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	The Long and Winding Road towards FAIR Data as an Integral Component of the Computational Modelling and Dissemination of Chemistry. Israel Journal of Chemistry, 2022, 62, .	1.0	2
2	A dataâ€oriented approach to making new molecules as a student experiment: artificial intelligenceâ€enabling FAIR publication of NMR data for organic esters. Magnetic Resonance in Chemistry, 2022, 60, 93-103.	1.1	9
3	CHAMP is a HPC Access and Metadata Portal. Journal of Open Source Software, 2022, 7, 3824.	2.0	4
4	A stereoselective hydride transfer reaction with contributions from attractive dispersion force control. Chemical Communications, 2022, , .	2.2	2
5	IUPAC specification for the FAIR management of spectroscopic data in chemistry (IUPAC FAIRSpec)Ââ€“ guiding principles. Pure and Applied Chemistry, 2022, 94, 623-636.	0.9	7
6	Routes involving no free C₂ in a DFT-computed mechanistic model for the reported room-temperature chemical synthesis of C₂. Physical Chemistry Chemical Physics, 2021, 23, 12630-12636.	1.3	8
7	Understanding the Diastereopreference of Intermediates in Aminocatalysis: Application to the Chiral Resolution of Lactols. Journal of Organic Chemistry, 2021, 86, 4326-4335.	1.7	0
8	A thermodynamic assessment of the reported room-temperature chemical synthesis of C2. Nature Communications, 2021, 12, 1241.	5.8	4
9	Cycloparaphenylene MÃ¶bius trefoils. Chemical Communications, 2020, 56, 13567-13570.	2.2	2
10	Bildung Stabiler Allâ€Silicium Varianten von 1,3â€Cyclobutandiyl im Gleichgewicht. Angewandte Chemie, 2020, 132, 15199-15204.	1.6	6
11	Equilibrium Formation of Stable Allâ€Silicon Versions of 1,3â€Cyclobutanediyl. Angewandte Chemie - International Edition, 2020, 59, 15087-15092.	7.2	34
12	Cycloaddition Reactions of Azides and Electronâ€Deficient Alkenes in Deep Eutectic Solvents: Pyrazolines, Aziridines and Other Surprises. Advanced Synthesis and Catalysis, 2020, 362, 1877-1886.	2.1	14
13	Epoxidation of Alkenes by Peracids: From Textbook Mechanisms to a Quantum Mechanically Derived Curlyâ€Arrow Depiction. ChemistryOpen, 2019, 8, 1244-1250.	0.9	11
14	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.	3.7	17
15	Elevated reaction order of 1,3,5-tri-tert-butylbenzene bromination as evidence of a clustered polybromide transition state: a combined kinetic and computational study. Organic and Biomolecular Chemistry, 2019, 17, 3781-3789.	1.5	7
16	A solid-supported arylboronic acid catalyst for direct amidation. Chemical Communications, 2019, 55, 2916-2919.	2.2	35
17	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
18	Monoâ€and Dicoordinate Germanium(0) as a Fourâ€Electron Donor. Chemistry - A European Journal, 2018, 24, 2873-2878.	1.7	12

#	Article	IF	Citations
19	Mechanistic insights into boron-catalysed direct amidation reactions. Chemical Science, 2018, 9, 1058-1072.	3.7	82
20	An Accessible Method for DFT Calculation of ¹¹B NMR Shifts of Organoboron Compounds. Journal of Organic Chemistry, 2018, 83, 8020-8025.	1.7	18
21	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.	4.6	30
22	Total Synthesis of (+)-Lophirone H and Its Pentamethyl Ether Utilizing an Oxoniumâ€“Prins Cyclization. Organic Letters, 2017, 19, 2486-2489.	2.4	33
23	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
24	Kinetic Resolution of 2â€Substituted Indolines by Nâ€sulfonylation using an Atropisomeric 4â€DMAPâ€Nâ€oxide Organocatalyst. Angewandte Chemie, 2017, 129, 5854-5858.	1.6	12
25	Tuning Azoheteroarene Photoswitch Performance through Heteroaryl Design. Journal of the American Chemical Society, 2017, 139, 1261-1274.	6.6	244
26	Synthesis and Reactions of Benzannulated Spiroaminals: Tetrahydrospirobiquinolines. ACS Omega, 2017, 2, 3241-3249.	1.6	5
27	A metadata-driven approach to data repository design. Journal of Cheminformatics, 2017, 9, 4.	2.8	17
28	The â˜Molecule of the Monthâ€™ Websiteâ€”An Extraordinary Chemistry Educational Resource Online for over 20 Years. Molecules, 2017, 22, 549.	1.7	4
29	InChI As a Research Data Management Tool. Chemistry International, 2016, 38, .	0.3	3
30	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
31	Stable bromoallene oxides. Chemical Communications, 2016, 52, 11219-11222.	2.2	4
32	Noncatalytic bromination of benzene: A combined computational and experimental study. Journal of Computational Chemistry, 2016, 37, 210-225.	1.5	16
33	How Many Water Molecules Does it Take to Dissociate HCl?. Chemistry - A European Journal, 2016, 22, 2812-2818.	1.7	42
34	Discovering More Chemical Concepts from 3D Chemical Information Searches of Crystal Structure Databases. Journal of Chemical Education, 2016, 93, 550-554.	1.1	16
35	Chemoselective Polymerizations from Mixtures of Epoxide, Lactone, Anhydride, and Carbon Dioxide. Journal of the American Chemical Society, 2016, 138, 4120-4131.	6.6	200
36	Standards-based metadata procedures for retrieving data for display or mining utilizing persistent (data-DOI) identifiers. Journal of Cheminformatics, 2015, 7, 37.	2.8	5

