Alexandru T Balaban

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/10540273/publications.pdf

Version: 2024-02-01

240 papers	8,010 citations	61945 43 h-index	64755 79 g-index
267 all docs	267 docs citations	267 times ranked	4197 citing authors

#	Article	IF	Citations
1	Criteria for ranking (poly)cyclic chemical constitutional graphs and their vertices via centrality measures. Journal of Mathematical Chemistry, 2020, 58, 439-457.	0.7	2
2	Two new topological indices based on graph adjacency matrix eigenvalues and eigenvectors. Journal of Mathematical Chemistry, 2019, 57, 1053-1074.	0.7	9
3	On pyrylium cations, molecular graphs, topological indices for QSAR, and various other structural problems. Structural Chemistry, 2019, 30, 1129-1139.	1.0	2
4	Local aromaticity and aromatic sextet theory beyond Clar. International Journal of Quantum Chemistry, 2018, 118, e25657.	1.0	22
5	Crystal and molecular structure of 1-picryl-2-phenyl-2-(4-picrylamidophenyl)-diazenium betaine: analogy between a picramido group and an oxygen atom. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 89-94.	0.3	6
6	Chemistry-Mathematics-Philosophy Brew: a Personal Approach. Journal of Computer Chemistry Japan, 2017, 16, 33-37.	0.0	0
7	Energies for cyclic and acyclic aggregations of adamantane and diamantane units sharing vertices, edges, or sixâ€membered rings. International Journal of Quantum Chemistry, 2016, 116, 113-122.	1.0	2
8	NMR spectral properties of the tetramantanes â€“ nanometerâ€sized diamondoids. Magnetic Resonance in Chemistry, 2015, 53, 1003-1018.	1.1	5
9	Cyclic Diamondoid Structures with Shared Vertices, Edges, or 6-membered Rings. Croatica Chemica Acta, 2015, 88, 7-14.	0.1	2
10	Aromaticity and Conjugation in 1,2-Benzoquinone Valence Isomers and Congeners. Advances in Heterocyclic Chemistry, 2014, 113, 111-142.	0.9	6
11	Helical [n]catamantanes and all-trans-perhydroacenic [n]perimantanes: structures and von Baeyer IUPAC numbering of carbon atoms. Arkivoc, 2014, 2014, 346-361.	0.3	3
12	Drug Design, Molecular Descriptors in. , 2014, , 1-31.		1
13	Bond-switch defects in carbon allotropes: Stone-Wales and connected exchange. Chemical Physics Letters, 2013, 566, 50-53.	1.2	2
14	Diamond hydrocarbons revisited: partitioned formula tables of diamondoids. Journal of Mathematical Chemistry, 2013, 51, 1043-1055.	0.7	7
15	Diamond Hydrocarbons and Related Structures. Carbon Materials, 2013, , 1-27.	0.2	5
16	Theoretical Study of Hole-Containing Macromolecular Diamond Lattices and Corona-Diamondoid Molecules or their Heteroatomic Derivatives. Croatica Chemica Acta, 2013, 86, 371-378.	0.1	0
17	Partitioned-Formula Periodic Tables for Diamond Hydrocarbons (Diamondoids). Journal of Chemical Information and Modeling, 2012, 52, 2856-2863.	2.5	9
18	Conjugated circuits currents in hexabenzocoronene and its derivatives formed by joining proximal carbons. Journal of Computational Chemistry, 2012, 33, 1111-1122.	1.5	7

#	Article	IF	Citations
19	Graphical Representation of Proteins. Chemical Reviews, 2011, 111, 790-862.	23.0	104
20	Defining rules of aromaticity: a unified approach to the HÃ¼ckel, Clar and RandiÄ‡ concepts. Physical Chemistry Chemical Physics, 2011, 13, 3737-3747.	1.3	26
21	Structural Approach to Aromaticity and Local Aromaticity in Conjugated Polycyclic Systems. Carbon Materials, 2011, , 159-204.	0.2	5
22	Using Clar sextets for two- and three-dimensional aromatic systems. Physical Chemistry Chemical Physics, 2011, 13, 20649.	1.3	25
23	Effect of benzo-annelation on cyclic conjugation. Monatshefte FÃ¼r Chemie, 2011, 142, 53-57.	0.9	12
24	Local aromaticity in benzo- and benzocyclobutadieno-annelated anthracenes. Monatshefte FÃ¼r Chemie, 2011, 142, 797-800.	0.9	9
25	Local Aromaticity in Benzo- and Benzocyclobutadieno-Annelated Phenanthrenes. Polycyclic Aromatic Compounds, 2011, 31, 339-349.	1.4	6
26	Nonconvex polyhedra by repeated truncation of semiregular polyhedra. Journal of Mathematical Chemistry, 2010, 47, 1177-1183.	0.7	0
27	N-Alkoxy-3,5-dinitro-4-aminobenzoic acid derivatives with controlled physico-chemical properties. Structural Chemistry, 2010, 21, 1227-1234.	1.0	3
28	Molecular and crystal structure of a self-assembling pyridinium cationic lipid. Journal of Molecular Structure, 2010, 984, 228-231.	1.8	8
29	Monocyclic Hetarenes with Ï€-Electron Aromatic Sextet. Advances in Heterocyclic Chemistry, 2010, 99, 61-105.	0.9	12
30	Correlations between Local Aromaticity Indices of Bipartite Conjugated Hydrocarbons. Journal of Physical Chemistry A, 2010, 114, 5870-5877.	1.1	26
31	A DFT Study on Push-Pull (Amino-Nitro) Fulminenes and Hexahelicenes. Polycyclic Aromatic Compounds, 2010, 30, 91-111.	1.4	4
32	Patterns of ring current in coronene isomers. Acta Chimica Slovenica, 2010, 57, 507-12.	0.2	19
33	Reactions of 2,2â€Diphenylâ€1â€picrylhydrazyl (DPPH) with Two Syringylic Phenols or One Aroxide Derivative. European Journal of Organic Chemistry, 2009, 2009, 626-634.	1.2	17
34	Protochirons and protohelices. Journal of Mathematical Chemistry, 2009, 45, 725-747.	0.7	1
35	Carbonic anhydrase inhibitors. Synthesis of 2,4,6-trimethylpyridinium derivatives of 2-(hydrazinocarbonyl)-3-aryl-1H-indole-5-sulfonamides acting as potent inhibitors of the tumor-associated isoform IX and XII. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 2931-2934.	1.0	16
36	Claromatic Carbon Nanostructures. Journal of Physical Chemistry C, 2009, 113, 19123-19133.	1.5	69

