Dage Matts Brje Sundholm

List of Publications by Year in Descending Order

168 papers	5,369 citations	38 h-index	65 g-index
181 ext. papers	5,989 ext. citations	4.1 avg, IF	6.14 L-index

#	Paper	IF	Citations
168	Aromatic Pathways in Porphyrinoids by Magnetically Induced Ring Currents. *Handbook of Porphyrin Science*, **2022**, 1-39	0.3	
167	Current density and molecular magnetic properties. *Chemical Communications*, **2021**, 57, 12362-12378	5.8	6
166	Magnetically Induced Ring-Current Strengths of Planar and Nonplanar Molecules: New Insights from the Pseudo-□Model. *Journal of Physical Chemistry A*, **2021**, 125, 5753-5764	2.8	5
165	Magnetically induced ring currents in naphthalene-fused heteroporphyrinoids. *Physical Chemistry Chemical Physics*, **2021**, 23, 16629-16634	3.6	0
164	Fast estimation of the internal conversion rate constant in photophysical applications. *Physical Chemistry Chemical Physics*, **2021**, 23, 6344-6348	3.6	5
163	Current density, current-density pathways, and molecular aromaticity **2021**, 155-194		0
162	Spatial Contributions to Nuclear Magnetic Shieldings. *Journal of Physical Chemistry A*, **2021**, 125, 1778-1788	2.8	8
161	Benchmarking Magnetizabilities with Recent Density Functionals. *Journal of Chemical Theory and Computation*, **2021**, 17, 1457-1468	6.4	19
160	Divergent Carbocatalytic Routes in Oxidative Coupling of Benzofused Heteroaryl Dimers: A Mechanistic Update. *Chemistry - A European Journal*, **2021**, 27, 5283-5291	4.8	4
159	Spatial Contributions to 1H NMR Chemical Shifts of Free-Base Porphyrinoids. *Chemistry*, **2021**, 3, 1005-1021	2.1	1
158	Aromaticity of Even-Number Cyclo□carbons (= 6-100). *Journal of Physical Chemistry A*, **2020**, 124, 10849-10855	2.8	12
157	Calculation of magnetic response properties of tetrazines.. *RSC Advances*, **2020**, 10, 18124-18130	3.7	4
156	Atoms and molecules in soft confinement potentials. *Molecular Physics*, **2020**, 118, e1730989	1.7	8
155	Interplay of Aromaticity and Antiaromaticity in N-Doped Nanographenes. *Journal of Physical Chemistry A*, **2020**, 124, 695-703	2.8	12
154	Calculation of vibrationally resolved absorption and fluorescence spectra of the rylenes. *Physical Chemistry Chemical Physics*, **2020**, 22, 2379-2385	3.6	7
153	A method for designing a novel class of gold-containing molecules. *Chemical Communications*, **2020**, 56, 5433-5436	5.8	2
152	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. *Journal of Chemical Theory and Computation*, **2020**, 16, 587-600	6.4	32

151	Perhalophenyl Three-Coordinate Gold(I) Complexes as TADF Emitters: A Photophysical Study from Experimental and Computational Viewpoints. *Inorganic Chemistry*, **2020**, 59, 14236-14244	5.1	8
150	The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids. *New Journal of Chemistry*, **2020**, 44, 20643-20650	3.6	2
149	When are Antiaromatic Molecules Paramagnetic?. *Journal of Physical Chemistry C*, **2020**, 124, 21027-21035	3.7	13
148	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. *Physical Chemistry Chemical Physics*, **2020**, 22, 22314-22323	3.6	15
147	Fully numerical electronic structure calculations on diatomic molecules in weak to strong magnetic fields. *Molecular Physics*, **2020**, 118, e1597989	1.7	10
146	Photophysical properties of the triangular [Au(HN[double bond, length as m-dash]COH)] complex and its dimer. *Physical Chemistry Chemical Physics*, **2020**, 22, 10314-10321	3.6	3
145	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. *Physical Chemistry Chemical Physics*, **2019**, 21, 21094-21103	3.6	26
144	Magnetically Induced Current Densities in Toroidal Carbon Nanotubes. *Journal of Physical Chemistry C*, **2019**, 123, 15354-15365	3.8	13
143	Deacetylation of per-acetatylated glycopyranosides: An overall pattern for acidic catalyzis. *Chemical Physics Letters*, **2019**, 723, 123-127	2.5	3
142	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. *Physical Chemistry Chemical Physics*, **2019**, 21, 6851-6858	3.6	12
141	Calculating rate constants for intersystem crossing and internal conversion in the Franck-Condon and Herzberg-Teller approximations. *Physical Chemistry Chemical Physics*, **2019**, 21, 18495-18500	3.6	22
140	Ab Initio Study of Phosphorescence of Hetero[8]Circulenes. *Russian Physics Journal*, **2019**, 62, 406-410	0.7	1
139	Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling. *Journal of Physical Chemistry Letters*, **2019**, 10, 6701-6705	6.4	57
138	Aromatic and Antiaromatic Pathways in Triphyrin(2.1.1) Annelated with Benzo[b]heterocycles. *Chemistry - A European Journal*, **2019**, 25, 15477-15482	4.8	8
137	Predicting Stable Molecular Structures for (RNC)2AuIX Complexes. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2019**, 645, 1127-1134	1.3	
136	Aromatic Pathways in Porphycene Derivatives Based on Current-Density Calculations. *Journal of Physical Chemistry A*, **2019**, 123, 284-292	2.8	0
135	First-principles method for calculating the rate constants of internal-conversion and intersystem-crossing transitions. *Physical Chemistry Chemical Physics*, **2018**, 20, 6121-6133	3.6	50
134	Insights into Molecular Structures and Optical Properties of Stacked [Au(RN?CR')] Complexes. *Inorganic Chemistry*, **2018**, 57, 718-730	5.1	12

