Rainer Koch

List of Publications by Year
in descending order

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88	2,007	201674	302126
papers	citations	27 h-index	39 g-index

99	99	99	2007
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Optimization and application of lithium parameters for PM3. Journal of Computational Chemistry, 1993, 14, 1301-1312.	3.3	180
2	Experimental and theoretical Raman and surfaceâ€enhanced Raman scattering study of cysteine. Journal of Raman Spectroscopy, 2009, 40, 632-638.	2.5	90
3	Investigation of Reactive Intermediates of Chemical Reactions in Solution by Electrospray Ionization Mass Spectrometry: Radical Cation Chain Reactions. Angewandte Chemie - International Edition, 2003, 42, 4700-4703.	13.8	71
4	Mechanism of the Intramolecular Hydroamination of Alkenes Catalyzed by Neutral Indenyltitanium Complexes: A DFT Study. Chemistry - A European Journal, 2008, 14, 10430-10436.	3.3	56
5	Nanofibers from functionalized para-phenylene molecules. Applied Physics Letters, 2005, 86, 153107.	3.3	55
6	Study of the Interaction of Pollutant Nitro Polycyclic Aromatic Hydrocarbons with Different Metallic Surfaces by Surface-Enhanced Vibrational Spectroscopy (SERS and SEIR). Journal of Physical Chemistry A, 2003, 107, 9611-9619.	2.5	52
7	PM3-MO Calculations of Monolithiated Sulfones, Sulfoxides, and 1,3-Dithianes: Comparison with ab Initio or X-ray Results. Journal of Organic Chemistry, 1994, 59, 4529-4534.	3.2	50
8	Two Different Structural Motifs Observed for Dimeric Dialkylaluminum and Dialkylgallium Alkynides [R2E-C?C-C6H5]2. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2004, 630, 1839-1845.	1.2	45
9	The First Structurally Authenticated Organomercury(1+) Thioether Complexesâ^' Mercuryâ^'Carbon Bond Activation Related to the Mechanism of the Bacterial Enzyme Organomercurial Lyase. European Journal of Inorganic Chemistry, 2004, 2004, 2301-2312.	2.0	41
10	Intramolecular Concerted Insertion of Vinyl Cations into Cï£¿H Bonds: Hydroalkylating Cyclization of Alkynes with Alkyl Chloroformates To Give Cyclopentanes. Angewandte Chemie - International Edition, 2006, 45, 3076-3079.	13.8	39
11	Initiation of Radical Chain Reactions of Thiol Compounds and Alkenes without any Added Initiator: Thiolâ€Catalyzed cis/trans Isomerization of Methyl Oleate. Chemistry - A European Journal, 2012, 18, 8201-8207.	3.3	39
12	Facile 1,3- and 1,5-Chlorine Migration. Journal of Organic Chemistry, 1996, 61, 6809-6813.	3.2	38
13	Theoretical group 14 chemistry. Part 2. Si4R6: a theoretical approach. Computational and Theoretical Chemistry, 2004, 680, 91-97.	1.5	38
14	Theoretical Study of the Deprotonation of Nitriles, RCH2CN:Â Ab Initio and PM3 Calculations of Intermediate Aggregates and Transition States. Journal of Organic Chemistry, 1996, 61, 2523-2529.	3.2	37
15	Di(Î¼-acetato)dialkyldigallium as starting compound for the facile syntheses of digallium derivatives containing bridged or terminally co-ordinated Gaâ€“Ga single bonds. Journal of the Chemical Society Dalton Transactions, 1999, , 2385-2392.	1.1	37
16	Synthesis of an Aluminatacyclopropene Derivative with an AlC2Heterocycle and an Exocyclic AlR2Substituent:Â Evidence for a Nonclassical Bonding Situation. Organometallics, 1999, 18, 4598-4602.	2.3	36
