Haruyuki Nakano

List of Publications by Year
in descending order

123 papers	4,320 citations	117453 34 h-index	118652 62 g-index
127 all docs	127 docs citations	127 times ranked	2909 citing authors

#	Article	IF	Citations
1	Copper(II) Complexes of 10,20-Diaryl-5,15-diazaporphyrin: Alternative Synthesis, Excited State Dynamics, and Substituent Effect on the 1O2-Generation Efficiency. Bulletin of the Chemical Society of Japan, 2022, 95, 427-432.	2.0	4
2	Computational Analysis of the SARS-CoV-2 RBDâ€“ACE2-Binding Process Based on MD and the 3D-RISM Theory. Journal of Chemical Information and Modeling, 2022, 62, 2889-2898.	2.5	4
3	9â€(Diphenylphosphoryl)â€10â€(phenylethynyl)anthracene Derivatives: Synthesis and Implications for the Substituent and Solvent Effects on the Lightâ€Emitting Properties. ChemPhotoChem, 2022, 6, .	1.5	3
4	Doubly Strapped Redox-Switchable 5,10,15,20-Tetraaryl-5,15-diazaporphyrinoids: Promising Platforms for the Evaluation of Paratropic and Diatropic Ring-Current Effects. Journal of Organic Chemistry, 2021, 86, 2283-2296.	1.7	12
5	A computational method to simulate global conformational changes of proteins induced by cosolvent. Journal of Computational Chemistry, 2021, 42, 552-563.	1.5	4
6	Relativistic two-electron repulsion operator formulas for the Douglasâ€“Kroll method. Chemical Physics Letters, 2021, 762, 138158.	1.2	5
7	Synthesis, Optical Properties, and Electrochemical Behavior of 5,10,15,20â€Tetraarylâ€5,15â€diazaporphyrinâ€Amine Hybrids. ChemPlusChem, 2021, 86, 1476-1486.	1.3	5
8	Recent Developments of Computational Methods for pKa Prediction Based on Electronic Structure Theory with Solvation Models. J, 2021, 4, 849-864.	0.6	7
9	Synthesis and optical, magnetic, and electrochemical properties of 5,10,15,20-tetraaryl-5,15-diazaporphyrin â€” tertiary amine conjugates. Journal of Porphyrins and Phthalocyanines, 2020, 24, 286-297.	0.4	5
10	Effect of Molecular Orientational Correlations on Solvation Free Energy Computed by Reference Interaction Site Model Theory. Journal of Chemical Information and Modeling, 2019, 59, 3770-3781.	2.5	24
11	Implementation of state-averaged MCSCF method to RISM- and 3D-RISM-SCF schemes. Chemical Physics Letters, 2019, 730, 179-185.	1.2	5
12	Three-Dimensional Reference Interaction Site Model Self-Consistent Field Study on the Coordination Structure and Excitation Spectra of Cu(II)â€“Water Complexes in Aqueous Solution. Journal of Physical Chemistry A, 2019, 123, 3344-3354.	1.1	6
13	Synthesis of Redoxâ€switchable 5,15â€Dialkylâ€10,20â€diarylâ€5,15â€diazaporphyrins and Diversification of their Nâ€Alkyl Groups. Asian Journal of Organic Chemistry, 2019, 8, 352-355.	1.3	17
14	Distinct ionic adsorption sites in defective Prussian blue: a 3D-RISM study. Physical Chemistry Chemical Physics, 2019, 21, 22569-22576.	1.3	6
15	Direct and Regioselective Amination of Î²â€Unsubstituted 5,15â€Diazaporphyrins with Amines: A Convenient Route to Nearâ€Infraredâ€Responsive Diazaporphyrin Sensitizers. Angewandte Chemie, 2018, 130, 3859-3862.	1.6	2
16	Direct and Regioselective Amination of Î²â€Unsubstituted 5,15â€Diazaporphyrins with Amines: A Convenient Route to Nearâ€Infraredâ€Responsive Diazaporphyrin Sensitizers. Angewandte Chemie - International Edition, 2018, 57, 3797-3800.	7.2	15
17	Redox switchable 19Ï€ and 18Ï€ 5,10,20-triaryl-5,15-diazaporphyrinoidâ€“nickel(II) complexes. Journal of Porphyrins and Phthalocyanines, 2018, 22, 542-551.	0.4	21
18	Synthesis and properties of redoxâ€switchable zinc complexes of 10,15,20â€triarylâ€15â€azaâ€5â€oxaporphyrin. Heteroatom Chemistry, 2018, 29, .	0.4	9

