

# Rainer Koch

## List of Publications by Year in descending order

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88  
papers

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201674

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docs citations

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times ranked

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#	ARTICLE	IF	CITATIONS
1	Why is an experimental regioselectivity of Fischer indole syntheses observed: A mechanistic model DFT study. <i>Tetrahedron</i> , 2021, 91, 132116.	1.9	1
2	Bacteriorhodopsin Enhances Efficiency of Perovskite Solar Cells. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 30728-30734.	8.0	30
3	Remote-controlled nucleophilicity III: A valuable model to explain and predict the observed regioselectivity of the electrophilic attack on substituted 4-methylpyridine anions. <i>Journal of Organometallic Chemistry</i> , 2019, 900, 120919.	1.8	2
4	Alkene Assisted Homolysis of the Si-H, Ge-H, and Sn-H Bond: New Examples of Molecule Assisted Homolysis (MAH). <i>European Journal of Organic Chemistry</i> , 2019, 2019, 3599-3604.	2.4	4
5	USING MOLECULAR ELECTROSTATIC POTENTIALS AND FRONTIER ORBITALS FOR THE SURFACE-ENHANCED RAMAN INTERPRETATION OF FLUOXETINE. <i>Journal of the Chilean Chemical Society</i> , 2019, 64, 4627-4632.	1.2	1
6	Simulation of NMR chemical shifts in heterocycles: a method evaluation. <i>Journal of Molecular Modeling</i> , 2017, 23, 9.	1.8	5
7	Twisted C=C Double Bonds with Very Low Rotational Barriers in Dioxanediones and Isoxazolones Determined by Low-Temperature Dynamic NMR Spectroscopy and Computational Chemistry. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 4985-4990.	2.4	5
8	$\hat{\pm}$ -Oxo-Iminoxyls of Isoxazolones, Pyrazolones and 1,2,3-Triazolone. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 5143-5149.	2.4	3
9	'Green' Synthesis of 2-Substituted 6-Hydroxy-[3H]-pyrimidin-4-ones and 4,6-Dichloropyrimidines: Improved Strategies and Mechanistic Study. <i>Australian Journal of Chemistry</i> , 2015, 68, 814.	0.9	1
10	Raman and SERS study of N-acetyl-5-methoxytryptamine, melatonin: The influence of the different molecular fragments on the SERS effect. <i>Vibrational Spectroscopy</i> , 2015, 80, 70-78.	2.2	14
11	Oximes in the Isoxazolone, Pyrazolone, and 1,2,3-Triazolone Series: Experimental and Computational Investigation of Energies and Structures of E/Z Isomers of $\hat{\pm}$ -Oxo-Oximes in the Gas Phase and in Solution. <i>Australian Journal of Chemistry</i> , 2015, 68, 1329.	0.9	5
12	Formation of Allenyl Ketones, 3-Ethynylcoumarins, and Arylfurans, Furylfurans, and Furylthiophenes by Flash Vacuum Thermolysis of 3-Methylidene-furan-2(3H)-ones. <i>Journal of Organic Chemistry</i> , 2014, 79, 65-71.	3.2	21
13	Ketene-Ketene Interconversion. 6-Carbonylcyclohexa-2,4-dienone-Hepta-1,2,4,6-tetraene-1,7-dione-6-Oxocyclohexa-2,4-dienylidene and Wolff Rearrangement to Fulven-6-one. <i>Journal of Organic Chemistry</i> , 2014, 79, 6978-6986.	3.2	29
14	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 $\rightleftharpoons$ RCX-NCY $\rightleftharpoons$ RCY-NCX $\rightleftharpoons$ RCY-XCN (X and Y = O, S, NR <sup>2</sup> ). <i>Journal of Organic Chemistry</i> , 2013, 78, 1802-1810.	3.2	11
15	IR, Raman and SERS spectral analysis and DFT calculations on the Herbicide O,S-Dimethyl phosphoramidothioate, metamidophos. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 114, 120-128.	3.9	6
16	Zwitterionic 1,3-Shift Intermediates in the Interconversions of (Thio)carbamoyl Isocyanates and Carbamoyl Iso(thio)cyanates, R <sub>2</sub> N-CX-NCO $\rightleftharpoons$ R <sub>2</sub> N-CO-NCX, and in Carbamoylketenes R <sub>2</sub> N-CO-CH=C=O. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 7914-7921.	2.4	4
17	[3,3]-Sigmatropic Shifts and Retro-ene Rearrangements in Cyanates, Isocyanates, Thiocyanates, and Isothiocyanates of the Form RX-YCN and RX-NCY. <i>Journal of Organic Chemistry</i> , 2012, 77, 1749-1759.	3.2	29
18	Initiation of Radical Chain Reactions of Thiol Compounds and Alkenes without any Added Initiator: Thiol-Catalyzed <i>cis</i> / <i>trans</i> Isomerization of Methyl Oleate. <i>Chemistry - A European Journal</i> , 2012, 18, 8201-8207.	3.3	39

