Haruo Hosoya

List of Publications by Year
in descending order

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119 papers	3,912 citations	159585 30 h-index	128289 60 g-index
127 all docs	127 docs citations	127 times ranked	1108 citing authors

#	Article	IF	Citations
1	Topological Index. A Newly Proposed Quantity Characterizing the Topological Nature of Structural Isomers of Saturated Hydrocarbons. Bulletin of the Chemical Society of Japan, 1971, 44, 2332-2339.	3.2	1,082
2	On some counting polynomials in chemistry. Discrete Applied Mathematics, 1988, 19, 239-257.	0.9	301
3	Graphical enumeration of the coefficients of the secular polynomials of the Hï¿½ckel molecular orbitals. Theoretica Chimica Acta, 1972, 25, 215-222.	0.8	139
4	A topological index for the total?-electron energy. Theoretica Chimica Acta, 1975, 38, 37-47.	0.8	139
5	Sextet polynomial. A new enumeration and proof technique for the resonance theory applied to the aromatic hydrocarbons.. Tetrahedron Letters, 1975, 16, 4659-4662.	1.4	111
6	Graph-theoretical analysis of the clar's aromatic sextet. Tetrahedron, 1981, 37, 1113-1122.	1.9	89
7	Operator technique for obtaining the recursion formulas of characteristic and matching polynomials as applied to polyhex graphs. Journal of Computational Chemistry, 1983, 4, 585-593.	3.3	80
8	Topological Index and Thermodynamic Properties. I. Empirical Rules on the Boiling Point of Saturated Hydrocarbons. Bulletin of the Chemical Society of Japan, 1972, 45, 3415-3421.	3.2	74
9	Topological Index as a Sorting Device for Coding Chemical Structures. Journal of Chemical Documentation, 1972, 12, 181-183.	0.3	72
10	Matching and symmetry of graphs. Computers and Mathematics With Applications, 1986, 12, 271-290.	2.7	70
11	Ultraviolet absorption spectra of monomer and dimer of benzoic acid. Journal of Molecular Spectroscopy, 1962, 8, 257-275.	1.2	69
12	Topological index as applied to Ï€â€electronic systems. III. Mathematical relations among various bond orders. Journal of Chemical Physics, 1976, 64, 1065-1073.	3.0	67
13	Topological dependency of the aromatic sextets in polycyclic benzenoid hydrocarbons. Recursive relations of the sextet polynomial. Theoretica Chimica Acta, 1983, 64, 153-170.	0.8	65
14	King and domino polynomials for polyomino graphs. Journal of Mathematical Physics, 1977, 18, 1485-1490.	1.1	59
15	Parameterized valence bond calculations for benzenoid hydrocarbons using clar structure. Tetrahedron, 1984, 40, 3987-3995.	1.9	59
16	Ultra-violet absorption spectra of tropone, troponium ion, tropolone and 2,4,6-octatrienal. Tetrahedron, 1962, 18, 859-874.	1.9	53
17	Spherical Aromaticity of Buckminsterfullerene. Bulletin of the Chemical Society of Japan, 1988, 61, 2657-2659.	3.2	48
18	Ultraviolet Absorption Spectra of Aqueous Solutions and Single Crystals of Thioacetamide and Thiourea. Bulletin of the Chemical Society of Japan, 1960, 33, 850-860.	3.2	47