133	Magnetically Induced Ring-Current Strengths in M□bius Twisted Annulenes. *Journal of Physical Chemistry Letters*, **2018**, 9, 1627-1632	6.4	11
132	The argon nuclear quadrupole moments. *Molecular Physics*, **2018**, 116, 1682-1686	1.7	2
131	On the Mechanism of the Reactivity of 1,3-Dialkylimidazolium Salts under Basic to Acidic Conditions: A Combined Kinetic and Computational Study. *Angewandte Chemie*, **2018**, 130, 11787-11791	3.6	4
130	On the Mechanism of the Reactivity of 1,3-Dialkylimidazolium Salts under Basic to Acidic Conditions: A Combined Kinetic and Computational Study. *Angewandte Chemie - International Edition*, **2018**, 57, 11613-11617	16.4	10
129	[Hg Te (Te)] : A Heavy Metal Porphyrinoid Embedded in a Lamellar Structure. *Angewandte Chemie - International Edition*, **2018**, 57, 8770-8774	16.4	17
128	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. *Journal of Physical Chemistry A*, **2018**, 122, 4756-4767	2.8	33
127	Tensor decompositions for the bubbles and cube numerical framework. *Computer Physics Communications*, **2018**, 232, 98-103	4.2	2
126	[Hg4Te8(Te2)4]8□ein Schwermetall-Porphyrinoid in einer lamellaren Struktur. *Angewandte Chemie* , **2018**, 130, 8906-8910	3.6	7
125	The aromatic character of [10]annulenes and dicupra[10]annulenes from current density calculations. *Physical Chemistry Chemical Physics*, **2018**, 20, 1337-1346	3.6	11
124	Relations between the aromaticity and magnetic dipole transitions in the electronic spectra of hetero[8]circulenes. *Physical Chemistry Chemical Physics*, **2018**, 20, 30239-30246	3.6	10
123	The aromaticity of verdazyl radicals and their closed-shell charged species. *New Journal of Chemistry*, **2018**, 42, 19987-19994	3.6	5
122	Density Functional Theory under the Bubbles and Cube Numerical Framework. *Journal of Chemical Theory and Computation*, **2018**, 14, 4237-4245	6.4	3
121	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. *Physical Chemistry Chemical Physics*, **2018**, 20, 17705-17713	3.6	17
120	A Generalized Grid-Based Fast Multipole Method for Integrating Helmholtz Kernels. *Journal of Chemical Theory and Computation*, **2017**, 13, 654-665	6.4	7
119	Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials. *Physical Chemistry Chemical Physics*, **2017**, 19, 7124-7131	3.6	29
118	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays. *Physical Chemistry Chemical Physics*, **2017**, 19, 12794-12803	3.6	14
117	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	11.5	52
116	Aromaticity introduced by antiferromagnetic ligand mediated metal□metal interactions. Insights from the induced magnetic response in [Cu6(dmPz)6(OH)6]. *Inorganic Chemistry Frontiers*, **2017**, 4, 986-993	6.8	8