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19	Vibrational and scaled quantum chemical study of O,O-dimethyl S-methylcarbamoylmethyl phosphorodithioate, dimethoate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 222-230.	3.9	7
20	Rearrangements and Interconversions of Heteroatom-Substituted Isocyanates, Isothiocyanates, Nitrile Oxides, and Nitrile Sulfides, $RX\hat{=}NCY$ and $RY\hat{=}CNX$ . <i>Journal of Organic Chemistry</i> , 2011, 76, 6024-6029.	3.2	16
21	The SAMP alkylation: A computational study. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 2885.	2.8	5
22	Arginine interactions with anatase TiO <sub>2</sub> (100) surface and the perturbation of <sup>49</sup> Ti NMR chemical shifts – a DFT investigation: relevance to Renu-Seeram bio solar cell. <i>Journal of Molecular Modeling</i> , 2011, 17, 1467-1472.	1.8	26
23	Raman, infrared, SERS and theoretical study of 3-(1-phenylpropan-2-ylamino) propanenitrile, fenproporex. <i>Journal of Raman Spectroscopy</i> , 2011, 42, 1497-1504.	2.5	2
24	Amino-, Alkoxy-, and Alkylthio-Isocyanates and Isothiocyanates, $RX\hat{=}NCY$ , their Isomers $RX\hat{=}YCN$ and $RX\hat{=}CNY$ , and their Rearrangements. <i>Current Organic Chemistry</i> , 2011, 15, 1745-1759.	1.6	34
25	Cumulene Rearrangements: Ketene-Ketene, Isocyanate-Isocyanate, Thioketene-Ketene, Imidoylketene-Ketenimine, and Ketene-Allene Rearrangements. <i>Current Organic Chemistry</i> , 2010, 14, 1586-1599.	1.6	27
26	Surface-enhanced Raman scattering and density functional theory studies of bis(4-aminophenyl)sulfone. <i>Journal of Raman Spectroscopy</i> , 2010, 41, 160-166.	2.5	9
27	Accurate Calculated Optical Properties of Substituted Quaterphenylene Nanofibers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 474-480.	2.5	7
28	Experimental and theoretical Raman and surface-enhanced Raman scattering study of cysteine. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 632-638.	2.5	90
29	Highly Twisted C=C Double Bonds in 4-Methyleneisoxazolones. <i>Australian Journal of Chemistry</i> , 2009, 62, 1068.	0.9	7
30	Theoretical study on the nonlinear optical properties of phenylenes and influencing factors. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 954-962.	1.9	18
31	Mechanism of the Intramolecular Hydroamination of Alkenes Catalyzed by Neutral Indenyltitanium Complexes: A DFT Study. <i>Chemistry - A European Journal</i> , 2008, 14, 10430-10436.	3.3	56
32	Theoretical surface-enhanced Raman spectra study of substituted benzenes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1049-1055.	3.9	34
33	Theoretical surface-enhanced Raman spectra study of substituted benzenes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1074-1079.	3.9	15
34	Reaction of Iminopropadienones with Amines – Formation of Zwitterionic Intermediates, Ketenes, and Ketenimines. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9742-9750.	2.5	5
35	Reaction of Iminopropadienones with Amines: Mechanistic Explanations of Zwitterionic Intermediate, Ketene and Ketenimine Formation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8999-9004.	2.5	6
36	Twisted Push - Pull Ethylenes. <i>Australian Journal of Chemistry</i> , 2008, 61, 805.	0.9	9

