Peter Politzer

List of Publications by Year
in descending order

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		3515	3638
356	35,826	90	180
papers	citations	h-index	g-index

369	369	369	11933
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The conceptual power of the Hellmannâ€“Feynman theorem. Structural Chemistry, 2023, 34, 17-21.	1.0	3
2	Electronegativity: A continuing enigma. Journal of Physical Organic Chemistry, 2023, 36, .	0.9	5
3	Some molecular and crystalline factors that affect the sensitivities of explosives. Theoretical and Computational Chemistry, 2022, , 173-194.	0.2	1
4	Interpreting the variations in the kinetic and potential energies in the formation of a covalent bond. Physical Chemistry Chemical Physics, 2022, , .	1.3	1
5	Tetrel and Pnictogen Bonds Complement Hydrogen and Halogen Bonds in Framing the Interactional Landscape of Barbituric Acids. Crystal Growth and Design, 2021, 21, 642-652.	1.4	26
6	The use and misuse of van der Waals radii. Structural Chemistry, 2021, 32, 623-629.	1.0	42
7	The Ï€-hole revisited. Physical Chemistry Chemical Physics, 2021, 23, 16458-16468.	1.3	41
8	Oxatriazoles: Potential Frameworks for Energetic Compounds?. Propellants, Explosives, Pyrotechnics, 2021, 46, 222-232.	1.0	3
9	Can Counterâ€Intuitive Halogen Bonding Be Coulombic?. ChemPhysChem, 2021, 22, 1201-1207.	1.0	33
10	Identifying the most energetic electrons in a molecule: The highest occupied molecular orbital and the average local ionization energy. Computational and Theoretical Chemistry, 2021, 1199, 113192.	1.1	41
11	The Neglected Nuclei. Molecules, 2021, 26, 2982.	1.7	16
12	The many faces of fluorine: Some noncovalent interactions of fluorine compounds. Journal of Chemical Thermodynamics, 2021, 156, 106382.	1.0	21
13	Electrostatic potentials at the nuclei of atoms and molecules. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	24
14	Are HOMOâ€“LUMO gaps reliable indicators of explosive impact sensitivity?. Journal of Molecular Modeling, 2021, 27, 327.	0.8	8
15	Electrostatics and Polarization in Ïƒâ€•and Ï€â€Hole Noncovalent Interactions: An Overview. ChemPhysChem, 2020, 21, 579-588.	1.0	78
16	Hydrogen Bonding: A Coulombic Ïƒ-Hole Interaction. Journal of the Indian Institute of Science, 2020, 100, 21-30.	0.9	41
17	A general model for the solubilities of gases in liquids. Journal of Molecular Modeling, 2020, 26, 244.	0.8	2
18	Interaction and Polarization Energy Relationships in Ïƒ-Hole and Ï€-Hole Bonding. Crystals, 2020, 10, 76.	1.0	58

#	Article	IF	Citations
19	Explicit Inclusion of Polarizing Electric Fields in Ïƒ- and Ï€-Hole Interactions. Journal of Physical Chemistry A, 2019, 123, 10123-10130.	1.1	24
20	A look at bonds and bonding. Structural Chemistry, 2019, 30, 1153-1157.	1.0	29
21	Ïƒ-Holes vs. Buildups of Electronic Density on the Extensions of Bonds to Halogen Atoms. Inorganics, 2019, 7, 71.	1.2	3
22	The Kamletâ€Jacobs Parameter Ït: A Measure of Intrinsic Detonation Potential. Propellants, Explosives, Pyrotechnics, 2019, 44, 844-849.	1.0	9
23	Ïƒ-Holes and SiÂ·Â·Â·N intramolecular interactions. Journal of Molecular Modeling, 2019, 25, 101.	0.8	23
24	An Overview of Strengths and Directionalities of Noncovalent Interactions: Ïƒ-Holes and Ï€-Holes. Crystals, 2019, 9, 165.	1.0	94
25	The role of â€˜Excludedâ€™ electronic charge in noncovalent interactions. Molecular Physics, 2019, 117, 2260-2266.	0.8	9
26	Cyanine dyes: synergistic action of hydrogen, halogen and chalcogen bonds allows discrete I₄^{2â^’} anions in crystals. New Journal of Chemistry, 2018, 42, 10463-10466.	1.4	8
27	Ïƒâ€holes and Ï€â€holes: Similarities and differences. Journal of Computational Chemistry, 2018, 39, 464-471.	1.5	127
28	In search of the â€˜impenetrableâ€™ volume of a molecule in a noncovalent complex. Molecular Physics, 2018, 116, 570-577.	0.8	8
29	A perspective on quantum mechanics and chemical concepts in describing noncovalent interactions. Physical Chemistry Chemical Physics, 2018, 20, 30076-30082.	1.3	135
30	An Occamâ€™s razor approach to chemical hardness: lex parsimoniae. Journal of Molecular Modeling, 2018, 24, 332.	0.8	26
31	The Ïƒâ€Hole Coulombic Interpretation of Trihalide Anion Formation. ChemPhysChem, 2018, 19, 3044-3049.	1.0	42
32	The Hellmann-Feynman theorem: a perspective. Journal of Molecular Modeling, 2018, 24, 266.	0.8	42
33	Electronegativityâ€”a perspective. Journal of Molecular Modeling, 2018, 24, 214.	0.8	43
34	Sensitivities of ionic explosives. Molecular Physics, 2017, 115, 497-509.	0.8	9
35	Computational analysis of polyazoles and their N-oxides. Structural Chemistry, 2017, 28, 1045-1063.	1.0	16
36	Close contacts and noncovalent interactions in crystals. Faraday Discussions, 2017, 203, 113-130.	1.6	62

