Marcel Swart

List of Publications by Year in Descending Order

173 papers	7,217 citations	46 h-index	78 g-index
200 ext. papers	7,967 ext. citations	5.5 avg, IF	6.35 L-index

#	Paper	IF	Citations
173	Modulation of a η1,2-Peroxo Dicopper(II) Intermediate by Strong Interaction with Alkali Metal Ions. *Journal of the American Chemical Society*, **2021**, 143, 17751-17760	16.4	3
172	Stable, but still reactive Investigations on the effects of Lewis acid binding on copper nitrene intermediates. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2021**, 647, 1495-1502	1.3	1
171	A Pseudotetrahedral Terminal Oxoiron(IV) Complex: Mechanistic Promiscuity in C-H Bond Oxidation Reactions. *Angewandte Chemie - International Edition*, **2021**, 60, 6752-6756	16.4	7
170	A Pseudotetrahedral Terminal Oxoiron(IV) Complex: Mechanistic Promiscuity in CH Bond Oxidation Reactions. *Angewandte Chemie*, **2021**, 133, 6826-6830	3.6	2
169	NWChem: Past, present, and future. *Journal of Chemical Physics*, **2020**, 152, 184102	3.9	187
168	Stoichiometric Formation of an Oxoiron(IV) Complex by a Soluble Methane Monooxygenase Type Activation of O at an Iron(II)-Cyclam Center. *Journal of the American Chemical Society*, **2020**, 142, 5924-5928	16.4	19
167	Dealing with Spin States in Computational Organometallic Catalysis. *Topics in Organometallic Chemistry*, **2020**, 191-226	0.6	5
166	Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs. *ChemPhysChem*, **2020**, 21, 2112-2126	3.2	8
165	Sc-Promoted O-O Bond Cleavage of a (η1,2-Peroxo)diiron(III) Species Formed from an Iron(II) Precursor and O to Generate a Complex with an Fe(O) Core. *Journal of the American Chemical Society*, **2020**, 142, 4285-4297	16.4	16
164	Sequential oxidations of phenylchalcogenides by H2O2: insights into the redox behavior of selenium via DFT analysis. *New Journal of Chemistry*, **2020**, 44, 6724-6731	3.6	12
163	Density functional approximations for consistent spin and oxidation states of oxoiron complexes. *International Journal of Quantum Chemistry*, **2020**, 120, e26121	2.1	6
162	Computational NMR Spectra of o-Benzyne and Stable Guests and Their Hemicarceplexes. *Chemistry - A European Journal*, **2020**, 26, 2626-2634	4.8	2
161	A Unified Framework for Understanding Nucleophilicity and Protophilicity in the S 2/E2 Competition. *Chemistry - A European Journal*, **2020**, 26, 15538-15548	4.8	13
160	Spin-resolved charge displacement analysis as an intuitive tool for the evaluation of cPCET and HAT scenarios. *Chemical Communications*, **2020**, 56, 12146-12149	5.8	1
159	Bond orders in metalloporphyrins. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	2
158	Trapping of a Highly Reactive Oxoiron(IV) Complex in the Catalytic Epoxidation of Olefins by Hydrogen Peroxide. *Angewandte Chemie - International Edition*, **2019**, 58, 4012-4016	16.4	29
157	The Irony of Manganocene: An Interplay between the Jahn-Teller Effect and Close-Lying Electronic and Spin States. *Journal of Chemical Information and Modeling*, **2019**, 59, 1806-1810	6.1	2

156	Directed Hydroxylation of sp and sp C-H Bonds Using Stoichiometric Amounts of Cu and HO. *Inorganic Chemistry*, **2019**, 58, 7584-7592	5.1	11
155	Four-component relativistic P NMR calculations for trans-platinum(ii) complexes: importance of the solvent and dynamics in spectral simulations. *Dalton Transactions*, **2019**, 48, 8076-8083	4.3	13
154	Computational Versus Experimental Spectroscopy for Transition Metals. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 161-183	0.7	1