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37	Synthesis of Monofunctionalized p-Quaterphenyls. <i>Synthesis</i> , 2008, 2008, 2446-2450.	2.3	4
38	An Unusual Reaction of the Natural Compound Benaphthamycin B: A Theoretical Study of a Model System. <i>Journal of Organic Chemistry</i> , 2006, 71, 1074-1079.	3.2	3
39	Novel acyclic nitroxides for nitroxide-mediated polymerization: Kinetic, electron paramagnetic resonance spectroscopic, X-ray diffraction, and molecular modeling investigations. <i>Journal of Polymer Science Part A</i> , 2006, 44, 1926-1940.	2.3	29
40	Theoretical studies on titanium pentafulvene complexes. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4539-4544.	1.8	22
41	Theoretical study of the syn and anti thiophene-2-aldehyde conformers using density functional theory and normal coordinate analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 935-945.	3.9	15
42	Theoretical <sup>49</sup> Ti NMR chemical shifts. <i>Journal of Molecular Modeling</i> , 2006, 12, 723-729.	1.8	8
43	Intramolecular Concerted Insertion of Vinyl Cations into C≡C-H Bonds: Hydroalkylating Cyclization of Alkynes with Alkyl Chloroformates To Give Cyclopentanes. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 3076-3079.	13.8	39
44	SERS spectrum and DFT calculations of 6-nitrochrysene on silver islands. <i>Vibrational Spectroscopy</i> , 2005, 37, 153-160.	2.2	15
45	Theoretical group 14 chemistry, Part 3. A DFT study of Ge <sub>4</sub> R <sub>6</sub> . <i>Computational and Theoretical Chemistry</i> , 2005, 714, 109-115.	1.5	15
46	Nanofibers from functionalized para-phenylene molecules. <i>Applied Physics Letters</i> , 2005, 86, 153107.	3.3	55
47	Theoretical Group 14 Chemistry. 4. Cyclotriplobanes: Relativistic and Substituents Effects. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1298-1303.	5.3	5
48	Ketene-acetylene [2 + 2] cycloadditions: cyclobutenone and/or oxete formation?. <i>Organic and Biomolecular Chemistry</i> , 2004, 2, 195-199.	2.8	14
49	Two Different Structural Motifs Observed for Dimeric Dialkylaluminum and Dialkylgallium Alkynides [R <sub>2</sub> E-C≡C-C <sub>6</sub> H <sub>5</sub> ] <sub>2</sub> . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2004, 630, 1839-1845.	1.2	45
50	The First Structurally Authenticated Organomercury(1+) Thioether Complexes: Mercury-Carbon Bond Activation Related to the Mechanism of the Bacterial Enzyme Organomercurial Lyase. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 2301-2312.	2.0	41
51	Theoretical group 14 chemistry. Part 2. Si <sub>4</sub> R <sub>6</sub> : a theoretical approach. <i>Computational and Theoretical Chemistry</i> , 2004, 680, 91-97.	1.5	38
52	Iminopropadienones: NCCCO and carbon suboxide, C <sub>3</sub> O <sub>2</sub> . Theoretical and experimental <sup>13</sup> C NMR spectra. <i>Computational and Theoretical Chemistry</i> , 2004, 686, 31-36.	1.5	11
53	Silylene and Germylene Additions to 1,3-Diynes: Bis(silacyclopropenes) versus Germaethenes Formation, a DFT Study. <i>Organometallics</i> , 2004, 23, 1570-1575.	2.3	8
54	1H-1,3-Diazepines, 5H-1,3-diazepines, 1,3-diazepinones, and 2,4-diazabicyclo[3.2.0]heptenes. <i>Organic and Biomolecular Chemistry</i> , 2004, 2, 1227-1238.	2.8	29

