Henry S Rzepa

List of Publications by Year
in descending order

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292 papers	10,916 citations	36303 51 h-index	45317 90 g-index
324 all docs	324 docs citations	324 times ranked	8040 citing authors

#	Article	IF	Citations
1	Some influences of fluorine in bioorganic chemistry. Chemical Communications, 1997, , 645-652.	4.1	454
2	The Blue Obeliskâ€”Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998.	5.4	366
3	MNDO parameters for third period elements. Journal of the American Chemical Society, 1978, 100, 3607-3607.	13.7	339
4	MÃ¶bius Aromaticity and Delocalization. Chemical Reviews, 2005, 105, 3697-3715.	47.7	328
5	Tuning Azoheteroarene Photoswitch Performance through Heteroaryl Design. Journal of the American Chemical Society, 2017, 139, 1261-1274.	13.7	244
6	A Tricyclic Aromatic Isomer of Hexasilabenzene. Science, 2010, 327, 564-566.	12.6	242
7	Synthetic, Structural, Mechanistic, and Computational Studies on Single-Site Î²-Diketiminate Tin(II) Initiators for the Polymerization ofrac-Lactide. Journal of the American Chemical Society, 2006, 128, 9834-9843.	13.7	209
8	Chemoselective Polymerizations from Mixtures of Epoxide, Lactone, Anhydride, and Carbon Dioxide. Journal of the American Chemical Society, 2016, 138, 4120-4131.	13.7	200
9	Quadruple bonding in C2 and analogous eight-valence electron species. Nature Chemistry, 2012, 4, 195-200.	13.6	198
10	Chemical Markup, XML, and the Worldwide Web. 1. Basic Principles. Journal of Chemical Information and Computer Sciences, 1999, 39, 928-942.	2.8	196
11	A Computational Analysis of the Ring-Opening Polymerization of rac-Lactide Initiated by Single-Site Î²-Diketiminate Metal Complexes:â€‰ Defining the Mechanistic Pathway and the Origin of Stereocontrol. Journal of the American Chemical Society, 2005, 127, 6048-6051.	13.7	196
12	Ground states of molecules. 40. MNDO results for molecules containing fluorine. Journal of the American Chemical Society, 1978, 100, 58-67.	13.7	183
13	The Houkâ€“List transition states for organocatalytic mechanisms revisited. Chemical Science, 2014, 5, 2057-2071.	7.4	154
14	A Stable Derivative of the Global Minimum on the Si₆H₆ Potential Energy Surface. Angewandte Chemie - International Edition, 2011, 50, 7936-7939.	13.8	136
15	Design, Synthesis, and Evaluation of a Helicenoidal DMAP Lewis Base Catalyst. Organic Letters, 2011, 13, 1250-1253.	4.6	133
16	One Molecule, Two Atoms, Three Views, Four Bonds?. Angewandte Chemie - International Edition, 2013, 52, 3020-3033.	13.8	129
17	Calculations of electron affinities using the MNDO semiempirical SCF-MO method. Journal of the American Chemical Society, 1978, 100, 784-790.	13.7	126
18	Crocker, Not Armit and Robinson, Begat the Six Aromatic Electrons. Chemical Reviews, 2005, 105, 3436-3447.	47.7	126

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19	Experimental and Computational Investigation of the Mechanism of Carbon Dioxide/Cyclohexene Oxide Copolymerization Using a Dizinc Catalyst. Macromolecules, 2012, 45, 6781-6795.	4.8	123
20	Ground states of molecules. 49. MINDO/3 study of the retro-Diels-Alder reaction of cyclohexene. Journal of the American Chemical Society, 1978, 100, 5650-5659.	13.7	121
21	Title is missing!. Tetrahedron, 1987, 43, 2805-2815.	1.9	113
22	Equilibrium between a cyclotrisilene and an isolable base adduct of a disilenyl silylene. Nature Chemistry, 2013, 5, 876-879.	13.6	111
23	Intrinsically Chiral Aromaticity. Rules Incorporating Linking Number, Twist, and Writhe for Higher-Twist MÃ¶bius Annulenes. Journal of the American Chemical Society, 2008, 130, 7613-7619.	13.7	108