153	Trapping of a Highly Reactive Oxoiron(IV) Complex in the Catalytic Epoxidation of Olefins by Hydrogen Peroxide. *Angewandte Chemie*, **2019**, 131, 4052-4056	3.6	12
152	Lewis versus Brønsted Acid Activation of a Mn(IV) Catalyst for Alkene Oxidation. *Inorganic Chemistry*, **2019**, 58, 14924-14930	5.1	15
151	Understanding the Catalase-Like Activity of a Bioinspired Manganese(II) Complex with a Pentadentate NSNSN Ligand Framework. A Computational Insight into the Mechanism. *ACS Catalysis*, **2018**, 8, 2944-2958	13.1	6
150	Nucleophilic Substitution (SN2): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. *ChemPhysChem*, **2018**, 19, 1248-1248	3.2	2
149	Nucleophilic Substitution (S 2): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. *ChemPhysChem*, **2018**, 19, 1315-1330	3.2	85
148	Rotating Iron and Titanium Sandwich Complexes. *Chemistry - A European Journal*, **2018**, 24, 5070-5073	4.8	1
147	Why the Flavin Adenine Dinucleotide (FAD) Cofactor Needs To Be Covalently Linked to Complex II of the Electron-Transport Chain for the Conversion of FADH into FAD. *Chemistry - A European Journal*, **2018**, 24, 5246-5252	4.8	10
146	Catalytic Aerobic Oxidation of Alcohols by Copper Complexes Bearing Redox-Active Ligands with Tunable H-Bonding Groups. *Journal of the American Chemical Society*, **2018**, 140, 16625-16634	16.4	30
145	HO Oxidation by Fe-OOH Intermediates and Its Effect on Catalytic Efficiency. *ACS Catalysis*, **2018**, 8, 9665-9674	13.1	31
144	The influence of substituents and the environment on the NMR shielding constants of supramolecular complexes based on A-T and A-U base pairs. *Physical Chemistry Chemical Physics*, **2017**, 19, 13496-13502	3.6	9
143	Electrochemical Polymerization of Iron(III) Polypyridyl Complexes through C-C Coupling of Redox Non-innocent Phenolato Ligands. *Inorganic Chemistry*, **2017**, 56, 470-479	5.1	13
142	A Highly Reactive Oxoiron(IV) Complex Supported by a Bioinspired N O Macrocyclic Ligand. *Angewandte Chemie - International Edition*, **2017**, 56, 14384-14388	16.4	32
141	A Highly Reactive Oxoiron(IV) Complex Supported by a Bioinspired N3O Macrocyclic Ligand. *Angewandte Chemie*, **2017**, 129, 14576-14580	3.6	10
140	The role of spin states in the catalytic mechanism of the intra- and extradiol cleavage of catechols by O. *Organic and Biomolecular Chemistry*, **2017**, 15, 7860-7868	3.9	6
139	Transient Formation and Reactivity of a High-Valent Nickel(IV) Oxido Complex. *Journal of the American Chemical Society*, **2017**, 139, 8718-8724	16.4	38

138	Indirect evidence for a Ni-oxyl oxidant in the reaction of a Ni complex with peracid. *Dalton Transactions*, **2017**, 47, 246-250	4.3	9
137	Reactivity of an Fe-Oxo Complex with Protons and Oxidants. *Journal of the American Chemical Society*, **2016**, 138, 13143-13146	16.4	37
136	Tuning the Reactivity of Terminal Nickel(III)-Oxygen Adducts for C-H Bond Activation. *Journal of the American Chemical Society*, **2016**, 138, 14362-14370	16.4	50
135	Spinning around in Transition-Metal Chemistry. *Accounts of Chemical Research*, **2016**, 49, 2690-2697	24.3	92
134	Unique mononuclear Mn(II) complexes of an end-off compartmental Schiff base ligand: experimental and theoretical studies on their bio-relevant catalytic promiscuity. *Dalton Transactions*, **2016**, 45, 12409-22	4.3	46
133	Rapid determination of polarizability exaltation in fullerene-based nanostructures. *Journal of Materials Chemistry C*, **2015**, 3, 23-25	7.1	10