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19	Î²-Functionalization of 5,15-Diazaporphyrins with Phosphorus, Oxygen, and Sulfur-Containing Substituents. Bulletin of the Chemical Society of Japan, 2018, 91, 1264-1266.	2.0	10
20	A computational scheme of pK_a values based on the three-dimensional reference interaction site model self-consistent field theory coupled with the linear fitting correction scheme. Physical Chemistry Chemical Physics, 2018, 20, 27272-27279.	1.3	11
21	Nitrogenâ€Bridged Metallodiazaporphyrin Dimers: Synergistic Effects of Nitrogen Bridges and mesoâ€Nitrogen Atoms on Structure and Properties. Chemistry - an Asian Journal, 2017, 12, 816-821.	1.7	15
22	Unsymmetrically Substituted Donorâ€“Ïâ€“Acceptorâ€Type 5,15â€Diazaporphyrin Sensitizers: Synthesis, Optical and Photovoltaic Properties. ChemPlusChem, 2017, 82, 695-704.	1.3	8
23	Syntheses, Properties, and Catalytic Activities of Metal(II) Complexes and Free Bases of Redoxâ€Switchable 20Ï€, 19Ï€, and 18Ï€ 5,10,15,20â€Tetraarylâ€5,15â€diazaporphyrinoids. Chemistry - A European Journal, 2017, 23, 16364-16373.	3.7	38
24	Solvatochromism and preferential solvation of Brooker's merocyanine in waterâ€“methanol mixtures. Journal of Computational Chemistry, 2017, 38, 2411-2419.	1.5	12
25	Size-dependent adsorption sites in a Prussian blue nanoparticle: A 3D-RISM study. Chemical Physics Letters, 2017, 684, 117-125.	1.2	15
26	Redoxâ€Switchable 20Ï€â€, 19Ï€â€, and 18Ï€â€Electron 5,10,15,20â€Tetraarylâ€5,15â€diazaporphyrinoid Nickel(II) Complexes. Angewandte Chemie, 2016, 128, 2275-2278.	1.6	28
27	The ion dependence of carbohydrate binding of CBM36: an MD and 3D-RISM study. Journal of Physics Condensed Matter, 2016, 28, 344005.	0.7	10
28	Redoxâ€Switchable 20Ï€â€, 19Ï€â€, and 18Ï€â€Electron 5,10,15,20â€Tetraarylâ€5,15â€diazaporphyrinoid Nickel(II) Complexes. Angewandte Chemie - International Edition, 2016, 55, 2235-2238.	7.2	70
29	Theoretical analysis of complex formation of p-carboxybenzeneboronic acid with a monosaccharide. Journal of Molecular Liquids, 2016, 217, 93-98.	2.3	9
30	Three-dimensional reference interaction site model self-consistent field analysis of solvent and substituent effects on the absorption spectra of Brooker's merocyanine. Journal of Computational Chemistry, 2015, 36, 1655-1663.	1.5	7
31	Comparison of electronic effects of Î²-aryl substituents on optical and electrochemical properties of 5,15-diazaporphyrin Ï€-systems. Journal of Porphyrins and Phthalocyanines, 2015, 19, 775-785.	0.4	11
32	Synthesis and Photophysical Properties of Two Diazaporphyrinâ€“Porphyrin Hetero Dimers in Polar and Nonpolar Solutions. Journal of Physical Chemistry B, 2015, 119, 7328-7337.	1.2	13
33	9,9â€²-Anthryl-anthroxyl radicals: strategic stabilization of highly reactive phenoxyl radicals. Chemical Communications, 2015, 51, 6734-6737.	2.2	16
34	Theoretical analysis of co-solvent effect on the proton transfer reaction of glycine in a waterâ€“acetonitrile mixture. Journal of Chemical Physics, 2015, 142, 204103.	1.2	7
35	Optical, Electrochemical, and Magnetic Properties of Pyrroleâ€and Thiopheneâ€Bridged 5,15â€Diazaporphyrin Dimers. Chemistry - A European Journal, 2015, 21, 2003-2010.	1.7	18
36	N,S,Pâ€Hybrid Donorâ€“Ïâ€“Acceptor Organic Dyes for Dyeâ€Sensitized Solar Cell: Synthesis, Optical Properties, and Photovoltaic Performances. Heteroatom Chemistry, 2014, 25, 533-547.	0.4	21

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37	Synthesis and photoreactivity of Î±-diketone-type precursors of acenes and their use in organic-device fabrication. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2014, 18, 50-70.	5.6	62
38	Covalently Linked 5,15â€Diazaporphyrin Dimers: Promising Scaffolds for a Highly Conjugated Azaporphyrin Ï€ System. Chemistry - A European Journal, 2014, 20, 3342-3349.	1.7	27