24	Correlation of Metal Spin State with Catalytic Reactivity: Polymerizations Mediated by Î±-Diimineâ€“Iron Complexes. Angewandte Chemie - International Edition, 2006, 45, 1241-1244.	13.8	106
25	Ground states of molecules. 45. MNDO results for molecules containing beryllium. Journal of the American Chemical Society, 1978, 100, 777-784.	13.7	104
26	Gaseous ions. 4. MINDO/3 calculations for some simple organic cations and for their hydrogen elimination reactions. Journal of the American Chemical Society, 1977, 99, 7432-7439.	13.7	101
27	Semiempirical calculations of molecular vibrational frequencies: The MNDO method. Journal of Molecular Structure, 1978, 43, 135-138.	3.6	101
28	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
29	Chemical Markup, XML, and the World Wide Web. 4. CML Schema. Journal of Chemical Information and Computer Sciences, 2003, 43, 757-772.	2.8	95
30	Delineating Origins of Stereocontrol in Asymmetric Pd-Catalyzed Î±-Hydroxylation of 1,3-Ketoesters. Journal of Organic Chemistry, 2010, 75, 3085-3096.	3.2	92
31	Fluoridation of heteroaromatic iodonium saltsâ€”experimental evidence supporting theoretical prediction of the selectivity of the process. Chemical Communications, 2000, , 649-650.	4.1	89
32	A Study in Mauve: Unveiling Perkin's Dye in Historic Samples. Chemistry - A European Journal, 2008, 14, 8507-8513.	3.3	85
33	Mechanistic insights into boron-catalysed direct amidation reactions. Chemical Science, 2018, 9, 1058-1072.	7.4	82
34	Stereoselective Synthesis of cis- and trans-2,3-Disubstituted Tetrahydrofurans via Oxoniumâ€Prins Cyclization: Access to the Cordigol Ring System. Organic Letters, 2010, 12, 900-903.	4.6	79
35	The Cope rearrangement. MINDO/3 studies of the rearrangements of 1,5-hexadiene and bicyclo[2.2.0]hexane. Journal of the American Chemical Society, 1977, 99, 5069-5073.	13.7	78
36	Enhancement of the chemical semantic web through the use of InChI identifiers. Organic and Biomolecular Chemistry, 2005, 3, 1832.	2.8	78

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37	Contraction and Expansion of the Silicon Scaffold of Stable Si₆R₆ Isomers. Journal of the American Chemical Society, 2012, 134, 16008-16016.	13.7	78
38	The Nature of the Fourth Bond in the Ground State of C₂: The Quadruple Bond Conundrum. Chemistry - A European Journal, 2014, 20, 6220-6232.	3.3	77
39	Nâ€Heterocyclic Carbene Coordinated Neutral and Cationic Heavier Cyclopropylidenes. Angewandte Chemie - International Edition, 2014, 53, 9953-9956.	13.8	76
40	The preferred conformation of Î±-fluoroamides. Journal of the Chemical Society Perkin Transactions II, 1999, , 2409-2411.	0.9	75
41	Ground states of molecules. 53.MNDO calculations for molecules containing chlorine. Journal of Computational Chemistry, 1983, 4, 158-169.	3.3	73
42	Development of chemical markup language (CML) as a system for handling complex chemical content. New Journal of Chemistry, 2001, 25, 618-634.	2.8	69
43	Structural Reassignment of Obtusallenes V, VI, and VII by GIAO-Based Density Functional Prediction. Journal of Natural Products, 2008, 71, 728-730.	3.0	64
44	Lemniscular Hexaphyrins as Examples of Aromatic and Antiaromatic Double-Twist MÃ¶bius Molecules. Organic Letters, 2008, 10, 949-952.	4.6	64
45	Chemical Markup, XML and the World-Wide Web. 2. Information Objects and the CMLDOM. Journal of Chemical Information and Computer Sciences, 2001, 41, 1113-1123.	2.8	63
46	Catalytic and Computational Studies of N-Heterocyclic Carbene or Phosphine-Containing Copper(I) Complexes for the Synthesis of 5-Iodo-1,2,3-Triazoles. ACS Catalysis, 2014, 4, 2274-2287.	11.2	62
47	Ground states of molecules. Journal of Molecular Structure, 1977, 40, 145-149.	3.6	58
