

Haruyuki Nakano

List of Publications by Year in descending order

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123
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117453

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127
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127
times ranked

2909
citing authors

#	ARTICLE	IF	CITATIONS
1	Quasidegenerate perturbation theory with multiconfigurational self-consistent field reference functions. <i>Journal of Chemical Physics</i> , 1993, 99, 7983-7992.	1.2	871
2	MCSCF reference quasidegenerate perturbation theory with Epstein-Nesbet partitioning. <i>Chemical Physics Letters</i> , 1993, 207, 372-378.	1.2	265
3	Theoretical Study of the Q and B Bands of Free-Base, Magnesium, and Zinc Porphyrins, and Their Derivatives. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1894-1904.	1.1	157
4	Theoretical study of the π^* excited states of linear polyenes: The energy gap between $11B_u^+$ and $21A_g^?$ states and their character. <i>International Journal of Quantum Chemistry</i> , 1998, 66, 157-175.	1.0	146
5	Theoretical study of the valence π^* excited states of polyacenes: Benzene and naphthalene. <i>Journal of Chemical Physics</i> , 1996, 104, 6244-6258.	1.2	133
6	Quasi-degenerate perturbation theory with general multiconfiguration self-consistent field reference functions. <i>Journal of Computational Chemistry</i> , 2002, 23, 1166-1175.	1.5	106
7	A complete active space valence bond (CASVB) method. <i>Journal of Chemical Physics</i> , 1996, 105, 9227-9239.	1.2	87
8	Theoretical study of the valence π^* excited states of polyacenes: anthracene and naphthalene. <i>Theoretical Chemistry Accounts</i> , 1999, 102, 49-64.	0.5	81
9	Theoretical study of the excitation spectra of five-membered ring compounds: Cyclopentadiene, furan, and pyrrole. <i>Journal of Chemical Physics</i> , 1996, 104, 2312-2320.	1.2	80
10	Study of low-lying electronic states of ozone by multireference Møller-Plesset perturbation method. <i>Journal of Chemical Physics</i> , 1995, 103, 6520-6528.	1.2	78
11	Transition state barrier height for the reaction $H_2CO + H_2 \rightarrow CO + H_2$ studied by multireference Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 1997, 106, 4912-4917.	1.2	77
12	Redox-Switchable 20-, 19-, and 18-Electron 5,10,15,20-Tetraaryl-5,15-diazaporphyrinoid Nickel(II) Complexes. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2235-2238.	7.2	70
13	The π^* excited states of long linear polyenes studied by the CASCI-MRMP method. <i>Chemical Physics Letters</i> , 2004, 400, 425-429.	1.2	64
14	Redox-Coupled Complexation of 23-Phospho-21-thiaporphyrin with Group 10 Metals: A Convenient Access to Stable Core-Modified Isophlorin α -Metal Complexes. <i>Journal of the American Chemical Society</i> , 2008, 130, 16446-16447.	6.6	63
15	Free Base and Metal Complexes of 5,15-Diaza-10,20-dimesitylporphyrins: Synthesis, Structures, Optical and Electrochemical Properties, and Aromaticities. <i>Inorganic Chemistry</i> , 2012, 51, 12879-12890.	1.9	63
16	Nickel(II) and Copper(II) Complexes of Unsubstituted 5,15-Diazaporphyrins and Pyridazine-Fused Diazacorrinoids: Metal-Template Syntheses and Peripheral Functionalizations. <i>Chemistry - A European Journal</i> , 2012, 18, 6208-6216.	1.7	63
17	Synthesis and photoreactivity of β -diketone-type precursors of acenes and their use in organic-device fabrication. <i>Journal of Photochemistry and Photobiology C: Photochemistry Reviews</i> , 2014, 18, 50-70.	5.6	62
18	Synthesis of a Phosphorus-Containing Hybrid Porphyrin. <i>Organic Letters</i> , 2006, 8, 5713-5716.	2.4	60

