Tore Brinck

List of Publications by Year in descending order

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142	9,289	41344	42399
papers	citations	49 h-index	92 g-index

160	160	160	7751
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Machine learning meets mechanistic modelling for accurate prediction of experimental activation energies. Chemical Science, 2021, 12, 1163-1175.	7.4	102
2	Improving the Stability of Trinitramide by Chemical Substitution: N(NF₂)₃ has Higher Stability and Excellent Propulsion Performance. Propellants, Explosives, Pyrotechnics, 2021, 46, 245-252.	1.6	4
3	Acetic acid conversion to ketene on Cu2O(1 0 0): Reaction mechanism deduced from experimental observations and theoretical computations. Journal of Catalysis, 2021, 402, 154-165.	6.2	3
4	Utilizing the Surface Electrostatic Potential to Predict the Interactions of Pt and Ni Nanoparticles with Lewis Acids and Basesâ€"Ïƒ-Lumps and Ïƒ-Holes Govern the Catalytic Activities. Journal of Physical Chemistry C, 2020, 124, 14696-14705.	3.1	13
5	The Surface Structure of Cu2O(100): Nature of Defects. Journal of Physical Chemistry C, 2019, 123, 7696-7704.	3.1	13
6	The local electron attachment energy and the electrostatic potential as descriptors of surfaceâ€“adsorbate interactions. Physical Chemistry Chemical Physics, 2019, 21, 17001-17009.	2.8	10
7	Asymmetric Synthesis of Adjacent Triâ€•and Tetrasubstituted Carbon Stereocenters: Organocatalytic Aldol Reaction of an Hydantoin Surrogate with Azaarene 2â€€arbaldehydes. Chemistry - A European Journal, 2019, 25, 12431-12438.	3.3	15
8	Interaction of Atomic Hydrogen with the Cu₂O(100) and (111) Surfaces. Journal of Physical Chemistry C, 2019, 123, 22172-22180.	3.1	13
9	Electrostatics and polarization determine the strength of the halogen bond: a red card for charge transfer. Journal of Molecular Modeling, 2019, 25, 125.	1.8	42
10	The Molecular Surface Property Approach: A Guide to Chemical Interactions in Chemistry, Medicine, and Material Science. Advanced Theory and Simulations, 2019, 2, 1800149.	2.8	36
11	Chemical Reactivity: The Molecular Surface Property Approach: A Guide to Chemical Interactions in Chemistry, Medicine, and Material Science (Adv. Theory Simul. 1/2019). Advanced Theory and Simulations, 2019, 2, 1970003.	2.8	1
12	Theoretical Investigation into Rate-Determining Factors in Electrophilic Aromatic Halogenation. Journal of Physical Chemistry A, 2018, 122, 3270-3279.	2.5	22
13	Mechanism and regioselectivity of electrophilic aromatic nitration in solution: the validity of the transition state approach. Journal of Molecular Modeling, 2018, 24, 15.	1.8	29
14	Ïƒ-Holes and Ïƒ-lumps direct the Lewis basic and acidic interactions of noble metal nanoparticles: introducing regium bonds. Physical Chemistry Chemical Physics, 2018, 20, 2676-2692.	2.8	99
15	Nucleophilic Aromatic Substitution Reactions Described by the Local Electron Attachment Energy. Journal of Organic Chemistry, 2017, 82, 3072-3083.	3.2	38
16	Interaction of Sulfur Dioxide and Near-Ambient Pressures of Water Vapor with Cuprous Oxide Surfaces. Journal of Physical Chemistry C, 2017, 121, 24011-24024.	3.1	11
17	On the Kinetic and Thermodynamic Properties of Aryl Radicals Using Electrochemical and Theoretical Approaches. ChemElectroChem, 2017, 4, 3212-3221.	3.4	12
18	Computational analysis of the early stage of cuprous oxide sulphidation: a top-down process. Corrosion Engineering Science and Technology, 2017, 52, 50-53.	1.4	13

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19	Extending the Ïƒ-Hole Concept to Metals: An Electrostatic Interpretation of the Effects of Nanostructure in Gold and Platinum Catalysis. Journal of the American Chemical Society, 2017, 139, 11012-11015.	13.7	136
20	MD Simulations Reveal Complex Water Paths in Squaleneâ€“Hopene Cyclase: Tunnel-Obstructing Mutations Increase the Flow of Water in the Active Site. ACS Omega, 2017, 2, 8495-8506.	3.5	6