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19	Topological Index and Thermodynamic Properties. 5.â€How Can We Explain the Topological Dependency of Thermodynamic Properties of Alkanes with the Topology of Graphs?. Journal of Chemical Information and Computer Sciences, 1999, 39, 192-196.	2.8	46
20	Analysis of the topological dependency of the characteristic polynomial in its chebyshev expansion. Theoretica Chimica Acta, 1983, 63, 473-495.	0.8	45
21	Mo- and Vb-benzene characters. Tetrahedron, 1980, 36, 1317-1326.	1.9	44
22	An effective algorithm for obtaining polynomials for dimer statistics. Application of operator technique on the topological index to twoâ€•and threeâ€dimensional rectangular and torus lattices. Journal of Mathematical Physics, 1985, 26, 157-167.	1.1	41
23	Clar's aromatic sextet and sextet polynomial. Topics in Current Chemistry, 1990, , 255-272.	4.0	39
24	Topological Index as Applied to Ï€-Electronic Systems. II. Topological Bond Order. Bulletin of the Chemical Society of Japan, 1975, 48, 3512-3517.	3.2	38
25	Electronic structures of the Meisenheimer and Janovsky complexes. Theoretica Chimica Acta, 1968, 12, 117-126.	0.8	36
26	Aromatic character of graphite and carbon nanotubes. Synthetic Metals, 1994, 64, 309-313.	3.9	35
27	On the calculation of the acyclic polynomial. Theoretica Chimica Acta, 1978, 48, 279-286.	0.8	34
28	Ab initio MO study of electronic structures of closo-borane anions BnHn2- and closo-carboranes C2Bn-2Hn. The Journal of Physical Chemistry, 1992, 96, 6962-6969.	2.9	34
29	Analysis of the ?-electronic structure of infinitely large networks. I. Some remarks on the characteristic polynomial and density of states of large polycyclic aromatic hydrocarbons. Journal of Computational Chemistry, 1987, 8, 358-366.	3.3	32
30	Spectroscopic and Theoretical Studies of Charge-Transfer Type Molecular Complexes between MonoÃ¶lefins and Metal Ions: Selective Complex Formation Abilities of Copper(I), Silver(I) and Mercury(II) Ions. Bulletin of the Chemical Society of Japan, 1964, 37, 249-265.	3.2	30
31	Topological Index and Thermodynamic Properties. II. Analysis of the Topological Factors on the Absolute Entropy of Acyclic Saturated Hydrocarbons. Bulletin of the Chemical Society of Japan, 1980, 53, 1228-1237.	3.2	30
32	Topological Index and Thermodynamic Properties. III. Classification of Various Topological Aspects of Properties of Acyclic Saturated Hydrocarbons. Bulletin of the Chemical Society of Japan, 1985, 58, 1778-1786.	3.2	28
33	Topological Index and Thermodynamic Properties. IV. Size Dependency of the Structure-Activity Correlation of Alkanes. Bulletin of the Chemical Society of Japan, 1988, 61, 3093-3102.	3.2	28
34	Hierarchical Structure of the Atomic Orbital Wave Functions ofD-Dimensional Atom. Journal of Physical Chemistry A, 1997, 101, 418-421.	2.5	27
35	Aromaticity Index Can Predict and Explain the Stability of Polycyclic Conjugated Hydrocarbons. Monatshefte FÃ¼r Chemie, 2005, 136, 1037-1054.	1.8	25
36	The Basicities of Tropone and Tropolone. Bulletin of the Chemical Society of Japan, 1966, 39, 1414-1418.	3.2	24

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37	Exact dimer statistics and characteristic polynomials of cacti lattices. Theoretica Chimica Acta, 1989, 76, 315-329.	0.8	24
38	Aromaticity of Multiply Charged Fullerene Ions. Bulletin of the Chemical Society of Japan, 1993, 66, 1955-1958.	3.2	23
39	On the matching properties of three fence graphs. Journal of Mathematical Chemistry, 1993, 12, 211-218.	1.5	22
40	The Relation between the Eigenvalue Sum and the Topological IndexZRevisited. Bulletin of the Chemical Society of Japan, 2002, 75, 1723-1727.	3.2	22
41	Topological Index as Applied to Ï€-Electronic Systems. IV. On the Topological Factors Causing Non-Uniform Ï€-Electron Charge Distribution in Non-Alternant Hydrocarbons. Bulletin of the Chemical Society of Japan, 1976, 49, 1811-1816.	3.2	21
42	Development of Neural Network Simulator for Structureâ^'Activity Correlation of Molecules (NECO). Prediction of Endo/Exo Substitution of Norbornane Derivatives and of Carcinogenic Activity of PAHs from13C-NMR Shifts. Journal of Chemical Information and Computer Sciences, 1996, 36, 286-293.	2.8	21
43	ULTRAVIOLET, INFRARED, AND RAMAN SPECTRA OF PROTONATED CARBOXYLIC ACIDS. Canadian Journal of Chemistry, 1966, 44, 1961-1965.	1.1	20
44	Wheland Polynomial. I. Graph-theoretical Analysis of the Contribution of the Excited Resonance Structures to the Ground State of Acyclic Polyenes. Bulletin of the Chemical Society of Japan, 1979, 52, 1624-1633.	3.2	19
45	Analysis of the oxidation state and oxidation number by ab initio molecular orbital calculations: chlorine and sulfur compounds. Journal of the American Chemical Society, 1982, 104, 3998-4005.	13.7	19
46	Factorization and recursion relations of the matching and characteristic polynomials of periodic polymer networks. Journal of Mathematical Chemistry, 1991, 7, 289-305.	1.5	19
47	Cross-Conjugation at the Heart of Understanding the Electronic Theory of Organic Chemistry. Current Organic Chemistry, 2015, 19, 293-310.	1.6	19
48	On the construction of the matching polynomial for unbranched catacondensed benzenoids. Journal of Computational Chemistry, 1989, 10, 683-697.	3.3	17
49	Computational algorithms for matching polynomials of graphs from the characteristic polynomials of edge-weighted graphs. Journal of Computational Chemistry, 1989, 10, 698-710.	3.3	17
50	Mathematical foundation of the organic electron theory â€" how do Ï€-electrons flow in conjugated systems?. Computational and Theoretical Chemistry, 1999, 461-462, 473-482.	1.5	17
51	Kekulï¿½ structure counts: General formulations for primitive coronoid hydrocarbons. Monatshefte FÃ¼r Chemie, 1991, 122, 435-444.	1.8	15
52	From How to Why. Graph-Theoretical Verification of Quantum-Mechanical Aspects of Ï€-Electron Behaviors in Conjugated Systems. Bulletin of the Chemical Society of Japan, 2003, 76, 2233-2252.	3.2	15
53	The electronic structure and spectrum of tropone. Theoretica Chimica Acta, 1967, 8, 319-333.	0.8	13
54	Quantum chemical interpretation of oxidation number as applied to carbon and oxygen compounds. Numerical analysis of the electron distribution with ab initio molecular orbital wave functions. Journal of the American Chemical Society, 1984, 106, 2787-2792.	13.7	13