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19	Relativistic quasidegenerate perturbation theory with four-component general multiconfiguration reference functions. <i>Journal of Chemical Physics</i> , 2006, 124, 044101.	1.2	60
20	A quasi-complete active space self-consistent field method. <i>Chemical Physics Letters</i> , 2000, 317, 90-96.	1.2	55
21	Theoretical study of electronic and geometric structures of a series of lanthanide trihalides LnX ₃ (Ln=La–Lu; X=Cl, F). <i>Computational and Theoretical Chemistry</i> , 1999, 461-462, 203-222.	1.5	54
22	Second-order quasi-degenerate perturbation theory with quasi-complete active space self-consistent field reference functions. <i>Journal of Chemical Physics</i> , 2001, 114, 1133-1141.	1.2	54
23	Efficient implementation of relativistic and non-relativistic quasidegenerate perturbation theory with general multiconfigurational reference functions. <i>Chemical Physics Letters</i> , 2007, 442, 164-169.	1.2	52
24	Analytic energy gradients for multiconfigurational self-consistent field second-order quasidegenerate perturbation theory (MC-QDPT). <i>Journal of Chemical Physics</i> , 1998, 108, 5660-5669.	1.2	51
25	Monophosphaporphyrins: Oxidative π -Extension at the Peripherally Fused Carbocycle of the Phosphaporphyrin Ring. <i>Organic Letters</i> , 2008, 10, 553-556.	2.4	50
26	A study of the ground state of manganese dimer using quasidegenerate perturbation theory. <i>Journal of Chemical Physics</i> , 2006, 124, 124302.	1.2	48
27	Theoretical study of valence and Rydberg excited states of benzene revisited. <i>Computational and Theoretical Chemistry</i> , 1998, 451, 25-33.	1.5	45
28	Synthesis and Reactions of Phosphaporphyrins: Reconstruction of π -Skeleton Triggered by Oxygenation of a Core Phosphorus Atom. <i>Journal of Organic Chemistry</i> , 2010, 75, 375-389.	1.7	45
29	Theoretical study of the $\pi^* \pi^*$ excited states of linear polyene radical cations and dications. <i>Chemical Physics Letters</i> , 1997, 267, 82-90.	1.2	43
30	Theoretical study of the electronic ground state of iron(II) porphine. <i>Chemical Physics Letters</i> , 1998, 295, 380-388.	1.2	39
31	Multireference perturbation theory with optimized partitioning. I. Theoretical and computational aspects. <i>Journal of Chemical Physics</i> , 2003, 118, 8197-8206.	1.2	39
32	Syntheses, Properties, and Catalytic Activities of Metal(II) Complexes and Free Bases of Redox-Switchable 20 π , 19 π , and 18 π 5,10,15,20-tetraaryl-, 5,15-diazaporphyrinoids. <i>Chemistry - A European Journal</i> , 2017, 23, 16364-16373.		38
33	Templating Effects on the Mineralization of Layered Inorganic Compounds: (1) Density Functional Calculations of the Formation of Single-Layered Magnesium Hydroxide as a Brucite Model. <i>Langmuir</i> , 2003, 19, 7120-7126.	1.6	37
34	A complete active space valence bond method with nonorthogonal orbitals. <i>Journal of Chemical Physics</i> , 1997, 107, 9966-9974.	1.2	36
35	Diverse Structures and Remarkable Oxidizing Ability of Triarylbiuthane Oxides. Comparative Study on the Structure and Reactivity of a Series of Triarylpnictogen Oxides. <i>Organometallics</i> , 2004, 23, 5471-5480.	1.1	36
36	A study of FeCO ⁺ with correlated wavefunctions. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 967-975.	1.3	31