21	Local Lewis Acidity of (TiO₂)_n (n = 7â€“10) Nanoparticles Characterized by DFT-Based Descriptors: Tools for Catalyst Design. Journal of Physical Chemistry C, 2017, 121, 27483-27492.	3.1	14
22	Dehydrogenation of methanol on Cu2O(100) and (111). Journal of Chemical Physics, 2017, 146, 244702.	3.0	23
23	Ïƒ-Holes on Transition Metal Nanoclusters and Their Influence on the Local Lewis Acidity. Crystals, 2017, 7, 222.	2.2	16
24	Local Electron Attachment Energy and Its Use for Predicting Nucleophilic Reactions and Halogen Bonding. Journal of Physical Chemistry A, 2016, 120, 10023-10032.	2.5	27
25	Fragment molecular orbital study of the cAMP-dependent protein kinase catalyzed phosphoryl transfer: a comparison with the differential transition state stabilization method. Physical Chemistry Chemical Physics, 2016, 18, 15153-15161.	2.8	5
26	Reactivity at the Cu₂O(100):Cuâ€“H₂O interface: a combined DFT and PES study. Physical Chemistry Chemical Physics, 2016, 18, 30570-30584.	2.8	21
27	Aqueous Solvation and Surface Oxidation of the Cu₇ Nanoparticle: Insights from Theoretical Modeling. Journal of Physical Chemistry C, 2016, 120, 1977-1988.	3.1	12
28	Surface Reactions of H₂O₂, H₂, and O₂ in Aqueous Systems Containing ZrO₂. Journal of Physical Chemistry C, 2016, 120, 1609-1614.	3.1	16
29	Dual Lewis Acid/Lewis Base Catalyzed Acylcyanation of Aldehydes: A Mechanistic Study. Chemistry - A European Journal, 2016, 22, 3821-3829.	3.3	9
30	The Surface Structure of Cu₂O(100). Journal of Physical Chemistry C, 2016, 120, 4373-4381.	3.1	46
31	Application of reactivity descriptors to the catalytic decomposition of hydrogen peroxide at oxide surfaces. Computational and Theoretical Chemistry, 2015, 1070, 108-116.	2.5	18
32	Novel Approach for Identifying Key Residues in Enzymatic Reactions: Proton Abstraction in Ketosteroid Isomerase. Journal of Physical Chemistry B, 2014, 118, 13050-13058.	2.6	14
33	Binder Materials for Green Propellants. , 2014, , 205-234.		3
34	Some Perspectives on Sensitivity to Initiation of Detonation. , 2014, , 45-62.		20
35	Searching for the thermodynamic limit â€“ a DFT study of the step-wise water oxidation of the bipyramidal Cu₇cluster. Physical Chemistry Chemical Physics, 2014, 16, 2452-2464.	2.8	24
36	Ionization of ammonium dinitramide: decomposition pathways and ionization products. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	9

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37	Reactivity of metal oxide clusters with hydrogen peroxide and water â€“ a DFT study evaluating the performance of different exchangeâ€“correlation functionals. Physical Chemistry Chemical Physics, 2013, 15, 5539.	2.8	73
38	In situ confocal Raman micro-spectroscopy and electrochemical studies of mussel adhesive protein and ceria composite film on carbon steel in salt solutions. Electrochimica Acta, 2013, 107, 276-291.	5.2	31
39	On the method-dependence of transition state asynchronicity in Dielsâ€“Alder reactions. Physical Chemistry Chemical Physics, 2013, 15, 5108.	2.8	76
40	Control of the ambident reactivity of the nitrite ion. Organic and Biomolecular Chemistry, 2013, 11, 648-653.	2.8	33
41	In situ investigations of Fe3+ induced complexation of adsorbed Mefp-1 protein film on iron substrate. Journal of Colloid and Interface Science, 2013, 404, 62-71.	9.4	28
42	Utilizing the Ï*f*-complex stability for quantifying reactivity in nucleophilic substitution of aromatic fluorides. Beilstein Journal of Organic Chemistry, 2013, 9, 791-799.	2.2	19
43	â€œAdapted Linear Interaction Energyâ€• A Structure-Based LIE Parametrization for Fast Prediction of Proteinâ€“Ligand Affinities. Journal of Chemical Theory and Computation, 2013, 9, 1230-1239.	5.3	5
44	Mechanism of H₂O₂ Decomposition on Transition Metal Oxide Surfaces. Journal of Physical Chemistry C, 2012, 116, 9533-9543.	3.1	223
45	Envisioning an enzymatic Dielsâ€“Alder reaction by in situ acidâ€“base catalyzed diene generation. Chemical Communications, 2012, 48, 5665.	4.1	12
46	Computational design of a Dielsâ€“Alderase from a thermophilic esterase: the importance of dynamics. Journal of Computer-Aided Molecular Design, 2012, 26, 1079-1095.	2.9	12