#	Article	IF	Citations
37	Chiroptical Properties of Streptorubin B: The Synergy Between Theory and Experiment. Chirality, 2015, 27, 745-751.	1.3	9
38	Chiroptical Studies on Brevianamide B: Vibrational and Electronic Circular Dichroism Confronted. Journal of Organic Chemistry, 2015, 80, 3359-3367.	1.7	7
39	Syntheses and Structures of Pseudo-Mauveine Picrate and 3-Phenylamino-5-(2-Methylphenyl)-7-Amino-8-Methylphenazinium Picrate Ethanol Mono-Solvate: The First Crystal Structures of a Mauveine Chromophore and a Synthetic Derivative. Journal of Chemical Research, 2015, 39, 711-718.	0.6	10
40	Standards-based curation of a decade-old digital repository dataset of molecular information. Journal of Cheminformatics, 2015, 7, 43.	2.8	8
41	A Multiply Functionalized Baseâ€Coordinated Ge^{II} Compound and Its Reversible Dimerization to the Digermene. Angewandte Chemie - International Edition, 2015, 54, 289-292.	7.2	42
42	A Molecular Complex with a Formally Neutral Iron Germanide Motif (Fe₂Ge₂). Organometallics, 2015, 34, 2130-2133.	1.1	28
43	Asymmetric Epoxidation: A Twinned Laboratory and Molecular Modeling Experiment for Upper-Level Organic Chemistry Students. Journal of Chemical Education, 2015, 92, 1385-1389.	1.1	13
44	Dual wavelength asymmetric photochemical synthesis with circularly polarized light. Chemical Science, 2015, 6, 3853-3862.	3.7	58
45	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
46	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	1.1	99
47	The Nature of the Fourth Bond in the Ground State of C₂: The Quadruple Bond Conundrum. Chemistry - A European Journal, 2014, 20, 6220-6232.	1.7	77
48	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
49	Nâ€Heterocyclic Carbene Coordinated Neutral and Cationic Heavier Cyclopropylidenes. Angewandte Chemie - International Edition, 2014, 53, 9953-9956.	7.2	76
50	The Houkâ€“List transition states for organocatalytic mechanisms revisited. Chemical Science, 2014, 5, 2057-2071.	3.7	154
51	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
52	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.	1.7	37
53	Equilibrium between a cyclotrisilene and an isolable base adduct of a disilenyl silylene. Nature Chemistry, 2013, 5, 876-879.	6.6	111
54	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.	1.7	17

#	Article	IF	Citations
55	Epoxidation of bromoallenes connects red algae metabolites by an intersecting bromoallene oxide â€“ Favorskii manifold. Chemical Communications, 2013, 49, 11176.	2.2	10
56	Lowâ€Valent Ge₂ and Ge₄ Species Trapped by Nâ€Heterocyclic Gallylene. Angewandte Chemie - International Edition, 2013, 52, 450-454.	7.2	50
57	Chemical datuments as scientific enablers. Journal of Cheminformatics, 2013, 5, 6.	2.8	12
58	A Computational Evaluation of the Evidence for the Synthesis of 1,3â€Dimethylcyclobutadiene in the Solid State and Aqueous Solution. Chemistry - A European Journal, 2013, 19, 4932-4937.	1.7	3
59	One Molecule, Two Atoms, Three Views, Four Bonds?. Angewandte Chemie - International Edition, 2013, 52, 3020-3033.	7.2	129
60	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
61	A HÃ¼ckel Theory Perspective on MÃ¶bius Aromaticity. Organic Letters, 2013, 15, 3432-3435.	2.4	21
62	N-heteroatom substitution effect in 3-aza-cope rearrangements. Chemistry Central Journal, 2013, 7, 94.	2.6	9
63	The Cp*Si+ cation as a stoichiometric source of silicon. Chemical Communications, 2012, 48, 7820.	2.2	25
64	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
65	Contraction and Expansion of the Silicon Scaffold of Stable Si₆R₆ Isomers. Journal of the American Chemical Society, 2012, 134, 16008-16016.	6.6	78
66	Semantic physical science. Journal of Cheminformatics, 2012, 4, 14.	2.8	3
67	Verification of stereospecific dyotropic racemisation of enantiopure d and l-1,2-dibromo-1,2-diphenylethane in non-polar media. Chemical Communications, 2012, 48, 8943.	2.2	13
68	Quadruple bonding in C2 and analogous eight-valence electron species. Nature Chemistry, 2012, 4, 195-200.	6.6	198
69	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
70	Can 1,3-dimethylcyclobutadiene and carbon dioxide co-exist inside a supramolecular cavity?. Chemical Communications, 2011, 47, 1851-1853.	2.2	13
71	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
72	Design, Synthesis, and Evaluation of a Helicenoidal DMAP Lewis Base Catalyst. Organic Letters, 2011, 13, 1250-1253.	2.4	133