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37	Molecular electrostatic potentials and noncovalent interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1326.	6.2	231
38	The Ïƒ-hole revisited. Physical Chemistry Chemical Physics, 2017, 19, 32166-32178.	1.3	319
39	Fluorination promotes chalcogen bonding in crystalline solids. CrystEngComm, 2017, 19, 4955-4959.	1.3	53
40	Ïƒ-Hole Interactions: Perspectives and Misconceptions. Crystals, 2017, 7, 212.	1.0	145
41	Halogen bonding in hypervalent iodine and bromine derivatives: halonium salts. IUCrJ, 2017, 4, 411-419.	1.0	80
42	Nitro Groups vs. N-Oxide Linkages: Effects Upon Some Key Determinants of Detonation Performance. Central European Journal of Energetic Materials, 2017, 14, 3-25.	0.5	12
43	Electrostatic Potentials, Intralattice Attractive Forces and Crystal Densities of Nitrogen-Rich C,H,N,O Salts. Crystals, 2016, 6, 7.	1.0	24
44	High Performance, Low Sensitivity: Conflicting or Compatible?. Propellants, Explosives, Pyrotechnics, 2016, 41, 414-425.	1.0	189
45	Hydrogen Bonding between Metalâ€ion Complexes and Noncoordinated Water: Electrostatic Potentials and Interaction Energies. ChemPhysChem, 2016, 17, 2035-2042.	1.0	22
46	Comparative analysis of electrostatic potential maxima and minima on molecular surfaces, as determined by three methods and a variety of basis sets. Journal of Computational Science, 2016, 17, 273-284.	1.5	62
47	Perspectives on the crystal densities and packing coefficients of explosive compounds. Structural Chemistry, 2016, 27, 401-408.	1.0	26
48	A Unified View of Halogen Bonding, Hydrogen Bonding and Other Ïƒ-Hole Interactions. Challenges and Advances in Computational Chemistry and Physics, 2015, , 291-321.	0.6	21
49	Some molecular/crystalline factors that affect the sensitivities of energetic materials: molecular surface electrostatic potentials, lattice free space and maximum heat of detonation per unit volume. Journal of Molecular Modeling, 2015, 21, 25.	0.8	124
50	Mathematical modeling and physical reality in noncovalent interactions. Journal of Molecular Modeling, 2015, 21, 52.	0.8	234
51	Quantitative Analyses of Molecular Surface Electrostatic Potentials in Relation to Hydrogen Bonding and Co-Crystallization. Crystal Growth and Design, 2015, 15, 3767-3774.	1.4	74
52	Intuitive and counterintuitive noncovalent interactions of aromatic Ï€ regions with the hydrogen and the nitrogen of HCN. Journal of Computational Science, 2015, 10, 209-216.	1.5	83
53	Impact sensitivity and the maximum heat of detonation. Journal of Molecular Modeling, 2015, 21, 262.	0.8	107
54	Correct electrostatic treatment of noncovalent interactions: the importance of polarization. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 169-177.	6.2	97