48	Dual wavelength asymmetric photochemical synthesis with circularly polarized light. Chemical Science, 2015, 6, 3853-3862.	7.4	58
49	A Double-Twist MÃ¶bius-Aromatic Conformation of [14]Annulene. Organic Letters, 2005, 7, 4637-4639.	4.6	56
50	A Response to the Critical Comments on â€œOne Molecule, Two Atoms, Three Views, Four Bonds?â€• Angewandte Chemie - International Edition, 2013, 52, 5926-5928.	13.8	55
51	Silverâ€Catalysed Enantioselective Addition of Oï£¿H and Nï£¿H Bonds to Allenes: A New Model for Stereoselectivity Based on Noncovalent Interactions. Chemistry - A European Journal, 2012, 18, 11317-11324.	3.3	54
52	Experimental and Computational Study of Î²-H Transfer between Cobalt(I) Alkyl Complexes and 1-Alkenes. Organometallics, 2004, 23, 5503-5513.	2.3	53
53	An AM1 and PM3 molecular orbital and self-consistent reaction-field study of the aqueous solvation of glycine, alanine and proline in their neutral and zwitterionic forms. Journal of the Chemical Society Perkin Transactions II, 1991, , 531.	0.9	52
54	Chemical Markup, XML, and the World Wide Web. 6. CMLReact, an XML Vocabulary for Chemical Reactions. Journal of Chemical Information and Modeling, 2006, 46, 145-157.	5.4	51

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55	Enantiomerically Pure Alenoâ€“Acetylenic Macrocycles: Synthesis, Solidâ€State Structures, Chiroptical Properties, and Electron Localization Function Analysis. Chemistry - A European Journal, 2010, 16, 9796-9807.	3.3	51
56	SPECTRa: The Deposition and Validation of Primary Chemistry Research Data in Digital Repositories. Journal of Chemical Information and Modeling, 2008, 48, 1571-1581.	5.4	50
57	Lowâ€Valent Ge₂ and Ge₄ Species Trapped by Nâ€Heterocyclic Gallylene. Angewandte Chemie - International Edition, 2013, 52, 450-454.	13.8	50
58	Kinetic Resolution of 2â€Substituted Indolines by Nâ€Sulfonylation using an Atropisomeric 4â€DMAPâ€Nâ€oxide Organocatalyst. Angewandte Chemie - International Edition, 2017, 56, 5760-5764.	13.8	48
59	A computational study of the mechanism of palladium insertion into alkynyl and aryl carbonâ€“fluorine bondsElectronic supplementary information (ESI) available: full coordinates for all geometries and normal mode animations. See http://www.rsc.org/suppdata/p2/b1/b108727b/. Perkin Transactions II RSC, 2002, , 576-581.	1.1	47
60	The vicinal difluoro motif: The synthesis and conformation of erythro- and threo- diastereoisomers of 1,2-difluorodiphenylethanes, 2,3-difluorosuccinic acids and their derivatives. Beilstein Journal of Organic Chemistry, 2006, 2, 19.	2.2	46
61	Ring Currents in the Dismutational Aromatic Si₆R₆. Angewandte Chemie - International Edition, 2010, 49, 10006-10009.	13.8	46
62	A crystallographic AM1 and PM3 SCF-MO investigation of strong OH â‹¯Ï€-alkene and alkyne hydrogen bonding interactions. Journal of the Chemical Society Perkin Transactions II, 1994, , 703-707.	0.9	44
63	An ab initio and MNDO-d SCF-MO computational study of stereoelectronic control in extrusion reactions of R2Iâ€“F iodine(III) intermediatesâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 2707-2714.	0.9	43
64	The importance of being bonded. Nature Chemistry, 2009, 1, 510-512.	13.6	43
65	Representation and use of chemistry in the global electronic age. Organic and Biomolecular Chemistry, 2004, 2, 3192.	2.8	42
66	Chiral Aromaticities. AIM and ELF Critical Point and NICS Magnetic Analyses of MÃ¶bius-Type Aromaticity and Homoaromaticity in Lemniscular Annulenes and Hexaphyrins. Journal of Organic Chemistry, 2008, 73, 6615-6622.	3.2	42
67	The Geometry and Electronic Topology of Higher-Order Charged MÃ¶bius Annulenes. Journal of Physical Chemistry A, 2009, 113, 11619-11629.	2.5	42