115	Optimization of numerical orbitals using the Helmholtz kernel. *Journal of Chemical Physics*, **2017**, 146, 084102	3.9	5
114	Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules. *Journal of Chemical Theory and Computation*, **2017**, 13, 1952-1962	6.4	7
113	Closed-shell paramagnetic porphyrinoids. *Chemical Communications*, **2017**, 53, 9866-9869	5.8	31
112	Relation Between Ring Currents and Hydrogenation Enthalpies for Assessing the Degree of Aromaticity. *Journal of Physical Chemistry A*, **2017**, 121, 7282-7289	2.8	32
111	Optical and magnetic properties of antiaromatic porphyrinoids. *Physical Chemistry Chemical Physics*, **2017**, 19, 25979-25988	3.6	17
110	Relation between molecular electronic structure and nuclear spin-induced circular dichroism. *Scientific Reports*, **2017**, 7, 46617	4.9	3
109	The influence of heteroatoms on the aromatic character and the current pathways of BN-dibenzo[a,e]pentalenes. *Physical Chemistry Chemical Physics*, **2017**, 19, 20213-20223	3.6	12
108	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	3.7	21
107	Gauge-Origin Independent Calculations of the Anisotropy of the Magnetically Induced Current Densities. *Journal of Physical Chemistry A*, **2016**, 120, 5658-64	2.8	35
106	Magnetic response properties of gaudiene - a cavernous and aromatic carbocage. *Physical Chemistry Chemical Physics*, **2016**, 18, 18880-6	3.6	12
105	Analysis of the magnetically induced current density of molecules consisting of annelated aromatic and antiaromatic hydrocarbon rings. *Physical Chemistry Chemical Physics*, **2016**, 18, 15934-42	3.6	43
104	Tuning the Protein-Induced Absorption Shifts of Retinal in Engineered Rhodopsin Mimics. *Chemistry - A European Journal*, **2016**, 22, 8254-61	4.8	17
103	Evaluating Shielding-Based Ring-Current Models by Using the Gauge-Including Magnetically Induced Current Method. *Journal of the Chinese Chemical Society*, **2016**, 63, 93-100	1.5	14
102	Thiolate-protected golden fullerenes. A 32-ve core involving a hollow Au32 cage. *RSC Advances*, **2016**, 6, 21332-21336	3.7	8
101	New insights into aromatic pathways of carbachlorins and carbaporphyrins based on calculations of magnetically induced current densities. *Physical Chemistry Chemical Physics*, **2016**, 18, 11932-41	3.6	26
100	Aromaticity of the doubly charged [8]circulenes. *Physical Chemistry Chemical Physics*, **2016**, 18, 8980-92	3.6	27
99	Calculations of magnetically induced current densities: theory and applications. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 639-678	7.9	174
98	Double Jahn-Teller Distortion in AuGe Complexes Leading to a Dual Blue-Orange Emission. *ChemPlusChem*, **2016**, 81, 176-186	2.8	6

97	Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 2644-51	6.4	26
96	Importance of Vibronic Effects in the UV-Vis Spectrum of the 7,7,8,8-Tetracyanoquinodimethane Anion. *Journal of Chemical Theory and Computation*, **2016**, 12, 5058-5066	6.4	25
95	Calculations of the light absorption spectra of porphyrinoid chromophores for dye-sensitized solar cells. *Physical Chemistry Chemical Physics*, **2016**, 18, 27877-27884	3.6	6
94	Double Jahn-Teller Distortion in AuGe Complexes Leading to a Dual Blue-Orange Emission. *ChemPlusChem*, **2016**, 81, 156	2.8	
93	The Excitation Spectra of Naphthalene Dimers: Frenkel and Charge-transfer Excitons. *Journal of the Chinese Chemical Society*, **2016**, 63, 20-32	1.5	3
92	Construction of the Fock Matrix on a Grid-Based Molecular Orbital Basis Using GPGPUs. *Journal of Chemical Theory and Computation*, **2015**, 11, 2053-62	6.4	9
91	Predicting the degree of aromaticity of novel carbaporphyrinoids. *Physical Chemistry Chemical Physics*, **2015**, 17, 14215-22	3.6	24
90	Protein-Induced Color Shift of Carotenoids in □Crustacyanin. *Angewandte Chemie - International Edition*, **2015**, 54, 11564-6	16.4	42
89	Novel hollow all-carbon structures. *Nanoscale*, **2015**, 7, 15886-94	7.7	24
88	Antiaromatic character of 16 □electron octaethylporphyrins: magnetically induced ring currents from DFT-GIMIC calculations. *Journal of Physical Chemistry A*, **2015**, 119, 2344-50	2.8	23
87	The grid-based fast multipole method--a massively parallel numerical scheme for calculating two-electron interaction energies. *Physical Chemistry Chemical Physics*, **2015**, 17, 31480-90	3.6	12
86	Computational studies of a paramagnetic planar dibenzotetraaza[14]annulene Ni(II) complex. *Journal of Physical Chemistry A*, **2015**, 119, 5189-96	2.8	1
85	Aromatic pathways in carbathiaporphyrins. *Journal of Physical Chemistry A*, **2015**, 119, 1201-7	2.8	23
84	Coupled-cluster studies of extensive green fluorescent protein models using the reduced virtual space approach. *Journal of Physical Chemistry B*, **2015**, 119, 2933-45	3.4	28
83	Coupled-cluster and density functional theory studies of the electronic 0-0 transitions of the DNA bases. *Physical Chemistry Chemical Physics*, **2014**, 16, 6931-41	3.6	14
82	Coupled-cluster calculations of the lowest 0-0 bands of the electronic excitation spectrum of naphthalene. *Physical Chemistry Chemical Physics*, **2014**, 16, 9859-65	3.6	14
81	Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2014**, 16, 22309-20	3.6	5
80	A comment to □atalyst Induced Hydrino Transition (CIHT) electrochemical cell□ *International Journal of Energy Research*, **2014**, 38, 1766-1766	4.5	