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55	Insights into some Dielsâ€“Alder cycloadditions via the electrostatic potential and the reaction force constant. Computational and Theoretical Chemistry, 2015, 1053, 270-280.	1.1	21
56	Ïƒ-Hole Interactions of Covalently-Bonded Nitrogen, Phosphorus and Arsenic: A Survey of Crystal Structures. Crystals, 2014, 4, 12-31.	1.0	149
57	Role of Polarization in Halogen Bonds. Australian Journal of Chemistry, 2014, 67, 451.	0.5	66
58	Ïƒ-Hole Bonding: A Physical Interpretation. Topics in Current Chemistry, 2014, 358, 19-42.	4.0	133
59	Detonation Performance and Sensitivity. Advances in Quantum Chemistry, 2014, 69, 1-30.	0.4	70
60	Some Perspectives on Sensitivity to Initiation of Detonation. , 2014, , 45-62.		20
61	Revisiting the seemingly straightforward hydrogen cyanide/hydrogen isocyanide isomerisation. Molecular Physics, 2014, 112, 349-354.	0.8	17
62	Driving and retarding forces in a chemical reaction. Journal of Molecular Modeling, 2014, 20, 2351.	0.8	25
63	Complementarity of reaction force and electron localization function analyses of asynchronicity in bond formation in Dielsâ€“Alder reactions. Physical Chemistry Chemical Physics, 2014, 16, 6726.	1.3	62
64	Impact sensitivity and crystal lattice compressibility/free space. Journal of Molecular Modeling, 2014, 20, 2223.	0.8	121
65	Some interesting aspects of N-oxides. Molecular Physics, 2014, 112, 719-725.	0.8	27
66	Factors affecting the strengths of Ïƒ-hole electrostatic potentials. Journal of Computational Science, 2014, 5, 590-596.	1.5	76
67	Perspectives on the reaction force constant. Journal of Molecular Modeling, 2013, 19, 4111-4118.	0.8	45
68	Trends in Ïƒ-hole strengths and interactions of F3MX molecules (M = C, Si, Ge and X = F, Cl, Br, I). Journal of Molecular Modeling, 2013, 19, 2739-2746.	0.8	219
69	Enthalpy and entropy factors in gas phase halogen bonding: compensation and competition. CrystEngComm, 2013, 15, 3145.	1.3	42
70	Halogen Bonding: An Interim Discussion. ChemPhysChem, 2013, 14, 278-294.	1.0	620
71	Directional Noncovalent Interactions: Repulsion and Dispersion. Journal of Chemical Theory and Computation, 2013, 9, 2264-2275.	2.3	64
72	Halogen bonding and other Ïƒ-hole interactions: a perspective. Physical Chemistry Chemical Physics, 2013, 15, 11178.	1.3	1,401

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73	Computational analysis of relative stabilities of polyazine N-oxides. Structural Chemistry, 2013, 24, 1965-1974.	1.0	37
74	The reaction force constant as an indicator of synchronicity/nonsynchronicity in [4+2] cycloaddition processes. Physical Chemistry Chemical Physics, 2013, 15, 7311.	1.3	53
75	Fine structure in the transition region: reaction force analyses of water-assisted proton transfers. Journal of Molecular Modeling, 2013, 19, 2689-2697.	0.8	36
76	Halogen bond tunability II: the varying roles of electrostatic and dispersion contributions to attraction in halogen bonds. Journal of Molecular Modeling, 2013, 19, 4651-4659.	0.8	190
77	Definition of the halogen bond (IUPAC Recommendations 2013). Pure and Applied Chemistry, 2013, 85, 1711-1713.	0.9	1,554
78	Perspectives on the Reaction Force. Advances in Quantum Chemistry, 2012, 64, 189-209.	0.4	36
79	Hydrogenation and Fluorination of Graphene Models: Analysis via the Average Local Ionization Energy. Journal of Physical Chemistry A, 2012, 116, 8644-8652.	1.1	54
80	Perspectives on halogen bonding and other Ïƒ-hole interactions: Lex parsimoniae (Occamâ€™s Razor). Computational and Theoretical Chemistry, 2012, 998, 2-8.	1.1	333
81	The reaction force constant: an indicator of the synchronicity in double proton transfer reactions. Physical Chemistry Chemical Physics, 2012, 14, 11125.	1.3	54
82	Polarization-induced Ïƒ-holes and hydrogen bonding. Journal of Molecular Modeling, 2012, 18, 2461-2469.	0.8	121
83	Halogen bonding and beyond: factors influencing the nature of CNâ€“R and SiNâ€“R complexes with Fâ€“Cl and Cl2. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	102
84	Ïƒ-Holes, Ï€-holes and electrostatically-driven interactions. Journal of Molecular Modeling, 2012, 18, 541-548.	0.8	545
85	Fluorine-Centered Halogen Bonding: A Factor in Recognition Phenomena and Reactivity. Crystal Growth and Design, 2011, 11, 4238-4246.	1.4	225
86	The fluorine atom as a halogen bond donor, viz. a positive site. CrystEngComm, 2011, 13, 6593.	1.3	217
87	Average Local Ionization Energies as a Route to Intrinsic Atomic Electronegativities. Journal of Chemical Theory and Computation, 2011, 7, 377-384.	2.3	55
88	Non-hydrogen-Bonding Intramolecular Interactions: Important but Often Overlooked. , 2011, , 479-496.		1
89	The electrostatic potential: an overview. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 153-163.	6.2	1,049
90	Molecular surface electrostatic potentials as guides to Si-O-N angle contraction: tunable Ïƒ-holes. Journal of Molecular Modeling, 2011, 17, 2151-2157.	0.8	27