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37	Effect of removing the no-virtual pair approximation on the correlation energy of the He isoelectronic sequence. II. Point nuclear charge model. <i>Journal of Chemical Physics</i> , 2010, 132, 124105.	1.2	30
38	Synthesis, Structure, and Reactions of (Acylimino)triaryl-5-bismuthanes: A First Comparative Study of the (Acylimino)pnictorane Series. <i>Journal of the American Chemical Society</i> , 2001, 123, 10954-10965.	6.6	28
39	Effect of removing the no-virtual-pair approximation on the correlation energy of the He isoelectronic sequence. <i>Journal of Chemical Physics</i> , 2007, 126, 174105.	1.2	28
40	Redox-switchable 20 ⁺ , 19 ⁺ , and 18 ⁺ Electron 5,10,15,20-tetraaryl-5,15-diazaporphyrinoid Nickel(II) Complexes. <i>Angewandte Chemie</i> , 2016, 128, 2275-2278.	1.6	28
41	Covalently Linked 5,15-Diazaporphyrin Dimers: Promising Scaffolds for a Highly Conjugated Azaporphyrin π System. <i>Chemistry - A European Journal</i> , 2014, 20, 3342-3349.	1.7	27
42	Ring Opening of Silacyclobutane. <i>Journal of the American Chemical Society</i> , 1997, 119, 11966-11973.	6.6	26
43	Multireference perturbation theory with optimized partitioning. II. Applications to molecular systems. <i>Journal of Computational Chemistry</i> , 2003, 24, 1390-1400.	1.5	26
44	UTChem – A Program for ab initio Quantum Chemistry. <i>Lecture Notes in Computer Science</i> , 2003, , 84-95.	1.0	26
45	Multireference MÅller-Plesset perturbation treatment for valence and Rydberg excited states of benzene. <i>Chemical Physics Letters</i> , 1995, 235, 430-435.	1.2	25
46	Identification of geometrical isomers using vibrational circular dichroism spectroscopy: a series of mixed-ligand complexes of diamagnetic Co(III) ions. <i>Dalton Transactions</i> , 2011, 40, 1332-1337.	1.6	25
47	New algorithm for electron repulsion integrals oriented to the general contraction scheme. <i>International Journal of Quantum Chemistry</i> , 2000, 76, 396-406.	1.0	24
48	Synthesis and Aggregation Behavior of <i>meso</i> -Sulfinylporphyrins: Evaluation of Chirality Effects on the Self-Organization to Oxo-tethered Cofacial Porphyrin Dimers. <i>Chemistry - an Asian Journal</i> , 2007, 2, 1417-1429.	1.7	24
49	Effect of Molecular Orientational Correlations on Solvation Free Energy Computed by Reference Interaction Site Model Theory. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3770-3781.	2.5	24
50	Retro-Diels-Alder Approach to the Synthesis of Expanded Azuliporphyrins and Their Porphyrinoid Aromaticity. <i>Chemistry - A European Journal</i> , 2012, 18, 12854-12863.	1.7	21
51	N,S-Hybrid Donor-Acceptor Organic Dyes for Dye-Sensitized Solar Cell: Synthesis, Optical Properties, and Photovoltaic Performances. <i>Heteroatom Chemistry</i> , 2014, 25, 533-547.	0.4	21
52	Redox switchable 19 ⁺ and 18 ⁺ 5,10,20-triaryl-5,15-diazaporphyrinoid nickel(II) complexes. <i>Journal of Porphyrins and Phthalocyanines</i> , 2018, 22, 542-551.	0.4	21
53	Solvent effect on the absorption spectra of coumarin 120 in water: A combined quantum mechanical and molecular mechanical study. <i>Journal of Chemical Physics</i> , 2011, 134, 014501.	1.2	18
54	Optical, Electrochemical, and Magnetic Properties of Pyrrole- and Thiophene-Bridged 5,15-Diazaporphyrin Dimers. <i>Chemistry - A European Journal</i> , 2015, 21, 2003-2010.	1.7	18

