Dage Sundholm

List of Publications by Year
in descending order

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207	8,922	36303	60623
papers	citations	51 h-index	81 g-index

211	211	211	5062
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Integration of global ring currents using the AmpÃ¨reâ€“Maxwell law. Physical Chemistry Chemical Physics, 2022, 24, 624-628.	2.8	15
2	Magnetically induced ring currents in metallocenothiaporphyrins. Physical Chemistry Chemical Physics, 2022, 24, 1666-1674.	2.8	9
3	Non-intersecting ring currents in [12]infinitene. Physical Chemistry Chemical Physics, 2022, 24, 6404-6409.	2.8	23
4	Magnetically Induced Current Densities in Zinc Porphyrin Nanoshells. Journal of Physical Chemistry A, 2022, 126, 1936-1945.	2.5	7
5	Core-electron contributions to the molecular magnetic response. Physical Chemistry Chemical Physics, 2022, 24, 12158-12166.	2.8	13
6	Odd-Number Cyclo[n]Carbons Sustaining Alternating Aromaticity. Journal of Physical Chemistry A, 2022, 126, 2445-2452.	2.5	7
7	Diagnosing Ring Current(s) in Figure-Eight Skeletons: A 3D Through-Space Conjugation in the Two-Loops Crossing. Organic Letters, 2022, 24, 4876-4880.	4.6	4
8	Magnetically induced ring currents in naphthalene-fused heteroporphyrinoids. Physical Chemistry Chemical Physics, 2021, 23, 16629-16634.	2.8	2
9	Current density, current-density pathways, and molecular aromaticity. , 2021, , 155-194.		4
10	Spatial Contributions to Nuclear Magnetic Shieldings. Journal of Physical Chemistry A, 2021, 125, 1778-1786.	2.5	17
11	Benchmarking Magnetizabilities with Recent Density Functionals. Journal of Chemical Theory and Computation, 2021, 17, 1457-1468.	5.3	43
12	Divergent Carbocatalytic Routes in Oxidative Coupling of Benzofused Heteroaryl Dimers: A Mechanistic Update. Chemistry - A European Journal, 2021, 27, 5283-5291.	3.3	7
13	Magnetically Induced Ring-Current Strengths of Planar and Nonplanar Molecules: New Insights from the Pseudo-Ï€ Model. Journal of Physical Chemistry A, 2021, 125, 5753-5764.	2.5	17
14	Spatial Contributions to 1H NMR Chemical Shifts of Free-Base Porphyrinoids. Chemistry, 2021, 3, 1005-1021.	2.2	6
15	Current density and molecular magnetic properties. Chemical Communications, 2021, 57, 12362-12378.	4.1	39
16	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. Journal of Chemical Theory and Computation, 2020, 16, 587-600.	5.3	69
17	Perhalophenyl Three-Coordinate Gold(I) Complexes as TADF Emitters: A Photophysical Study from Experimental and Computational Viewpoints. Inorganic Chemistry, 2020, 59, 14236-14244.	4.0	15
18	The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids. New Journal of Chemistry, 2020, 44, 20643-20650.	2.8	4

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19	When are Antiaromatic Molecules Paramagnetic?. Journal of Physical Chemistry C, 2020, 124, 21027-21035.	3.1	18
20	Aromaticity of Even-Number Cyclo[n]carbons (n = 6â€“100). Journal of Physical Chemistry A, 2020, 124, 10849-10855.	2.5	30
21	Calculation of magnetic response properties of tetrazines. RSC Advances, 2020, 10, 18124-18130.	3.6	10
22	Interplay of Aromaticity and Antiaromaticity in N-Doped Nanographenes. Journal of Physical Chemistry A, 2020, 124, 695-703.	2.5	17
23	Calculation of vibrationally resolved absorption and fluorescence spectra of the rylenes. Physical Chemistry Chemical Physics, 2020, 22, 2379-2385.	2.8	13
24	A method for designing a novel class of gold-containing molecules. Chemical Communications, 2020, 56, 5433-5436.	4.1	5
25	Photophysical properties of the triangular [Au(HNî€COH)]₃ complex and its dimer. Physical Chemistry Chemical Physics, 2020, 22, 10314-10321.	2.8	3