39	Theoretical analysis of salt effect on intramolecular proton transfer reaction of glycine in aqueous NaCl solution. Journal of Molecular Liquids, 2014, 200, 32-37.	2.3	8
40	Solvent effect on excited states of merocyanines: A theoretical study using the RISMâ€“SCF method. Chemical Physics Letters, 2013, 583, 69-73.	1.2	7
41	Three-Dimensional Reference Interaction Site Model Self-Consistent Field Study of the Electronic Structure of [Cr(H₂O)₆]³⁺ in Aqueous Solution. Journal of Physical Chemistry A, 2013, 117, 8314-8322.	1.1	8
42	Solvent Effect on the Fluorescence Spectra of Coumarin 120 in Water: A Combined Quantum Mechanical and Molecular Mechanical Study. Journal of the Physical Society of Japan, 2012, 81, SA024.	0.7	1
43	Free Base and Metal Complexes of 5,15-Diaza-10,20-dimesitylporphyrins: Synthesis, Structures, Optical and Electrochemical Properties, and Aromaticities. Inorganic Chemistry, 2012, 51, 12879-12890.	1.9	63
44	Retroâ€Dielsâ€“Alder Approach to the Synthesis of Ï€â€Expanded Azuliporphyrins and Their Porphyrinoid Aromaticity. Chemistry - A European Journal, 2012, 18, 12854-12863.	1.7	21
45	Nickel(II) and Copper(II) Complexes of Î²â€Unsubstituted 5,15â€Diazaporphyrins and Pyridazineâ€Fused Diazacorrinoids: Metalâ€“Template Syntheses and Peripheral Functionalizations. Chemistry - A European Journal, 2012, 18, 6208-6216.	1.7	63
46	A combined quantum mechanical and molecular mechanical method using modified generalized hybrid orbitals: implementation for electronic excited states. Physical Chemistry Chemical Physics, 2011, 13, 11731.	1.3	10
47	Identification of geometrical isomers using vibrational circular dichroism spectroscopy: a series of mixed-ligand complexes of diamagnetic Co(<scp>iii</scp>) ions. Dalton Transactions, 2011, 40, 1332-1337.	1.6	25
48	Parallel Implementation of the Four-Component Relativistic Quasidegenerate Perturbation Theory with General Multiconfigurational Reference Functions. Journal of Chemical Theory and Computation, 2011, 7, 998-1005.	2.3	6
49	Solvent effect on the absorption spectra of coumarin 120 in water: A combined quantum mechanical and molecular mechanical study. Journal of Chemical Physics, 2011, 134, 014501.	1.2	18
50	Effect of removing the no-virtual pair approximation on the correlation energy of the He isoelectronic sequence. II. Point nuclear charge model. Journal of Chemical Physics, 2010, 132, 124105.	1.2	30
51	Low-Lying Excited States of C120 and C151: A Multireference Perturbation Theory Study. Journal of Physical Chemistry A, 2010, 114, 12363-12368.	1.1	11
52	Synthesis and Reactions of Phosphaporphyrins: Reconstruction of Ï€-Skeleton Triggered by Oxygenation of a Core Phosphorus Atom. Journal of Organic Chemistry, 2010, 75, 375-389.	1.7	45
53	Electronic structure of LaO based on frozen-core four-component relativistic multiconfigurational quasidegenerate perturbation theory. Journal of Chemical Physics, 2010, 132, 124310.	1.2	12
54	Valence-bond description of chemical reactions on Bornâ€“Oppenheimer molecular dynamics trajectories. Journal of Chemical Physics, 2009, 130, 154309.	1.2	1

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55	Molecular spinors suitable for fourâ€component relativistic correlation calculations: Studies of LaF⁺ and LaF using multiconfigurational quasiâ€degenerate perturbation theory. International Journal of Quantum Chemistry, 2009, 109, 1898-1904.	1.0	7
56	Lowâ€lying excited states of 7â€aminocoumarin derivatives: A theoretical study. International Journal of Quantum Chemistry, 2009, 109, 1940-1949.	1.0	13
57	Study on Chemical Reactivity Control of Liquid Sodium: Development of Nano-Fluid and Its Property and Applicability to FBR Plant. , 2008, , .		0