68	A Multiply Functionalized Baseâ€Coordinated Ge^{II} Compound and Its Reversible Dimerization to the Digermene. Angewandte Chemie - International Edition, 2015, 54, 289-292.	13.8	42
69	How Many Water Molecules Does it Take to Dissociate HCl?. Chemistry - A European Journal, 2016, 22, 2812-2818.	3.3	42
70	Chemical Markup, XML, and the World-Wide Web. 3. Toward a Signed Semantic Chemical Web of Trust. Journal of Chemical Information and Computer Sciences, 2001, 41, 1124-1130.	2.8	40
71	Unusual regiodivergence in metal-catalysed intramolecular cyclisation of Î³-allenols. Chemical Communications, 2009, , 7125-7127.	4.1	39
72	A quantitative molecular-orbital study of the structures and vibrational spectra of the hydrogen-bonded complexes H2OÂ·NH3, H2COÂ·NH3and (H2O)n, n= 2â€“4. Journal of the Chemical Society Perkin Transactions II, 1990, , 943-951.	0.9	38

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73	Double aromaticity and anti-aromaticity in small carbon rings. Chemical Communications, 2000, , 1503-1504.	4.1	38
74	Chemical Markup, XML, and the World Wide Web. 5. Applications of Chemical Metadata in RSS Aggregators. Journal of Chemical Information and Computer Sciences, 2004, 44, 462-469.	2.8	38
75	In Search of the Bailar and RÃ¢yâ^'Dutt Twist Mechanisms That Racemize Chiral Trischelates:â€‰ A Computational Study of Sc^{III}, Ti^{IV}, Co^{III}, Zn^{II}, Ga^{III}, and Ge^{IV} Complexes of a Ligand Analogue of Acetylacetonate. Inorganic Chemistry, 2007, 46, 8024-8031.	4.0	37
76	Mechanistic Diversity in Thermal Fragmentation Reactions: A Computational Exploration of CO and CO₂ Extrusions from Five-Membered Rings. Journal of Organic Chemistry, 2013, 78, 7565-7574.	3.2	37
77	HÃ¼ckel and MÃ¶bius aromaticity and trimerous transition state behaviour in the pericyclic reactions of [10], [14], [16] and [18]annulenesâ€Šâ€. Perkin Transactions II RSC, 2000, , 1415-1417.	1.1	36
78	CML: Evolution and design. Journal of Cheminformatics, 2011, 3, 44.	6.1	36
79	The rational design of helium bonds. Nature Chemistry, 2010, 2, 390-393.	13.6	35
80	A solid-supported arylboronic acid catalyst for direct amidation. Chemical Communications, 2019, 55, 2916-2919.	4.1	35
81	Aromaticity rules for cycles with arbitrary numbers of half-twists. Physical Chemistry Chemical Physics, 2006, 8, 1775.	2.8	34
82	Equilibrium Formation of Stable Allâ€Šilicon Versions of 1,3â€Cyclobutanediyl. Angewandte Chemie - International Edition, 2020, 59, 15087-15092.	13.8	34
83	Tetrahedral intermediates formed by nitrogen and oxygen attack of aromatic hydroxylamines on acetyl cyanide. Journal of Organic Chemistry, 1987, 52, 2925-2927.	3.2	33
84	? Facial hydrogen bonding in the chiral resolving agent (S)-2,2,2-trifluoro-1-(9-anthryl)ethanol and its racemic modification. Journal of the Chemical Society Chemical Communications, 1991, , 765.	2.0	33
85	The Application of Chemical Multipurpose Internet Mail Extensions (Chemical MIME) Internet Standards to Electronic Mail and World Wide Web Information Exchange. Journal of Chemical Information and Computer Sciences, 1998, 38, 976-982.	2.8	33
86	The aromaticity and MÃ¶bius characteristics of carbeno[8]heteroannulenes and triplet state annulenesElectronic supplementary information (ESI) available: due to the two printed page length restriction on this communication, energies and coordinates for all the systems studied can be viewed via the ESI. See http://www.rsc.org/suppdata/cc/b1/b110626k/. Chemical Communications, 2002, , 642-643.	4.1	33
87	Total Synthesis of (+)-Lophirone H and Its Pentamethyl Ether Utilizing an Oxoniumâ€"Prins Cyclization. Organic Letters, 2017, 19, 2486-2489.	4.6	33