#	Article	IF	Citations
37	Are Thermodynamic and Kinetic Stabilities Correlated? A Topological Index of Reactivity toward Electrophiles Used as a Criterion of Aromaticity of Polycyclic Benzenoid Hydrocarbons. Journal of Chemical Information and Modeling, 2009, 49, 369-376.	2.5	38
38	CYCLIC CONJUGATION IN FLUORANTHENE AND ITS BENZO-DERIVATIVES. PART 1. CATACONDENSED SYSTEMS. Polycyclic Aromatic Compounds, 2009, 29, 90-102.	1.4	24
39	Discovery of Low Nanomolar and Subnanomolar Inhibitors of the Mycobacterial Î²-Carbonic Anhydrases Rv1284 and Rv3273. Journal of Medicinal Chemistry, 2009, 52, 4063-4067.	2.9	82
40	A REGULARITY FOR CYCLIC CONJUGATION IN ACENAPHYHYLENE, FLUORANTHENE AND THEIR CONGENERS. Polycyclic Aromatic Compounds, 2009, 29, 3-11.	1.4	29
41	COMMENTS ON Ï€-ELECTRON CONJUGATION IN THE FIVE-MEMBERED RING OF BENZO-DERIVATIVES OF CORANNULENE. Polycyclic Aromatic Compounds, 2009, 29, 185-208.	1.4	12
42	Drug Design, Molecular Descriptors in. , 2009, , 2196-2215.		3
43	Partition of Ï€-electrons between faces of polyhedral carbon aggregates. Journal of Mathematical Chemistry, 2008, 43, 773-779.	0.7	8
44	Note on ordering and complexity of Platonic and Archimedean polyhedra based on solid angles. Journal of Mathematical Chemistry, 2008, 44, 725-730.	0.7	4
45	Ring signatures for benzenoids with up to seven rings, Part 2: Pericondensed systems. International Journal of Quantum Chemistry, 2008, 108, 898-926.	1.0	12
46	Ring signatures for benzenoids with up to seven rings, Part 1: Catacondensed systems. International Journal of Quantum Chemistry, 2008, 108, 865-897.	1.0	14
47	Synthesis and electron paramagnetic resonance study of a nitroxide free radical covalently bonded on aminopropyl-silica gel. Applied Surface Science, 2008, 254, 1904-1908.	3.1	9
48	Statistical investigation of new topological indices based on the molecular path code. Chemical Physics Letters, 2008, 464, 155-159.	1.2	4
49	EFFECT OF HETEROATOMS ON PARTITIONING OF Ï€-ELECTRONS IN RINGS OF CATAFUSENES. Polycyclic Aromatic Compounds, 2008, 28, 85-97.	1.4	8
50	Correlations between various ways of accounting for the distribution of Ï€-electrons in benzenoids. New Journal of Chemistry, 2008, 32, 1071.	1.4	10
51	New Chessboard (8×8) Representation of the Standard Genetic Code, and Its Application for Representing Primary Structures of Proteins. , 2008, , .		0
52	A New Yardstick for Benzenoid Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2008, 112, 11769-11776.	1.1	5
53	Ï€-Electron Partitions, Signatures, and Clar Structures of Selected Benzenoid Hydrocarbons. Journal of Physical Chemistry A, 2008, 112, 4148-4157.	1.1	13
54	3,5-Dinitro-N-(4â€™-benzo-15-crown-5)-benzamide derivatives. Synthesis and properties. Arkivoc, 2008, 2008, 307-321.	0.3	2