#	Article	IF	Citations
73	CML: Evolution and design. Journal of Cheminformatics, 2011, 3, 44.	2.8	36
74	The past, present and future of Scientific discourse. Journal of Cheminformatics, 2011, 3, 46.	2.8	9
75	A Stable Derivative of the Global Minimum on the Si₆H₆ Potential Energy Surface. Angewandte Chemie - International Edition, 2011, 50, 7936-7939.	7.2	136
76	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
77	Racemization of Isobornyl Chloride via Carbocations: A Nonclassical Look at a Classic Mechanism. Journal of Chemical Education, 2010, 87, 221-228.	1.1	12
78	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
79	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
80	Inside Cover: Enantiomerically Pure Alleno-Acetylenic Macrocycles: Synthesis, Solid-State Structures, Chiroptical Properties, and Electron Localization Function Analysis (Chem. Eur. J. 32/2010). Chemistry - A European Journal, 2010, 16, 9694-9694.	1.7	0
81	Ring Currents in the Dismutational Aromatic Si₆R₆. Angewandte Chemie - International Edition, 2010, 49, 10006-10009.	7.2	46
82	The rational design of helium bonds. Nature Chemistry, 2010, 2, 390-393.	6.6	35
83	Using Semantically-Enabled Components for Social Web-Based Scientific Collaborations. ACS Symposium Series, 2010, , 41-63.	0.5	1
84	Chiral Aziridination of Olefins Using a Chiral Sulfinamide as the Nitrogen Source. Synlett, 2010, 2010, 145-149.	1.0	1
85	Successful Computational Modeling of Isobornyl Chloride Ion-Pair Mechanisms. Journal of Organic Chemistry, 2010, 75, 5164-5169.	1.7	22
86	SPECTRa-T: Machine-Based Data Extraction and Semantic Searching of Chemistry e-Theses. Journal of Chemical Information and Modeling, 2010, 50, 251-261.	2.5	7
87	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
88	A Tricyclic Aromatic Isomer of Hexasilabenzene. Science, 2010, 327, 564-566.	6.0	242
89	Wormholes in chemical space connecting torus knot and torus link Ï€-electron density topologies. Physical Chemistry Chemical Physics, 2009, 11, 1340-1345.	1.3	8
90	The importance of being bonded. Nature Chemistry, 2009, 1, 510-512.	6.6	43

#	Article	IF	Citations
91	A dramatic effect of double bond configuration in N-oxy-3-aza Cope rearrangementsâ€"a simple synthesis of functionalised allenes. Tetrahedron Letters, 2009, 50, 3446-3449.	0.7	7
92	The Chiro-optical Properties of a Lemniscular Octaphyrin. Organic Letters, 2009, 11, 3088-91.	2.4	27
93	Unusual regiodivergence in metal-catalysed intramolecular cyclisation of Î³-allenols. Chemical Communications, 2009, , 7125-7127.	2.2	39
94	The Geometry and Electronic Topology of Higher-Order Charged MÃ¶bius Annulenes. Journal of Physical Chemistry A, 2009, 113, 11619-11629.	1.1	42
95	The distortivity of Ï€-electrons in conjugated boron rings. Physical Chemistry Chemical Physics, 2009, 11, 10042.	1.3	6
96	A Study in Mauve: Unveiling Perkin's Dye in Historic Samples. Chemistry - A European Journal, 2008, 14, 8507-8513.	1.7	85
97	Reaction of aromatic nitroso compounds with chemical models of â€˜thiamine active aldehydeâ€™. Tetrahedron, 2008, 64, 7759-7770.	1.0	6
98	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
99	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
100	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
101	Chiral Aromaticities. A Topological Exploration of MÃ¶bius Homoaromaticity. Journal of Chemical Theory and Computation, 2008, 4, 1841-1848.	2.3	23
102	Linking number analysis of a self-assembled lemniscular MÃ¶bius-metallamacrocycle. New Journal of Chemistry, 2008, 32, 1831.	1.4	13
103	A computational investigation of the structure of polythiocyanogen. Dalton Transactions, 2008, , 6925-6932.	1.6	6
104	Visualizing Metal Tris Chelates: Visualizations to Examine the Structure and Symmetry of Metal Tris Chelates: Symmetry Operations, Chirality, and Mechanisms (Bailar Twist and RÃ¢y-Dutt) that Racemize the Î" and Î› Isomers. Journal of Chemical Education, 2008, 85, 750.	1.1	4
105	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
106	Linking Number Analysis of a Pentadecanuclear Metallamacrocycle: A MÃ¶bius-Craig System Revealed. Inorganic Chemistry, 2008, 47, 8932-8934.	1.9	21
107	Lemniscular Hexaphyrins as Examples of Aromatic and Antiaromatic Double-Twist MÃ¶bius Molecules. Organic Letters, 2008, 10, 949-952.	2.4	64
108	Chemical Markup, XML and the World-Wide Web. 8. Polymer Markup Language. Journal of Chemical Information and Modeling, 2008, 48, 2118-2128.	2.5	25