58	Redox-Coupled Complexation of 23-Phospha-21-thiaporphyrin with Group 10 Metals: A Convenient Access to Stable Core-Modified Isophlorinâ€'Metal Complexes. Journal of the American Chemical Society, 2008, 130, 16446-16447.	6.6	63
59	Monophosphaporphyrins:â€‰ Oxidative Ï€-Extension at the Peripherally Fused Carbocycle of the Phosphaporphyrin Ring. Organic Letters, 2008, 10, 553-556.	2.4	50
60	Electronic Structure of LaF+ and LaF from Frozen-Core Four-Component Relativistic Multiconfigurational Quasidegenerate Perturbation Theory. Journal of Physical Chemistry A, 2008, 112, 2683-2692.	1.1	9
61	Electronic structure of CeF from frozen-core four-component relativistic multiconfigurational quasidegenerate perturbation theory. Journal of Chemical Physics, 2008, 128, 214901.	1.2	11
62	Effect of removing the no-virtual-pair approximation on the correlation energy of the He isoelectronic sequence. Journal of Chemical Physics, 2007, 126, 174105.	1.2	28
63	Heavy mass effect on excited-state double-proton transfer in the 7-azaindole dimer by Cl substitution. Chemical Physics Letters, 2007, 441, 176-180.	1.2	3
64	Efficient implementation of relativistic and non-relativistic quasidegenerate perturbation theory with general multiconfigurational reference functions. Chemical Physics Letters, 2007, 442, 164-169.	1.2	52
65	Remarkable suppression of the excited-state double-proton transfer in the 7-azaindole dimer due to substitution of the dimethylamino group studied by electronic spectroscopy in the gas phase. Chemical Physics Letters, 2007, 443, 194-198.	1.2	9
66	Synthesis and Aggregation Behavior of mesoâ€Sulfinylporphyrins: Evaluation of Sâ€Chirality Effects on the Selfâ€Organization to Sâ€“Oxoâ€Tethered Cofacial Porphyrin Dimers. Chemistry - an Asian Journal, 2007, 2, 1417-1429.	1.7	24
67	Synthesis of a Phosphorus-Containing Hybrid Porphyrin. Organic Letters, 2006, 8, 5713-5716.	2.4	60
68	A model two-dimensional potential for internal rotation of 9-methylanthracene studied by electronic spectroscopy and DFT calculations. Chemical Physics, 2006, 328, 190-196.	0.9	9
69	Relativistic quasidegenerate perturbation theory with four-component general multiconfiguration reference functions. Journal of Chemical Physics, 2006, 124, 044101.	1.2	60
70	A study of the ground state of manganese dimer using quasidegenerate perturbation theory. Journal of Chemical Physics, 2006, 124, 124302.	1.2	48
71	Internal rotation of methyl group in 2- and 1-methylanthracene studied by electronic spectroscopy and DFT calculations. Chemical Physics, 2005, 316, 178-184.	0.9	12
72	Recent advances in ab initio, density functional theory, and relativistic electronic structure theory. , 2005, , 507-557.		14

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73	A Microscopic Model for Helical Twisting Power by the Optical Isomers of an Octahedral Metal Complex. Japanese Journal of Applied Physics, 2005, 44, 4067-4072.	0.8	8
74	The Ï€â†'Ï€* excited states of long linear polyenes studied by the CASCI-MRMP method. Chemical Physics Letters, 2004, 400, 425-429.	1.2	64
75	The Most Stable Structure of SiC3Studied by Multireference Perturbation Theory with General Multiconfiguration Self-Consistent Field Reference Functionsâ€. Journal of Physical Chemistry A, 2004, 108, 3064-3067.	1.1	10
76	Selective Catalytic Reduction of Nitric Oxide by Ammonia:Â The Activation Mechanism. Journal of Physical Chemistry B, 2004, 108, 12264-12266.	1.2	13
77	Diverse Structures and Remarkable Oxidizing Ability of Triarylbismuthane Oxides. Comparative Study on the Structure and Reactivity of a Series of Triarylpnictogen Oxides. Organometallics, 2004, 23, 5471-5480.	1.1	36