26	Calculating rate constants for intersystem crossing and internal conversion in the Franckâ€“Condon and Herzbergâ€“Teller approximations. Physical Chemistry Chemical Physics, 2019, 21, 18495-18500.	2.8	38
27	Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling. Journal of Physical Chemistry Letters, 2019, 10, 6701-6705.	4.6	103
28	Aromatic and Antiaromatic Pathways in Triphyrin(2.1.1) Annelated with Benzo[b]heterocycles. Chemistry - A European Journal, 2019, 25, 15477-15482.	3.3	18
29	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. Physical Chemistry Chemical Physics, 2019, 21, 21094-21103.	2.8	47
30	Magnetically Induced Current Densities in Toroidal Carbon Nanotubes. Journal of Physical Chemistry C, 2019, 123, 15354-15365.	3.1	20
31	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. Physical Chemistry Chemical Physics, 2019, 21, 6851-6858.	2.8	16
32	Aromatic Pathways in Porphycene Derivatives Based on Current-Density Calculations. Journal of Physical Chemistry A, 2019, 123, 284-292.	2.5	1
33	Insights into Molecular Structures and Optical Properties of Stacked [Au₃(RNâ•CRâ€²)₃]_n Complexes. Inorganic Chemistry, 2018, 57, 718-730.	4.0	13
34	Magnetically Induced Ring-Current Strengths in MÃ¶bius Twisted Annulenes. Journal of Physical Chemistry Letters, 2018, 9, 1627-1632.	4.6	19
35	The argon nuclear quadrupole moments. Molecular Physics, 2018, 116, 1682-1686.	1.7	2
36	The aromatic character of [10]annulenes and dicupra[10]annulenes from current density calculations. Physical Chemistry Chemical Physics, 2018, 20, 1337-1346.	2.8	14

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37	The aromaticity of verdazyl radicals and their closed-shell charged species. New Journal of Chemistry, 2018, 42, 19987-19994.	2.8	5
38	Density Functional Theory under the Bubbles and Cube Numerical Framework. Journal of Chemical Theory and Computation, 2018, 14, 4237-4245.	5.3	6
39	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. Physical Chemistry Chemical Physics, 2018, 20, 17705-17713.	2.8	21
40	[Hg 4 Te 8 (Te 2) 4] 8â˜ : A Heavy Metal Porphyrinoid Embedded in a Lamellar Structure. Angewandte Chemie - International Edition, 2018, 57, 8770-8774.	13.8	26
41	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. Journal of Physical Chemistry A, 2018, 122, 4756-4767.	2.5	41
42	[Hg 4 Te 8 (Te 2) 4] 8â˜ : ein Schwermetallâ€Porphyrinoid in einer lamellaren Struktur. Angewandte Chemie, 2018, 130, 8906-8910.	2.0	9
43	A Generalized Grid-Based Fast Multipole Method for Integrating Helmholtz Kernels. Journal of Chemical Theory and Computation, 2017, 13, 654-665.	5.3	9
44	Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials. Physical Chemistry Chemical Physics, 2017, 19, 7124-7131.	2.8	43
45	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays. Physical Chemistry Chemical Physics, 2017, 19, 12794-12803.	2.8	18
46	Energetics and dynamics of a light-driven sodium-pumping rhodopsin. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7043-7048.	7.1	73
47	Optimization of numerical orbitals using the Helmholtz kernel. Journal of Chemical Physics, 2017, 146, 084102.	3.0	7
48	Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1952-1962.	5.3	12
49	Closed-shell paramagnetic porphyrinoids. Chemical Communications, 2017, 53, 9866-9869.	4.1	40
50	Relation Between Ring Currents and Hydrogenation Enthalpies for Assessing the Degree of Aromaticity. Journal of Physical Chemistry A, 2017, 121, 7282-7289.	2.5	37
51	Optical and magnetic properties of antiaromatic porphyrinoids. Physical Chemistry Chemical Physics, 2017, 19, 25979-25988.	2.8	19