17	Theoretical surface-enhanced Raman spectra study of substituted benzenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1049-1055.	3.9	34
18	Amino-, Alkoxy-, and Alkylthio-Isocyanates and â€“ Isothiocyanates, RX-NCY, their Isomers RX-YCN and RX-CNY, and their Rearrangements. Current Organic Chemistry, 2011, 15, 1745-1759.	1.6	34

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19	Nitrilimines:Â Evidence for the Allenic Structure in Solution, Experimental andAb InitioStudies of the Barrier to Racemization, and First Diastereoselective [3 + 2]-Cycloaddition. Journal of the American Chemical Society, 1997, 119, 2819-2824.	13.7	32
20	Cycloaddition Reactions of an Acetylene-Linked Bis(germaethene)1,2. Organometallics, 2002, 21, 3990-3995.	2.3	32
21	Ab initio and PM3-MO calculations of lithiophosphonates. Journal of Organic Chemistry, 1995, 60, 5861-5866.	3.2	30
22	1,3-Stereoinduction in Radical Reactions:Â Radical Additions to Dialkyl 2-Alkyl-4-methyleneglutarates. Journal of the American Chemical Society, 2000, 122, 12458-12468.	13.7	30
23	Bacteriorhodopsin Enhances Efficiency of Perovskite Solar Cells. ACS Applied Materials & Interfaces, 2019, 11, 30728-30734.	8.0	30
24	1H-1,3-Diazepines, 5H-1,3-diazepines, 1,3-diazepinones, and 2,4-diazabicyclo[3.2.0]heptenes,. Organic and Biomolecular Chemistry, 2004, 2, 1227-1238.	2.8	29
25	Novel acyclic nitroxides for nitroxide-mediated polymerization: Kinetic, electron paramagnetic resonance spectroscopic, X-ray diffraction, and molecular modeling investigations. Journal of Polymer Science Part A, 2006, 44, 1926-1940.	2.3	29
26	[3,3]-Sigmatropic Shifts and Retro-ene Rearrangements in Cyanates, Isocyanates, Thiocyanates, and Isothiocyanates of the Form RX-YCN and RX-NCY. Journal of Organic Chemistry, 2012, 77, 1749-1759.	3.2	29
27	Keteneâ€“Ketene Interconversion. 6-Carbonylcyclohexa-2,4-dienoneâ€“Hepta-1,2,4,6-tetraene-1,7-dioneâ€“6-Oxocyclohexa-2,4-dienylidene and Wolff Rearrangement to Fulven-6-one. Journal of Organic Chemistry, 2014, 79, 6978-6986.	3.2	29
28	Retro-Ene Reactions in Acylallene Derivatives. Journal of Organic Chemistry, 1998, 63, 2619-2626.	3.2	28
29	A PM3 and MNDO Study on the Mechanism and the Regioselectivity of the Lithiation of Lithium Methyl-1- and Methyl-2-naphthylcarbamate, Lithium 1,2,3,4-Tetrahydroisoquinolinecarbamate and Toluene. Journal of Organic Chemistry, 1995, 60, 3743-3749.	3.2	27
30	Complete Defluorination of 1,2,3,4-Tetramethyl-5-(trifluoromethyl)cyclopentadiene by Titanium Tetrakis(dimethylamide)â€”Selective Formation of a Cyclic Hexanuclear Titanium Fluoroamide and 6,6-Dimethylaminotetramethylfulvene. Chemistry - A European Journal, 2001, 7, 622-626.	3.3	27
31	Cumulene Rearrangements: Ketene-Ketene, Isocyanate-Isocyanate, Thioketene-Ketene, Imidoylketene-Ketenimine, and Ketene-Allene Rearrangements. Current Organic Chemistry, 2010, 14, 1586-1599.	1.6	27
32	N-Mesityl-C-acylketenimines:â€‰ 1,5-Sigmatropic Shifts and Electrocyclization to Quinolines. Journal of Organic Chemistry, 1998, 63, 5779-5786.	3.2	26
33	Diastereoselective Lewis acid mediated hydrophosphonylation of heterocyclic imines: a stereoselective approach towards ÃŽÂ±-amino phosphonates. Journal of the Chemical Society, Perkin Transactions 1, 2001, , 2804-2816.	1.3	26