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55	Topological factors governing the HOMO-LUMO band gap of the density of states of periodic hydrocarbon polymer networks. Journal of Mathematical Chemistry, 1993, 12, 279-308.	1.5	13
56	Topological Twin Graphs. Smallest Pair of Isospectral Polyhedral Graphs with Eight Vertices. Journal of Chemical Information and Computer Sciences, 1994, 34, 428-431.	2.8	13
57	Efficient Way for Factorizing the Characteristic Polynomial of Highly Symmetrical Graphs Such as the Buckminsterfullerene. Fullerenes, Nanotubes, and Carbon Nanostructures, 1994, 2, 381-393.	0.6	13
58	On Construction of Clar Structures for Large Benzenoids. Polycyclic Aromatic Compounds, 1995, 4, 249-269.	2.6	13
59	Studies on Rydberg Orbitals. II. Calculation of the Rydberg Orbitals of Li(I)â€“F(I) and Their Isoelectronic Series. Journal of Chemical Physics, 1968, 48, 1380-1392.	3.0	12
60	Two Variants of the Topological Index and the Relations between Them. Bulletin of the Chemical Society of Japan, 1992, 65, 14-18.	3.2	12
61	An ab initio study of interactions of carbon monoxide and metal electrodes. Chemical Physics Letters, 1993, 209, 109-110.	2.6	12
62	Multilayered Cyclic Fence Graphs: Novel Cubic Graphs Related to the Graphite Network. Journal of Chemical Information and Computer Sciences, 1995, 35, 351-356.	2.8	12
63	Important Mathematical Structures of the Topological Index Z for Tree Graphs. Journal of Chemical Information and Modeling, 2007, 47, 744-750.	5.4	12
64	Proof of the generalized expressions for the number of perfect matchings of polycube graphs. Journal of Mathematical Chemistry, 1989, 3, 383-391.	1.5	11
65	An experience with super-linear speedup achieved by parallel computing on a workstation cluster: Parallel calculation of density of states of large scale cyclic polyacenes. Parallel Computing, 1995, 21, 1491-1504.	2.1	11
66	Spectroscopic and Theoretical Studies on the Protonation to Xanthone Derivatives. Bulletin of the Chemical Society of Japan, 1974, 47, 1596-1603.	3.2	9
67	Analysis of the Ï€-electronic structure of infinitely large networks. Computational and Theoretical Chemistry, 1989, 185, 123-137.	1.5	9
68	Analysis of the ?-electronic structure of infinitely large networks. Theoretica Chimica Acta, 1991, 81, 105-123.	0.8	9
69	Back-of-envelope derivation of the analytical formulas of the atomic wave functions of aD-dimensional atom. International Journal of Quantum Chemistry, 1997, 64, 35-42.	2.0	9
70	KekulÃ© structures of hexagonal chainsâ€”some unusual connections. Journal of Mathematical Chemistry, 2008, 44, 559-568.	1.5	9
71	Estimation of Elution Induce Time and 80% Elution Time of Polymer-Coated Manure by a Neural Network and Ck Interpolation Scheme. Development of a Neural Network Simulator for Structure-Activity Correlation of Molecules: Neco (5).. Journal of Chemical Software, 2001, 7, 115-128.	0.2	9
72	Abnormal Hyperchromism of the nâ†'Ï€*Absorption Band of Acetone in Protic Solvents. Bulletin of the Chemical Society of Japan, 1978, 51, 1708-1713.	3.2	8