47	Mechanistic Insights into the Stepwise Dielsâ€“Alder Reaction of 4,6-Dinitrobenzofuroxan. Organic Letters, 2012, 14, 118-121.	4.6	26
48	Electrochemical, atomic force microscopy and infrared reflection absorption spectroscopy studies of pre-formed mussel adhesive protein films on carbon steel for corrosion protection. Thin Solid Films, 2012, 520, 7136-7143.	1.8	18
49	Predicting Regioselectivity in Nucleophilic Aromatic Substitution. Journal of Organic Chemistry, 2012, 77, 3262-3269.	3.2	37
50	Stepwise Dielsâ€“Alder: More than Just an Oddity? A Computational Mechanistic Study. Journal of Organic Chemistry, 2012, 77, 6563-6573.	3.2	52
51	The Molecular Surface Structure of Ammonium and Potassium Dinitramide: A Vibrational Sum Frequency Spectroscopy and Quantum Chemical Study. Journal of Physical Chemistry C, 2011, 115, 10588-10596.	3.1	7
52	Designing a New Dielsâ€“Alderase: A Combinatorial, Semirational Approach Including Dynamic Optimization.. Journal of Chemical Information and Modeling, 2011, 51, 1906-1917.	5.4	11
53	Computational design of a lipase for catalysis of the Diels-Alder reaction. Journal of Molecular Modeling, 2011, 17, 833-849.	1.8	12
54	Experimental Detection of Trinitramide, N(NO₂)₃. Angewandte Chemie - International Edition, 2011, 50, 1145-1148.	13.8	38

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55	Racemase Activity of B. cepacia Lipase Leads to Dualâ€Function Asymmetric Dynamic Kinetic Resolution of Î±â€Aminonitriles. Angewandte Chemie - International Edition, 2011, 50, 6592-6595.	13.8	37
56	A pragmatic procedure for predicting regioselectivity in nucleophilic substitution of aromatic fluorides. Tetrahedron Letters, 2011, 52, 3150-3153.	1.4	18
57	On the formation of hydrogen gas on copper in anoxic water. Journal of Chemical Physics, 2011, 135, 084709.	3.0	24
58	Validation of a Computational Model for Predicting the Site for Electrophilic Substitution in Aromatic Systems. Journal of Organic Chemistry, 2010, 75, 4696-4705.	3.2	42
59	Generation of soluble oligomeric Î²-amyloid species via copper catalyzed oxidation with implications for Alzheimerâ€™s disease: A DFT study. Journal of Molecular Modeling, 2010, 16, 1103-1108.	1.8	5
60	Quantitative analysis of molecular surfaces: areas, volumes, electrostatic potentials and average local ionization energies. Journal of Molecular Modeling, 2010, 16, 1679-1691.	1.8	985
61	Kinetic Stability and Propellant Performance of Green Energetic Materials. Chemistry - A European Journal, 2010, 16, 6590-6600.	3.3	69
62	Diastereoselective One-Pot Tandem Synthesis of 3-Substituted Isoindolinones: A Mechanistic Investigation. Journal of Organic Chemistry, 2010, 75, 5882-5887.	3.2	38
63	On the Anomalous Decomposition and Reactivity of Ammonium and Potassium Dinitramide. Journal of Physical Chemistry A, 2010, 114, 2845-2854.	2.5	36
64	Synthesis and Mechanistic Studies of Organic Chromophores with Different Energy Levels for p-Type Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2010, 114, 4738-4748.	3.1	174
65	pH-Dependent Mutarotation of 1-Thioaldoses in Water. Unexpected Behavior of (2S)-d-Aldopyranoses. Journal of Organic Chemistry, 2010, 75, 6115-6121.	3.2	27
66	High Incident Photonâ€toâ€Current Conversion Efficiency of pâ€Type Dyeâ€Sensitized Solar Cells Based on NiO and Organic Chromophores. Advanced Materials, 2009, 21, 2993-2996.	21.0	173
67	Rhodaninedyes for dye-sensitized solar cellsâ€‰:â€‰ spectroscopy, energy levels and photovoltaic performance. Physical Chemistry Chemical Physics, 2009, 11, 133-141.	2.8	178
68	Symmetric and unsymmetric donor functionalization. comparing structural and spectral benefits of chromophores for dye-sensitized solar cells. Journal of Materials Chemistry, 2009, 19, 7232.	6.7	177
69	Molecular dynamics study of zinc binding to cysteines in a peptide mimic of the alcohol dehydrogenase structural zinc site. Physical Chemistry Chemical Physics, 2009, 11, 975-983.	2.8	54