34	Arginine interactions with anatase TiO2 (100) surface and the perturbation of 49Ti NMR chemical shifts â€“ a DFT investigation: relevance to Renu-Seeram bio solar cell. Journal of Molecular Modeling, 2011, 17, 1467-1472.	1.8	26
35	Dihydro-1,3-diazepinones and diazabicyclo[3.2.0]heptenones from pyridyl azides. Journal of the Chemical Society Perkin Transactions 1, 1998, , 2247-2250.	0.9	25
36	Aluminium Hydrazides: Reactions oftert-Butylaluminium Chlorides with Dilithium Bis(trimethylsilyl)hydrazide â€“ Formation of Iminoalanes and their Hydrazido Adducts. European Journal of Inorganic Chemistry, 1999, 1999, 2021-2027.	2.0	25

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37	Aluminium Hydrazides: Dimeric Bis(tert-butyl)aluminium Hydrazides withSix-Membered Al2N4 and Five-Membered Al2N3 Heterocycles. European Journal of Inorganic Chemistry, 2000, 2000, 2255-2262.	2.0	23
38	Theoretical studies on titanium pentafulvene complexes. Journal of Organometallic Chemistry, 2006, 691, 4539-4544.	1.8	22
39	Twisting and planarization in pushâ€“pull ethylenesElectronic supplementary information (ESI) available: tables of X-ray crystallographic bond lengths and angles of compounds 8â€“19 (including) Tj ETQq1 1 0.784314 rgBT /Overlock and 18 (Figs. S1â€“S5) and packing diagrams for 17Â·H2O and 19Â·H2O (Figs. S6â€“S7). See http://www.rsc.org/suppdata/p2/b1/b106624a/. Perkin Transactions II RSC, 2002, , 515-523.	1.1	21
40	Formation of Allenyl Ketones, 3-Ethynylcoumarins, and Arylfurans, Furylfurans, and Furylthiophenes by Flash Vacuum Thermolysis of 3-Methylidenefuran-2(3H)-ones. Journal of Organic Chemistry, 2014, 79, 65-71.	3.2	21
41	1,3-Stereoinduction in Radical Reactions. Angewandte Chemie - International Edition, 2000, 39, 2758-2761.	13.8	19
42	[Ga9(CMe3)9].â€”a Persistent Cluster Radical Anion, Boron-Analogous Chemistry with the Heavier Homologue Gallium. Angewandte Chemie - International Edition, 2003, 42, 2422-2423.	13.8	18
43	Theoretical study on the nonlinear optical properties of phenylenes and influencing factors. Journal of Physical Organic Chemistry, 2008, 21, 954-962.	1.9	18
44	Reactions of the Titanaallene Intermediate [Cp*2TiCCH2] with Isonitriles:â€‰ An Approach to the Chemistry of Radialene Type Molecules. Organometallics, 2001, 20, 1354-1359.	2.3	17
45	Rearrangements and Interconversions of Heteroatom-Substituted Isocyanates, Isothiocyanates, Nitrile Oxides, and Nitrile Sulfides, RXâ€“NCY and RYâ€“CNX. Journal of Organic Chemistry, 2011, 76, 6024-6029.	3.2	16
46	SERS spectrum and DFT calculations of 6-nitrochrysene on silver islands. Vibrational Spectroscopy, 2005, 37, 153-160.	2.2	15
47	Theoretical group 14 chemistry, Part 3. A DFT study of Ge4R6. Computational and Theoretical Chemistry, 2005, 714, 109-115.	1.5	15
48	Theoretical study of the syn and anti thiophene-2-aldehyde conformers using density functional theory and normal coordinate analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 935-945.	3.9	15
49	Theoretical surface-enhanced Raman spectra study of substituted benzenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1074-1079.	3.9	15
50	13C NMR calculations on azepines and diazepines. Journal of the Chemical Society Perkin Transactions II, 1997, , 1851-1860.	0.9	14