52	The influence of heteroatoms on the aromatic character and the current pathways of B₂N₂-dibenzo[a,e]pentalenes. Physical Chemistry Chemical Physics, 2017, 19, 20213-20223.	2.8	15
53	Electronic and optical properties of metalloporphyrins of zinc on TiO₂ cluster in dye-sensitized solar-cells (DSSC). A quantum chemistry study. RSC Advances, 2017, 7, 42677-42684.	3.6	29
54	Calculations of magnetically induced current densities: theory and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 639-678.	14.6	244

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55	Double Jahnâ€“Teller Distortion in AuGe Complexes Leading to a Dual Blueâ€“Orange Emission. ChemPlusChem, 2016, 81, 176-186.	2.8	6
56	Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. Journal of Chemical Theory and Computation, 2016, 12, 2644-2651.	5.3	32
57	Importance of Vibronic Effects in the UVâ€“Vis Spectrum of the 7,7,8,8-Tetracyanoquinodimethane Anion. Journal of Chemical Theory and Computation, 2016, 12, 5058-5066.	5.3	35
58	Calculations of the light absorption spectra of porphyrinoid chromophores for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2016, 18, 27877-27884.	2.8	8
59	Gauge-Origin Independent Calculations of the Anisotropy of the Magnetically Induced Current Densities. Journal of Physical Chemistry A, 2016, 120, 5658-5664.	2.5	44
60	Analysis of the magnetically induced current density of molecules consisting of annelated aromatic and antiaromatic hydrocarbon rings. Physical Chemistry Chemical Physics, 2016, 18, 15934-15942.	2.8	61
61	Tuning the Proteinâ€Induced Absorption Shifts of Retinal in Engineered Rhodopsin Mimics. Chemistry - A European Journal, 2016, 22, 8254-8261.	3.3	17
62	Evaluating Shieldingâ€Based Ringâ€Current Models by Using the Gaugeâ€Including Magnetically Induced Current Method. Journal of the Chinese Chemical Society, 2016, 63, 93-100.	1.4	15
63	New insights into aromatic pathways of carbachlorins and carbaporphyrins based on calculations of magnetically induced current densities. Physical Chemistry Chemical Physics, 2016, 18, 11932-11941.	2.8	28
64	Aromaticity of the doubly charged [8]circulenes. Physical Chemistry Chemical Physics, 2016, 18, 8980-8992.	2.8	34
65	The grid-based fast multipole method â€“ a massively parallel numerical scheme for calculating two-electron interaction energies. Physical Chemistry Chemical Physics, 2015, 17, 31480-31490.	2.8	13
66	Real-space numerical grid methods in quantum chemistry. Physical Chemistry Chemical Physics, 2015, 17, 31357-31359.	2.8	23
67	Computational Studies of a Paramagnetic Planar Dibenzotetraaza[14]annulene Ni(II) Complex. Journal of Physical Chemistry A, 2015, 119, 5189-5196.	2.5	4
68	Aromatic Pathways in Carbathiaporphyrins. Journal of Physical Chemistry A, 2015, 119, 1201-1207.	2.5	23
69	Coupled-Cluster Studies of Extensive Green Fluorescent Protein Models Using the Reduced Virtual Space Approach. Journal of Physical Chemistry B, 2015, 119, 2933-2945.	2.6	30
70	Construction of the Fock Matrix on a Grid-Based Molecular Orbital Basis Using GPGPUs. Journal of Chemical Theory and Computation, 2015, 11, 2053-2062.	5.3	11
71	Predicting the degree of aromaticity of novel carbaporphyrinoids. Physical Chemistry Chemical Physics, 2015, 17, 14215-14222.	2.8	27
72	Proteinâ€Induced Color Shift of Carotenoids in Î²â€Crustacyanin. Angewandte Chemie - International Edition, 2015, 54, 11564-11566.	13.8	57

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73	Novel hollow all-carbon structures. Nanoscale, 2015, 7, 15886-15894.	5.6	27
74	Antiaromatic Character of 16 Ï€ Electron Octaethylporphyrins: Magnetically Induced Ring Currents from DFT-GIMIC Calculations. Journal of Physical Chemistry A, 2015, 119, 2344-2350.	2.5	23