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55	Synthesis of Redox-switchable 5,15-Dialkyl-10,20-diaryl-5,15-diazaporphyrins and Diversification of their Alkyl Groups. <i>Asian Journal of Organic Chemistry</i> , 2019, 8, 352-355.	1.3	17
56	9,9- ² -Anthryl-anthroxyl radicals: strategic stabilization of highly reactive phenoxyl radicals. <i>Chemical Communications</i> , 2015, 51, 6734-6737.	2.2	16
57	Nitrogen-Bridged Metallodiazaporphyrin Dimers: Synergistic Effects of Nitrogen Bridges and meso-Nitrogen Atoms on Structure and Properties. <i>Chemistry - an Asian Journal</i> , 2017, 12, 816-821.	1.7	15
58	Size-dependent adsorption sites in a Prussian blue nanoparticle: A 3D-RISM study. <i>Chemical Physics Letters</i> , 2017, 684, 117-125.	1.2	15
59	Direct and Regioselective Amination of Unsubstituted 5,15-Diazaporphyrins with Amines: A Convenient Route to Near-Infrared-Responsive Diazaporphyrin Sensitizers. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3797-3800.	7.2	15
60	Recent advances in ab initio, density functional theory, and relativistic electronic structure theory. , 2005, , 507-557.		14
61	Research activities of the theoretical chemistry group at the University of Tokyo. <i>Computational and Theoretical Chemistry</i> , 2001, 573, 91-128.	1.5	13
62	Selective Catalytic Reduction of Nitric Oxide by Ammonia: The Activation Mechanism. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12264-12266.	1.2	13
63	Low-lying excited states of 7-aminocoumarin derivatives: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1940-1949.	1.0	13
64	Synthesis and Photophysical Properties of Two Diazaporphyrin-Porphyrin Hetero Dimers in Polar and Nonpolar Solutions. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7328-7337.	1.2	13
65	Stability of multiply charged anions of lanthanide hexafluorides LnF ₆ ²⁻ and LnF ₆ ³⁻ (Ln=Ce to Lu). <i>Computational and Theoretical Chemistry</i> , 2001, 537, 107-115.	1.5	12
66	Internal rotation of methyl group in 2- and 1-methylanthracene studied by electronic spectroscopy and DFT calculations. <i>Chemical Physics</i> , 2005, 316, 178-184.	0.9	12
67	Electronic structure of LaO based on frozen-core four-component relativistic multiconfigurational quasidegenerate perturbation theory. <i>Journal of Chemical Physics</i> , 2010, 132, 124310.	1.2	12
68	Solvatochromism and preferential solvation of Brooker's merocyanine in water-methanol mixtures. <i>Journal of Computational Chemistry</i> , 2017, 38, 2411-2419.	1.5	12
69	Doubly Strapped Redox-Switchable 5,10,15,20-Tetraaryl-5,15-diazaporphyrinoids: Promising Platforms for the Evaluation of Paratropic and Diatropic Ring-Current Effects. <i>Journal of Organic Chemistry</i> , 2021, 86, 2283-2296.	1.7	12
70	Fluorescence and photoinversion reactions in solutions of chiral diaryl sulfoxides with various sizes of aromatic rings. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 1999, 122, 161-168.	2.0	11
71	Multireference Møller-Plesset perturbation theory using spin-dependent orbital energies. <i>Chemical Physics Letters</i> , 2001, 336, 529-535.	1.2	11
72	Electronic structure of CeF from frozen-core four-component relativistic multiconfigurational quasidegenerate perturbation theory. <i>Journal of Chemical Physics</i> , 2008, 128, 214901.	1.2	11