#	Article	IF	Citations
109	Chapter 7 Achieving a Holistic Web in the Chemistry Curriculum. Annual Reports in Computational Chemistry, 2007, , 99-133.	0.9	0
110	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
111	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.	1.9	37
112	The Aromaticity of Pericyclic Reaction Transition States. Journal of Chemical Education, 2007, 84, 1535.	1.1	28
113	Aromaticity rules for cycles with arbitrary numbers of half-twists. Physical Chemistry Chemical Physics, 2006, 8, 1775.	1.3	34
114	The Blue Obeliskâ€"Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998.	2.5	366
115	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
116	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
117	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
118	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
119	ChemSem:Â An Extensible and Scalable RSS-Based Seminar Alerting System for Scientific Collaboration. Journal of Chemical Information and Modeling, 2006, 46, 985-990.	2.5	3
120	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
121	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
122	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
123	Crocker, Not Armit and Robinson, Begat the Six Aromatic Electrons. ChemInform, 2006, 37, no.	0.1	0
124	Moebius Aromaticity and Delocalization. ChemInform, 2006, 37, no.	0.1	0
125	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
126	Chemistry in bioinformatics. BMC Bioinformatics, 2005, 6, 141.	1.2	12

#	Article	IF	Citations
127	Representation and Use of Chemistry in the Global Electronic Age.. ChemInform, 2005, 36, no.	0.1	0
128	A global resource for computational chemistry. Journal of Molecular Modeling, 2005, 11, 532-541.	0.8	16
129	Communication and re-use of chemical information in bioscience. BMC Bioinformatics, 2005, 6, 180.	1.2	15
130	Crocker, Not Armit and Robinson, Begat the Six Aromatic Electrons. Chemical Reviews, 2005, 105, 3436-3447.	23.0	126
131	Aromaticity on the edge of chaos: anAb initioCCSD(T) study of the bimodal balance between aromatic and non-aromatic structures for 10-Ï€-diheterocins and heteronins. Molecular Physics, 2005, 103, 401-405.	0.8	10
132	An Animated Interactive Overview of Molecular Symmetry. Journal of Chemical Education, 2005, 82, 1742.	1.1	10
133	MÃ¶bius Aromaticity and Delocalization. Chemical Reviews, 2005, 105, 3697-3715.	23.0	328
134	A solid-state structural and theoretical study on the 1 âˆ¶ 1 addition compounds of thioethers with dihalogens and interhalogens Iâ€“X (X = I, Br, Cl). New Journal of Chemistry, 2005, 29, 315-319.	1.4	10
135	Enhancement of the chemical semantic web through the use of InChI identifiers. Organic and Biomolecular Chemistry, 2005, 3, 1832.	1.5	78
136	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
137	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
138	A Double-Twist MÃ¶bius-Aromatic Conformation of [14]Annulene. Organic Letters, 2005, 7, 4637-4639.	2.4	56
139	Double-twist MÃ¶bius aromaticity in a 4n+ 2 electron electrocyclic reaction. Chemical Communications, 2005, , 5220.	2.2	27
140	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. ChemInform, 2004, 35, no.	0.1	0
141	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
142	Representation and use of chemistry in the global electronic age. Organic and Biomolecular Chemistry, 2004, 2, 3192.	1.5	42
143	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
144	Experimental and Computational Study of Î²-H Transfer between Cobalt(I) Alkyl Complexes and 1-Alkenes. Organometallics, 2004, 23, 5503-5513.	1.1	53

#	Article	IF	Citations
145	Foliacenes:Â Ab Initio Modeling of Metallocomplexes Exhibiting a Unique Form of 16-Electron, Metal-Induced Aromaticity. Journal of the American Chemical Society, 2004, 126, 14865-14870.	6.6	5
146	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
147	Chemical Machine Vision:â€‰Automated Extraction of Chemical Metadata from Raster Images. Journal of Chemical Information and Computer Sciences, 2003, 43, 1342-1355.	2.8	12
148	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
149	MÃ¶bius bis and tris-spiroaromatic systems. Organic and Biomolecular Chemistry, 2003, 1, 182-185.	1.5	17
150	XML for scientific publishing. OCLC Systems & Services, 2003, 19, 162-169.	0.4	4
151	Chemistry Preprints. Journal of Chemical Information and Computer Sciences, 2002, 42, 767-767.	2.8	1
152	An ab initio computational study of monodentate palladium ligand complexes with MÃ¶bius-aromatic chiral character. Dalton Transactions RSC, 2002, , 2421.	2.3	16
153	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
154	MÃ¶bius and HÃ¼ckel spiroaromatic systems. Perkin Transactions II RSC, 2002, , 1499-1501.	1.1	23
155	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
156	ChemDig: new approaches to chemically significant indexing and searching of distributed web collectionsElectronic supplementary information (ESI) available: list of less common chemical MIME media types, output template definitions and stylesheets associated with Table 4. See http://www.rsc.org/suppdata/nj/b1/b110693g/. New Journal of Chemistry, 2002, 26, 656-666.	1.4	5
157	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
158	Diastereoselective Reactions in Glycine Templates Containing anent-Ardeemin Fragment. Journal of Organic Chemistry, 2002, 67, 2013-2018.	1.7	7
159	STMML. A markup language for scientific, technical and medical publishing. Data Science Journal, 2002, 1, 128-192.	0.6	17
160	Scientific publications in XML - towards a global knowledge base. Data Science Journal, 2002, 1, 84-98.	0.6	20
161	A robot-based resource discovery tool for adding chemical meta-information and value to web-based documents. New Journal of Chemistry, 2001, 25, 635-638.	1.4	3
162	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

