-Substitution; erste Kristallstrukturanalyse einer aliphatischen Diazoniumverbindung: ß-Diethoxy-ethendiazonium-hexachloroantimonat. *Angewandte Chemie*, **1992**, 104, 749-752	3.6	11
13	Heterosubstituted diazonium ions FNN+, HONN+, and H2NNN+. Automerization, dediazoniation, and deprotonation. *The Journal of Physical Chemistry*, **1991**, 95, 7682-7693		14
12	Analysis of the remarkable difference in the stabilities of methyl- and ethyldiazonium ions. *Journal of the American Chemical Society*, **1991**, 113, 1109-1120	16.4	25
11	Stereochemistry of metalated aldimines. 1. An ab initio study of the potential energy surfaces of isolated acetaldimine anions, their monomeric lithium and sodium ion pairs, and mechanistic consequences. *Journal of Organic Chemistry*, **1991**, 56, 6612-6624	4.2	16
10	Stereochemistry of metalated aldimines. 2. A theoretical study of dimeric ion-pair aggregates of isomeric lithioacetaldimines and of their kinetically controlled reaction with formaldehyde. *Journal of Organic Chemistry*, **1991**, 56, 6625-6637	4.2	10
9	The effects of the first- and second-row substituents on the structures and energies of PH4X phosphoranes. An ab initio study. *Journal of the American Chemical Society*, **1991**, 113, 55-64	16.4	70
8	Diazonium ions. Topological electron density analysis of cyclopropeniumyldiazonium dications and of their stability toward dediazoniation. *Journal of Computational Chemistry*, **1990**, 11, 663-679	3.5	13
7	Charge transfers and polarizations in bonds to silicon. Organosilanes and the SN2(Si) reaction of silane with fluoride. An ab initio study. *Journal of the American Chemical Society*, **1989**, 111, 3111-3117	16.4	52
6	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. *Journal of Organic Chemistry*, **1989**, 54, 5491-5502	4.2	3
5	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. *Journal of the American Chemical Society*, **1989**, 111, 8799-8809	16.4	7
4	Configurational and conformational preferences in oximes and oxime carbanions. Ab initio study of the syn effect in reactions of oxyimine enolate equivalents. *Journal of the American Chemical Society*, **1989**, 111, 7340-7348	16.4	38
3	Semipolar phosphorus-oxygen and phosphorus-carbon bonds. A theoretical study of hypophosphite and related methylenephosphoranes. *Journal of the American Chemical Society*, **1987**, 109, 4184-4188	16.4	70

2	Theoretical study of structures and relative energies of isomeric metalated acetaldoximes, models for metalated oxime ethers. *Journal of the American Chemical Society*, **1987**, 109, 1258-1260	16.4	23
1	Software for the Synergistic Integration of Science with ICT Education. *Journal of Information Technology Education:Research*,3, 325-339		3