78	Maximum radius of convergence perturbation theory: test calculations on Be, Ne, H 2 and HF. Theoretical Chemistry Accounts, 2003, 110, 185-189.	0.5	3
79	A non-orthogonal Kohn-Sham method using partially fixed molecular orbitals. Theoretical Chemistry Accounts, 2003, 110, 328-337.	0.5	2
80	Multireference perturbation theory with optimized partitioning. II. Applications to molecular systems. Journal of Computational Chemistry, 2003, 24, 1390-1400.	1.5	26
81	Templating Effects on the Mineralization of Layered Inorganic Compounds:Â (1) Density Functional Calculations of the Formation of Single-Layered Magnesium Hydroxide as a Brucite Model. Langmuir, 2003, 19, 7120-7126.	1.6	37
82	UTChem â€" A Program for ab initio Quantum Chemistry. Lecture Notes in Computer Science, 2003, , 84-95.	1.0	26
83	Multireference perturbation theory with optimized partitioning. I. Theoretical and computational aspects. Journal of Chemical Physics, 2003, 118, 8197-8206.	1.2	39
84	Recent Advances in Multireference-Based Perturbation Theory. Bulletin of the Korean Chemical Society, 2003, 24, 812-816.	1.0	4
85	RECENT ADVANCES IN ELECTRONIC STRUCTURE THEORY. Journal of Theoretical and Computational Chemistry, 2002, 01, 109-136.	1.8	8
86	Complete active space valence bond (CASVB) method and its application to chemical reactions. Theoretical and Computational Chemistry, 2002, , 55-77.	0.2	6
87	Quasi-degenerate perturbation theory withgeneral multiconfiguration self-consistent field reference functions. Journal of Computational Chemistry, 2002, 23, 1166-1175.	1.5	106
88	Synthesis, Structure, and Reactions of (Acylimino)triaryl-Î»5-bismuthanes:Â First Comparative Study of the (Acylimino)pnictorane Series. Journal of the American Chemical Society, 2001, 123, 10954-10965.	6.6	28
89	Multireference MÃ¸llerâ€“Plesset perturbation theory using spin-dependent orbital energies. Chemical Physics Letters, 2001, 336, 529-535.	1.2	11
90	Stability of multiply charged anions of lanthanide hexafluorides LnF62â^' and LnF63â^' (Ln=Ce to Lu). Computational and Theoretical Chemistry, 2001, 537, 107-115.	1.5	12

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91	Research activities of the theoretical chemistry group at the University of Tokyo. Computational and Theoretical Chemistry, 2001, 573, 91-128.	1.5	13
92	Second-order quasi-degenerate perturbation theory with quasi-complete active space self-consistent field reference functions. Journal of Chemical Physics, 2001, 114, 1133-1141.	1.2	54
93	New algorithm for electron repulsion integrals oriented to the general contraction scheme. International Journal of Quantum Chemistry, 2000, 76, 396-406.	1.0	24
94	A quasi-complete active space self-consistent field method. Chemical Physics Letters, 2000, 317, 90-96.	1.2	55
95	On the performance of diagrammatic complete active space perturbation theory. Journal of Chemical Physics, 2000, 113, 7773-7778.	1.2	6
96	New algorithm for electron repulsion integrals oriented to the general contraction scheme. , 2000, 76, 396.		1
97	New algorithm for electron repulsion integrals oriented to the general contraction scheme. , 2000, 76, 396.		1
98	New algorithm for electron repulsion integrals oriented to the general contraction scheme. International Journal of Quantum Chemistry, 2000, 76, 396.	1.0	1
99	ANALYTIC ENERGY GRADIENTS FOR SECOND-ORDER MULTIREFERENCE PERTURBATION THEORY. Recent Advances in Computational, 1999, , 131-160.	0.8	7
100	Fluorescence and photoinversion reactions in solutions of chiral diaryl sulfoxides with various sizes of aromatic rings. Journal of Photochemistry and Photobiology A: Chemistry, 1999, 122, 161-168.	2.0	11