132	Terminal Metal□Oxo Species with Unusual Spin States **2015**, 203-227		2
131	Environment Effects on Spin States, Properties, and Dynamics from Multi-Level QM/MM Studies **2015**, 327-367		
130	General Introduction to Spin States **2015**, 1-5		1
129	Application of Density Functional and Density Functional Based Ligand Field Theory to Spin States **2015**, 7-34		6
128	Ab Initio Wavefunction Approaches to Spin States **2015**, 35-57		7
127	Experimental Techniques for Determining Spin States **2015**, 59-83		5
126	Molecular Discovery in Spin Crossover **2015**, 85-102		
125	Principles and Prospects of Spin-States Reactivity in Chemistry and Bioinorganic Chemistry **2015**, 131-156		13
124	**2015**,		33
123	Characterization and reactivity of a terminal nickel(III)-oxygen adduct. *Chemistry - A European Journal*, **2015**, 21, 3785-90	4.8	32
122	Experimental and theoretical investigation of octahedral and square-planar isothiocyanato complexes of Ni(II) with acylhydrazones of 2-(diphenylphosphino)benzaldehyde. *Polyhedron*, **2015**, 89, 271-279	2.7	10
121	Spin state relaxation of iron complexes: The case for OPBE and S12g. *Journal of the Serbian Chemical Society*, **2015**, 80, 1399-1410	0.9	14

120	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes. *Carbon Materials*, **2015**, 67-99		
119	Exploring the potential energy surface of E$_2$P$_2$ clusters (E=Group 13 element): the quest for inverse carbon-free sandwiches. *Chemistry - A European Journal*, **2014**, 20, 4583-90	4.8	17
118	Exploring the Potential Energy Surface of E2P4 Clusters (E=Group 13 Element): The Quest for Inverse Carbon-Free Sandwiches. *Chemistry - A European Journal*, **2014**, 20, 4497-4497	4.8	
117	Indenyl effect due to metal slippage? Computational exploration of rhodium-catalyzed acetylene [2+2+2] cyclotrimerization. *ChemPhysChem*, **2014**, 15, 219-28	3.2	24
116	A density functional study of the spin state energetics of polypyrazolylborato complexes of first-row transition metals. *Physical Chemistry Chemical Physics*, **2014**, 16, 14514-22	3.6	19
115	Synthesis, characterization, DFT calculation and biological activity of square-planar Ni(II) complexes with tridentate PNO ligands and monodentate pseudohalides. Part II. *European Journal of Medicinal Chemistry*, **2014**, 87, 284-97	6.8	17
114	Energetics of charges in organic semiconductors and at organic donor–acceptor interfaces. *Journal of Materials Chemistry C*, **2014**, 2, 3467-3475	7.1	16
113	Reaction Mechanisms for the Formation of Mono- And Dipropylene Glycol from the Propylene Oxide Hydrolysis over ZSM-5 Zeolite. *Journal of Physical Chemistry C*, **2014**, 118, 21952-21962	3.8	7
112	Electronic structure investigation and parametrization of biologically relevant iron-sulfur clusters. *Journal of Chemical Information and Modeling*, **2014**, 54, 613-20	6.1	22
111	Synthesis, characterization, DFT calculations, and antimicrobial activity of Pd(II) and Co(III) complexes with the condensation derivative of 2-(diphenylphosphino)benzaldehyde and Girard–T reagent. *Journal of Coordination Chemistry*, **2014**, 67, 3633-3648	1.6	6
110	The role of aromaticity in determining the molecular structure and reactivity of (endohedral metallo)fullerenes. *Chemical Society Reviews*, **2014**, 43, 5089-105	58.5	84
109	Combined Experimental and Theoretical Investigation of Ligand and Anion Controlled Complex Formation with Unprecedented Structural Features and Photoluminescence Properties of Zinc(II) Complexes. *Crystal Growth and Design*, **2014**, 14, 4111-4123	3.5	25
