# Henry S Rzepa

List of Publications by Year
in descending order



| 292 | 10,916 | 41627 | 51 | 51423 | 90 |
|---|---|---|---|---|---|
| papers | citations | | h-index | | g-index |

| 324 | 324 | 324 | 8871 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Some influences of fluorine in bioorganic chemistry. Chemical Communications, 1997, , 645-652. | 2.2 | 454 |
| 2 | The Blue Obeliskâ€”Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998. | 2.5 | 366 |
| 3 | MNDO parameters for third period elements. Journal of the American Chemical Society, 1978, 100, 3607-3607. | 6.6 | 339 |
| 4 | MÃ¶bius Aromaticity and Delocalization. Chemical Reviews, 2005, 105, 3697-3715. | 23.0 | 328 |
| 5 | Tuning Azoheteroarene Photoswitch Performance through Heteroaryl Design. Journal of the American Chemical Society, 2017, 139, 1261-1274. | 6.6 | 244 |
| 6 | A Tricyclic Aromatic Isomer of Hexasilabenzene. Science, 2010, 327, 564-566. | 6.0 | 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. | 6.6 | 209 |
| 8 | Chemoselective Polymerizations from Mixtures of Epoxide, Lactone, Anhydride, and Carbon Dioxide. Journal of the American Chemical Society, 2016, 138, 4120-4131. | 6.6 | 200 |
| 9 | Quadruple bonding in C2 and analogous eight-valence electron species. Nature Chemistry, 2012, 4, 195-200. | 6.6 | 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. | 6.6 | 196 |
| 12 | Ground states of molecules. 40. MNDO results for molecules containing fluorine. Journal of the American Chemical Society, 1978, 100, 58-67. | 6.6 | 183 |
| 13 | The Houkâ€“List transition states for organocatalytic mechanisms revisited. Chemical Science, 2014, 5, 2057-2071. | 3.7 | 154 |
| 14 | A Stable Derivative of the Global Minimum on the Si<sub>6</sub>H<sub>6</sub> Potential Energy Surface. Angewandte Chemie - International Edition, 2011, 50, 7936-7939. | 7.2 | 136 |
| 15 | Design, Synthesis, and Evaluation of a Helicenoidal DMAP Lewis Base Catalyst. Organic Letters, 2011, 13, 1250-1253. | 2.4 | 133 |
| 16 | One Molecule, Two Atoms, Three Views, Four Bonds?. Angewandte Chemie - International Edition, 2013, 52, 3020-3033. | 7.2 | 129 |
| 17 | Calculations of electron affinities using the MNDO semiempirical SCF-MO method. Journal of the American Chemical Society, 1978, 100, 784-790. | 6.6 | 126 |
| 18 | Crocker, Not Armit and Robinson, Begat the Six Aromatic Electrons. Chemical Reviews, 2005, 105, 3436-3447. | 23.0 | 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. | 2.2 | 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. | 6.6 | 121 |
| 21 | Title is missing!. Tetrahedron, 1987, 43, 2805-2815. | 1.0 | 113 |
| 22 | Equilibrium between a cyclotrisilene and an isolable base adduct of a disilenyl silylene. Nature Chemistry, 2013, 5, 876-879. | 6.6 | 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. | 6.6 | 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. | 7.2 | 106 |
| 25 | Ground states of molecules. 45. MNDO results for molecules containing beryllium. Journal of the American Chemical Society, 1978, 100, 777-784. | 6.6 | 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. | 6.6 | 101 |
| 27 | Semiempirical calculations of molecular vibrational frequencies: The MNDO method. Journal of Molecular Structure, 1978, 43, 135-138. | 1.8 | 101 |
| 28 | Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16. | 1.1 | 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. | 1.7 | 92 |
| 31 | Fluoridation of heteroaromatic iodonium saltsâ€”experimental evidence supporting theoretical prediction of the selectivity of the process. Chemical Communications, 2000, , 649-650. | 2.2 | 89 |
| 32 | A Study in Mauve: Unveiling Perkin's Dye in Historic Samples. Chemistry - A European Journal, 2008, 14, 8507-8513. | 1.7 | 85 |
| 33 | Mechanistic insights into boron-catalysed direct amidation reactions. Chemical Science, 2018, 9, 1058-1072. | 3.7 | 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. | 2.4 | 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. | 6.6 | 78 |
| 36 | Enhancement of the chemical semantic web through the use of InChI identifiers. Organic and Biomolecular Chemistry, 2005, 3, 1832. | 1.5 | 78 |