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91	Sensitivity and the available free space per molecule in the unit cell. Journal of Molecular Modeling, 2011, 17, 2569-2574.	0.8	127
92	Halogen bond tunability I: the effects of aromatic fluorine substitution on the strengths of halogen-bonding interactions involving chlorine, bromine, and iodine. Journal of Molecular Modeling, 2011, 17, 3309-3318.	0.8	374
93	Enhanced detonation sensitivities of silicon analogs of PETN: reaction force analysis and the role of Ïƒâ€“hole interactions. Theoretical Chemistry Accounts, 2010, 127, 345-354.	0.5	30
94	A possible crystal volume factor in the impact sensitivities of some energetic compounds. Journal of Molecular Modeling, 2010, 16, 895-901.	0.8	250
95	Quantitative analysis of molecular surfaces: areas, volumes, electrostatic potentials and average local ionization energies. Journal of Molecular Modeling, 2010, 16, 1679-1691.	0.8	985
96	Average local ionization energy: A review. Journal of Molecular Modeling, 2010, 16, 1731-1742.	0.8	328
97	The unique role of the nitro group in intramolecular interactions: chloronitromethanes. Structural Chemistry, 2010, 21, 139-146.	1.0	37
98	The principle of maximum hardness and structural effects of nonbonded interactions in chloronitromethanes. Computational and Theoretical Chemistry, 2010, 943, 53-58.	1.5	5
99	Directional tendencies of halogen and hydrogen bonds. International Journal of Quantum Chemistry, 2010, 110, 2823-2832.	1.0	243
100	Identification of pseudodiatomic behavior in polyatomic bond dissociation: Reaction force analysis. Journal of Chemical Physics, 2010, 132, 154308.	1.2	9
101	Reactivities of Sites on (5,5) Single-Walled Carbon Nanotubes with and without a Stone-Wales Defect. Journal of Chemical Theory and Computation, 2010, 6, 1351-1357.	2.3	126
102	Reaction Force and Its Link to Diabatic Analysis: A Unifying Approach to Analyzing Chemical Reactions. Journal of Physical Chemistry Letters, 2010, 1, 2858-2862.	2.1	46
103	Directional Weak Intermolecular Interactions: Ïƒ-Hole Bonding. Australian Journal of Chemistry, 2010, 63, 1598.	0.5	235
104	Halogen bonding: an electrostatically-driven highly directional noncovalent interaction. Physical Chemistry Chemical Physics, 2010, 12, 7748.	1.3	1,389
105	An electrostatic correction for improved crystal density predictions of energetic ionic compounds. Molecular Physics, 2010, 108, 1391-1396.	0.8	75
106	Molecular dynamics characterization of void defects in crystalline (1,3,5-trinitro-1,3,5-triazacyclohexane). Journal of Chemical Physics, 2009, 131, 204903.	1.2	29
107	Expansion of the Ïƒ-hole concept. Journal of Molecular Modeling, 2009, 15, 723-729.	0.8	669
108	Analysis of diatomic bond dissociation and formation in terms of the reaction force and the position-dependent reaction force constant. Journal of Molecular Modeling, 2009, 15, 701-706.	0.8	30