#	Article	IF	Citations
55	Four New Topological Indices Based on the Molecular Path Code. Journal of Chemical Information and Modeling, 2007, 47, 716-731.	2.5	21
56	PARTITIONING OF Ï€-ELECTRONS IN RINGS OF AZA-DERIVATIVES OF POLYCYCLIC BENZENOID HYDROCARBONS. Polycyclic Aromatic Compounds, 2007, 27, 51-63.	1.4	17
57	Synthesis and Characterization of Some Novel Homo- and Hetero-Diradicals of Hydrazyl and Nitroxide Type. Australian Journal of Chemistry, 2007, 60, 173.	0.5	7
58	QSPR for Physical Properties of cata-Condensed Benzenoids Using Two Simple Dualist-Based Descriptors. Journal of Physical Chemistry A, 2007, 111, 2448-2454.	1.1	9
59	Molecular Descriptors for Natural Diamondoid Hydrocarbons and Quantitative Structure-Property Relationships for Their Chromatographic Data. Open Organic Chemistry Journal, 2007, 1, 13-31.	0.9	16
60	QSPR correlations of half-wave reduction potentials of cata-condensed benzenoid hydrocarbons. Arkivoc, 2007, 2006, 104-119.	0.3	8
61	Reaction of 2-(Î±-bromoacetyl)-phenoxathiin with substituted o-, m-, or p-formyl-aroxides. Arkivoc, 2007, 2007, 8-22.	0.3	4
62	The Eight Classes of Positive-Curvature Graphitic Nanocones. Journal of Chemical Information and Modeling, 2006, 46, 307-320.	2.5	32
63	Partitioning of Ï€-Electrons in Rings for Clar Structures of Benzenoid Hydrocarbons. Journal of Chemical Information and Modeling, 2006, 46, 57-64.	2.5	43
64	Strain-Free Sextet-Resonant Benzenoids and Their Antisextet Dualists. Journal of Chemical Information and Modeling, 2006, 46, 1563-1579.	2.5	30
65	Lipophilic Pyrylium Salts in the Synthesis of Efficient Pyridinium-Based Cationic Lipids, Gemini Surfactants, and Lipophilic Oligomers for Gene Delivery. Journal of Medicinal Chemistry, 2006, 49, 3872-3887.	2.9	101
66	Is chemistry 'The Central Science'? How are different sciences related? Co-citations, reductionism, emergence, and posets. Scientometrics, 2006, 69, 615-637.	1.6	33
67	Crocker, Not Armit and Robinson, Begat the Six Aromatic Electrons. ChemInform, 2006, 37, no.	0.1	0
68	ALGORITHM FOR SIMULTANEOUS CALCULATION OF KEKULÃ‰ AND CLAR STRUCTURE COUNTS, AND CLAR NUMBER OF BENZENOID MOLECULES. Polycyclic Aromatic Compounds, 2006, 26, 17-35.	1.4	22
69	178. Structure-Activity Relationships in a Library of Pyridinium Non-Viral Vectors for Gene Delivery. Molecular Therapy, 2006, 13, S69.	3.7	0
70	Reaction of 2,2-Diphenyl-1-picrylhydrazyl with HOâ€¢, O2â€¢â€“, HOâ€“ ,and HOOâ€“ Radicals and Anions. International Journal of Molecular Sciences, 2006, 7, 130-143.	1.8	31
71	Study on supramolecular complexing ability vis-Ã-vis estimation of pKa of substituted sulfonamides: Dominating role of Balaban index (J). Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3966-3973.	1.0	23
72	Four-color map representation of DNA or RNA sequences and their numerical characterization. Chemical Physics Letters, 2005, 407, 205-208.	1.2	52

#	Article	IF	Citations
73	Partitioning of Ï€ -electrons in rings of polycyclic conjugated hydrocarbons: Part 6. Comparison with other methods for estimating the local aromaticity of rings in polycyclic benzenoids. Journal of Mathematical Chemistry, 2005, 37, 443-453.	0.7	40
74	Can topological indices transmit information on properties but not on structures?. Journal of Computer-Aided Molecular Design, 2005, 19, 651-660.	1.3	22
75	On the Complexity of Fullerenes and Nanotubes. , 2005, , 1-48.		2
76	Partitioning of Ï€-Electrons in Rings of Fibonacenes. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2005, 60, 171-176.	0.7	21
77	Ï€-ELECTRON CONTENTS OF RINGS IN THE DOUBLE-HEXAGONAL-CHAIN HOMOLOGOUS SERIES (PYRENE,) Tj ETQq1 1 0.784314 rgB	1.4	16
78	Crocker, Not Armit and Robinson, Begat the Six Aromatic Electrons. Chemical Reviews, 2005, 105, 3436-3447.	23.0	126
79	Pyridinium cationic lipids in gene delivery: an in vitro and in vivo comparison of transfection efficiency versus a tetraalkylammonium congener. Archives of Biochemistry and Biophysics, 2005, 435, 217-226.	1.4	72
80	Synthesis and properties of dinitrobenzamido-TEMPO derivatives. Arkivoc, 2005, 2005, 225-237.	0.3	5
81	Clar Formulas: How to Draw and How not to Draw Formulas of Polycyclic Aromatic Hydrocarbons. Polycyclic Aromatic Compounds, 2004, 24, 83-89.	1.4	32
82	Partitioning of Ï€-electrons in Rings of Polycyclic Conjugated Hydrocarbons. Part 4. Benzenoids with More Than One Geometric KekulÃ© Structure Corresponding to the Same Algebraic KekulÃ© Structure. Journal of Mathematical Chemistry, 2004, 36, 271-279.	0.7	30
83	QSAR study using topological indices for inhibition of carbonic anhydrase II by sulfanilamides and Schiff bases. Molecular Diversity, 2004, 8, 401-412.	2.1	26
84	Partitioning of Ï€-Electrons in Rings of Polycyclic Benzenoid Hydrocarbons. Part 2. Catacondensed Coronoids.. ChemInform, 2004, 35, no.	0.1	0
85	Aromaticity as a Cornerstone of Heterocyclic Chemistry. ChemInform, 2004, 35, no.	0.1	0
86	Partitioning of Ï€-Electrons in Rings of Polycyclic Conjugated Hydrocarbons. Part 5. Nonalternant Compounds.. ChemInform, 2004, 35, no.	0.1	0
87	Unique graphical representation of protein sequences based on nucleotide triplet codons. Chemical Physics Letters, 2004, 397, 247-252.	1.2	97
88	PARTITIONING OF Ï€-ELECTRONS IN RINGS OF POLYCYCLIC conjugated HYDROCARBONS. PART 1: CATACONDENSED BENZENOIDS. Polycyclic Aromatic Compounds, 2004, 24, 173-193.	1.4	55
89	Simple Synthesis of a Weak Nucleophilic Base (4-Ethyl-2,6-diisopropyl-3,5-dimethylpyridine) Evidencing a Double Janus Group Effect. Journal of Organic Chemistry, 2004, 69, 536-542.	1.7	16
90	Partitioning of Ï€-Electrons in Rings of Polycyclic Conjugated Hydrocarbons. 5. Nonalternant Compoundsâ€. Journal of Chemical Information and Computer Sciences, 2004, 44, 1701-1707.	2.8	47