79	The aromatic character of thienopyrrole-modified 20□electron porphyrinoids. *Physical Chemistry Chemical Physics*, **2014**, 16, 11010-6	3.6	25
78	Spectral tuning of rhodopsin and visual cone pigments. *Journal of the American Chemical Society*, **2014**, 136, 2723-6	16.4	40
77	On energetic prerequisites of attracting electrons. *Journal of Chemical Physics*, **2014**, 140, 234111	3.9	
76	Double Photoinduced Jahn-Teller Distortion of Tetrahedral Au ?Sn Complexes. *ChemPlusChem*, **2014**, 79, 67-76	2.8	17
75	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, 4631-7	?	4
74	Insights into magnetically induced current pathways and optical properties of isophlorins. *Journal of Physical Chemistry A*, **2013**, 117, 9062-8	2.8	37
73	An efficient algorithm to calculate three-electron integrals for Gaussian-type orbitals using numerical integration. *Molecular Physics*, **2013**, 111, 2536-2543	1.7	4
72	C72: gaudiene, a hollow and aromatic all-carbon molecule. *Physical Chemistry Chemical Physics*, **2013**, 15, 9025-8	3.6	29
71	Electrostatic spectral tuning mechanism of the green fluorescent protein. *Physical Chemistry Chemical Physics*, **2013**, 15, 4491-5	3.6	36
70	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	27
69	Computational studies of the corrosion-inhibition efficiency of iron by triazole surfactants. *International Journal of Quantum Chemistry*, **2013**, 113, 1365-1371	2.1	5
68	Aromatic pathways of porphins, chlorins, and bacteriochlorins. *Journal of Organic Chemistry*, **2012**, 77, 3408-14	4.2	69
67	Effect of fluorine substitution on the aromaticity of polycyclic hydrocarbons. *Journal of Physical Chemistry A*, **2012**, 116, 10257-68	2.8	50
66	Construction of the two-electron contribution to the Fock matrix by numerical integration. *Molecular Physics*, **2012**, 110, 2569-2578	1.7	5
65	The effect of protein environment on photoexcitation properties of retinal. *Journal of Physical Chemistry B*, **2012**, 116, 2249-58	3.4	39
64	Ab Initio Studies of Triplet-State Properties for Organic Semiconductor Molecules. *Journal of Physical Chemistry C*, **2012**, 116, 15203-15217	3.8	19
63	Computational methods for studies of semiconductor quantum dots and rings. *Annual Reports on the Progress of Chemistry Section C*, **2012**, 108, 96		7
62	Computational studies of photophysical properties of porphin, tetraphenylporphyrin and tetrabenzoporphyrin. *Physical Chemistry Chemical Physics*, **2012**, 14, 11508-17	3.6	51