51	Keteneâ€“acetylene [2 + 2] cycloadditions: cyclobutenone and/or oxete formation?. Organic and Biomolecular Chemistry, 2004, 2, 195-199.	2.8	14
52	Raman and SERS study of N-acetyl-5-methoxytryptamine, melatoninâ€”The influence of the different molecular fragments on the SERS effect. Vibrational Spectroscopy, 2015, 80, 70-78.	2.2	14
53	Benzotriazole-assisted Î²-lithiation of vinyl ethers. Tetrahedron, 1994, 50, 6005-6016.	1.9	13
54	A Spiropentasiladiene and Other Strained Silicon-Containing Rings. Angewandte Chemie - International Edition, 2002, 41, 1861.	13.8	13

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55	Highly diastereoselective hydrophosphonylation of cyclic imines using BINOL as source of chirality. Tetrahedron Letters, 2000, 41, 7285-7288.	1.4	11
56	The thioacyl isocyanateâ€“acyl isothiocyanate rearrangementâ€Šâ€. Perkin Transactions II RSC, 2000, , 1846-1850.	1.1	11
57	Iminopropadienones Râ€“NCCCO and carbon suboxide, C3O2. Theoretical and experimental 13C NMR spectra. Computational and Theoretical Chemistry, 2004, 686, 31-36.	1.5	11
58	Rearrangements of Acyl, Thioacyl, and Imidoyl (Thio)cyanates to Iso(thio)cyanates, Acyl Iso(thio)cyanates to (Thio)acyl Isocyanates, and Imidoyl Iso(thio)cyanates to (Thio)acyl Carbodiimides, RCX-YCN â‡Œ RCX-NCY â‡Œ RCY-NCX â‡Œ RCY-XCN (X and Y = O, S, NRâ€²). Journal of Organic Chemistry, 2013, 78, 1802-1810.	3.2	11
59	Coordination chemistry of lipoic acid and related compounds.. New Journal of Chemistry, 2002, 26, 560-566.	2.8	10
60	Ein Spiropentasiladien und andere gespannte Silicium-haltige Ringe. Angewandte Chemie, 2002, 114, 1941.	2.0	9
61	Twisted Push - Pull Ethylenes. Australian Journal of Chemistry, 2008, 61, 805.	0.9	9
62	Surfaceâ€enhanced Raman scattering and density functional theory studies of bis(4â€aminophenyl)sulfone. Journal of Raman Spectroscopy, 2010, 41, 160-166.	2.5	9
63	Silylene and Germylene Additions to 1,3-Diynes:Â Bis(silacyclopropenes) versus Germaethenes Formation, a DFT Study. Organometallics, 2004, 23, 1570-1575.	2.3	8
64	Theoretical 49Ti NMR chemical shifts. Journal of Molecular Modeling, 2006, 12, 723-729.	1.8	8
65	Collisionally Activated Dissociation of Some Bulkily Substituted Pyridinium Cations, II. Substituent Effect on Appearance Potential. Chemische Berichte, 1992, 125, 177-181.	0.2	7
66	Highly Twisted C=C Double Bonds in 4-Methyleneisoxazolones. Australian Journal of Chemistry, 2009, 62, 1068.	0.9	7
67	Accurate Calculated Optical Properties of Substituted Quaterphenylene Nanofibers. Journal of Physical Chemistry A, 2010, 114, 474-480.	2.5	7
68	Vibrational and scaled quantum chemical study of O,O-dimethyl S-methylcarbamoylmethyl phosphorodithioate, dimethoate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 89, 222-230.	3.9	7
69	Coordination Chemistry of Lipoic Acid and Related Compounds V [1]. New Heteroditopic Ligands Derived from Monoazacrown Ethers and Lipoic Acid. Monatshefte FÃ¼r Chemie, 2002, 133, 1097-1108.	1.8	6
70	Reaction of Iminopropadienones with Amines: Mechanistic Explanations of Zwitterionic Intermediate, Ketene and Ketenimine Formation. Journal of Physical Chemistry A, 2008, 112, 8999-9004.	2.5	6