#	Article	IF	Citations
91	Partitioning of Ï€-electrons in rings of polycyclic conjugated hydrocarbons. Part 3. Perifusenes. New Journal of Chemistry, 2004, 28, 800-806.	1.4	49
92	Partitioning of Ï€-Electrons in Rings of Polycyclic Benzenoid Hydrocarbons. 2.1Catacondensed Coronoids. Journal of Chemical Information and Computer Sciences, 2004, 44, 50-59.	2.8	61
93	Pyridinium Cationic Lipids in Gene Delivery:Â A Structureâ^'Activity Correlation Study. Journal of Medicinal Chemistry, 2004, 47, 3744-3754.	2.9	87
94	Aromaticity as a Cornerstone of Heterocyclic Chemistry. Chemical Reviews, 2004, 104, 2777-2812.	23.0	662
95	A Four-Dimensional Representation of DNA Primary Sequences.. ChemInform, 2003, 34, no.	0.1	1
96	Theoretical Examination of New Forms of Carbon Formed by Intra- or Intermolecular Dehydrogenation of Polycyclic Aromatic Hydrocarbons, Particularly Helicenes. ChemInform, 2003, 34, no.	0.1	0
97	DNA invariants based on nonoverlapping triplets of nucleotide bases. Chemical Physics Letters, 2003, 379, 147-154.	1.2	18
98	Synthesis of 2,4-dimethyl-6-oxo-2,4-heptadienoic acid derivatives from 2,4,6-trimethylpyrylium salts. Tetrahedron, 2003, 59, 3291-3295.	1.0	6
99	On a Four-Dimensional Representation of DNA Primary Sequences [J.Chem. Inf. Comput. Sci.43, 532â^'539 (2003)]. Journal of Chemical Information and Computer Sciences, 2003, 43, 1724-1724.	2.8	1
100	On A Four-Dimensional Representation of DNA Primary Sequences. Journal of Chemical Information and Computer Sciences, 2003, 43, 532-539.	2.8	117
101	Theoretical Examination of New Forms of Carbon Formed by Intra- or Intermolecular Dehydrogenation of Polycyclic Aromatic Hydrocarbons, Particularly Helicenes. Polycyclic Aromatic Compounds, 2003, 23, 277-296.	1.4	2
102	A Comparison Between Various Topological Indices, Particularly Between the Index J and Wiener's Index W. , 2002, , 89-112.		7
103	Applications of Topological Indices in the Property/Bioactivity/Toxicity Prediction of Chemicals. , 2002, , 113-184.		14
104	From Chemical Graphs to 3D Molecular Modeling. , 2002, , 1-24.		2
105	Cationic Lipids in Gene Delivery: Principles, Vector Design and Therapeutical Applications. Current Pharmaceutical Design, 2002, 8, 2441-2473.	0.9	59
106	Applications of Topological Indices in the Property/Bioactivity/Toxicity Prediction of Chemicals. , 2002, , 113-184.		4
107	Scavenging the hydroxyl radical by 2,2-diphenyl-1-picrylhydrazyl. Arkivoc, 2002, 2002, 123-132.	0.3	8
108	A Comparison Between Various Topological Indices, Particularly Between the Index J and Wiener's Index W. , 2002, , 89-112.		0

#	Article	IF	Citations
109	Wiener Index Extension by Counting Even/Odd Graph Distances. Journal of Chemical Information and Computer Sciences, 2001, 41, 536-549.	2.8	53
110	Prediction of Mutagenicity of Aromatic and Heteroaromatic Amines from Structure:â€‰ A Hierarchical QSAR Approach. Journal of Chemical Information and Computer Sciences, 2001, 41, 671-678.	2.8	86
111	Serendipitous, one-pot formation of 2,3,7-triphenylcyclopenta[c]pyran from 1,2-diphenylethanedione (Ã¢â‚¬Ã“benzilÃ¢â‚¬Â) and cyclopentadiene. New Journal of Chemistry, 2001, 25, 1472-1474.	1.4	11
112	Using Protochirons for Three-Dimensional Coding of Certain Chemical Structures. Journal of Chemical Information and Computer Sciences, 2001, 41, 1145-1149.	2.8	11
113	Recent developments in cationic lipid-mediated gene delivery and gene therapy. Expert Opinion on Therapeutic Patents, 2001, 11, 1729-1752.	2.4	34
114	On Structural Interpretation of Several Distance Related Topological Indices. Journal of Chemical Information and Computer Sciences, 2001, 41, 593-601.	2.8	42
115	Reactions of Pyrylium Salts with Nucleophiles. Part 26.1 the Reaction with the Cyanide Anion Revisited. Journal of Chemical Research, 2001, 2001, 170-172.	0.6	8
116	Evaluation in Quantitative Structureâ^'Property Relationship Models of Structural Descriptors Derived from Information-Theory Operators. Journal of Chemical Information and Computer Sciences, 2000, 40, 631-643.	2.8	33
117	Comparison of Weighting Schemes for Molecular Graph Descriptors:â€‰ Application in Quantitative Structureâ^'Retention Relationship Models for Alkylphenols in Gasâ^'Liquid Chromatography. Journal of Chemical Information and Computer Sciences, 2000, 40, 732-743.	2.8	33
118	Topological Indices:â€‰ Their Nature and Mutual Relatedness. Journal of Chemical Information and Computer Sciences, 2000, 40, 891-898.	2.8	117
119	Visual Chemistry: Three-Dimensional Perception of Chemical Structures. Journal of Science Education and Technology, 1999, 8, 251-255.	2.4	9
120	Correlation between Structure and Normal Boiling Points of Acyclic Carbonyl Compounds. Journal of Chemical Information and Computer Sciences, 1999, 39, 758-764.	2.8	22
121	Normal Boiling Points of 1,ï‰-Alkanedinitriles:â€‰ The Highest Increment in a Homologous Series. Journal of Chemical Information and Computer Sciences, 1999, 39, 769-774.	2.8	15
122	Selective (15N) nitration of 2,2-diphenyl-1-(2,4- or 2,6-dinitrophenyl)-hydrazines or -hydrazyls. Journal of Labelled Compounds and Radiopharmaceuticals, 1998, 41, 791-799.	0.5	6
123	Reaction of pyrylium salts with nucleophiles. Part 25. Formation of pyridine-1-oxides, 2-isoxazolines and 1-pyrazoline-1-oxides. Tetrahedron, 1998, 54, 9747-9764.	1.0	18
124	Quantitative structure-property relationship study of normal boiling points for halogen-/ oxygen-/ sulfur-containing organic compounds using the CODESSA program. Tetrahedron, 1998, 54, 9129-9142.	1.0	54
125	SYNTHESIS AND SPECTRAL DATA OF SOME NEW N-NITROSO-N-PHENYLHYDROXYLAMINE (CUPFERRON) DERIVATIVES. Organic Preparations and Procedures International, 1998, 30, 439-446.	0.6	33
126	Design of Topological Indices. Part 10. Parameters Based on Electronegativity and Covalent Radius for the Computation of Molecular Graph Descriptors for Heteroatom-Containing Molecules. Journal of Chemical Information and Computer Sciences, 1998, 38, 395-401.	2.8	69