101	Theoretical study of electronic and geometric structures of a series of lanthanide trihalides LnX3 (Ln=Laâ€“Lu; X=Cl, F). Computational and Theoretical Chemistry, 1999, 461-462, 203-222.	1.5	54
102	Theoretical study of the valence Ï€ â†' Ï€ * excited states of polyacenes: anthracene and naphthacene. Theoretical Chemistry Accounts, 1999, 102, 49-64.	0.5	81
103	Complete active space valence bond method applied to chemical reactions. Computational and Theoretical Chemistry, 1999, 461-462, 55-69.	1.5	6
104	A study of FeCO+ with correlated wavefunctions. Physical Chemistry Chemical Physics, 1999, 1, 967-975.	1.3	31
105	Theoretical Study of the Q and B Bands of Free-Base, Magnesium, and Zinc Porphyrins, and Their Derivatives. Journal of Physical Chemistry A, 1999, 103, 1894-1904.	1.1	157
106	Theoretical study of the electronic ground state of iron(II) porphine. Chemical Physics Letters, 1998, 295, 380-388.	1.2	39
107	Theoretical study of valence and Rydberg excited states of benzene revisited. Computational and Theoretical Chemistry, 1998, 451, 25-33.	1.5	45
108	Theoretical study of the ???* excited states of linear polyenes: The energy gap between 11Bu+ and 21Ag? states and their character. International Journal of Quantum Chemistry, 1998, 66, 157-175.	1.0	146

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109	Analytic energy gradients for multiconfigurational self-consistent field second-order quasidegenerate perturbation theory (MC-QDPT). Journal of Chemical Physics, 1998, 108, 5660-5669.	1.2	51
110	Theoretical study of the Ï€â†'Ï€* excited states of linear polyenes: The energy gap between 11Bu+ and 21Agâ^' states and their character. , 1998, 66, 157.		6
111	Transition state barrier height for the reaction H2COâ†'H2+CO studied by multireference Mo/llerâ€"Plesset perturbation theory. Journal of Chemical Physics, 1997, 106, 4912-4917.	1.2	77
112	A complete active space valence bond method with nonorthogonal orbitals. Journal of Chemical Physics, 1997, 107, 9966-9974.	1.2	36
113	Ring Opening of Silacyclobutane. Journal of the American Chemical Society, 1997, 119, 11966-11973.	6.6	26
114	Theoretical study of the Ï€ â†' Ï€â^— excited states of linear polyene radical cations and dications. Chemical Physics Letters, 1997, 267, 82-90.	1.2	43
115	Theoretical study of the valence Ï€â†'Ï€* excited states of polyacenes: Benzene and naphthalene. Journal of Chemical Physics, 1996, 104, 6244-6258.	1.2	133
116	A complete active space valence bond (CASVB) method. Journal of Chemical Physics, 1996, 105, 9227-9239.	1.2	87
117	Theoretical study of the excitation spectra of fiveâ€membered ring compounds: Cyclopentadiene, furan, and pyrrole. Journal of Chemical Physics, 1996, 104, 2312-2320.	1.2	80
118	Multireference MÃ¸ller-Plesset perturbation treatment for valence and Rydberg excited states of benzene. Chemical Physics Letters, 1995, 235, 430-435.	1.2	25
119	Study of lowâ€lying electronic states of ozone by multireference Mo/llerâ€"Plesset perturbation method. Journal of Chemical Physics, 1995, 103, 6520-6528.	1.2	78
120	MCSCF reference quasidegenerate perturbation theory with Epsteinâ€"Nesbet partitioning. Chemical Physics Letters, 1993, 207, 372-378.	1.2	265
121	Convergence property of multireference many-body perturbation theory analyzed by the use of a norm of effective Hamiltonian. Theoretica Chimica Acta, 1993, 86, 369-377.	0.9	2
122	Quasidegenerate perturbation theory with multiconfigurational selfâ€consistentâ€field reference functions. Journal of Chemical Physics, 1993, 99, 7983-7992.	1.2	871
123	Efficient and stable method of searching for optimum structures of molecules containing cyclic parts. Chemical Physics Letters, 1991, 177, 458-462.	1.2	6