108	B-DNA structure and stability: the role of hydrogen bonding, π-stacking interactions, twist-angle, and solvation. *Organic and Biomolecular Chemistry*, **2014**, 12, 4691-700	3.9	51
107	Spin states of (bio)inorganic systems: Successes and pitfalls. *International Journal of Quantum Chemistry*, **2013**, 113, 2-7	2.1	86
106	Aromaticity as the driving force for the stability of non-IPR endohedral metallofullerene Bingel-Hirsch adducts. *Chemical Communications*, **2013**, 49, 8767-9	5.8	21
105	Maximum aromaticity as a guiding principle for the most suitable hosting cages in endohedral metallofullerenes. *Angewandte Chemie - International Edition*, **2013**, 52, 9275-8	16.4	48
104	A new family of hybrid density functionals. *Chemical Physics Letters*, **2013**, 580, 166-171	2.5	76
103	Unraveling the origin of the relative stabilities of group 14 M2N2(2+) (M, N = C, Si, Ge, Sn, and Pb) isomer clusters. *Journal of Physical Chemistry A*, **2013**, 117, 10462-9	2.8	12

102	A change in the oxidation state of iron: scandium is not innocent. *Chemical Communications*, **2013**, 49, 6650-2	5.8	68
101	A complete guide on the influence of metal clusters in the Diels-Alder regioselectivity of I(h)-C80 endohedral metallofullerenes. *Chemistry - A European Journal*, **2013**, 19, 14931-40	4.8	36
100	Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. *Chemical Communications*, **2013**, 49, 1220-2	5.8	38
99	Self-assembled tetragonal prismatic molecular cage highly selective for anionic guests. *Chemistry - A European Journal*, **2013**, 19, 1445-56	4.8	29
98	Computational study of the spin-state energies and UV-Vis spectra of bis(1,4,7-triazacyclononane) complexes of some first-row transition metal cations. *Physical Chemistry Chemical Physics*, **2013**, 15, 6631-9	3.6	15
97	Diels-Alder and retro-Diels-Alder cycloadditions of (1,2,3,4,5-pentamethyl)cyclopentadiene to La@C(2v)-C(82): regioselectivity and product stability. *Chemistry - A European Journal*, **2013**, 19, 4468-79	4.8	25
96	Nuclear magnetic resonance shieldings of water clusters: is it possible to reach the complete basis set limit by extrapolation?. *Molecular Physics*, **2013**, 111, 1332-1344	1.7	4
95	Intramolecular halogen-halogen bonds?. *Physical Chemistry Chemical Physics*, **2013**, 15, 11543-53	3.6	53
94	Synthesis, characterization, DFT calculations and biological activity of derivatives of 3-acetylpyridine and the zinc(II) complex with the condensation product of 3-acetylpyridine and semicarbazide. *Inorganica Chimica Acta*, **2013**, 404, 5-12	2.7	12
93	Role of spin state and ligand charge in coordination patterns in complexes of 2,6-diacetylpyridinebis(semioxamazide) with 3d-block metal ions: a density functional theory study. *Inorganic Chemistry*, **2013**, 52, 13415-23	5.1	15
92	Maximum Aromaticity as a Guiding Principle for the Most Suitable Hosting Cages in Endohedral Metallofullerenes. *Angewandte Chemie*, **2013**, 125, 9445-9448	3.6	8
91	Benchmark study on the smallest bimolecular nucleophilic substitution reaction: H?+CH□>CH□H?. *Molecules*, **2013**, 18, 7726-38	4.8	2
90	Solvent effects on hydrogen bonds in Watson□rick, mismatched, and modified DNA base pairs. *Computational and Theoretical Chemistry*, **2012**, 998, 57-63	2	25
89	Product formation in the Prato reaction on Sc3N@D(5h)-C80: preference for [5,6]-bonds, and not pyracylenic bonds. *Chemical Communications*, **2012**, 48, 2486-8	5.8	26