61	A divide and conquer real-space approach for all-electron molecular electrostatic potentials and interaction energies. *Journal of Chemical Physics*, **2012**, 136, 214104	3.9	21
60	Calculation of spin-current densities using gauge-including atomic orbitals. *Journal of Chemical Physics*, **2011**, 134, 054123	3.9	65
59	The gauge including magnetically induced current method. *Physical Chemistry Chemical Physics*, **2011**, 13, 20500-18	3.6	231
58	Hydrogen-bond strengths by magnetically induced currents. *Physical Chemistry Chemical Physics*, **2011**, 13, 434-7	3.6	34
57	Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. *Journal of Chemical Physics*, **2011**, 134, 214114	3.9	52
56	Theoretical investigation of photoelectron spectra and magnetically induced current densities in ring-shaped transition-metal oxides. *Theoretical Chemistry Accounts*, **2011**, 129, 701-713	1.9	11
55	Aromatic pathways in conjugated rings connected by single bonds. *International Journal of Quantum Chemistry*, **2011**, 111, 848-857	2.1	16
54	Aromatic pathways in mono- and bisphosphorous singly M□bius twisted [28] and [30]hexaphyrins. *Physical Chemistry Chemical Physics*, **2011**, 13, 20659-65	3.6	37
53	Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. *Journal of Chemical Theory and Computation*, **2011**, 7, 2473-84	6.4	39
52	The direct approach to gravitation and electrostatics method for periodic systems. *Journal of Chemical Physics*, **2010**, 132, 024102	3.9	21
51	Magnetically induced currents in [n]cycloparaphenylenes, n = 6-11. *Journal of Organic Chemistry*, **2010**, 75, 5867-74	4.2	44
50	Aromatic pathways in twisted hexaphyrins. *Journal of Physical Chemistry A*, **2010**, 114, 7153-61	2.8	57
49	Calculation of absorption and emission spectra of [n]cycloparaphenylenes: the reason for the large Stokes shift. *Physical Chemistry Chemical Physics*, **2010**, 12, 2751-7	3.6	50
48	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	3.9	43
47	Magnetically induced current densities in aromatic, antiaromatic, homoaromatic, and nonaromatic hydrocarbons. *Journal of Physical Chemistry A*, **2009**, 113, 8668-76	2.8	138
46	Magnetically induced currents in bianthraquinodimethane-stabilized M□bius and H□kel [16]annulenes. *Journal of Organic Chemistry*, **2009**, 74, 6495-502	4.2	31
45	Calculation of magnetically induced currents in hydrocarbon nanorings. *Journal of Physical Chemistry A*, **2008**, 112, 13584-92	2.8	32
44	Polycyclic antiaromatic hydrocarbons. *Physical Chemistry Chemical Physics*, **2008**, 10, 6630-4	3.6	45

43	Exploring the Stability of Golden Fullerenes. *Journal of Physical Chemistry C*, **2008**, 112, 19311-19315	3.8	37
42	Parallel implementation of a direct method for calculating electrostatic potentials. *Journal of Chemical Physics*, **2007**, 126, 094101	3.9	25
41	On the Aromaticity of the Planar Hydrogen-Bonded (HF)3 Trimer. *Journal of Chemical Theory and Computation*, **2006**, 2, 761-4	6.4	22
40	Computational methods for studies of multiexciton complexes. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 4035-4045	1.3	9
39	Computational studies of 13C NMR chemical shifts of saccharides. *Physical Chemistry Chemical Physics*, **2005**, 7, 2561-9	3.6	28
38	Sphere currents of Buckminsterfullerene. *Angewandte Chemie - International Edition*, **2005**, 44, 1843-6	16.4	107
37	Sphere Currents of Buckminsterfullerene. *Angewandte Chemie*, **2005**, 117, 1877-1880	3.6	6
36	Universal method for computation of electrostatic potentials. *Journal of Chemical Physics*, **2005**, 122, 194107	3.9	23
35	Au32: a 24-carat golden fullerene. *Angewandte Chemie - International Edition*, **2004**, 43, 2678-81	16.4	261
34	Au32: A 24-Carat Golden Fullerene. *Angewandte Chemie*, **2004**, 116, 2732-2735	3.6	31
33	Properties of WAu12. *Physical Chemistry Chemical Physics*, **2004**, 6, 11-22	3.6	93
32	Density functional studies of the luminescence of Si29H36. *Physical Chemistry Chemical Physics*, **2004**, 6, 2044	3.6	26
31	Aromaticity Indices from Magnetic Shieldings **2004**, 395-407		8
30	Calculation of current densities using gauge-including atomic orbitals. *Journal of Chemical Physics*, **2004**, 121, 3952-63	3.9	298
29	Perturbation energy expansions based on two-component relativistic Hamiltonians. *Theoretical Chemistry Accounts*, **2003**, 110, 144-152	1.9	
28	Calculation of ring-current susceptibilities for potentially homoaromatic hydrocarbons. *Computational and Theoretical Chemistry*, **2003**, 633, 123-136		20
27	A density-functional-theory study of bacteriochlorophyll b. *Physical Chemistry Chemical Physics*, **2003**, 5, 4265	3.6	38
26	Full configuration interaction studies of phonon and photon transition rates in semiconductor quantum dots. *Molecular Physics*, **2002**, 100, 911-918	1.7	15