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| 37 | Contraction and Expansion of the Silicon Scaffold of Stable Si<sub>6</sub>R<sub>6</sub> Isomers. Journal of the American Chemical Society, 2012, 134, 16008-16016. | 6.6 | 78 |
| 38 | The Nature of the Fourth Bond in the Ground State of C<sub>2</sub>: The Quadruple Bond Conundrum. Chemistry - A European Journal, 2014, 20, 6220-6232. | 1.7 | 77 |
| 39 | Nâ€Heterocyclic Carbene Coordinated Neutral and Cationic Heavier Cyclopropylidenes. Angewandte Chemie - International Edition, 2014, 53, 9953-9956. | 7.2 | 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. | 1.5 | 73 |
| 42 | Development of chemical markup language (CML) as a system for handling complex chemical content. New Journal of Chemistry, 2001, 25, 618-634. | 1.4 | 69 |
| 43 | Structural Reassignment of Obtusallenes V, VI, and VII by GIAO-Based Density Functional Prediction. Journal of Natural Products, 2008, 71, 728-730. | 1.5 | 64 |
| 44 | Lemniscular Hexaphyrins as Examples of Aromatic and Antiaromatic Double-Twist MÃ¶bius Molecules. Organic Letters, 2008, 10, 949-952. | 2.4 | 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. | 5.5 | 62 |
| 47 | Ground states of molecules. Journal of Molecular Structure, 1977, 40, 145-149. | 1.8 | 58 |
| 48 | Dual wavelength asymmetric photochemical synthesis with circularly polarized light. Chemical Science, 2015, 6, 3853-3862. | 3.7 | 58 |
| 49 | A Double-Twist MÃ¶bius-Aromatic Conformation of [14]Annulene. Organic Letters, 2005, 7, 4637-4639. | 2.4 | 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. | 7.2 | 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. | 1.7 | 54 |
| 52 | Experimental and Computational Study of Î²-H Transfer between Cobalt(I) Alkyl Complexes and 1-Alkenes. Organometallics, 2004, 23, 5503-5513. | 1.1 | 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. | 2.5 | 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. | 1.7 | 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. | 2.5 | 50 |
| 57 | Lowâ€Valent Ge<sub>2</sub> and Ge<sub>4</sub> Species Trapped by Nâ€Heterocyclic Gallylene. Angewandte Chemie - International Edition, 2013, 52, 450-454. | 7.2 | 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. | 7.2 | 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. | 1.3 | 46 |
| 61 | Ring Currents in the Dismutational Aromatic Si<sub>6</sub>R<sub>6</sub>. Angewandte Chemie - International Edition, 2010, 49, 10006-10009. | 7.2 | 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. | 6.6 | 43 |
| 65 | Representation and use of chemistry in the global electronic age. Organic and Biomolecular Chemistry, 2004, 2, 3192. | 1.5 | 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. | 1.7 | 42 |
| 67 | The Geometry and Electronic Topology of Higher-Order Charged MÃ¶bius Annulenes. Journal of Physical Chemistry A, 2009, 113, 11619-11629. | 1.1 | 42 |
| 68 | A Multiply Functionalized Baseâ€Coordinated Ge<sup>II</sup> Compound and Its Reversible Dimerization to the Digermene. Angewandte Chemie - International Edition, 2015, 54, 289-292. | 7.2 | 42 |
| 69 | How Many Water Molecules Does it Take to Dissociate HCl?. Chemistry - A European Journal, 2016, 22, 2812-2818. | 1.7 | 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. | 2.2 | 39 |
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| 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<sup>III</sup>, Ti<sup>IV</sup>, Co<sup>III</sup>, Zn<sup>II</sup>, Ga<sup>III</sup>, and Ge<sup>IV</sup> Complexes of a Ligand Analogue of Acetylacetonate. Inorganic Chemistry, 2007, 46, 8024-8031. | 1.9 | 37 |
| 76 | Mechanistic Diversity in Thermal Fragmentation Reactions: A Computational Exploration of CO and CO<sub>2</sub> Extrusions from Five-Membered Rings. Journal of Organic Chemistry, 2013, 78, 7565-7574. | 1.7 | 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. | 2.8 | 36 |