#	Article	IF	Citations
163	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
164	JChemTidy:â€‰ A Tool for Converting Chemical Web Document Collections to an XHTML Representation. Journal of Chemical Information and Computer Sciences, 2001, 41, 253-258.	2.8	4
165	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
166	A new publishing paradigm: STM articles as part of the semantic web. Learned Publishing, 2001, 14, 177-182.	0.8	11
167	Double aromaticity and anti-aromaticity in small carbon rings. Chemical Communications, 2000, , 1503-1504.	2.2	38
168	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
169	MÃ¶bius aromatics arising from a Cî€†Cî€†C ring component. Chemical Communications, 2000, , 1089-1090.	2.2	26
170	A universal approach to web-based chemistry using XML and CML. Chemical Communications, 2000, , 1471-1472.	2.2	13
171	An ab initio and MNDO-d SCFâ€“MO computational study of the extrusion reactions of R2Iâ€“F iodine(III) via dimeric, trimeric and tetrameric transition statesâ€Šâ€. Perkin Transactions II RSC, 2000, , 2158-2161.	1.1	15
172	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
173	Fluoridation of heteroaromatic iodonium saltsâ€”experimental evidence supporting theoretical prediction of the selectivity of the process. Chemical Communications, 2000, , 649-650.	2.2	89
174	Twist localisation in single, double and triple twisted MÃ¶bius cyclacenesâ€. Perkin Transactions II RSC, 2000, , 2378-2381.	1.1	27
175	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
176	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
177	The preferred conformation of Î±-fluoroamides. Journal of the Chemical Society Perkin Transactions II, 1999, , 2409-2411.	0.9	75
178	Chemical Markup, XML, and the Worldwide Web. 1. Basic Principles. Journal of Chemical Information and Computer Sciences, 1999, 39, 928-942.	2.8	196
179	Authentication of Internet-Based Distributed Computing Resources in Chemistry. Journal of Chemical Information and Computer Sciences, 1999, 39, 483-490.	2.8	10
180	Moldanet: a network distributed molecular graphics and modelling program that integrates secure signed applet and Java 3D technologies. Journal of Molecular Graphics and Modelling, 1998, 16, 144-149.	1.3	4

#	Article	IF	Citations
181	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
182	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
183	Elemental and Molecular Heritage: An Internet-based Display. Molecules, 1998, 3, 94-99.	1.7	5
184	The World-Wide Web as a chemical information tool. Chemical Society Reviews, 1997, 26, 1.	18.7	22
185	Some influences of fluorine in bioorganic chemistry. Chemical Communications, 1997, , 645-652.	2.2	454
186	The Internet as a computational chemistry tool. Computational and Theoretical Chemistry, 1997, 398-399, 27-33.	1.5	1
187	Advanced VRML based chemistry applications: a 3D molecular hyperglossary. Computational and Theoretical Chemistry, 1996, 368, 49-55.	1.5	9
188	The World-Wide Web information system: chemical chaos or global scientific enabler?. Chemometrics and Intelligent Laboratory Systems, 1995, 31, 47-52.	0.2	1
189	Chemical collaboratories using World-Wide Web servers and EyeChem-based viewers. Journal of Molecular Graphics, 1995, 13, 268-270.	1.7	10
190	A theoretical mechanistic investigation of asymmetric aziridination by N-Aryl-O-acylhydroxylamines.. AIP Conference Proceedings, 1995, , .	0.3	0
191	A chemical collaboratory using Explorer EyeChem and the common client interface. Computer Graphics, 1995, 29, 52-54.	0.1	8
192	The case for content integrity in electronic chemistry journals: The CLIC project. New Review of Information Networking, 1995, 1, 61-69.	0.3	7
193	Studies of imidazole and pyrazole protonation using electrostatically trained neural networks. Journal of the Chemical Society Perkin Transactions II, 1995, , 431.	0.9	10
194	Photoelectron spectroscopic study of the thermal decomposition of 2-pyrrolidinone and 2-pyrrolidinethione. Journal of the Chemical Society Perkin Transactions II, 1995, , 427.	0.9	5
195	Hyperactive molecules and the World-Wide-Web information system. Journal of the Chemical Society Perkin Transactions II, 1995, , 7.	0.9	28
196	?-Facial hydrogen bonding in the chiral resolving agent 2,2,2-trifluoro-1-(9-anthryl)-ethanol and its racemic modification. Chirality, 1994, 6, 245-250.	1.3	5
197	EyeChem 1.0: A modular chemistry toolkit for collaborative molecular visualization. Journal of Molecular Graphics, 1994, 12, 226-230.	1.7	11
198	Chemical applications of the World-Wide-Web system. Journal of the Chemical Society Chemical Communications, 1994, , 1907.	2.0	22