75	On energetic prerequisites of attracting electrons. Journal of Chemical Physics, 2014, 140, 234111.	3.0	0
76	Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2014, 16, 22309-22320.	2.8	7
77	The aromatic character of thienopyrrole-modified 20Ï€-electron porphyrinoids. Physical Chemistry Chemical Physics, 2014, 16, 11010.	2.8	26
78	Spectral Tuning of Rhodopsin and Visual Cone Pigments. Journal of the American Chemical Society, 2014, 136, 2723-2726.	13.7	43
79	Computational and experimental studies of the electronic excitation spectra of EDTA and DTPA substituted tetraphenylporphyrins and their Lu complexes. Journal of Molecular Modeling, 2013, 19, 4631-4637.	1.8	5
80	Insights into Magnetically Induced Current Pathways and Optical Properties of Isophlorins. Journal of Physical Chemistry A, 2013, 117, 9062-9068.	2.5	38
81	Computational Studies of the Electronic Absorption Spectrum of [(2,2â€²;6â€²,2â€³-Terpyridine)â€“Pt(II)â€“OH] [7,7,8,8-Tetracyanoquinodimethane] Complex. Journal of Physical Chemistry A, 2013, 117, 12363-12373.	2.5	3
82	C72: gaudiene, a hollow and aromatic all-carbon molecule. Physical Chemistry Chemical Physics, 2013, 15, 9025.	2.8	33
83	Ab Initio, Density Functional Theory, and Semi-Empirical Calculations. Methods in Molecular Biology, 2013, 924, 3-27.	0.9	6
84	Electrostatic spectral tuning mechanism of the green fluorescent protein. Physical Chemistry Chemical Physics, 2013, 15, 4491.	2.8	47
85	Aromatic pathways in thieno-bridged porphyrins: understanding the influence of the direction of the thiophene ring on the aromatic character. Molecular Physics, 2013, 111, 1364-1372.	1.7	29
86	Aromatic Pathways of Porphins, Chlorins, and Bacteriochlorins. Journal of Organic Chemistry, 2012, 77, 3408-3414.	3.2	80
87	Effect of Fluorine Substitution on the Aromaticity of Polycyclic Hydrocarbons. Journal of Physical Chemistry A, 2012, 116, 10257-10268.	2.5	57
88	The Effect of Protein Environment on Photoexcitation Properties of Retinal. Journal of Physical Chemistry B, 2012, 116, 2249-2258.	2.6	43
89	Computational Studies of Nonstoichiometric Sodium Auride Clusters. Journal of Physical Chemistry A, 2012, 116, 5119-5128.	2.5	4
90	Ab Initio Studies of Triplet-State Properties for Organic Semiconductor Molecules. Journal of Physical Chemistry C, 2012, 116, 15203-15217.	3.1	20

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91	Computational methods for studies of semiconductor quantum dots and rings. Annual Reports on the Progress of Chemistry Section C, 2012, 108, 96.	4.4	7
92	Computational studies of photophysical properties of porphin, tetraphenylporphyrin and tetrabenzoporphyrin. Physical Chemistry Chemical Physics, 2012, 14, 11508.	2.8	56
93	Aromatic pathways in mono- and bisphosphorous singly MÃ¶bius twisted [28] and [30]hexaphyrins. Physical Chemistry Chemical Physics, 2011, 13, 20659.	2.8	41
94	Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. Journal of Chemical Theory and Computation, 2011, 7, 2473-2484.	5.3	40
95	Calculation of spin-current densities using gauge-including atomic orbitals. Journal of Chemical Physics, 2011, 134, 054123.	3.0	109
96	The gauge including magnetically induced current method. Physical Chemistry Chemical Physics, 2011, 13, 20500.	2.8	326
97	Hydrogen-bond strengths by magnetically induced currents. Physical Chemistry Chemical Physics, 2011, 13, 434-437.	2.8	35
98	Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. Journal of Chemical Physics, 2011, 134, 214114.	3.0	55
99	Theoretical investigation of photoelectron spectra and magnetically induced current densities in ring-shaped transition-metal oxides. Theoretical Chemistry Accounts, 2011, 129, 701-713.	1.4	11