88	Ab initio SCF-MO study of the Staudinger phosphorylation reaction between a phosphane and an azide to form a phosphazeneâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 1811-1814.	0.9	32
89	Studies in sigmatropic rearrangements of N-prenylindole derivatives ? a formal enantiomerically pure synthesis of tryprostatin B. Organic and Biomolecular Chemistry, 2006, 4, 3966.	2.8	31
90	Mechanisms That Interchange Axial and Equatorial Atoms in Fluxional Processes: Illustration of the Berry Pseudorotation, the Turnstile, and the Lever Mechanisms via Animation of Transition State Normal Vibrational Modes. Journal of Chemical Education, 2006, 83, 336.	2.3	31

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91	On the Determination of the Stereochemistry of Semisynthetic Natural Product Analogues using Chiroptical Spectroscopy: Desulfurization of Epidithiodioxopiperazine Fungal Metabolites. Chemistry - A European Journal, 2011, 17, 11868-11875.	3.3	31
92	Thermal azideâ€“alkene cycloaddition reactions: straightforward multi-gram access to Î”²-1,2,3-triazolines in deep eutectic solvents. Green Chemistry, 2018, 20, 4023-4035.	9.0	30
93	MNDO study of ozone and its decomposition into (O2 + 0). Chemical Physics Letters, 1977, 47, 80-84.	2.6	29
94	Hyperactive molecules and the World-Wide-Web information system. Journal of the Chemical Society Perkin Transactions II, 1995, , 7.	0.9	28
95	The Aromaticity of Pericyclic Reaction Transition States. Journal of Chemical Education, 2007, 84, 1535.	2.3	28
96	A Molecular Complex with a Formally Neutral Iron Germanide Motif (Fe₂Ge₂). Organometallics, 2015, 34, 2130-2133.	2.3	28
97	Structural reappraisal of the limonoid insect antifeedant azadirachtin. Journal of the Chemical Society Chemical Communications, 1985, , 968.	2.0	27
98	Theoretical calculations of benzoquinone redox potentials using the COSMO continuum solvation model. Journal of the Chemical Society Chemical Communications, 1993, , 1743-1744.	2.0	27
99	Twist localisation in single, double and triple twisted MÃ¶bius cyclacenesâ€. Perkin Transactions II RSC, 2000, , 2378-2381.	1.1	27
100	Solid state and theoretical evaluation of Î²-fluoroethyl esters indicate a fluorine-ester gauche effect. Journal of Fluorine Chemistry, 2004, 125, 19-25.	1.7	27
101	Double-twist MÃ¶bius aromaticity in a 4n+ 2 electron electrocyclic reaction. Chemical Communications, 2005, , 5220.	4.1	27
102	SemanticEye:â€‰ A Semantic Web Application to Rationalize and Enhance Chemical Electronic Publishing. Journal of Chemical Information and Modeling, 2006, 46, 2396-2411.	5.4	27
103	The Chiro-optical Properties of a Lemniscular Octaphyrin. Organic Letters, 2009, 11, 3088-91.	4.6	27
104	The mechanism of diazo-coupling to indoles and the effect of steric hindrance on the rate-limiting step. Journal of the Chemical Society Perkin Transactions II, 1975, , 1209.	0.9	26
105	VChemLab: A Virtual Chemistry Laboratory. The Storage, Retrieval, and Display of Chemical Information Using Standard Internet Tools. Journal of Chemical Information and Computer Sciences, 1998, 38, 1048-1053.	2.8	26
106	MÃ¶bius aromatics arising from a Cî€†Cî€†C ring component. Chemical Communications, 2000, , 1089-1090.	4.1	26
107	MÃ¶bius aromatic forms of 8-Ï€ electron heteropinesElectronic supplementary information (ESI) available: all coordinates as MDL Molfiles, together with 3D models of the orbitals expressed as 3DMF files. Diagrams are also available in SVG (high resolution) format. See http://www.rsc.org/suppdata/p2/b1/b111369k/. Perkin Transactions II RSC, 2002, , 388-392.	1.1	26
108	Modulation of Amide Bond Rotamers in 5-Acyl-6,7-dihydrothieno[3,2-c]pyridines. Journal of Organic Chemistry, 2015, 80, 4370-4377.	3.2	26