#	Article	IF	Citations
199	Stereoelectronic influence of fluorine in enzyme resolutions of Î±-fluoroesters. Journal of the Chemical Society Perkin Transactions II, 1994, , 3-4.	0.9	12
200	Stereospecific control of the citrate synthase mediated synthesis of (2R,3R)-3-fluorocitrate by the relative stabilities of the intermediate fluoroenolates. Journal of the Chemical Society Chemical Communications, 1994, , 2029.	2.0	8
201	An SCF-MO study of the dimerisation reaction of hemifullerene (C30H12) to the potential fullerene precursor C60H24. Journal of the Chemical Society Chemical Communications, 1994, , 1567.	2.0	11
202	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
203	Intermolecular interactions responsible for the absence of chiral recognition: aromatic Câ€“H â‹¯ O hydrogen bonding in the crystal structure of 3-chloro-9,13-dibutylamino-1-hydroxypropyl-6-trifluomethylphenanthrene propan-2-ol solvate hydrochloride. Journal of the Chemical Society Chemical Communications, 1994, , 1135-1137.	2.0	7
204	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
205	Theoretical study of the solvatochromic properties of rhodamines using the AM1 and PM3/COSMO solvation model. Journal of the Chemical Society Perkin Transactions II, 1994, , 1397-1398.	0.9	9
206	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
207	Electronic effects in Ï€-facially stereoselective epoxidation of phenyltrifluoromethylpropenol. Journal of the Chemical Society Chemical Communications, 1993, .	2.0	9
208	An MCSCF study of the effect of substituents and solvent on the [2 + 2]cycloaddition of tert-butylcyanoketene to phenylethene. Journal of the Chemical Society Perkin Transactions II, 1993, , 1499.	0.9	11
209	Reduction of nitrosobenzene by 2-(Î±-hydroxyethyl)-3,4-dimethylthiazolium Salts. Journal of the Chemical Society Chemical Communications, 1993, , 133-134.	2.0	7
210	Rank correlation of AM1 and PM3 derived molecular electrostatic potentials (RACEL) with Hammett Ïƒp-parameters. Journal of the Chemical Society Chemical Communications, 1992, , 37-39.	2.0	9
211	An unusual example of stereoelectronic control in the ring opening of 3,3-disubstituted 1,2-dichlorocyclopropenes. Journal of the Chemical Society Chemical Communications, 1992, , 1323.	2.0	9
212	A molecular orbital and crystallographic study of the structure and Ï€-facial regioselectivity of 9-chloro-1,4,5,8-tetrahydro-4a,8a-methanonaphthalene. Journal of the Chemical Society Perkin Transactions II, 1992, , 447-448.	0.9	6
213	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
214	Aryl group Ï€-facial electrostatic asymmetry as a contributing factor to chiral resolution on Î²-cyclodextrin HPLC phases. Journal of the Chemical Society Chemical Communications, 1992, , 1122-1124.	2.0	9
215	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
216	Prediction of the histidine-95 pK a perturbation in triosephosphate isomerase using an electrostatically trained neural network (SONNIC). Journal of the Chemical Society Chemical Communications, 1992, , 1178.	2.0	4

#	Article	IF	Citations
217	Transition-state structures for the reaction between styrene andtbutyl cyanoketene: Theoretical evidence for antarafacial characteristics in a ?2 + ?2 thermal cycloaddition. International Journal of Quantum Chemistry, 1992, 44, 469-476.	1.0	8
218	An AM1 and PM3 molecular orbital study of the pericyclic reactivity of aryl carbodiimides.. Tetrahedron, 1992, 48, 7425-7434.	1.0	12
219	? 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
220	2-Acyl thiazolium salts as selective agents for the O-acylation of aromatic hydroxylamines. Journal of the Chemical Society Chemical Communications, 1991, , 1127.	2.0	11
221	Transition state structure in cycloaddition reactions as a function of ring size and geometry. Journal of the Chemical Society Perkin Transactions II, 1991, , 939.	0.9	6
222	The preparation, X-ray crystal structure and theoretical study of [CoCp2][S3N3], (Cp =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 547 Td (cy of the Chemical Society Chemical Communications, 1991, .	2.0	22
223	Photodimerization of Aromatic Resin Acids. Journal of Natural Products, 1991, 54, 247-253.	1.5	1
224	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
225	Geometry optimisation at the semiempirical self-consistent-reaction-field level using the AMPAC and MOPAC programs. Journal of the Chemical Society Perkin Transactions II, 1991, , 635.	0.9	15
226	A PM3 SCF-MO study of the structure and bonding in the cage systems S4N4 and S4N4X (X = N+, Nâ¯, S,) Tj ETQq0 0 0 rgBT /Overlock	1.0	9
227	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
228	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
229	Vibrational spectra of sulphurâ€”nitrogen heterocycles: [S4N3]Cl and [S3N2Cl]Cl. Spectrochimica Acta Part A: Molecular Spectroscopy, 1989, 45, 367-369.	0.1	7
230	Photooxidation of Resin Acids. Journal of Natural Products, 1989, 52, 85-94.	1.5	14
231	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
232	A theoretical MNDO and AM1 SCF-MO study of dihydrogen transfer reactions. Journal of the Chemical Society Perkin Transactions II, 1989, , 475.	0.9	6
233	PM3 potential energy surfaces for phosphoryl transfer reactions. Journal of the Chemical Society Chemical Communications, 1989, , 1502.	2.0	9
234	A comparison of semi-empirical SCFâ€“MO and ab initio energy surfaces for the Beckmann rearrangement. Journal of the Chemical Society Chemical Communications, 1989, , 623-625.	2.0	16