| 79 | The rational design of helium bonds. Nature Chemistry, 2010, 2, 390-393. | 6.6 | 35 |
| 80 | A solid-supported arylboronic acid catalyst for direct amidation. Chemical Communications, 2019, 55, 2916-2919. | 2.2 | 35 |
| 81 | Aromaticity rules for cycles with arbitrary numbers of half-twists. Physical Chemistry Chemical Physics, 2006, 8, 1775. | 1.3 | 34 |
| 82 | Equilibrium Formation of Stable Allâ€Šilicon Versions of 1,3â€Cyclobutanediyl. Angewandte Chemie - International Edition, 2020, 59, 15087-15092. | 7.2 | 34 |
| 83 | Tetrahedral intermediates formed by nitrogen and oxygen attack of aromatic hydroxylamines on acetyl cyanide. Journal of Organic Chemistry, 1987, 52, 2925-2927. | 1.7 | 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. | 2.2 | 33 |
| 87 | Total Synthesis of (+)-Lophirone H and Its Pentamethyl Ether Utilizing an Oxoniumâ€"Prins Cyclization. Organic Letters, 2017, 19, 2486-2489. | 2.4 | 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. | 1.5 | 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. | 1.1 | 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. | 1.7 | 31 |
| 92 | Thermal azideâ€“alkene cycloaddition reactions: straightforward multi-gram access to Î”<sup>2</sup>-1,2,3-triazolines in deep eutectic solvents. Green Chemistry, 2018, 20, 4023-4035. | 4.6 | 30 |
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| 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. | 1.1 | 28 |
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| 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. | 0.9 | 27 |
| 101 | Double-twist MÃ¶bius aromaticity in a 4n+ 2 electron electrocyclic reaction. Chemical Communications, 2005, , 5220. | 2.2 | 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. | 2.5 | 27 |
| 103 | The Chiro-optical Properties of a Lemniscular Octaphyrin. Organic Letters, 2009, 11, 3088-91. | 2.4 | 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. | 2.2 | 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. | 1.7 | 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. | 6.6 | 25 |
| 110 | Triterpenoids of the fungus Pisolithus tinctorius*. Phytochemistry, 1988, 27, 3569-3574. | 1.4 | 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. | 1.9 | 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. | 2.5 | 25 |
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| 114 | The Cp*Si+ cation as a stoichiometric source of silicon. Chemical Communications, 2012, 48, 7820. | 2.2 | 25 |
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| 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. | 1.3 | 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. | 1.1 | 23 |
| 120 | Chiral Aromaticities. A Topological Exploration of MÃ¶bius Homoaromaticity. Journal of Chemical Theory and Computation, 2008, 4, 1841-1848. | 2.3 | 23 |
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| 123 | The World-Wide Web as a chemical information tool. Chemical Society Reviews, 1997, 26, 1. | 18.7 | 22 |
| 124 | Successful Computational Modeling of Isobornyl Chloride Ion-Pair Mechanisms. Journal of Organic Chemistry, 2010, 75, 5164-5169. | 1.7 | 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. | 1.9 | 21 |

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| 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. | 1.7 | 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. | 2.3 | 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. | 2.5 | 20 |
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| 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. | 1.6 | 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. | 6.6 | 18 |
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