#	Article	IF	Citations
127	Algorithm for the Direct Enumeration of Chiral and Achiral Skeletons of a Homosubstituted Derivative of a Monocyclic Cycloalkane with a Large and Factorizable Ring Sizen. Journal of Chemical Information and Computer Sciences, 1998, 38, 1145-1150.	2.8	5
128	Theoretical investigation of carbon nets and molecules. Theoretical and Computational Chemistry, 1998, , 381-404.	0.2	8
129	From Chemical Topology to 3D Geometryâ€. Journal of Chemical Information and Computer Sciences, 1997, 37, 645-650.	2.8	48
130	Generalizations of the Stone-Wales rearrangement for cage compounds, including fullerenes. Computational and Theoretical Chemistry, 1996, 363, 291-301.	1.5	26
131	EPR and Multiple Electron Resonance Spectroscopic Indication ofpara-Nitration of Aminyl Radicals. Magnetic Resonance in Chemistry, 1996, 34, 197-206.	1.1	6
132	Holes in diamond or carbon nitride lattices. International Journal of Quantum Chemistry, 1996, 60, 1065-1068.	1.0	8
133	Covalently-Bonded â€œOnion Typeâ€•Double Fullerenic Carbon Cages. Fullerenes, Nanotubes, and Carbon Nanostructures, 1996, 4, 467-476.	0.6	3
134	W. R. Hamilton: His Genius, His Circuits, and the IUPAC Nomenclature for Fulleranes. Journal of Chemical Education, 1995, 72, 693.	1.1	10
135	Hydrophobic supramolecular complexes of various cations with 18-crown-6 as the ligand and N-methoxy-picramide as the anion pair in a water/methylene chloride two-phase system: complexes with Î±-amino acids, their characteristics and conditions for formation. Supramolecular Science, 1995, 2, 37-40.	0.7	5
136	Chemical Graphs: Looking Back and Glimpsing Ahead. Journal of Chemical Information and Computer Sciences, 1995, 35, 339-350.	2.8	78
137	SYNTHESIS AND SPECTRA OF 3-(3,5-DIMETHYL-2-FUROYL)-4-ARYL-5-CARBETHOXY-Î”2-PYRAZOLINES. Heterocyclic Communications, 1994, 1, .	0.6	1
138	Molecular cyclicity and centricity of polycyclic graphs. I. Cyclicity based on resistance distances or reciprocal distances. International Journal of Quantum Chemistry, 1994, 50, 1-20.	1.0	141
139	Conjugatedâ€circuit computations on twoâ€dimensional carbon networks. Journal of Chemical Physics, 1994, 101, 5281-5292.	1.2	52
140	Modeling the anticarcinogenic action of retinoids by making use of the OASIS method. 3. Inhibition of the induction of ornithine decarboxylase by arotinoids. Journal of Medicinal Chemistry, 1994, 37, 2300-2307.	2.9	9
141	Correlation between Structure and Normal Boiling Points of Haloalkanes C1-C4 Using Neural Networks. Journal of Chemical Information and Computer Sciences, 1994, 34, 1118-1121.	2.8	56
142	Local versus Global (i.e. Atomic versus Molecular) Numerical Modeling of Molecular Graphs. Journal of Chemical Information and Computer Sciences, 1994, 34, 398-402.	2.8	37
143	Reaction Graphs. , 1994, , 137-180.		16
144	Search for nondegenerate real vertex invariants and derived topological indexes. Journal of Computational Chemistry, 1993, 14, 155-160.	1.5	7