#	Article	IF	Citations
235	A theoretical MNDO and AM1 SCF-MO study of dihydrogen elimination reactions. Journal of the Chemical Society Perkin Transactions II, 1989, , 367.	0.9	2
236	An ab initio self-consistent field molecular-orbital study of novel stereoelectronic effects in linear R2S3N2 and cyclic XS3N2 systems. Journal of the Chemical Society Dalton Transactions, 1989, , 1609.	1.1	8
237	Unusual Cis ring junction stereochemistry in a lactol derived from photo-oxygenation of abietic acid: An NMR and molecular modeling study. Tetrahedron Computer Methodology, 1988, 1, 133-139.	0.2	1
238	A study of the oxyanion effect in reactions of 2-methyl-2-propen-1-ol. Tetrahedron, 1988, 44, 1809-1823.	1.0	0
239	Triterpenoids of the fungus Pisolithus tinctorius*. Phytochemistry, 1988, 27, 3569-3574.	1.4	25
240	Enzymatic resolution of bicyclo[4.2.0]oct-2-en-7-ol and the preparation of some polysubstituted bicyclo[3.3.0]octan-2-ones via highly strained tricyclo[4.2.0.01,5]octan-8-ones. Journal of the Chemical Society Chemical Communications, 1988, , 470.	2.0	10
241	An essentially planar conformation determined for an arylsulphonylurea by low-temperature nuclear Overhauser effect spectroscopy. Journal of the Chemical Society Chemical Communications, 1988, , 1132.	2.0	2
242	Stereoelectronic effects in Râ€“NSNâ€“R systems. An MNDO and ab initio SCFMO study. Journal of the Chemical Society Dalton Transactions, 1988, , 3051-3053.	1.1	7
243	Thermally induced rearrangement of thiopheniobis(alkoxycarbonyl)methanides. Journal of the Chemical Society Perkin Transactions 1, 1988, , 803.	0.9	18
244	An ab initio SCF-MO study of the relative stability of carbonyl imines (R2Cî—»Oâ€”NR). Computational and Theoretical Chemistry, 1987, 149, 33-38.	1.5	7
245	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
246	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
247	The reaction between tetrasulphur tetranitride (S4N4) and electron-deficient alkynes. A molecular orbital study. Journal of the Chemical Society Perkin Transactions II, 1987, , 1669.	0.9	7
248	Volumes of reaction for the formation of some analogues of tetrahedral intermediates. Journal of the Chemical Society Perkin Transactions II, 1987, , 1477.	0.9	6
249	Hydrogen isotope effects in hydride transfer reactions of formaldehyde and glyoxal. An Ab initio and MNDO SCF-M.O. study. Journal of the Chemical Society Chemical Communications, 1987, , 998.	2.0	7
250	The base catalysed dimerisation of 2-methylpropenol. A MNDO SCF-MO model study of the reaction mechanism. Journal of the Chemical Society Chemical Communications, 1987, , 193.	2.0	2
251	The mechanism of phosphoryl to carbonyl migration of amino groups in mixed anhydrides. A MNDO SCF-MO study. Journal of the Chemical Society Perkin Transactions II, 1987, , 767.	0.9	5
252	Dihydrogen transfer reactions. An SCF-MO study of the relative energies of the concerted and stepwise pathways. Journal of the Chemical Society Chemical Communications, 1987, , 902.	2.0	9