70	The anomalous solid state decomposition of ammonium dinitramide: a matter of surface polarization. Chemical Communications, 2009, , 2896.	4.1	14
71	Synergistic activation of the Dielsâ€“Alder reaction by an organic catalyst and substituents: a computational study. Organic and Biomolecular Chemistry, 2009, 7, 1304.	2.8	18
72	Direct Epoxidation in Candida antarctica Lipase B Studied by Experiment and Theory. ChemBioChem, 2008, 9, 2443-2451.	2.6	78

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73	HCCI experiments with toluene reference fuels modeled by a semidetailed chemical kinetic model. Combustion and Flame, 2008, 155, 696-712.	5.2	195
74	Dinitraminic acid (HDN) isomerization and self-decomposition revisited. Chemical Physics, 2008, 348, 53-60.	1.9	17
75	Phosphine-catalyzed disulfide metathesis. Chemical Communications, 2008, , 6603.	4.1	85
76	Novel 1,3-Dipolar Cycloadditions of Dinitraminic Acid:â€‰ Implications for the Chemical Stability of Ammonium Dinitramide. Journal of Physical Chemistry A, 2008, 112, 2456-2463.	2.5	17
77	Supramolecular Control in Carbohydrate Epimerization: Discovery of a New Anion Hostâ'Guest System. Journal of the American Chemical Society, 2008, 130, 15270-15271.	13.7	26
78	Tuning the HOMO and LUMO Energy Levels of Organic Chromophores for Dye Sensitized Solar Cells. Journal of Organic Chemistry, 2007, 72, 9550-9556.	3.2	576
79	A combined molecular dynamics simulation and quantum chemical study on the mechanism for activation of the OxyR transcription factor by hydrogen peroxide. Organic and Biomolecular Chemistry, 2006, 4, 3468-3478.	2.8	18
80	Electrostatic potential as a measure of gas phase carbocation stability. International Journal of Quantum Chemistry, 2006, 106, 2904-2909.	2.0	15
81	Exploring the Active-Site of a Rationally Redesigned Lipase for Catalysis of Michael-Type Additions. ChemBioChem, 2005, 6, 331-336.	2.6	135
82	Elucidation of the Thermochemical Properties of Triphenyl- or Tributyl-Substituted Si-, Ge-, and Sn-Centered Radicals by Means of Electrochemical Approaches and Computations. Journal of the American Chemical Society, 2005, 127, 2677-2685.	13.7	22
83	Aldol additions with mutant lipase: analysis by experiments and theoretical calculations. Journal of Molecular Catalysis B: Enzymatic, 2004, 31, 123-128.	1.8	65
84	Thiol-ene coupling reaction of fatty acid monomers. Journal of Polymer Science Part A, 2004, 42, 6346-6352.	2.3	74
85	Polymer-assisted laser desorption/ionization analysis of small molecular weight compounds. Rapid Communications in Mass Spectrometry, 2004, 18, 841-852.	1.5	34
86	Computation of Franckâ€“Condon factors for many-atom systems: simulated photoelectron spectra of formic acid isotopologues. Chemical Physics, 2004, 302, 217-228.	1.9	6
87	The Stability of Arylpentazoles. Journal of Physical Chemistry A, 2004, 108, 7463-7467.	2.5	58
88	Computational Study of the Amination of Halobenzenes and Phenylpentazole. A Viable Route to Isolate the Pentazolate Anion?. Journal of Organic Chemistry, 2004, 69, 3222-3225.	3.2	14
89	Carbonâ'Carbon Bonds by Hydrolytic Enzymes. Journal of the American Chemical Society, 2003, 125, 874-875.	13.7	249
90	Segmental analysis of molecular surface electrostatic potentials: application to enzyme inhibition. Journal of Molecular Modeling, 2003, 9, 77-83.	1.8	20

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91	Rational design of a lipase to accommodate catalysis of Baeyer?Villiger oxidation with hydrogen peroxide. Journal of Molecular Modeling, 2003, 9, 164-171.	1.8	34
92	Detection of pentazolate anion (cyclo-N5â¯) from laser ionization and decomposition of solid p-dimethylaminophenylpentazole. Chemical Physics Letters, 2003, 379, 539-546.	2.6	114
93	Computational prediction of relative group polarizabilities. International Journal of Quantum Chemistry, 2003, 95, 632-637.	2.0	19
94	Thermochemistry of Arylselanyl Radicals and the Pertinent Ions in Acetonitrile. Journal of the American Chemical Society, 2003, 125, 2148-2157.	13.7	27