88	The Frozen Cage Model: A Computationally Low-Cost Tool for Predicting the Exohedral Regioselectivity of Cycloaddition Reactions Involving Endohedral Metallofullerenes. *Journal of Chemical Theory and Computation*, **2012**, 8, 1671-83	6.4	18
87	Density functional study on UV/VIS spectra of copper-protein active sites: the effect of mutations. *Chemistry and Biodiversity*, **2012**, 9, 1728-38	2.5	2
86	Chemical shifts in nucleic acids studied by density functional theory calculations and comparison with experiment. *Chemistry - A European Journal*, **2012**, 18, 12372-87	4.8	48
85	Chemical bonding in supermolecular flowers. *Physical Chemistry Chemical Physics*, **2012**, 14, 14905-10	3.6	8

84	The exohedral Diels-Alder reactivity of the titanium carbide endohedral metallofullerene Ti2C2@D(3h)-C78: comparison with D(3h)-C78 and M3N@D(3h)-C78 (M=Sc and Y) reactivity. *Chemistry - A European Journal*, **2012**, 18, 7141-54	4.8	47
83	Full exploration of the Diels-Alder cycloaddition on metallofullerenes M3N@C80 (M = Sc, Lu, Gd): the D(5h) versus I(h) isomer and the influence of the metal cluster. *Chemistry - A European Journal*, **2012**, 18, 8944-56	4.8	46
82	Ab initio absorption spectrum of NiO combining molecular dynamics with the embedded cluster approach in a discrete reaction field. *Physical Review B*, **2012**, 85,	3.3	35
81	The reactivity of endohedral fullerenes. What can be learnt from computational studies?. *Physical Chemistry Chemical Physics*, **2011**, 13, 3585-603	3.6	117
80	Dispersion corrections essential for the study of chemical reactivity in fullerenes. *Journal of Physical Chemistry A*, **2011**, 115, 3491-6	2.8	108
79	Selectivity in DNA replication. Interplay of steric shape, hydrogen bonds, π-stacking and solvent effects. *Chemical Communications*, **2011**, 47, 7326-8	5.8	47
78	A multi-scale approach to spin crossover in Fe(II) compounds. *Physical Chemistry Chemical Physics*, **2011**, 13, 10449-56	3.6	17
77	Atomic radii in molecules for use in a polarizable force field. *International Journal of Quantum Chemistry*, **2011**, 111, 1763-1772	2.1	8
76	Is the pig a good umami sensing model for humans? A comparative taste receptor study. *Flavour and Fragrance Journal*, **2011**, 26, 282-285	2.5	19
75	Inter- and intramolecular dispersion interactions. *Journal of Computational Chemistry*, **2011**, 32, 1117-27	3.5	32
74	Subtle effects control the polymerisation mechanism in α-diimine iron catalysts. *Dalton Transactions*, **2011**, 40, 8419-28	4.3	18
73	Nuclear shieldings with the SSB-D functional. *Journal of Physical Chemistry A*, **2011**, 115, 1250-6	2.8	16
72	The Chemical Reactivity of Fullerenes and Endohedral Fullerenes: A Theoretical Perspective. *Carbon Materials*, **2011**, 57-78		2
71	Density Functional Calculations of E2 and SN2 Reactions: Effects of the Choice of Method, Algorithm, and Numerical Accuracy. *Journal of Chemical Theory and Computation*, **2010**, 6, 3145-52	6.4	26
70	Magnetizabilities at Self-Interaction-Corrected Density Functional Theory Level. *Journal of Chemical Theory and Computation*, **2010**, 6, 3302-11	6.4	9
69	On the "Atomic" Polarizabilities in Small Sin Clusters and the Dielectric Constant of Bulk Silicon" *Journal of Physical Chemistry C*, **2010**, 114, 20547-20555	3.8	6
68	Spin-state-corrected Gaussian-type orbital basis sets. *Journal of Physical Chemistry A*, **2010**, 114, 7191-7	2.8	39
67	The minimum polarizability principle for spin states. *Journal of Computational Methods in Sciences and Engineering*, **2010**, 10, 609-614	0.3	