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73	Graph generators. Journal of Computational Chemistry, 1987, 8, 522-535.	3.3	8
74	An ab initio study of adsorbed carbon monoxide on a metal electrode by cluster model. Applied Surface Science, 1994, 75, 121-124.	6.1	8
75	Mathematical and Chemical Analysis of Wiener's Polarity Number. , 2002, , 38-57.		8
76	Mathematical Features of the Genealogy of Acyclic Conjugated Polyenes. Bulletin of the Chemical Society of Japan, 2019, 92, 205-215.	3.2	8
77	Generalized expression for the numbers of perfect matching of cylindrical mÃ—n graphs. Journal of Mathematical Physics, 1991, 32, 1885-1889.	1.1	7
78	Topological Indices of Unbranched Catacondensed Benzenoid Hydrocarbons. Bulletin of the Chemical Society of Japan, 1992, 65, 2011-2015.	3.2	7
79	Number and shapes of the atomic orbitals of four and higher dimensional atoms. Journal of Molecular Structure, 1995, 352-353, 561-565.	3.6	7
80	The Electronic Structures of the Protonated Benzoic Acid and the Related Ions. Bulletin of the Chemical Society of Japan, 1964, 37, 1500-1505.	3.2	6
81	Pascalâ€™s triangle, nonâ€adjacent numbers, and D-dimensional atomic orbitals. Journal of Mathematical Chemistry, 1998, 23, 169-178.	1.5	6
82	Development of NEural network simulator for structure-activity COrrelation of molecules:Neco. (3). Performance Evaluation of Self-organized Network and Perceptron.. Journal of Chemical Software, 1998, 4, 19-32.	0.2	6
83	Studies on Rydberg orbitals. IV. Basic formulas for the one-electron perturbation calculation of molecular Rydberg excited states. International Journal of Quantum Chemistry, 1972, 6, 801-817.	2.0	5
84	SemiempiricalMO study on the abnormal bond orders of large networks of highly branched polyenes. International Journal of Quantum Chemistry, 1979, 15, 243-257.	2.0	5
85	Analysis of the Ï€-electronic structure of infinitely large networks. Computational and Theoretical Chemistry, 1990, 206, 153-172.	1.5	5
86	Revisiting superdelocalizability. Mathematical stability of reactivity indices. Theoretical Chemistry Accounts, 1999, 102, 293-299.	1.4	5
87	A Concealed Property of the Topological IndexZ. Bulletin of the Chemical Society of Japan, 2004, 77, 491-496.	3.2	5
88	How Can We Explain the Stability of Conjugated Hydrocarbon- and Heterosubstituted Networks by Topological Descriptors?. Current Computer-Aided Drug Design, 2010, 6, 225-234.	1.2	5
89	Mathematical and Chemical Analysis of Wiener's Polarity Number. , 2002, , 38-57.		4
90	Studies on Rydberg Orbitals. I. Slaterâ€"Condon Parameters and Valenceâ€State Energies for Rydberg Excitations Determined from Atomic Spectra of Beâ€"F. Journal of Chemical Physics, 1967, 47, 4190-4198.	3.0	3