95	Reaction of Peroxyl Radicals with Ozone in Water. Journal of Physical Chemistry A, 2003, 107, 676-681.	2.5	25
96	Electronic structure calculations as a tool in the quest for experimental verification of N4. Theoretical and Computational Chemistry, 2003, , 421-439.	0.4	6
97	Solvation of Sulfur-Centered Cations and Anions in Acetonitrile. Journal of Physical Chemistry A, 2002, 106, 8827-8833.	2.5	23
98	Prediction of Solubility of Solid Organic Compounds in Solvents by UNIFAC. Industrial & Engineering Chemistry Research, 2002, 41, 5114-5124.	3.7	98
99	A theoretical study of the azide (N3) doublet states. A new route to tetraazatetrahedrane (N4): N+N3â†'N4. Journal of Chemical Physics, 2002, 116, 9740-9748.	3.0	50
100	A Theoretical Study of the Uncatalyzed and BF3-Assisted Baeyerâ¯Villiger Reactions. Journal of Organic Chemistry, 2001, 66, 1193-1199.	3.2	53
101	How Does Methyllithium Invert? A Density Functional Study. Organometallics, 2001, 20, 5134-5138.	2.3	10
102	Ab initio study of the ground state and the first excited state of the rectangular (D2h)N4 molecule. Chemical Physics Letters, 2001, 347, 220-228.	2.6	26
103	Theoretical study of the singlet electronically excited states of N4. Chemical Physics Letters, 2001, 340, 597-603.	2.6	23
104	Theoretical Study of the Triplet N4Potential Energy Surface. Journal of Physical Chemistry A, 2000, 104, 11999-12005.	2.5	45
105	Solvation of Carbanions in Organic Solvents:â€‰ A Test of the Polarizable Continuum Model. Journal of Physical Chemistry B, 2000, 104, 9887-9893.	2.6	24
106	Two potential energetic compounds: Ammonium superoxide and ammonium ozonide. Journal of Energetic Materials, 2000, 18, 89-95.	2.0	1
107	The catalytic effect of water in basic hydrolysis of methyl acetate: a theoretical study. Computational and Theoretical Chemistry, 1999, 459, 85-93.	1.5	34
108	Quantum Chemical Studies on the Thermochemistry of Alkyl and Peroxyl Radicals. Journal of Physical Chemistry A, 1999, 103, 7094-7104.	2.5	65

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109	Theoretical Studies of the Hydrolysis of the Methyl Phosphate Anion. Journal of Physical Chemistry A, 1999, 103, 5379-5386.	2.5	100
110	Ab initio and density functional theory studies of the catalytic mechanism for ester hydrolysis in serine hydrolases. International Journal of Quantum Chemistry, 1998, 69, 89-103.	2.0	54
111	The use of the electrostatic potential for analysis and prediction of intermolecular interactions. Theoretical and Computational Chemistry, 1998, , 51-93.	0.4	21
112	Modified Interaction Properties Function for the Analysis and Prediction of Lewis Basicities. Journal of Physical Chemistry A, 1997, 101, 3408-3415.	2.5	18
113	A Computational Analysis of Substituent Effects on the Oâ^'H Bond Dissociation Energy in Phenols:Â Polar Versus Radical Effects. Journal of the American Chemical Society, 1997, 119, 4239-4244.	13.7	170
114	Prediction of waterâ€“octanol partition coefficients using theoretical descriptors derived from the molecular surface area and the electrostatic potential. Journal of the Chemical Society Perkin Transactions II, 1997, , 289-294.	0.9	42
115	Force field parameterization of copper(I)-olefin systems from density functional calculations. Computational and Theoretical Chemistry, 1997, 397, 39-50.	1.5	19
116	Computational Analysis of Substituent Effects in Para-Substituted Phenoxide Ions. The Journal of Physical Chemistry, 1996, 100, 10116-10120.	2.9	30
117	Relationships of molecular surface electrostatic potentials to some macroscopic properties. Chemical Physics, 1996, 204, 289-299.	1.9	85
118	Analytical Representation and Prediction of Macroscopic Properties. ACS Symposium Series, 1995, , 109-118.	0.5	6
119	Family-independent relationships between computed molecular surface quantities and solute hydrogen bond acidity/basicity and solute-induced methanol Oâ€“H infrared frequency shifts. Canadian Journal of Chemistry, 1995, 73, 483-488.	1.1	164