66	Accurate Description of Spin States and its Implications for Catalysis **2010**, 551-583		10
65	Adenine versus guanine quartets in aqueous solution: dispersion-corrected DFT study on the differences in stacking and hydrogen-bonding behavior. *Theoretical Chemistry Accounts*, **2010**, 125, 245-252	1.9	110
64	Differential stabilization of adenine quartets by anions and cations. *Journal of Biological Inorganic Chemistry*, **2010**, 15, 387-97	3.7	16
63	On the mechanism of action of fullerene derivatives in superoxide dismutation. *Chemistry - A European Journal*, **2010**, 16, 3207-14	4.8	39
62	Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C60 and Ng2@C60 (Ng=He Xe). *Chemistry - A European Journal*, **2010**, 16, 3878-3878	4.8	5
61	Spin-state splittings of iron(II) complexes with trispyrazolyl ligands. *Polyhedron*, **2010**, 29, 84-93	2.7	39
60	A new all-round density functional based on spin states and S(N)2 barriers. *Journal of Chemical Physics*, **2009**, 131, 094103	3.9	104
59	Switching between OPTX and PBE exchange functionals. *Journal of Computational Methods in Sciences and Engineering*, **2009**, 9, 69-77	0.3	18
58	A Ditopic Ion-Pair Receptor Based on Stacked Nucleobase Quartets. *Angewandte Chemie*, **2009**, 121, 3335-3337	3.6	23
57	Rare tautomers of 1-methyluracil and 1-methylthymine: tuning relative stabilities through coordination to PtII complexes. *Chemistry - A European Journal*, **2009**, 15, 209-18	4.8	29
56	Reactivity and regioselectivity of noble gas endohedral fullerenes Ng@C(60) and Ng(2)@C(60) (Ng=He-Xe). *Chemistry - A European Journal*, **2009**, 15, 13111-23	4.8	42
55	Homolytic versus heterolytic dissociation of alkalimetal halides: the effect of microsolvation. *ChemPhysChem*, **2009**, 10, 2955-65	3.2	13
54	Role of the variable active site residues in the function of thioredoxin family oxidoreductases. *Journal of Computational Chemistry*, **2009**, 30, 710-24	3.5	11
53	A ditopic ion-pair receptor based on stacked nucleobase quartets. *Angewandte Chemie - International Edition*, **2009**, 48, 3285-7	16.4	64
52	The Diels-Alder reaction on endohedral Y3N@C78: the importance of the fullerene strain energy. *Journal of the American Chemical Society*, **2009**, 131, 129-39	16.4	69
51	Stepwise walden inversion in nucleophilic substitution at phosphorus. *Physical Chemistry Chemical Physics*, **2009**, 11, 259-67	3.6	41
50	Chemical bonding and aromaticity in metalloporphyrins,. *Canadian Journal of Chemistry*, **2009**, 87, 1063-1073	0.9	27
49	Accurate Spin-State Energies for Iron Complexes. *Journal of Chemical Theory and Computation*, **2008**, 4, 2057-66	6.4	289

48	Importance of the basis set for the spin-state energetics of iron complexes. *Journal of Physical Chemistry A*, **2008**, 112, 6384-91	2.8	115
47	Mechanism of thioredoxin-catalyzed disulfide reduction. Activation of the buried thiol and role of the variable active-site residues. *Journal of Physical Chemistry B*, **2008**, 112, 2511-23	3.4	34
46	Chemical reactivity of D3h C78 (metallo)fullerene: regioselectivity changes induced by Sc3N encapsulation. *Journal of the American Chemical Society*, **2008**, 130, 6206-14	16.4	70
45	QUILD: QUantum-regions interconnected by local descriptions. *Journal of Computational Chemistry*, **2008**, 29, 724-34	3.5	114
44	The Discrete Reaction Field approach for calculating solvent effects. *Challenges and Advances in Computational Chemistry and Physics*, **2008**, 39-102	0.7	7