25	Full Configuration Interaction Calculations of Electron–Hole Correlation Effects in Strain-Induced Quantum Dots. *Physica Status Solidi (B): Basic Research*, **2001**, 224, 775-779	1.3	12
24	Tetraberyllium-μ4-oxo-hexa(arylcarboxylates). *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **2001**, 56, 979-989	1	27
23	The aromaticity and antiaromaticity of dehydroannulenes. *Physical Chemistry Chemical Physics*, **2001**, 3, 2433-2437	3.6	57
22	The quest for beryllium peroxides. *Inorganic Chemistry*, **2001**, 40, 2270-4	5.1	8
21	Carrier–Carrier Correlations in Strain-Induced Quantum Dots. *Physica Status Solidi (B): Basic Research*, **2000**, 221, 37-41	1.3	10
20	A modified variation–perturbation approach to zero-point vibrational motion. *Theoretical Chemistry Accounts*, **2000**, 103, 365-373	1.9	34
19	Interpretation of the electronic absorption spectrum of free-base porphin using time-dependent density-functional theory. *Physical Chemistry Chemical Physics*, **2000**, 2, 2275-2281	3.6	104
18	Luminescent Characterization of Solution Oligomerization Process Mediated Gold–Gold Interactions. DFT Calculations on [Au2Ag2R4L2]n Moieties. *Journal of the American Chemical Society*, **2000**, 122, 7287-7293	16.4	126
17	The aromatic character of magnesium porphyrins. *Journal of Organic Chemistry*, **2000**, 65, 5233-7	4.2	79
16	The aromatic pathways of porphins, chlorins and bacteriochlorins. *Physical Chemistry Chemical Physics*, **2000**, 2, 2145-2151	3.6	88
15	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	4.8	10
14	Ab initio determination of the induced ring current in aromatic molecules. *Physical Chemistry Chemical Physics*, **1999**, 1, 3429-3435	3.6	154
13	Relativistic multiconfiguration Hartree–Fock by means of direct perturbation theory. *International Journal of Quantum Chemistry*, **1997**, 65, 151-158	2.1	2
12	A numerical Hartree-Fock program for diatomic molecules. *Computer Physics Communications*, **1996**, 98, 346-358	4.2	115
11	Finite element multiconfiguration Hartree–Fock determination of the nuclear quadrupole moments of chlorine, potassium, and calcium isotopes. *Journal of Chemical Physics*, **1993**, 98, 7152-7158	3.9	48
10	The exactness of the extended Koopmans' theorem: A numerical study. *Journal of Chemical Physics*, **1993**, 98, 3999-4002	3.9	34
9	Response to 'Comment on 'The exactness of the extended Koopmans' theorem: A numerical study' [J. Chem. Phys. 99, 6221 (1993)]. *Journal of Chemical Physics*, **1993**, 99, 6222-6223	3.9	11
8	Large multiconfiguration Hartree–Fock calculations on the hyperfine structure of B(2P) and the nuclear quadrupole moments of 10B and 11B. *Journal of Chemical Physics*, **1991**, 94, 5051-5055	3.9	65

7	Two Fully Numerical Methods in Quantum Chemistry. *International Journal of Modern Physics C*, **1991**, 02, 455-457	1.1	2
6	Large multiconfigurational Hartree-Fock calculations on the hyperfine structure of Li(2S) and Li(2P). *Physical Review A*, **1990**, 42, 2614-2621	2.6	64
5	Two-dimensional, fully numerical molecular calculations. *Molecular Physics*, **1987**, 60, 597-604	1.7	44
4	Fully numerical hartree-fock methods for molecules. *Computer Physics Reports*, **1986**, 4, 313-344		229
3	Two-dimensional, fully numerical molecular calculations. *Molecular Physics*, **1985**, 55, 627-635	1.7	28
2	Two-dimensional, fully numerical molecular calculations. *Molecular Physics*, **1985**, 56, 1411-1418	1.7	106
1	Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. *Chemical Modelling*,1-42	2	25