#	Article	IF	Citations
253	A comparison of the MNDO and AM1 SCF-MO energy surfaces for dipolar cycloaddition and [3,3] sigmatropic reactions. Journal of the Chemical Society Chemical Communications, 1987, , 1779.	2.0	11
254	Characterizing a tetrahedral intermediate in an acyl transfer reaction: An undergraduate 1H NMR demonstration. Journal of Chemical Education, 1987, 64, 725.	1.1	2
255	Title is missing!. Tetrahedron, 1987, 43, 2805-2815.	1.0	113
256	Concerted dihydrogen exchange between methanol and formaldehyde: a theoretical study. Journal of the American Chemical Society, 1986, 108, 5793-5798.	6.6	18
257	The structure of an abietic acid dimer. Journal of the Chemical Society Chemical Communications, 1986, , 1038.	2.0	9
258	Novel triterpenoids from the fungus. Tetrahedron Letters, 1985, 26, 2589-2592.	0.7	10
259	Tetrahedral intermediates formed during acyl transfer. Reactions of acetyl cyanide. Journal of the Chemical Society Chemical Communications, 1985, , 1113.	2.0	16
260	Electronic and crystallographic structures of trithiadiazepines. Journal of the Chemical Society Chemical Communications, 1985, , 398.	2.0	14
261	2H-thiopyrans as intermediates in the rearrangement of thiophenium bisalkoycarbonylmethylides to thiophene-2-malonates; the crystal and molecular structure of 2,2-bis-t-butoxycarbonyl-5-bromo-2H-thiopyran and 2,2-bis-t-butoxycarbonyl-6-bromo-2H-thiopyran. Journal of the Chemical Society Chemical Communications, 1985, , 1590.	2.0	9
262	Structural reappraisal of the limonoid insect antifeedant azadirachtin. Journal of the Chemical Society Chemical Communications, 1985, , 968.	2.0	27
263	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
264	An MNDO SCF-MO study of the mechanism of the Cannizzaro reaction. Journal of the Chemical Society Perkin Transactions II, 1985, , 717.	0.9	15
265	A 1H n.m.r. and ab initio SCF-MO study of thiophenium methylides. Journal of the Chemical Society Chemical Communications, 1984, , 859.	2.0	3
266	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
267	C-substitution reactions of c,n-diaryl nitrones. Tetrahedron, 1983, 39, 3833-3841.	1.0	16
268	Ground states of molecules. 53.MNDO calculations for molecules containing chlorine. Journal of Computational Chemistry, 1983, 4, 158-169.	1.5	73
269	A MNDO SCF-MO theoretical study of the mechanism of [1,2] migrations in free radicals as a model for coenzyme B12 mediated rearrangement reactions. Journal of the Chemical Society Chemical Communications, 1983, , 625.	2.0	7
270	MNDO SCF-MO calculations of equilibrium isotope effects. Journal of the Chemical Society, Faraday Transactions 2, 1982, 78, 671.	1.1	10

#	Article	IF	Citations
271	Two-dimensional Î´/J-resolved31P n.m.r. spectroscopy of [bis(diphenylphosphino)methane](trimethylphosphine)chlororhodium(I). Journal of the Chemical Society Chemical Communications, 1982, , 482-484.	2.0	6
272	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.	1.0	19
273	MNDO SCF-MO calculations of kinetic isotope effects for dehydrochlorination reactions of chloroalkanes. Journal of the Chemical Society Chemical Communications, 1981, , 939.	2.0	9
274	Assignment of the structure of dihydrodaphnine diacetate by nuclear Overhauser effect difference spectroscopy. Tetrahedron Letters, 1981, 22, 2933-2936.	0.7	12
275	MNDO study of transient species: the IR spectrum of benzyne. Journal of Molecular Structure, 1979, 51, 275-279.	1.8	17
276	Ground states of molecules. 52. A MNDO SCF-MO study of the coordination of beryllium-indenyl and -fluorenyl complexes. Inorganic Chemistry, 1979, 18, 602-605.	1.9	7
277	Semiempirical calculations of molecular vibrational frequencies: The MNDO method. Journal of Molecular Structure, 1978, 43, 135-138.	1.8	101
278	Ground states of molecules. 45. MNDO results for molecules containing beryllium. Journal of the American Chemical Society, 1978, 100, 777-784.	6.6	104
279	MNDO parameters for third period elements. Journal of the American Chemical Society, 1978, 100, 3607-3607.	6.6	339
280	Ground states of molecules. 40. MNDO results for molecules containing fluorine. Journal of the American Chemical Society, 1978, 100, 58-67.	6.6	183
281	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
282	Calculations of electron affinities using the MNDO semiempirical SCF-MO method. Journal of the American Chemical Society, 1978, 100, 784-790.	6.6	126
283	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
284	Electrocyclic ring opening of 1Î±,4Î±- and 1Î±,4Î²-bicyclo[2.2.0]hexa-2,5-dienes (cis and trans Dewar benzenes): MNDO (modified neglect of diatomic overlap) semiempirical molecular orbital calculations. Journal of the Chemical Society Chemical Communications, 1977, , 728-730.	2.0	7
285	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
286	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
287	Ground states of molecules. Journal of Molecular Structure, 1977, 40, 145-149.	1.8	58
288	An MNDO study of the structures, vibrational frequencies, and ionization energies of the first five poly-ynes. Chemical Physics Letters, 1977, 50, 262-265.	1.2	9

#	Article	IF	Citations
289	MNDO study of ozone and its decomposition into (O2 + 0). Chemical Physics Letters, 1977, 47, 80-84.	1.2	29
290	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
291	FAIR enough?. Spectroscopy Europe, 0, , 25.	0.0	2
292	Open publishing FAIR spectra for and by students. Spectroscopy Europe, 0, , 22.	0.0	1