#	Article	IF	Citations
145	Chemical graphs with degenerate topological indices based on information on distances. Journal of Mathematical Chemistry, 1993, 14, 21-33.	0.7	24
146	Central vertices versus central rings in polycyclic systems. Journal of Mathematical Chemistry, 1993, 14, 287-304.	0.7	9
147	Design of topological indices. Part 4. Reciprocal distance matrix, related local vertex invariants and topological indices. Journal of Mathematical Chemistry, 1993, 12, 309-318.	0.7	243
148	Solved and Unsolved Problems in Chemical Graph Theory. Annals of Discrete Mathematics, 1993, , 109-126.	1.4	13
149	Real number vertex invariants: Regressive distance sums and related topological indexes. Journal of Chemical Information and Computer Sciences, 1993, 33, 421-428.	2.8	23
150	Benzenoids with maximum Kekule structure counts for given numbers of hexagons. Journal of Chemical Information and Computer Sciences, 1993, 33, 429-436.	2.8	15
151	Correlations between chemical structure and normal boiling points of halogenated alkanes C1-C4. Journal of Chemical Information and Computer Sciences, 1992, 32, 233-237.	2.8	48
152	Correlations between chemical structure and normal boiling points of acyclic ethers, peroxides, acetals, and their sulfur analogs. Journal of Chemical Information and Computer Sciences, 1992, 32, 237-244.	2.8	48
153	Using real numbers as vertex invariants for third-generation topological indexes. Journal of Chemical Information and Computer Sciences, 1992, 32, 23-28.	2.8	85
154	Relative stabilities of pyrylium anhydrobases (Î±/Î³-methylenepyrans) and their N-methylpyridinium congeners. Tetrahedron, 1992, 48, 6799-6806.	1.0	6
155	Nonisomorphic graphs with identical atomic counts of self-returning walks: Isocodal graphs. Journal of Mathematical Chemistry, 1992, 11, 155-167.	0.7	12
156	Recurrence relationships for the computation of the number of Kekulï¿½ structures. Journal of Mathematical Chemistry, 1992, 11, 169-177.	0.7	7
157	Carbonic Anhydrase Inhibitors. V: Pyrylium Salts in the Synthesis of Isozyme-Specific Inhibitors. Journal of Pharmaceutical Sciences, 1992, 81, 716-719.	1.6	41
158	Theoretical studies of aza analogues of platonic hydrocarbons.. Computational and Theoretical Chemistry, 1991, 228, 47-60.	1.5	19
159	Molecular topology. IV. Regressive vertex degrees (new graph invariants) and derived topological indices. Journal of Computational Chemistry, 1991, 12, 527-535.	1.5	37
160	Crystal and molecular structure of 1-(3,5-dimethyl-2-furyl)-3-(p-tolyl) -prop-2-en-1-one. Structural Chemistry, 1991, 2, 651-654.	1.0	5
161	New vertex invariants and topological indices of chemical graphs based on information on distances. Journal of Mathematical Chemistry, 1991, 8, 383-397.	0.7	86
162	Theoretical studies of aza analogues of platonic hydrocarbons. Computational and Theoretical Chemistry, 1990, 206, 67-75.	1.5	33

#	Article	IF	Citations
163	Theoretical studies on aza-analogs of platonic hydrocarbons. Computational and Theoretical Chemistry, 1990, 208, 63-77.	1.5	18
164	Stereoisomerism due to restricted rotation in N-substituted 2,6-di-ortho-tolylpyridirium cations. A molecular design enabling unambiguous identification of isomers. Tetrahedron Letters, 1990, 31, 5645-5648.	0.7	4
165	Chemical Graphs. Part 51.¹Enumeration of Nonbranched Catafusenes According to the Numbers of Benzenoid Rings in the Catafusene and in its Longest Linearly Condensed Portion. Polycyclic Aromatic Compounds, 1990, 1, 171-189.	1.4	13
166	Benzo[c] Pyrlium Salts: Syntheses, Reactions, and Physical Properties. Advances in Heterocyclic Chemistry, 1990, 50, 157-254.	0.9	57
167	Factors Affecting Stability and Equilibria of Free Radicals, XVII⁺ EPR Evidence for Formation of N-Alkoxypicramides on Oxidation of N-Alkoxy-dinitroanilines. Electronic Structure of Aminyl Radicals. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1989, 44, 1459-1463.	0.3	9
168	Use of solvent vapour pressure to evacuate the installation in carbonations of grignard reagents. Journal of Labelled Compounds and Radiopharmaceuticals, 1989, 27, 971-976.	0.5	2
169	Iterative procedure for the generalized graph center in polycyclic graphs. Journal of Chemical Information and Computer Sciences, 1989, 29, 91-97.	2.8	36
170	Catalytic automerization of phenanthrene. Journal of the American Chemical Society, 1989, 111, 734-735.	6.6	17
171	Title is missing!. Die Makromolekulare Chemie, 1988, 189, 863-870.	1.1	4
172	2-benzopyrylium salts. XXXVII. Oxygen analogs of reissert compounds : molecular structure and reactions with sodium hydroxide. Tetrahedron, 1988, 44, 6217-6224.	1.0	11
173	Alternating 6-cycles in perfect matchings of graphs representing condensed benzenoid hydrocarbons. Discrete Applied Mathematics, 1988, 19, 5-16.	0.5	11
174	SYNTHESIS OF ALKYL INDOLIZINES FROM PYRYLIUM SALTS. Organic Preparations and Procedures International, 1988, 20, 237-243.	0.6	4
175	4-PHENYL-Î”3-DIHYDROPYRANS BY REDUCTION OF PYRILIUM SALTS WITH SODIUM BOROHYDRIDE IN ACETIC ACID. Organic Preparations and Procedures International, 1988, 20, 231-236.	0.6	7
176	Topological indices and their uses: A new approach for the coding of alkanes. Computational and Theoretical Chemistry, 1988, 165, 243-253.	1.5	32
177	The number of alkanes having n carbons and a longest chain of length d: An application of a theorem of Polya. Journal of Chemical Education, 1988, 65, 304.	1.1	33
178	3,4-Connected carbon nets: through-space and through-bond interactions in the solid state. Journal of the American Chemical Society, 1987, 109, 6742-6751.	6.6	113
179	2-benzopyrylium salts. xxxi. Tetrahedron, 1987, 43, 409-414.	1.0	7
180	Î”3-Dihydropyrans and tetrahydropyrans by reduction of pyrylium salts with sodium borohydride in acetic acid. Tetrahedron Letters, 1987, 28, 1341-1344.	0.7	21