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91	MATCHING AND SYMMETRY OF GRAPHS. , 1986, , 271-290.		3
92	Generalized expression of the perfect matching number for 2Ã—3Ã—n lattices. Journal of Mathematical Physics, 1993, 34, 1043-1051.	1.1	3
93	Graph-Theoretical Analysis of Tunneling Electron Transfer in Large Polycyclic Aromatic Hydrocarbon Networks. Journal of Chemical Information and Computer Sciences, 2001, 41, 512-516.	2.8	3
94	Distance Polynomial and the Related Counting Polynomials. Croatica Chemica Acta, 2013, 86, 443-451.	0.4	3
95	Genealogy of Conjugated Acyclic Polyenes. Molecules, 2017, 22, 896.	3.8	3
96	Development of a Neural Network Simulator for Structure-Activity Correlation of Molecules: Neco. (6). Estimation of Mechanical Properties of Cr-Mo Steel, Ni Steel, Ni-Cr Steel and Ni-Cr-Mo Steel.. Journal of Chemical Software, 2001, 7, 179-190.	0.2	3
97	Studies on Rydberg Orbitals. III. Calculation of the 4s, 4p, and 4dOrbitals of Carbon Atom. Bulletin of the Chemical Society of Japan, 1971, 44, 3464-3465.	3.2	2
98	Modified oxidation number as applied to carbon compounds: electron number analysis with ab initio molecular orbital wave functions. The Journal of Physical Chemistry, 1988, 92, 4869-4875.	2.9	2
99	An expression for the perfect matching number of cubic 2 ï¿½m ï¿½n lattices and their asymptotic values. Journal of Mathematical Chemistry, 1994, 16, 221-228.	1.5	2
100	Analysis of the Relationship among the Graphs Isomorphic to Multilayered Cyclic Fence Graphs (MLCFG). Journal of Chemical Information and Computer Sciences, 2002, 42, 1004-1010.	2.8	2
101	Spectroscopic Studies on the Protonation to Compounds Containing Groups. Nippon Kagaku Zassi, 1967, 88, 797-809.	0.2	1
102	Modified oxidation number as applied to organic compounds containing nitrogen atoms: electron number analysis with ab initio molecular orbital wave functions. The Journal of Physical Chemistry, 1990, 94, 2820-2828.	2.9	1
103	Expressions for the perfect matching numbers of cubicl x m x n lattices and their asymptotic values. Journal of Mathematical Chemistry, 1996, 20, 67-77.	1.5	1
104	A quarter century history of Quantum Chemistry Literature Database (QCLDB). Journal of Information Processing and Management, 2000, 43, 288-293.	0.0	1
105	A Hybrid Data Base: Quantum Chemistry Literature Data Base IIâ€"New Concept and New Methodologyâ€". Bulletin of the Chemical Society of Japan, 2010, 83, 660-666.	3.2	1
106	Reconstruction of Organic Electron Theory. II. Cross-Conjugation.. Journal of Computer Chemistry Japan, 2014, 13, 165-166.	0.1	1
107	Spherical Charge Analysis with Ab Initio Wave Functions: Modified Oxidation Number of Open Shell Molecule, CH2. Bulletin of the Chemical Society of Japan, 1995, 68, 1551-1557.	3.2	0
108	Some properties of the topological bond order. Chemical Physics Letters, 2005, 407, 73-77.	2.6	0

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109	Visualization of Four Dimensional Atomic Orbitals. Molecular Crystals and Liquid Crystals, 2005, 431, 345-350.	0.9	0
110	What a Mathematical Chemist is Thinking. Molecular Science, 2007, 1, A0013-A0013.	0.2	0
111	Analysis of the Genealogy of Conjugated Polyenes.. Journal of Computer Chemistry Japan, 2016, 14, 177-178.	0.1	0
112	The Bright Side of Mathematical Chemistry. Journal of Computer Chemistry Japan, 2017, 16, 47-51.	0.1	0
113	Development of a Computer-Aided-Education System of Polyhedra. Journal of Chemical Software, 2002, 8, 61-68.	0.2	0
114	Quantum Chemical Interpretation of Oxidation Number with Ab Initio Molecular Orbital Wavefunctions. , 1986, , 375-393.		0
115	Introduction to Graph Theory. , 1994, , 1-36.		0
116	Multi-Layered Cyclic Fence Graphs. Discovery of New Series of Graphs with Exceedingly High Symmetry. , 1996, , 195-200.		0
117	Development of Graphical Characteristics Data Base:GCDB. Graphical Characteristics of Multi-Layerd Cyclic Fence Graph.. Journal of Chemical Software, 1999, 5, 137-146.	0.2	0
118	Discovery of â€œdormantâ€•Generating Isospectral Pair of Tree Graphs (II). Journal of Computer Chemistry Japan, 2017, 16, 139-140.	0.1	0
119	Discovery of â€œDormantâ€•Generating Isospectral Pair of Tree Graphs. Journal of Computer Chemistry Japan, 2017, 16, 106-107.	0.1	0