100	Aromatic pathways in conjugated rings connected by single bonds. International Journal of Quantum Chemistry, 2011, 111, 848-857.	2.0	19
101	Interpretation of the photoluminescence spectrum of double quantum rings. Physical Review B, 2010, 82, .	3.2	5
102	Magnetically Induced Currents in [n]Cycloparaphenylenes, n = 6â^'11. Journal of Organic Chemistry, 2010, 75, 5867-5874.	3.2	56
103	Aromatic Pathways in Twisted Hexaphyrins. Journal of Physical Chemistry A, 2010, 114, 7153-7161.	2.5	65
104	Calculation of absorption and emission spectra of [n]cycloparaphenylenes: the reason for the large Stokes shift. Physical Chemistry Chemical Physics, 2010, 12, 2751.	2.8	53
105	Coupled-cluster and density functional theory studies of the electronic excitation spectra of trans-1,3-butadiene and trans-2-propeniminium. Journal of Chemical Physics, 2009, 131, 024301.	3.0	44
106	Magnetically Induced Current Densities in Aromatic, Antiaromatic, Homoaromatic, and Nonaromatic Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 8668-8676.	2.5	164
107	The chemistry of the CuB site in cytochrome c oxidase and the importance of its unique Hisâ€“Tyr bond. Biochimica Et Biophysica Acta - Bioenergetics, 2009, 1787, 221-233.	1.0	47
108	Magnetically Induced Currents in Bianthraquinodimethane-Stabilized MÃ¶bius and HÃ¼ckel [16]Annulenes. Journal of Organic Chemistry, 2009, 74, 6495-6502.	3.2	36

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109	Excited State Potential Energy Surfaces of Polyenes and Protonated Schiff Bases. Journal of Chemical Theory and Computation, 2009, 5, 2401-2414.	5.3	36
110	The molecular structure of a curl-shaped retinal isomer. Journal of Molecular Modeling, 2008, 14, 717-726.	1.8	15
111	Computational studies of semiconductor quantum dots. Physical Chemistry Chemical Physics, 2008, 10, 4535.	2.8	37
112	Calculation of Magnetically Induced Currents in Hydrocarbon Nanorings. Journal of Physical Chemistry A, 2008, 112, 13584-13592.	2.5	33
113	Dynamics and magnetic resonance properties of Sc3C2@C80 and its monoanion. Physical Chemistry Chemical Physics, 2008, 10, 7158.	2.8	31
114	Polycyclic antiaromatic hydrocarbons. Physical Chemistry Chemical Physics, 2008, 10, 6630.	2.8	49
115	Exploring the Stability of Golden Fullerenes. Journal of Physical Chemistry C, 2008, 112, 19311-19315.	3.1	37
116	Parallel implementation of a direct method for calculating electrostatic potentials. Journal of Chemical Physics, 2007, 126, 094101.	3.0	27
117	Stairway to the Conical Intersection:Â A Computational Study of the Retinal Isomerization. Journal of Physical Chemistry A, 2007, 111, 8766-8773.	2.5	63
118	The Role of the Î²-Ionone Ring in the Photochemical Reaction of Rhodopsin. Journal of Physical Chemistry A, 2007, 111, 27-33.	2.5	38
119	Coupled-cluster studies of the lowest excited states of the 11-cis-retinal chromophore. Physical Chemistry Chemical Physics, 2007, 9, 2862.	2.8	46
120	A Photoelectron Spectroscopic and Computational Study of Sodium Auride Clusters, NanAun-(n= 1â^'3). Journal of Physical Chemistry A, 2007, 111, 7555-7561.	2.5	16
121	Bright luminescence from silane substituted and bridged silicon nanoclusters. Physical Chemistry Chemical Physics, 2006, 8, 4228.	2.8	10
122	On the Aromaticity of the Planar Hydrogen-Bonded (HF)3Trimer. Journal of Chemical Theory and Computation, 2006, 2, 761-764.	5.3	26
123	Experimental and Computational Studies of Alkali-Metal Coinage-Metal Clusters. Journal of Physical Chemistry A, 2006, 110, 4244-4250.	2.5	70
124	Coupled-cluster studies of the electronic excitation spectra of silanes. Journal of Chemical Physics, 2006, 125, 144314.	3.0	15