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109	The reaction force and the transition region of a reaction. Journal of Molecular Modeling, 2009, 15, 707-710.	0.8	101
110	Reaction force analyses of nitro-aci tautomerizations of trinitromethane, the elusive trinitromethanol, picric acid and 2,4-dinitro-1H-imidazole. Theoretical Chemistry Accounts, 2009, 124, 355-363.	0.5	29
111	A comparative analysis of the electrostatic potentials of some polycyclic aromatic hydrocarbons. International Journal of Quantum Chemistry, 2009, 12, 317-325.	1.0	0
112	Epoxide-Nucleophile interactions: Acid-catalyzed reaction of ethylene oxide with water. International Journal of Quantum Chemistry, 2009, 14, 291-299.	1.0	1
113	The role of hydrogen bonding in some diol epoxides. International Journal of Quantum Chemistry, 2009, 16, 47-53.	1.0	1
114	Computed effects of electric fields upon the Cï£¿NO₂ and Nï£¿NO₂ bonds of nitromethane and dimethylnitramine. International Journal of Quantum Chemistry, 2009, 109, 3-7.	1.0	24
115	Computational determination of effects of electric fields upon â€œtrigger linkagesâ€• of prototypical energetic molecules. International Journal of Quantum Chemistry, 2009, 109, 534-539.	1.0	31
116	Electrostatically driven complexes of SiF₄ with amines. International Journal of Quantum Chemistry, 2009, 109, 3773-3780.	1.0	43
117	Chlorotrinitromethane and its exceptionally short carbonâ€“chlorine bond. Nature Chemistry, 2009, 1, 229-235.	6.6	65
118	An electrostatic interaction correction for improved crystal density prediction. Molecular Physics, 2009, 107, 2095-2101.	0.8	365
119	Links between surface electrostatic potentials of energetic molecules, impact sensitivities and Câ€“NO₂/Nâ€“NO₂ bond dissociation energies. Molecular Physics, 2009, 107, 89-97.	0.8	280
120	BrÂ·Â·Â·O Complexes as Probes of Factors Affecting Halogen Bonding: Interactions of Bromobenzenes and Bromopyrimidines with Acetone. Journal of Chemical Theory and Computation, 2009, 5, 155-163.	2.3	303
121	Reaction Force Analysis of Solvent Effects in the Addition of HCl to Propene. Journal of Physical Chemistry A, 2009, 113, 6500-6503.	1.1	32
122	Average Local Ionization Energies in the Hartreeâ^'Fock and Kohnâ^'Sham Theories. Journal of Physical Chemistry A, 2009, 113, 1384-1389.	1.1	32
123	An Overview of Ïƒ-Hole Bonding, an Important and Widely-Occurring Noncovalent Interaction. , 2009, , 149-163.		16
124	Intra- and intermolecular electrostatic interactions and their significance for the structure, acidity, and tautomerization behavior of trinitromethane. Journal of Chemical Physics, 2009, 130, 104304.	1.2	17
125	The Electrostatic Potential as a Guide to Molecular Interactive Behavior. , 2009, , .		5
126	Reaction Force. , 2009, , .		5