#	Article	IF	Citations
181	Formation of 6,6-dimethyl-2,4-cyclohexadienylidene-1-imines from primary amines and 2,6-diisopropylpyrylium salts. Tetrahedron Letters, 1987, 28, 3143-3144.	0.7	5
182	Synthesis of indolizines starting from pyrylium salts. Tetrahedron Letters, 1987, 28, 3145-3146.	0.7	14
183	Factors affecting the stability and equilibria of free radicals. XIII. N-alkoxy- and N-aralkoxypicrylamines and ESR spectra of the corresponding capto-dative persistent aminyls. Journal of Magnetic Resonance, 1987, 75, 63-72.	0.5	6
184	Model mndo calculations for rotamers of Î±-acylnitroxides and of N-nitrosonitroxides. Tetrahedron, 1987, 43, 405-408.	1.0	11
185	[55] Measurement of transmembrane proton movements with nitroxide spin probes. Methods in Enzymology, 1986, 127, 738-745.	0.4	6
186	Symmetry in chemical structures and reactions. Computers and Mathematics With Applications, 1986, 12, 999-1020.	1.4	6
187	SYMMETRY IN CHEMICAL STRUCTURES AND REACTIONS. , 1986, , 999-1020.		3
188	Factors affecting the interaction of lanthanide shift reagents with substituted pyridines. Tetrahedron Letters, 1985, 26, 4669-4672.	0.7	9
189	Janus-type isopropyl groups revealed by 1H-NMR spectra of alkylpyridines with lanthanide shift reagents (LSR). Tetrahedron Letters, 1985, 26, 4673-4676.	0.7	15
190	Unique description of chemical structures based on hierarchically ordered extended connectivities. VII. Condensed benzenoid hydrocarbons and their 1H NMR chemical shifts. Journal of Magnetic Resonance, 1985, 63, 1-13.	0.5	4
191	Applications of graph theory in chemistry. Journal of Chemical Information and Computer Sciences, 1985, 25, 334-343.	2.8	305
192	Unique description of chemical structures based on hierarchically ordered extended connectivities (HOC procedures). I. Algorithms for finding graph orbits and canonical numbering of atoms. Journal of Computational Chemistry, 1985, 6, 538-551.	1.5	59
193	Unique description of chemical structures on hierarchically ordered extended connectivities (HOC) Tj ETQq1 1 0.784314 rgBT /Overlo 1985, 6, 552-561.	1.5	14
194	Unique description of chemical structures based on hierarchically ordered extended connectivities (HOC procedures). III. Topological, chemical, and stereochemical coding of molecular structure. Journal of Computational Chemistry, 1985, 6, 562-569.	1.5	14
195	Unique description of chemical structures based on hierarchically ordered extended connectivities (HOC procedures). VIII. General principles for computer implementation. Journal of Computational Chemistry, 1985, 6, 587-591.	1.5	7
196	Chiral Rotamers of N-(1-Indanyl)-pyridinium Salts and their Restricted Rotation Around the C(sp³)â€"N⁺(sp²) Single Bond. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1985, 40, 1555-1557.	0.3	4
197	CorrÃ©lation entre possibilitÃ© d'effet laser et force oscillatrice de la transition fluorescente : cas des sels de pyrylium. Canadian Journal of Physics, 1985, 63, 191-194.	0.4	20
198	Graph theory and theoretical chemistry. Computational and Theoretical Chemistry, 1985, 120, 117-142.	1.5	46

#	Article	IF	Citations
199	Symbolic computation and chemistry. Lecture Notes in Computer Science, 1985, , 68-79.	1.0	2
200	Steric Versus Electronic Components of Secondary Deuterium Isotope Effects Depend on the Size of Electrophilic Probes. , 1985, , 655-663.		1
201	Schemes and transformations in the (CH)2k series: Valence isomers of [8]- and [10]annulene. Journal of Chemical Education, 1984, 61, 766.	1.1	21
202	Unique description of chemical structures based on hierarchically ordered extended connectivities (HOC procedures). V. New topological indices, ordering of graphs, and recognition of graph similarity. Journal of Computational Chemistry, 1984, 5, 629-639.	1.5	21
203	Oxygen-18 isotope effect in carbon-13 nuclear magnetic resonance spectroscopy. 8. Oxygen exchange of 2,4,6-trimethylpyrylium cation. Journal of the American Chemical Society, 1984, 106, 7836-7840.	6.6	13
204	Gear effectâ€"10. Tetrahedron, 1983, 39, 4209-4219.	1.0	27
205	Factors affecting stability and equilibria of free radicals-XII. Tetrahedron, 1983, 39, 3943-3945.	1.0	13
206	Doubly Vinylogous 4Hâ€Pyrones from Pyrylium Salts and Aryl Î²â€Chlorovinyl Ketones. Liebigs Annalen Der Chemie, 1983, 1983, 1807-1817.	0.8	5
207	The aryl group controls the Î±/Î³ regioselectivity in deuterations of 2-(p-substituted) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 42 20, 1097-1104.	0.5	2
208	Regioselective deuteration kinetics of 2,3,6-trimethyl-4-phenylpyrylium and 2,6-dimethyl-3,4-diphenylpyrylium salts (1). Journal of Labelled Compounds and Radiopharmaceuticals, 1983, 20, 1105-1112.	0.5	4
209	Electron impact mass spectra of 3,5,7-triaryl-and -trialkyl-4H-1,2-diazepines. Organic Mass Spectrometry, 1983, 18, 433-437.	1.3	2
210	Factors affecting the stability and equilibria of free radicals. Part 11. 1-Benzoyl-2,2-bis-(3,5-di-t-butylphenyl)hydrazyl and its temperature-dependent electron spin resonance spectrum. Journal of the Chemical Society Perkin Transactions II, 1983, , 591-594.	0.9	11
211	Topological indices for structure-activity correlations. , 1983, , 21-55.		256
212	Carbenium-carbonium structures, H2C+-CH4+, for the ethane dication. Journal of the American Chemical Society, 1982, 104, 3771-3773.	6.6	33
213	PREPARATION OF 2,3,4,6-TETRAMETHYLPYRYLIUM PERCHLORATE AND OF 2,3,4,6-TETRAMETHYLPYRIDINE. Organic Preparations and Procedures International, 1982, 14, 31-38.	0.6	11
214	Synthesis of new radical-cations with 2,2,6,6-tetramethylpiperidine-N-oxyl and pyridinium moieties. Canadian Journal of Chemistry, 1982, 60, 1512-1513.	0.6	10
215	Regioselective deuteriation kinetics of 2-, 4-, and 6-methyl groups in D2O solutions of pyrylium and N-methylpyridinium perchlorates possessing also 3-methyl or 3-phenyl groups. Journal of Labelled Compounds and Radiopharmaceuticals, 1982, 19, 783-794.	0.5	4
216	Highly discriminating distance-based topological index. Chemical Physics Letters, 1982, 89, 399-404.	1.2	935