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73	Low-Lying Excited States of C120 and C151: A Multireference Perturbation Theory Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12363-12368.	1.1	11
74	Comparison of electronic effects of \hat{I}^2 -aryl substituents on optical and electrochemical properties of 5,15-diazaporphyrin I^{\ominus} -systems. <i>Journal of Porphyrins and Phthalocyanines</i> , 2015, 19, 775-785.	0.4	11
75	A computational scheme of p_{K_a} values based on the three-dimensional reference interaction site model self-consistent field theory coupled with the linear fitting correction scheme. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27272-27279.	1.3	11
76	The Most Stable Structure of SiC ₃ Studied by Multireference Perturbation Theory with General Multiconfiguration Self-Consistent Field Reference Functions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3064-3067.	1.1	10
77	A combined quantum mechanical and molecular mechanical method using modified generalized hybrid orbitals: implementation for electronic excited states. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11731.	1.3	10
78	The ion dependence of carbohydrate binding of CBM36: an MD and 3D-RISM study. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 344005.	0.7	10
79	\hat{I}^2 -Functionalization of 5,15-Diazaporphyrins with Phosphorus, Oxygen, and Sulfur-Containing Substituents. <i>Bulletin of the Chemical Society of Japan</i> , 2018, 91, 1264-1266.	2.0	10
80	A model two-dimensional potential for internal rotation of 9-methylantracene studied by electronic spectroscopy and DFT calculations. <i>Chemical Physics</i> , 2006, 328, 190-196.	0.9	9
81	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. <i>Chemical Physics Letters</i> , 2007, 443, 194-198.	1.2	9
82	Electronic Structure of LaF ⁺ and LaF from Frozen-Core Four-Component Relativistic Multiconfigurational Quasidegenerate Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2683-2692.	1.1	9
83	Theoretical analysis of complex formation of p-carboxybenzeneboronic acid with a monosaccharide. <i>Journal of Molecular Liquids</i> , 2016, 217, 93-98.	2.3	9
84	Synthesis and properties of redox-switchable zinc complexes of 10,15,20-triaryl-5-oxaporphyrin. <i>Heteroatom Chemistry</i> , 2018, 29, .	0.4	9
85	RECENT ADVANCES IN ELECTRONIC STRUCTURE THEORY. <i>Journal of Theoretical and Computational Chemistry</i> , 2002, 01, 109-136.	1.8	8
86	A Microscopic Model for Helical Twisting Power by the Optical Isomers of an Octahedral Metal Complex. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 4067-4072.	0.8	8
87	Three-Dimensional Reference Interaction Site Model Self-Consistent Field Study of the Electronic Structure of [Cr(H ₂ O) ₆] ³⁺ in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8314-8322.	1.1	8
88	Theoretical analysis of salt effect on intramolecular proton transfer reaction of glycine in aqueous NaCl solution. <i>Journal of Molecular Liquids</i> , 2014, 200, 32-37.	2.3	8
89	Unsymmetrically Substituted Donor-Acceptor Type 5,15-Diazaporphyrin Sensitizers: Synthesis, Optical and Photovoltaic Properties. <i>ChemPlusChem</i> , 2017, 82, 695-704.	1.3	8
90	ANALYTIC ENERGY GRADIENTS FOR SECOND-ORDER MULTIREFERENCE PERTURBATION THEORY. <i>Recent Advances in Computational</i> , 1999, , 131-160.	0.8	7