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127	Why are dimethyl sulfoxide and dimethyl sulfone such good solvents?. Journal of Molecular Modeling, 2008, 14, 689-697.	0.8	159
128	Ïƒ-hole bonding between like atoms; a fallacy of atomic charges. Journal of Molecular Modeling, 2008, 14, 659-665.	0.8	368
129	Blue shifts vs red shifts in Ïƒ-hole bonding. Journal of Molecular Modeling, 2008, 14, 699-704.	0.8	231
130	Computational characterization of the hydroxylamino (ï£¿NHï£¿OH) group. Journal of Physical Organic Chemistry, 2008, 21, 155-162.	0.9	9
131	Simultaneous Ïƒâ€hole and hydrogen bonding by sulfurâ€•and seleniumâ€containing heterocycles. International Journal of Quantum Chemistry, 2008, 108, 2770-2781.	1.0	172
132	Reaction force constant and projected force constants of vibrational modes along the path of an intramolecular proton transfer reaction. Chemical Physics Letters, 2008, 456, 135-140.	1.2	80
133	The Position-Dependent Reaction Force Constant in Bond Dissociation/Formation. Collection of Czechoslovak Chemical Communications, 2008, 73, 822-830.	1.0	12
134	Chapter 3 Charge delocalization in (n, 0) model carbon nanotubes. Theoretical and Computational Chemistry, 2007, 17, 82-95.	0.2	1
135	Molecular Electrostatic Potentials and Chemical Reactivity. Reviews in Computational Chemistry, 2007, , 273-312.	1.5	153
136	An Operational Definition of Relative Hardness. Collection of Czechoslovak Chemical Communications, 2007, 72, 51-63.	1.0	12
137	Chapter 8 The average local ionization energy: concepts and applications. Theoretical and Computational Chemistry, 2007, 19, 119-137.	0.2	35
138	Reaction Force Decomposition of Activation Barriers To Elucidate Solvent Effects. Journal of Physical Chemistry A, 2007, 111, 2455-2457.	1.1	71
139	A predicted new type of directional noncovalent interaction. International Journal of Quantum Chemistry, 2007, 107, 2286-2292.	1.0	341
140	A noteworthy feature of bond dissociation/formation reactions. International Journal of Quantum Chemistry, 2007, 107, 2153-2157.	1.0	30
141	Ïƒ-Hole bonding and hydrogen bonding: Competitive interactions. International Journal of Quantum Chemistry, 2007, 107, 3046-3052.	1.0	305
142	Halogen bonding: the Ïƒ-hole. Journal of Molecular Modeling, 2007, 13, 291-296.	0.8	2,004
143	Molecular surface electrostatic potentials and anesthetic activity. Journal of Molecular Modeling, 2007, 13, 313-318.	0.8	62
144	An overview of halogen bonding. Journal of Molecular Modeling, 2007, 13, 305-311.	0.8	1,284

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145	Halogen bonding and the design of new materials: organic bromides, chlorides and perhaps even fluorides as donors. Journal of Molecular Modeling, 2007, 13, 643-650.	0.8	342
146	Ï*f*-hole bonding: molecules containing group VI atoms. Journal of Molecular Modeling, 2007, 13, 1033-1038.	0.8	475
147	The Remarkable Capacities of (6,0) Carbon and Carbon/Boron/Nitrogen Model Nanotubes for Transmission of Electronic Effects. Challenges and Advances in Computational Chemistry and Physics, 2007, , 487-504.	0.6	1
148	Analysis of the Reaction Force for a Gas Phase SN2 Process:Â CH3Cl + H2O â†' CH3OH + HClâ€. Journal of Physical Chemistry A, 2006, 110, 756-761.	1.1	59
149	Computational determination of the relative polarizabilities of molecular components. International Journal of Quantum Chemistry, 2006, 106, 2347-2355.	1.0	12
150	Electrostatic potential as a measure of gas phase carbocation stability. International Journal of Quantum Chemistry, 2006, 106, 2904-2909.	1.0	15
151	A link between the ionization energy ratios of an atom and its electronegativity and hardness. Chemical Physics Letters, 2006, 431, 195-198.	1.2	23
152	Quantitative Approaches to Solute-Solvent Interactions. , 2006, , 1-63.		6
153	The Use of the Molecular Electrostatic Potential in Medicinal Chemistry. Methods and Principles in Medicinal Chemistry, 2005, , 233-254.	0.3	5
154	Effects of different caps on model nanotube surface properties. Microelectronic Engineering, 2005, 81, 485-493.	1.1	14
155	Connection between the average local ionization energy and the Fukui function. Chemical Physics Letters, 2005, 407, 143-146.	1.2	34
156	Comparative analysis of surface electrostatic potentials of carbon, boron/nitrogen and carbon/boron/nitrogen model nanotubes. Journal of Molecular Modeling, 2005, 11, 1-7.	0.8	57
157	An unusual feature of end-substituted model carbon (6,0) nanotubes. Journal of Molecular Modeling, 2005, 11, 258-264.	0.8	25
158	The reaction force: Three key points along an intrinsic reaction coordinate. Journal of Chemical Sciences, 2005, 117, 467-472.	0.7	122
159	Computational prediction of standard gas, liquid, and solid-phase heats of formation and heats of vaporization and sublimation. International Journal of Quantum Chemistry, 2005, 105, 341-347.	1.0	119
160	Atomic energies from electrostatic potentials at nuclei: direct evaluation. Molecular Physics, 2005, 103, 2105-2108.	0.8	3
161	Electronegativity and Average Local Ionization Energy. Collection of Czechoslovak Chemical Communications, 2005, 70, 550-558.	1.0	20
162	Electronic Density Approaches to the Energetics of Noncovalent Interactions. International Journal of Molecular Sciences, 2004, 5, 130-140.	1.8	4