125	Optical properties of sila-adamantane nanoclusters from density-functional theory. Physical Review B, 2006, 74, .	3.2	18
126	Sphere Currents of Buckminsterfullerene. Angewandte Chemie - International Edition, 2005, 44, 1843-1846.	13.8	113

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127	Sphere Currents of Buckminsterfullerene. Angewandte Chemie, 2005, 117, 1877-1880.	2.0	6
128	A Non-Iterative Numerical Solver of Poisson and Helmholtz Equations Using High-Order Finite-Element Functions. Advances in Quantum Chemistry, 2005, 50, 235-247.	0.8	8
129	Magnetically induced current densities in Al42â˜ and Al44â˜ species studied at the coupled-cluster level. Journal of Chemical Physics, 2005, 122, 214308.	3.0	87
130	Computational studies of 13C NMR chemical shifts of saccharides. Physical Chemistry Chemical Physics, 2005, 7, 2561.	2.8	31
131	Density-functional studies of excited states of silicon nanoclusters. Physical Review B, 2005, 72, .	3.2	34
132	Au32: A 24-Carat Golden Fullerene. Angewandte Chemie - International Edition, 2004, 43, 2678-2681.	13.8	285
133	Properties of WAu12.. ChemInform, 2004, 35, no.	0.0	0
134	Properties of WAu12. Physical Chemistry Chemical Physics, 2004, 6, 11-22.	2.8	97
135	Density functional studies of the luminescence of Si29H36. Physical Chemistry Chemical Physics, 2004, 6, 2044.	2.8	27
136	Calculation of current densities using gauge-including atomic orbitals. Journal of Chemical Physics, 2004, 121, 3952-3963.	3.0	393
137	Spin and charge distribution in iron porphyrin models: A coupled cluster and density-functional study. Journal of Chemical Physics, 2004, 120, 3229-3236.	3.0	37
138	Calculation of ring-current susceptibilities for potentially homoaromatic hydrocarbons. Computational and Theoretical Chemistry, 2003, 633, 123-136.	1.5	21
139	First Principles Calculations of the Absorption Spectrum of Si29H36. Nano Letters, 2003, 3, 847-849.	9.1	23
140	A density-functional-theory study of bacteriochlorophyll b. Physical Chemistry Chemical Physics, 2003, 5, 4265.	2.8	40
141	The Spin Distribution in Low-Spin Iron Porphyrins. Journal of the American Chemical Society, 2002, 124, 11771-11780.	13.7	64
142	Change in electron and spin density upon electron transfer to haem. Biochimica Et Biophysica Acta - Bioenergetics, 2002, 1553, 183-187.	1.0	49
143	The aromaticity and antiaromaticity of dehydroannulenes. Physical Chemistry Chemical Physics, 2001, 3, 2433-2437.	2.8	61
144	Magnetic-Shielding Calculations on Al42-and Analogues. A New Family of Aromatic Molecules?. Journal of Physical Chemistry A, 2001, 105, 9939-9944.	2.5	103

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145	Tetraberyllium-Î·⁴-oxo-hexa(arylcarboxylates). Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2001, 56, 979-989.	0.7	31
146	Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. Physical Review A, 2001, 64, .	2.5	46
147	Comparison of the electronic excitation spectra of chlorophyll a and pheophytin a calculated at density functional theory level. Chemical Physics Letters, 2000, 317, 545-552.	2.6	87
148	A modified variation-perturbation approach to zero-point vibrational motion. Theoretical Chemistry Accounts, 2000, 103, 365-373.	1.4	38
149	Interpretation of the electronic absorption spectrum of free-base porphin using time-dependent density-functional theory. Physical Chemistry Chemical Physics, 2000, 2, 2275-2281.	2.8	109
150	Luminescent Characterization of Solution Oligomerization Process Mediated Goldâ^'Gold Interactions. DFT Calculations on [Au2Ag2R4L2]nMoieties. Journal of the American Chemical Society, 2000, 122, 7287-7293.	13.7	140
151	The Aromatic Character of Magnesium Porphyrins. Journal of Organic Chemistry, 2000, 65, 5233-5237.	3.2	83