43	Conformational behavior of basic monomeric building units of glycosaminoglycans: isolated systems and solvent effect. *Journal of Physical Chemistry B*, **2007**, 111, 2313-21	3.4	12
42	Energy landscapes of nucleophilic substitution reactions: a comparison of density functional theory and coupled cluster methods. *Journal of Computational Chemistry*, **2007**, 28, 1551-1560	3.5	87
41	Proton Affinities in Water of Maingroup-Element Hydrides Effects of Hydration and Methyl Substitution. *European Journal of Inorganic Chemistry*, **2007**, 2007, 3646-3654	2.3	82
40	Nucleophilic substitution at phosphorus centers (SN2@p). *ChemPhysChem*, **2007**, 8, 2452-63	3.2	55
39	Metal ligand bonding in metallocenes: Differentiation between spin state, electrostatic and covalent bonding. *Inorganica Chimica Acta*, **2007**, 360, 179-189	2.7	167
38	Pi-pi stacking tackled with density functional theory. *Journal of Molecular Modeling*, **2007**, 13, 1245-57	2	111
37	Proton affinities of maingroup-element hydrides and noble gases: trends across the periodic table, structural effects, and DFT validation. *Journal of Computational Chemistry*, **2006**, 27, 1486-93	3.5	38
36	DRF90: a polarizable force field. *Molecular Simulation*, **2006**, 32, 471-484	2	56
35	Nucleophilic substitution at phosphorus (S(N)2@P): disappearance and reappearance of reaction barriers. *Journal of the American Chemical Society*, **2006**, 128, 10738-44	16.4	126
34	Proton Affinities of Anionic Bases: Trends Across the Periodic Table, Structural Effects, and DFT Validation. *Journal of Chemical Theory and Computation*, **2006**, 2, 281-7	6.4	46
33	Circular dichroism spectrum of [Co(en)3]3+ in water: A discrete solvent reaction field study. *International Journal of Quantum Chemistry*, **2006**, 106, 2479-2488	2.1	30
32	Optimization of strong and weak coordinates. *International Journal of Quantum Chemistry*, **2006**, 106, 2536-2544	2.1	92
31	Performance of various density functionals for the hydrogen bonds in DNA base pairs. *Chemical Physics Letters*, **2006**, 426, 415-421	2.5	141

30	Theoretical study of structure, pKa, lipophilicity, solubility, absorption, and polar surface area of some centrally acting antihypertensives. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 1715-28	3.4	70
29	QM/MM study of the role of the solvent in the formation of the charge separated excited state in 9,9'-bianthryl. *Journal of the American Chemical Society*, **2005**, 127, 11019-28	16.4	50
28	Study of Hg22+ and complexes of NpO2+ and UO22+ in solution. examples of cation-cation interactions. *Inorganic Chemistry*, **2005**, 44, 6975-82	5.1	31
27	Electronic ground states of iron porphyrin and of the first species in the catalytic reaction cycle of cytochrome P450s. *Journal of Physical Chemistry A*, **2005**, 109, 3411-7	2.8	95
26	Substrate binding in the active site of cytochrome P450cam. *Chemical Physics Letters*, **2005**, 403, 35-41	2.5	9
25	Multicomponent synthesis of 2-imidazolines. *Journal of Organic Chemistry*, **2005**, 70, 3542-53	4.2	141
24	Calculation of the redox potential of the protein azurin and some mutants. *ChemBioChem*, **2005**, 6, 738-46	3.8	46
23	Microscopic and macroscopic polarization within a combined quantum mechanics and molecular mechanics model. *Journal of Chemical Physics*, **2005**, 122, 34103	3.9	36
22	Polarizabilities of amino acid residues. *Journal of Computational Methods in Sciences and Engineering*, **2004**, 4, 419-425	0.3	16