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163	Computational Determination of Nitroaromatic Solid Phase Heats of Formation. Structural Chemistry, 2004, 15, 469-478.	1.0	32
164	Local ionization energy and local polarizability. International Journal of Quantum Chemistry, 2004, 96, 394-401.	1.0	43
165	Noncovalent intermolecular energetics: RDX crystal. International Journal of Quantum Chemistry, 2004, 100, 733-739.	1.0	13
166	Calculation of electrostatic and polarization energies from electron densities. Journal of Chemical Physics, 2004, 120, 3152-3157.	1.2	12
167	Analysis of two intramolecular proton transfer processes in terms of the reaction force. Journal of Chemical Physics, 2004, 121, 4570-4576.	1.2	78
168	Nitroacetylene:Â Computed Heats of Formation and Analysis of Reaction Mechanisms with Vinyl Ethers. Journal of Physical Chemistry A, 2004, 108, 3493-3498.	1.1	2
169	Density Functional Tight-Binding Studies of Carbon Nanotube Structures. Structural Chemistry, 2003, 14, 431-443.	1.0	44
170	Segmental analysis of molecular surface electrostatic potentials: application to enzyme inhibition. Journal of Molecular Modeling, 2003, 9, 77-83.	0.8	20
171	Electrostatic potentials and covalent radii. Journal of Computational Chemistry, 2003, 24, 505-511.	1.5	34
172	Computational prediction of relative group polarizabilities. International Journal of Quantum Chemistry, 2003, 95, 632-637.	1.0	19
173	Characterization of Surface Electrostatic Potentials of some (5,5) and (n,1) Carbon and Boron/Nitrogen Model Nanotubes. Nano Letters, 2003, 3, 21-28.	4.5	124
174	Computational approaches to heats of formation. Theoretical and Computational Chemistry, 2003, 12, 247-277.	0.2	4
175	Sensitivity Correlations. Theoretical and Computational Chemistry, 2003, , 5-23.	0.2	18
176	Some Exact Energy Relationships. , 2003, , 631-638.		2
177	Molecular Electrostatic Potentials. , 2003, , .		1
178	THE FUNDAMENTAL SIGNIFICANCE OF ELECTROSTATIC POTENTIALS AT NUCLEI. , 2002, , 63-84.		3
179	Atomic polarizability, volume and ionization energy. Journal of Chemical Physics, 2002, 117, 8197-8202.	1.2	82
180	The fundamental nature and role of the electrostatic potential in atoms and molecules. Theoretical Chemistry Accounts, 2002, 108, 134-142.	0.5	965

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181	Atomic and molecular energies in terms of electrostatic potentials at nuclei. International Journal of Quantum Chemistry, 2002, 90, 459-463.	1.0	23
182	The complementary roles of molecular surface electrostatic potentials and average local ionization energies with respect to electrophilic processes. International Journal of Quantum Chemistry, 2002, 88, 19-27.	1.0	166
183	Molecular Dynamics Simulations of Energetic Solids. Structural Chemistry, 2002, 13, 105-113.	1.0	38
184	Energetics of Aluminum Combustion. Journal of Physical Chemistry A, 2001, 105, 7473-7480.	1.1	56
185	Comparison of Quantum Chemical Parameters and Hammett Constants in Correlating pKaValues of Substituted Anilines. Journal of Organic Chemistry, 2001, 66, 6919-6925.	1.7	158
186	Computational prediction of condensed phase properties from statistical characterization of molecular surface electrostatic potentials. Fluid Phase Equilibria, 2001, 185, 129-137.	1.4	89
187	Computed molecular surface electrostatic potentials of two groups of reverse transcriptase inhibitors: Relationships to anti-HIV-1 activities. International Journal of Quantum Chemistry, 2001, 83, 115-121.	1.0	16
188	Computational characterization of nucleotide bases: Molecular surface electrostatic potentials and local ionization energies, and local polarization energies. International Journal of Quantum Chemistry, 2001, 83, 245-254.	1.0	50
189	Molecular surface electrostatic potentials in relation to noncovalent interactions in biological systems. International Journal of Quantum Chemistry, 2001, 85, 676-684.	1.0	217
190	Electronegativities, electrostatic potentials and covalent radii. Computational and Theoretical Chemistry, 2001, 549, 69-76.	1.5	32
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