#	Article	IF	Citations
217	Topological centric coding and nomenclature of polycyclic hydrocarbons. 1. Condensed benzenoid systems (polyhexes, fusenes). Journal of Chemical Information and Computer Sciences, 1981, 21, 223-229.	2.8	35
218	Preparation of selectively side-chain deuteriated pyridines via pyrylium salts. Journal of Labelled Compounds and Radiopharmaceuticals, 1981, 18, 1621-1632.	0.5	11
219	The graph center concept for polycyclic graphs. International Journal of Quantum Chemistry, 1981, 19, 61-82.	1.0	33
220	Molecular structure and tautomerism of the 1,3,2-benzodioxaarsole ether of tropolone. Tetrahedron, 1981, 37, 421-427.	1.0	5
221	¹Hâ€NMR Conformational Study of 2â€Acylâ€3,5â€dialkylfurans Using Lanthanide Shift Reagents. Israel Journal of Chemistry, 1980, 20, 168-172.	1.0	6
222	Graph theoretical characterization and computer generation of certain carcinogenic benzenoid hydrocarbons and identification of bay regions. Journal of Computational Chemistry, 1980, 1, 149-157.	1.5	79
223	Graph-theoretical analysis of the bonding topology in polyhedral organic cations. Tetrahedron, 1980, 36, 1851-1855.	1.0	11
224	Methyl chemical shifts in 1H-NMR spectra of 1-R-2,4,6-trimethylpyridinium salts as simple probes for the existence and magnitude of ring current in group R. Tetrahedron Letters, 1979, 20, 437-440.	0.7	12
225	Chemical graphs. Theoretica Chimica Acta, 1979, 53, 355-375.	0.9	167
226	Systematic classification and nomenclature of diamond hydrocarbonsâ€"I. Tetrahedron, 1978, 34, 3599-3609.	1.0	100
227	IMPROVED SYNTHESIS OF 2,6-DI-t-BUTYL-4-METHYLPYRYLIUM CHLOROSTANNATE AND PERCHLORATE AND OF 2,6-DI-t-BUTYL-4-METHYLPYRIDINE. Organic Preparations and Procedures International, 1977, 9, 125-130.	0.6	16
228	Steric origin of isotope effects in nuclear magnetic resonance shifts induced by lanthanide shift reagents; effect of deuteriation of methyl substituted pyridines. Journal of the Chemical Society Chemical Communications, 1976, , 984.	2.0	11
229	Molecular complexes with aromatic cations as electron-acceptorsâ€"III. Charge-transfer spectra of substituted pyrylium thiocyanates, selenocyanates and iodides. Spectrochimica Acta Part A: Molecular Spectroscopy, 1976, 32, 1311-1318.	0.1	6
230	N-arenesulphonyl-N-(2,2,6,6-tetramethylpiperidyl-1)-aminyls, hydrazyls with no nitrogen-bonded aromatic groups. Tetrahedron Letters, 1973, 14, 1879-1880.	0.7	9
231	Notizen: Push-Pull Nitrogen Free Radicals from Benzenesulphonanilides or Benzanilides with Donor para-Substituents. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1973, 28, 543-544.	0.3	11
232	Mass spectrometry in structural and stereochemical problemsâ€"CC A study of the fragmentation processes of some pyrilium salts. Organic Mass Spectrometry, 1971, 5, 87-93.	1.3	17
233	Heteroaromatic Boron Compounds. V. On the Synthesis of a Dithienoborepin.. Acta Chemica Scandinavica, 1969, 23, 2927-2930.	0.7	14
234	Seven-Membered Heterocyclic Rings. I. Formation of Substituted 4H-1,2-Diazepines from 2,4,6-Triarylpyrylium Salts and Hydrazine.. Acta Chemica Scandinavica, 1969, 23, 3125-3138.	0.7	35

#	Article	IF	Citations
235	Automerization of Naphthalene in the Presence of Aluminum Chloride. Journal of the American Chemical Society, 1967, 89, 1958-1960.	6.6	54
236	Steric hindrance revealed by absorption spectra of 2-acyl-3,5-dialkylfurans and of their polynitrophenylhydrazones. Spectrochimica Acta, 1963, 19, 367-378.	1.3	6
237	TRITIATION OF AROMATICS BY HTO-PROMOTED ALUMINUM CHLORIDE. Canadian Journal of Chemistry, 1963, 41, 2120-2121.	0.6	11
238	Ringverengung von Pyryliumsalzen zu Furanderivaten. Chemische Berichte, 1960, 93, 599-602.	0.2	40
239	Aluminiumchloridâ€Katalysen, XXVII Eine Synthese von Pyryliumsalzen aus SÃurechloriden und Olefinen. Justus Liebigs Annalen Der Chemie, 1959, 625, 74-88.	0.5	84
240	Correlations between Topological Ring-Currents, Ï€-Electron Partitions, and Six-Centre Delocalisation Indices in Benzenoid Hydrocarbons. Croatica Chemica Acta, 0, , 37-52.	0.1	5