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55	[Ga9(CMe3)9]·a Persistent Cluster Radical Anion, Boron-Analogous Chemistry with the Heavier Homologue Gallium. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 2422-2423.	13.8	18
56	Investigation of Reactive Intermediates of Chemical Reactions in Solution by Electrospray Ionization Mass Spectrometry: Radical Cation Chain Reactions. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 4700-4703.	13.8	71
57	Study of the Interaction of Pollutant Nitro Polycyclic Aromatic Hydrocarbons with Different Metallic Surfaces by Surface-Enhanced Vibrational Spectroscopy (SERS and SEIR). <i>Journal of Physical Chemistry A</i> , 2003, 107, 9611-9619.	2.5	52
58	Cycloaddition Reactions of an Acetylene-Linked Bis(germaethene)1,2. <i>Organometallics</i> , 2002, 21, 3990-3995.	2.3	32
59	Coordination chemistry of lipoic acid and related compounds.. <i>New Journal of Chemistry</i> , 2002, 26, 560-566.	2.8	10
60	Twisting and planarization in push-pull ethylenesElectronic supplementary information (ESI) available: tables of X-ray crystallographic bond lengths and angles of compounds 8-19 (including) and 18 (Figs. S1-S5) and packing diagrams for 17·H2O and 19·H2O (Figs. S6-S7). See <a href="http://www.rsc.org/suppdata/p2/b1/b109624a/">http://www.rsc.org/suppdata/p2/b1/b109624a/</a> . <i>Perkin Transactions II RSC</i> , 2002, , 515-523.	1.1	21
61	Synthesis, Characterization, and Modelling of Novel Multifunctional Acryloyl-Based Monomers: An Experimental and Computational Study. <i>Australian Journal of Chemistry</i> , 2002, 55, 675.	0.9	4
62	Ein Spiropentasiladien und andere gespannte Silicium-haltige Ringe. <i>Angewandte Chemie</i> , 2002, 114, 1941.	2.0	9
63	A Spiropentasiladiene and Other Strained Silicon-Containing Rings. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1861.	13.8	13
64	Coordination Chemistry of Lipoic Acid and Related Compounds V [1]. New Heteroditopic Ligands Derived from Monoazacrown Ethers and Lipoic Acid. <i>Monatshefte für Chemie</i> , 2002, 133, 1097-1108.	1.8	6
65	Diastereoselective Lewis acid mediated hydrophosphonylation of heterocyclic imines: a stereoselective approach towards $\alpha,\alpha$ -amino phosphonates. <i>Journal of the Chemical Society, Perkin Transactions 1</i> , 2001, , 2804-2816.	1.3	26
66	Reactions of the Titanaallene Intermediate [Cp*2TiCCH2] with Isonitriles: An Approach to the Chemistry of Radialene Type Molecules. <i>Organometallics</i> , 2001, 20, 1354-1359.	2.3	17
67	Complete Defluorination of 1,2,3,4-Tetramethyl-5-(trifluoromethyl)cyclopentadiene by Titanium Tetrakis(dimethylamide) Selective Formation of a Cyclic Hexanuclear Titanium Fluoroamide and 6,6-Dimethylaminotetramethylfulvene. <i>Chemistry - A European Journal</i> , 2001, 7, 622-626.	3.3	27
68	1,3-Stereoiduction in Radical Reactions. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 2758-2761.	13.8	19
69	Aluminium Hydrazides: Dimeric Bis(tert-butyl)aluminium Hydrazides with Six-Membered Al2N4 and Five-Membered Al2N3 Heterocycles. <i>European Journal of Inorganic Chemistry</i> , 2000, 2000, 2255-2262.	2.0	23
70	Highly diastereoselective hydrophosphonylation of cyclic imines using BINOL as source of chirality. <i>Tetrahedron Letters</i> , 2000, 41, 7285-7288.	1.4	11
71	The thioacyl isocyanate acyl isothiocyanate rearrangement. <i>Perkin Transactions II RSC</i> , 2000, , 1846-1850.	1.1	11
72	1,3-Stereoiduction in Radical Reactions: Radical Additions to Dialkyl 2-Alkyl-4-methyleneglutarates. <i>Journal of the American Chemical Society</i> , 2000, 122, 12458-12468.	13.7	30