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109	Ground states of molecules. 51. MNDO (modified neglect of diatomic overlap) calculations of kinetic isotope effects. Journal of the American Chemical Society, 1978, 100, 7832-7836.	13.7	25
110	Triterpenoids of the fungus Pisolithus tinctorius*. Phytochemistry, 1988, 27, 3569-3574.	2.9	25
111	A Computational Study of the Nondissociative Mechanisms that Interchange Apical and Equatorial Atoms in Square Pyramidal Molecules. Inorganic Chemistry, 2006, 45, 3958-3963.	4.0	25
112	Chemical Markup, XML, and the World Wide Web. 7. CMLSpect, an XML Vocabulary for Spectral Data. Journal of Chemical Information and Modeling, 2007, 47, 2015-2034.	5.4	25
113	Chemical Markup, XML and the World-Wide Web. 8. Polymer Markup Language. Journal of Chemical Information and Modeling, 2008, 48, 2118-2128.	5.4	25
114	The Cp*Si+ cation as a stoichiometric source of silicon. Chemical Communications, 2012, 48, 7820.	4.1	25
115	X-Ray crystallographic and NMR evidence for a uniquely strong OH ? N hydrogen bond in the solid state and solution. Journal of the Chemical Society Chemical Communications, 1989, , 1722.	2.0	23
116	Electrostatic vs. orbital control in Ï€-facial diasteroselection: a PM3 SCF-MO study of electrophilic reactivity in 7-methylenenorbornanes. Journal of the Chemical Society Chemical Communications, 1992, , 998-1000.	2.0	23
117	MÃ¶bius and HÃ¼ckel spiroaromatic systems. Perkin Transactions II RSC, 2002, , 1499-1501.	1.1	23
118	Aromaticity on the edge of chaos: An ab initio study of the bimodal balance between aromatic and non-aromatic structures for 10Ï€-dihetero[8]annulenes. Physical Chemistry Chemical Physics, 2004, 6, 310-313.	2.8	23
119	The Use of the Free, Open-Source Program Jmol To Generate an Interactive Web Site To Teach Molecular Symmetry. Journal of Chemical Education, 2005, 82, 1736.	2.3	23
120	Chiral Aromaticities. A Topological Exploration of MÃ¶bius Homoaromaticity. Journal of Chemical Theory and Computation, 2008, 4, 1841-1848.	5.3	23
121	The preparation, X-ray crystal structure and theoretical study of [CoCp2][S3N3], (Cp =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 2 of the Chemical Society Chemical Communications, 1991, .	2.0	22
122	Chemical applications of the World-Wide-Web system. Journal of the Chemical Society Chemical Communications, 1994, , 1907.	2.0	22
123	The World-Wide Web as a chemical information tool. Chemical Society Reviews, 1997, 26, 1.	38.1	22
124	Successful Computational Modeling of Isobornyl Chloride Ion-Pair Mechanisms. Journal of Organic Chemistry, 2010, 75, 5164-5169.	3.2	22
125	Selective Ï€-facial binding of metal cations to triindenotriphenylene as a possible catalytic route to C60precursors: a MNDO, PM3 and ab initio SCF-MO study. Journal of the Chemical Society Perkin Transactions II, 1994, , 399-400.	0.9	21
126	Linking Number Analysis of a Pentadecanuclear Metallamacrocycle: A MÃ¶bius-Craig System Revealed. Inorganic Chemistry, 2008, 47, 8932-8934.	4.0	21

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127	A HÃ¼ckel Theory Perspective on MÃ¶bius Aromaticity. Organic Letters, 2013, 15, 3432-3435.	4.6	21
128	Epimeric Face-Selective Oxidations and Diastereodivergent Transannular Oxonium Ion Formation Fragmentations: Computational Modeling and Total Syntheses of 12-Epoxyobtusallene IV, 12-Epoxyobtusallene II, Obtusallene X, Marilzabicycloallene C, and Marilzabicycloallene D. Journal of Organic Chemistry, 2016, 81, 9539-9552.	3.2	21
129	MÃ¶bius and HÃ¼ckel molecular orbitals arising from Cî€†Cî€†C components in annulene ringsâ€Šâ€. Perkin Transactions II RSC, 2000, , 2372-2377.	1.1	20