120	Statistically-based interaction indices derived from molecular surface electrostatic potentials: a general interaction properties function (GIPF). Computational and Theoretical Chemistry, 1994, 307, 55-64.	1.5	183
121	Molecular surface electrostatic potentials and local ionization energies of Group V-VII hydrides and their anions: Relationships for aqueous and gas-phase acidities. International Journal of Quantum Chemistry, 1993, 48, 73-88.	2.0	146
122	Some proposed criteria for simulants in supercritical systems. Computational and Theoretical Chemistry, 1993, 281, 107-111.	1.5	12
123	Relationships between solute molecular properties and solubility in supercritical carbon dioxide. The Journal of Physical Chemistry, 1993, 97, 729-732.	2.9	48
124	Relationships of critical constants and boiling points to computed molecular surface properties. The Journal of Physical Chemistry, 1993, 97, 9369-9373.	2.9	81
125	Octanol/water partition coefficients expressed in terms of solute molecular surface areas and electrostatic potentials. Journal of Organic Chemistry, 1993, 58, 7070-7073.	3.2	69
126	Relationships between computed molecular properties and solute-solvent interactions in supercritical solutions. The Journal of Physical Chemistry, 1993, 97, 5144-5148.	2.9	38

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127	Polarizability and volume. Journal of Chemical Physics, 1993, 98, 4305-4306.	3.0	216
128	Partition coefficients of nitroaromatics expressed in terms of their molecular surface areas and electrostatic potentials. The Journal of Physical Chemistry, 1993, 97, 13807-13809.	2.9	31
129	A computational analysis of the bonding in boron trifluoride and boron trichloride and their complexes with ammonia. Inorganic Chemistry, 1993, 32, 2622-2625.	4.0	94
130	Calculated electrostatic potentials and local surface ionization energies of para-substituted anilines as measures of substituent effects. Canadian Journal of Chemistry, 1992, 70, 2209-2214.	1.1	66
131	Surface electrostatic potentials of halogenated methanes as indicators of directional intermolecular interactions. International Journal of Quantum Chemistry, 1992, 44, 57-64.	2.0	370
132	Quantitative determination of the total local polarity (charge separation) in molecules. Molecular Physics, 1992, 76, 609-617.	1.7	118
133	Investigation of relationships between solute molecule surface electrostatic potentials and solubilities in supercritical fluids. The Journal of Physical Chemistry, 1992, 96, 7938-7943.	2.9	62
134	Applications of calculated local surface ionization energies to chemical reactivity. Computational and Theoretical Chemistry, 1992, 255, 271-281.	1.5	62
135	Correlations between molecular electrostatic potentials and some experimentally-based indices of reactivity. Computational and Theoretical Chemistry, 1992, 256, 29-45.	1.5	114
136	Electrostatic potentials on the molecular surfaces of cyclic ureides. The Journal of Physical Chemistry, 1991, 95, 844-848.	2.9	49
137	Relationships between the aqueous acidities of some carbon, oxygen, and nitrogen acids and the calculated surface local ionization energies of their conjugate bases. Journal of Organic Chemistry, 1991, 56, 5012-5015.	3.2	74
138	A relationship between experimentally determined pKas and molecular surface ionization energies for some azines and azoles. Journal of Organic Chemistry, 1991, 56, 2934-2936.	3.2	68
139	Surface local ionization energies and electrostatic potentials of the conjugate bases of a series of cyclic hydrocarbons in relation to their aqueous acidities. International Journal of Quantum Chemistry, 1991, 40, 91-98.	2.0	25
140	Radial behavior of the average local ionization energies of atoms. Journal of Chemical Physics, 1991, 95, 6699-6704.	3.0	88
141	The use of the electrostatic potential at the molecular surface in recognition interactions: Dibenzo-p-dioxinsand related systems. Journal of Molecular Graphics, 1990, 8, 81-85.	1.1	37
142	Average local ionization energies on the molecular surfaces of aromatic systems as guides to chemical reactivity. Canadian Journal of Chemistry, 1990, 68, 1440-1443.	1.1	363