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73	Aluminium Hydrazides: Reactions of tert-Butylaluminium Chlorides with Dilithium Bis(trimethylsilyl)hydrazide – Formation of Iminoalanes and their Hydrazido Adducts. <i>European Journal of Inorganic Chemistry</i> , 1999, 1999, 2021-2027.	2.0	25
74	Di( $\eta^4$ -acetato)dialkyldigallium as starting compound for the facile syntheses of digallium derivatives containing bridged or terminally co-ordinated Ga–Ga single bonds. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 2385-2392.	1.1	37
75	Synthesis of an Aluminatecyclopropene Derivative with an AlC <sub>2</sub> Heterocycle and an Exocyclic AlR <sub>2</sub> Substituent: Evidence for a Nonclassical Bonding Situation. <i>Organometallics</i> , 1999, 18, 4598-4602.	2.3	36
76	Retro-Ene Reactions in Acylallene Derivatives. <i>Journal of Organic Chemistry</i> , 1998, 63, 2619-2626.	3.2	28
77	Dihydro-1,3-diazepinones and diazabicyclo[3.2.0]heptenones from pyridyl azides. <i>Journal of the Chemical Society Perkin Transactions 1</i> , 1998, , 2247-2250.	0.9	25
78	N-Mesityl-C-acylketenimines: 1,5-Sigmatropic Shifts and Electrocyclization to Quinolines. <i>Journal of Organic Chemistry</i> , 1998, 63, 5779-5786.	3.2	26
79	<sup>13</sup> C NMR calculations on azepines and diazepines. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 1851-1860.	0.9	14
80	Nitrilimines: Evidence for the Allenic Structure in Solution, Experimental and Ab Initio Studies of the Barrier to Racemization, and First Diastereoselective [3 + 2]-Cycloaddition. <i>Journal of the American Chemical Society</i> , 1997, 119, 2819-2824.	13.7	32
81	Facile 1,3- and 1,5-Chlorine Migration. <i>Journal of Organic Chemistry</i> , 1996, 61, 6809-6813.	3.2	38
82	Theoretical Study of the Deprotonation of Nitriles, RCH <sub>2</sub> CN: Ab Initio and PM3 Calculations of Intermediate Aggregates and Transition States. <i>Journal of Organic Chemistry</i> , 1996, 61, 2523-2529.	3.2	37
83	Ab initio and PM3-MO calculations of lithiophosphonates. <i>Journal of Organic Chemistry</i> , 1995, 60, 5861-5866.	3.2	30
84	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. <i>Journal of Organic Chemistry</i> , 1995, 60, 3743-3749.	3.2	27
85	Benzotriazole-assisted $\eta^2$ -lithiation of vinyl ethers. <i>Tetrahedron</i> , 1994, 50, 6005-6016.	1.9	13
86	PM3-MO Calculations of Monolithiated Sulfones, Sulfoxides, and 1,3-Dithianes: Comparison with ab Initio or X-ray Results. <i>Journal of Organic Chemistry</i> , 1994, 59, 4529-4534.	3.2	50
87	Optimization and application of lithium parameters for PM3. <i>Journal of Computational Chemistry</i> , 1993, 14, 1301-1312.	3.3	180
88	Collisionally Activated Dissociation of Some Bulkily Substituted Pyridinium Cations, II. Substituent Effect on Appearance Potential. <i>Chemische Berichte</i> , 1992, 125, 177-181.	0.2	7