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91	Molecular spinors suitable for four-component relativistic correlation calculations: Studies of LaF ⁺ and LaF using multiconfigurational quasi-degenerate perturbation theory. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1898-1904.	1.0	7
92	Solvent effect on excited states of merocyanines: A theoretical study using the RISM-SCF method. <i>Chemical Physics Letters</i> , 2013, 583, 69-73.	1.2	7
93	Three-dimensional reference interaction site model self-consistent field analysis of solvent and substituent effects on the absorption spectra of Brooker's merocyanine. <i>Journal of Computational Chemistry</i> , 2015, 36, 1655-1663.	1.5	7
94	Theoretical analysis of co-solvent effect on the proton transfer reaction of glycine in a water-acetonitrile mixture. <i>Journal of Chemical Physics</i> , 2015, 142, 204103.	1.2	7
95	Recent Developments of Computational Methods for pKa Prediction Based on Electronic Structure Theory with Solvation Models. <i>J.</i> , 2021, 4, 849-864.	0.6	7
96	Efficient and stable method of searching for optimum structures of molecules containing cyclic parts. <i>Chemical Physics Letters</i> , 1991, 177, 458-462.	1.2	6
97	Complete active space valence bond method applied to chemical reactions. <i>Computational and Theoretical Chemistry</i> , 1999, 461-462, 55-69.	1.5	6
98	On the performance of diagrammatic complete active space perturbation theory. <i>Journal of Chemical Physics</i> , 2000, 113, 7773-7778.	1.2	6
99	Complete active space valence bond (CASVB) method and its application to chemical reactions. <i>Theoretical and Computational Chemistry</i> , 2002, , 55-77.	0.2	6
100	Parallel Implementation of the Four-Component Relativistic Quasidegenerate Perturbation Theory with General Multiconfigurational Reference Functions. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 998-1005.	2.3	6
101	Three-Dimensional Reference Interaction Site Model Self-Consistent Field Study on the Coordination Structure and Excitation Spectra of Cu(II)-Water Complexes in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3344-3354.	1.1	6
102	Distinct ionic adsorption sites in defective Prussian blue: a 3D-RISM study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22569-22576.	1.3	6
103	Theoretical study of the $\tilde{\epsilon}^*$ excited states of linear polyenes: The energy gap between $11B_u^+$ and $21A_g^+$ states and their character. , 1998, 66, 157.		6
104	Implementation of state-averaged MCSCF method to RISM- and 3D-RISM-SCF schemes. <i>Chemical Physics Letters</i> , 2019, 730, 179-185.	1.2	5
105	Synthesis and optical, magnetic, and electrochemical properties of 5,10,15,20-tetraaryl-5,15-diazaporphyrin tertiary amine conjugates. <i>Journal of Porphyrins and Phthalocyanines</i> , 2020, 24, 286-297.	0.4	5
106	Relativistic two-electron repulsion operator formulas for the Douglas-Kroll method. <i>Chemical Physics Letters</i> , 2021, 762, 138158.	1.2	5
107	Synthesis, Optical Properties, and Electrochemical Behavior of 5,10,15,20-Tetraaryl-5,15-diazaporphyrin-Amine Hybrids. <i>ChemPlusChem</i> , 2021, 86, 1476-1486.	1.3	5
108	A computational method to simulate global conformational changes of proteins induced by cosolvent. <i>Journal of Computational Chemistry</i> , 2021, 42, 552-563.	1.5	4

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109	Recent Advances in Multireference-Based Perturbation Theory. Bulletin of the Korean Chemical Society, 2003, 24, 812-816.	1.0	4
110	Copper(II) Complexes of 10,20-Diaryl-5,15-diazaporphyrin: Alternative Synthesis, Excited State Dynamics, and Substituent Effect on the IO ₂ -Generation Efficiency. Bulletin of the Chemical Society of Japan, 2022, 95, 427-432.	2.0	4
111	Computational Analysis of the SARS-CoV-2 RBD-ACE2-Binding Process Based on MD and the 3D-RISM Theory. Journal of Chemical Information and Modeling, 2022, 62, 2889-2898.	2.5	4
112	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
113	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
114	9-(Diphenylphosphoryl)-10-(phenylethynyl)anthracene Derivatives: Synthesis and Implications for the Substituent and Solvent Effects on the Light-Emitting Properties. ChemPhotoChem, 2022, 6, .	1.5	3
115	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
116	A non-orthogonal Kohn-Sham method using partially fixed molecular orbitals. Theoretical Chemistry Accounts, 2003, 110, 328-337.	0.5	2
117	Direct and Regioselective Amination of β -Unsubstituted 5,15-Diazaporphyrins with Amines: A Convenient Route to Near-Infrared-Responsive Diazaporphyrin Sensitizers. Angewandte Chemie, 2018, 130, 3859-3862.	1.6	2
118	Valence-bond description of chemical reactions on Born-Oppenheimer molecular dynamics trajectories. Journal of Chemical Physics, 2009, 130, 154309.	1.2	1
119	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
120	New algorithm for electron repulsion integrals oriented to the general contraction scheme. , 2000, 76, 396.		1
121	New algorithm for electron repulsion integrals oriented to the general contraction scheme. , 2000, 76, 396.		1
122	New algorithm for electron repulsion integrals oriented to the general contraction scheme. International Journal of Quantum Chemistry, 2000, 76, 396.	1.0	1
123	Study on Chemical Reactivity Control of Liquid Sodium: Development of Nano-Fluid and Its Property and Applicability to FBR Plant. , 2008, , .		0