71	IR, Raman and SERS spectral analysis and DFT calculations on the Herbicide O,S-Dimethyl phosphoramidothioate, metamidophos. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 120-128.	3.9	6
72	Theoretical Group 14 Chemistry. 4. Cyclotriplumbanes:â€‰ Relativistic and Substituents Effects. Journal of Chemical Theory and Computation, 2005, 1, 1298-1303.	5.3	5

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73	Reaction of Iminopropadienones with Aminesâ€"Formation of Zwitterionic Intermediates, Ketenes, and Ketenimines. Journal of Physical Chemistry A, 2008, 112, 9742-9750.	2.5	5
74	The SAMP alkylation: A computational study. Organic and Biomolecular Chemistry, 2011, 9, 2885.	2.8	5
75	Oximes in the Isoxazolone, Pyrazolone, and 1,2,3-Triazolone Series: Experimental and Computational Investigation of Energies and Structures of E/Z Isomers of Î±-Oxo-Oximes in the Gas Phase and in Solution. Australian Journal of Chemistry, 2015, 68, 1329.	0.9	5
76	Twisted C=C Double Bonds with Very Low Rotational Barriers in Dioxanediones and Isoxazolones Determined by Lowâ€Temperature Dynamic NMR Spectroscopy and Computational Chemistry. European Journal of Organic Chemistry, 2016, 2016, 4985-4990.	2.4	5
77	Simulation of NMR chemical shifts in heterocycles: a method evaluation. Journal of Molecular Modeling, 2017, 23, 9.	1.8	5
78	Synthesis, Characterization, and Modelling of Novel Multifunctional Acryloyl-Based Monomers: An Experimental and Computational Study. Australian Journal of Chemistry, 2002, 55, 675.	0.9	4
79	Synthesis of Monofunctionalized p-Quaterphenyls. Synthesis, 2008, 2008, 2446-2450.	2.3	4
80	Zwitterionic 1,3â€Shift Intermediates in the Interconversions of (Thio)carbamoyl Isocyanates and Carbamoyl Iso(thio)cyanates, R₂Nâ€“CXâ€“NCOâ€‰â‡Œâ€‰R₂Nâ€“COâ€“NCX, and in Carbamoylketenes R₂Nâ€“COâ€“CH=C=O. European Journal of Organic Chemistry, 2013, 2013, 7914-7921.	2.4	4
81	Alkene Assisted Homolysis of the Siâ€H, Geâ€H, and Snâ€H Bond: New Examples of Molecule Assisted Homolysis (MAH). European Journal of Organic Chemistry, 2019, 2019, 3599-3604.	2.4	4
82	An Unusual Reaction of the Natural Compound Benaphthamycin B:Â Theoretical Study of a Model Systemâ€. Journal of Organic Chemistry, 2006, 71, 1074-1079.	3.2	3
83	Î±â€Oxoâ€Iminoxyls of Isoxazolones, PyrazolÂones and 1,2,3â€Triazolone. European Journal of Organic Chemistry, 2015, 2015, 5143-5149.	2.4	3
84	Raman, infrared, SERS and theoretical study of 3â€(1â€phenylpropanâ€2â€ylamino) propanenitrile, fenproporex. Journal of Raman Spectroscopy, 2011, 42, 1497-1504.	2.5	2
85	Remote-controlled nucleophilicity III: A valuable model to explain and predict the observed regioselectivity of the electrophilic attack on substituted 4-methylpyridine anions. Journal of Organometallic Chemistry, 2019, 900, 120919.	1.8	2
86	â€˜Green' Synthesis of 2-Substituted 6-Hydroxy-[3H]-pyrimidin-4-ones and 4,6-Dichloropyrimidines: Improved Strategies and Mechanistic Study. Australian Journal of Chemistry, 2015, 68, 814.	0.9	1
87	Why is an experimental regioselectivity of Fischer indole syntheses observed: A mechanistic model DFT study. Tetrahedron, 2021, 91, 132116.	1.9	1
88	USING MOLECULAR ELECTROSTATIC POTENTIALS AND FRONTIER ORBITALS FOR THE SURFACE-ENHANCED RAMAN INTERPRETATION OF FLUOXETINE. Journal of the Chilean Chemical Society, 2019, 64, 4627-4632.	1.2	1