152	The aromatic pathways of porphins, chlorins and bacteriochlorins. Physical Chemistry Chemical Physics, 2000, 2, 2145-2151.	2.8	99
153	Finite-element multiconfiguration Hartree-Fock calculations of the atomic quadrupole moment ofAr+(2P3/2). Physical Review A, 1999, 59, 3355-3358.	2.5	4
154	Ab initiocalculations of the ground-state electron affinities of gallium and indium. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 5853-5859.	1.5	17
155	Density functional theory calculations of the visible spectrum of chlorophyll a. Chemical Physics Letters, 1999, 302, 480-484.	2.6	170
156	Electric quadrupole moment of the 27Al nucleus: Converging results from the AlF and AlCl molecules and the Al atom. Chemical Physics Letters, 1999, 304, 414-422.	2.6	73
157	An Ab Initio Study of Structure and Energetics of Free-Base Bonellin-Dimethylester Isomers and Transition States. Chemistry - A European Journal, 1999, 5, 267-273.	3.3	11
158	Ab initio determination of the induced ring current in aromatic molecules. Physical Chemistry Chemical Physics, 1999, 1, 3429-3435.	2.8	173
159	On perturbation expansions of the extended Koopmans' theorem. Chemical Physics Letters, 1998, 288, 282-288.	2.6	27
160	Nuclear quadrupole moments of gallium isotopes obtained from finite-element MCHF calculations on the 4p2P3/2 state of Ga. Chemical Physics Letters, 1998, 291, 414-418.	2.6	20
161	Isotope and temperature effects on nuclear magnetic shieldings and spin-rotation constants calculated at the coupled-cluster level. Molecular Physics, 1997, 92, 1007-1014.	1.7	47
162	Coupled-cluster calculations of spin-rotation constants. Molecular Physics, 1997, 91, 449-458.	1.7	46

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163	The nuclear quadrupole moment of 14N obtained from finite-element MCHF calculationson N2+ (2p;) Tj ETQq1 1 0.784314 rgBT /Ove	2.6	61
164	A numerical Hartree-Fock program for diatomic molecules. Computer Physics Communications, 1996, 98, 346-358.	7.5	123
165	Rovibrationally averaged nuclear magnetic shielding tensors calculated at the coupledâ€cluster level. Journal of Chemical Physics, 1996, 105, 11051-11059.	3.0	169
166	Finite-element multiconfiguration Hartree-Fock calculations of electron affinities of manganese. Chemical Physics Letters, 1995, 233, 115-122.	2.6	4
167	The electron correlation contribution to the nuclear magnetic shielding tensor of the hydrogen molecule. Chemical Physics Letters, 1995, 243, 264-268.	2.6	29
168	Numerical multiconfigurational Hartreeâ€“Fock calculations of spin and charge densities using the Hillerâ€“Sucherâ€“Feinberg operator identity. Journal of Chemical Physics, 1995, 102, 4895-4903.	3.0	7
169	A multiconfiguration selfâ€consistentâ€field response study of oneâ€and twoâ€photon dipole transitions between the Xâ€‰1Î£+ and Aâ€‰1Î states of CO. Journal of Chemical Physics, 1995, 102, 4143-4150.	3.0	15
170	Multiconfiguration selfâ€consistent field quadratic response calculations of the twoâ€photon transition probability rate constants for argon. Journal of Chemical Physics, 1994, 101, 4931-4935.	3.0	17
171	Finite-element multiconfiguration Hartree-Fock calculations of the atomic quadrupole moments ofC+(2P) andNe+(2P). Physical Review A, 1994, 49, 3453-3456.	2.5	18
172	Coreâ€”valence correlation effects on the ground state electron affinity of calcium. Chemical Physics Letters, 1994, 217, 451-455.	2.6	26
173	Fully numerical soluti ons of molecular Dirac equations for highly charged one-electron homonuclear diatomic molecules. Chemical Physics Letters, 1994, 223, 469-473.	2.6	17
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