21	Hydrogen bonds of RNA are stronger than those of DNA, but NMR monitors only presence of methyl substituent in uracil/thymine. *Journal of the American Chemical Society*, **2004**, 126, 16718-9	16.4	81
20	Active site modeling in copper azurin molecular dynamics simulations. *Journal of Molecular Modeling*, **2004**, 10, 25-31	2	18
19	Accuracy of geometries: influence of basis set, exchange□correlation potential, inclusion of core electrons, and relativistic corrections. *Theoretical Chemistry Accounts*, **2004**, 111, 56-56	1.9	12
18	Performance of the OPBE exchange-correlation functional. *Molecular Physics*, **2004**, 102, 2467-2474	1.7	330
17	Validation of Exchange□Correlation Functionals for Spin States of Iron Complexes. *Journal of Physical Chemistry A*, **2004**, 108, 5479-5483	2.8	353
16	Simulation of the substrate cavity dynamics of quercetinase. *Journal of Molecular Biology*, **2004**, 344, 725-38	6.5	9
15	Theoretical Study of Molecular Structure, Tautomerism, and Geometrical Isomerism of N-Methyl- and N-Phenyl-Substituted Cyclic Imidazolines, Oxazolines, and Thiazolines. *Structural Chemistry*, **2003**, 14, 271-278	1.8	22
14	Accuracy of geometries: influence of basis set, exchange□correlation potential, inclusion of core electrons, and relativistic corrections. *Theoretical Chemistry Accounts*, **2003**, 110, 34-41	1.9	96
13	AddRemove: A new link model for use in QM/MM studies. *International Journal of Quantum Chemistry*, **2003**, 91, 177-183	2.1	40

12	Collision effects in the nonlinear Raman response of liquid carbon disulfide. *Journal of Chemical Physics*, **2002**, 116, 3277-3285	3.9	25
11	Polarizabilities in the condensed phase and the local fields problem: A direct reaction field formulation. *Journal of Chemical Physics*, **2002**, 117, 8442-8453	3.9	42
10	Medium perturbations on the molecular polarizability calculated within a localized dipole interaction model. *Journal of Chemical Physics*, **2002**, 117, 3316-3320	3.9	35
9	Theoretical and experimental studies of the opto-electronic properties of positively charged oligo(phenylene vinylene)s: Effects of chain length and alkoxy substitution. *Journal of Chemical Physics*, **2002**, 117, 11366-11378	3.9	61
8	A charge analysis derived from an atomic multipole expansion. *Journal of Computational Chemistry*, **2001**, 22, 79-88	3.5	154
7	Solvent Induced Charge Separation in the Excited States of Symmetrical Ethylene:A Direct Reaction Field Study. *Journal of Physical Chemistry A*, **2001**, 105, 3583-3590	2.8	11
6	Some applications of the direct reaction field approach. *Computational and Theoretical Chemistry*, **1999**, 464, 191-198		10
5	IodineBenzene charge-transfer complex: Potential energy surface and transition probabilities studied at several levels of theory **1999**, 75, 709-723		44
4	Mean polarizabilities of organic molecules. A comparison of Restricted Hartree Fock, Density Functional Theory and Direct Reaction Field results. *Computational and Theoretical Chemistry*, **1998**, 458, 11-17		22
3	Molecular and Atomic Polarizabilities: Thole's Model Revisited. *Journal of Physical Chemistry A*, **1998**, 102, 2399-2407	2.8	438
2	Quantum Mechanical-Molecular Mechanical Calculations of (Hyper-)Polarizabilities with the Direct Reaction Field Approach. *ACS Symposium Series*, **1998**, 220-232	0.4	3
1	Thole's interacting polarizability model in computational chemistry practice. *Journal of Electron Spectroscopy and Related Phenomena*, **1997**, 86, 49-55	1.7	18