130	Nature of the Carbonâ^'Sulfur Bond in the Species Hâ^'CSâ^'OH. Journal of Chemical Theory and Computation, 2011, 7, 97-102.	5.3	20
131	Digital Data Repositories in Chemistry and Their Integration with Journals and Electronic Notebooks. Journal of Chemical Information and Modeling, 2014, 54, 2627-2635.	5.4	20
132	Scientific publications in XML - towards a global knowledge base. Data Science Journal, 2002, 1, 84-98.	1.3	20
133	Bis(diphenylphosphino)methane trimethylphosphine alkyl and Î·5-cyclopentadienyl compounds of rhodium(I); 31P{1H} two dimensional Î'J resolved and Overhauser effect nuclear magnetic resonance spectroscopy. Polyhedron, 1982, 1, 809-817.	2.2	19
134	X-Ray and SCFâ€"MO model study of the complex formed between N-bromosuccinimide and 1,4-diazabicyclo[2.2.2]octane. Journal of the Chemical Society Chemical Communications, 1984, , 276-278.	2.0	19
135	Molecular orbital studies of molecular exciplexes. Part 1: AM1 and PM3 calculations of the ammoniaâ€"oxygen complex and its solvation by water. Journal of the Chemical Society Perkin Transactions II, 1990, , 877-883.	0.9	19
136	Origins of the regioselectivity of cyclopropylcarbinyl ring opening reactions in bicyclo [n.1.0] systems. Journal of the Chemical Society Chemical Communications, 1992, , 942.	2.0	19
137	Workflows Allowing Creation of Journal Article Supporting Information and Findable, Accessible, Interoperable, and Reusable (FAIR)-Enabled Publication of Spectroscopic Data. ACS Omega, 2019, 4, 3280-3286.	3.5	19
138	A novel hydrogen-bonded complex formed by reaction between bromine and 1,4-diazabicyclo[2.2.2]octane in dichloromethane solution. Journal of the Chemical Society Chemical Communications, 1985, , 1127.	2.0	18
139	Concerted dihydrogen exchange between methanol and formaldehyde: a theoretical study. Journal of the American Chemical Society, 1986, 108, 5793-5798.	13.7	18
140	Thermally induced rearrangement of thiopheniobis(alkoxycarbonyl)methanides. Journal of the Chemical Society Perkin Transactions 1, 1988, , 803.	0.9	18
141	An Accessible Method for DFT Calculation of ¹¹B NMR Shifts of Organoboron Compounds. Journal of Organic Chemistry, 2018, 83, 8020-8025.	3.2	18
142	MNDO study of transient species: the IR spectrum of benzyne. Journal of Molecular Structure, 1979, 51, 275-279.	3.6	17
143	MÃ¶bius bis and tris-spiroaromatic systems. Organic and Biomolecular Chemistry, 2003, 1, 182-185.	2.8	17
144	Mechanistic and Chiroptical Studies on the Desulfurization of Epidithiodioxopiperazines Reveal Universal Retention of Configuration at the Bridgehead Carbon Atoms. Journal of Organic Chemistry, 2013, 78, 11646-11655.	3.2	17

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145	A metadata-driven approach to data repository design. Journal of Cheminformatics, 2017, 9, 4.	6.1	17
146	Reversibility and reactivity in an acid catalyzed cyclocondensation to give furanochromanes â€“ a reaction at the â€˜oxonium-Prinsâ€™ vs. â€˜ortho-quinone methide cycloadditionâ€™ mechanistic nexus. Chemical Science, 2019, 10, 406-412.	7.4	17
147	STMML. A markup language for scientific, technical and medical publishing. Data Science Journal, 2002, 1, 128-192.	1.3	17
148	C-substitution reactions of c,n-diaryl nitrones. Tetrahedron, 1983, 39, 3833-3841.	1.9	16
149	Tetrahedral intermediates formed during acyl transfer. Reactions of acetyl cyanide. Journal of the Chemical Society Chemical Communications, 1985, , 1113.	2.0	16
150	An MNDO SCF-MO study of the mechanism of the benzilic acid and related rearrangements. Journal of the Chemical Society Perkin Transactions II, 1987, , 1819.	0.9	16
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