Jane S Murray

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/10240931/publications.pdf

Version: 2024-02-01

165 papers	23,760 citations	15504 65 h-index	7348 152 g-index
174 all docs	174 docs citations	174 times ranked	8904 citing authors

#	Article	IF	Citations
1	Electronegativity: A continuing enigma. Journal of Physical Organic Chemistry, 2023, 36, .	1.9	5
2	Interpreting the variations in the kinetic and potential energies in the formation of a covalent bond. Physical Chemistry Chemical Physics, 2022, , .	2.8	1
3	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.	3.0	26
4	The use and misuse of van der Waals radii. Structural Chemistry, 2021, 32, 623-629.	2.0	42
5	The Ï€-hole revisited. Physical Chemistry Chemical Physics, 2021, 23, 16458-16468.	2.8	41
6	Oxatriazoles: Potential Frameworks for Energetic Compounds?. Propellants, Explosives, Pyrotechnics, 2021, 46, 222-232.	1.6	3
7	Can Counterâ€Intuitive Halogen Bonding Be Coulombic?. ChemPhysChem, 2021, 22, 1201-1207.	2.1	33
8	The Neglected Nuclei. Molecules, 2021, 26, 2982.	3.8	16
9	Electrostatic potentials at the nuclei of atoms and molecules. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	24
10	Are HOMOâ€“LUMO gaps reliable indicators of explosive impact sensitivity?. Journal of Molecular Modeling, 2021, 27, 327.	1.8	8
11	Electrostatics and Polarization in Ïƒâ€•and Ï€â€Hole Noncovalent Interactions: An Overview. ChemPhysChem, 2020, 21, 579-588.	2.1	78
12	Hydrogen Bonding: A Coulombic Ïƒ-Hole Interaction. Journal of the Indian Institute of Science, 2020, 100, 21-30.	1.9	41
13	A general model for the solubilities of gases in liquids. Journal of Molecular Modeling, 2020, 26, 244.	1.8	2
14	Interaction and Polarization Energy Relationships in Ïƒ-Hole and Ï€-Hole Bonding. Crystals, 2020, 10, 76.	2.2	58
15	â€œConformation pinningâ€•by anion attachment enabling separation of isomeric steroid monomers by ion mobility spectrometry. Journal of Mass Spectrometry, 2020, 55, .	1.6	7
16	Explicit Inclusion of Polarizing Electric Fields in Ïƒ- and Ï€-Hole Interactions. Journal of Physical Chemistry A, 2019, 123, 10123-10130.	2.5	24
17	A look at bonds and bonding. Structural Chemistry, 2019, 30, 1153-1157.	2.0	29
18	Ïƒ-Holes vs. Buildups of Electronic Density on the Extensions of Bonds to Halogen Atoms. Inorganics, 2019, 7, 71.	2.7	3

#	Article	IF	Citations
19	The Kamletâ€Jacobs Parameter Ï†: A Measure of Intrinsic Detonation Potential. Propellants, Explosives, Pyrotechnics, 2019, 44, 844-849.	1.6	9
20	Ïƒ-Holes and SiÂ·Â·Â·N intramolecular interactions. Journal of Molecular Modeling, 2019, 25, 101.	1.8	23
21	An Overview of Strengths and Directionalities of Noncovalent Interactions: Ïƒ-Holes and Ï€-Holes. Crystals, 2019, 9, 165.	2.2	94
22	Chalcogen Bonds in Crystals of Bis(o-anilinium)diselenide Salts. Crystal Growth and Design, 2019, 19, 1149-1154.	3.0	16
23	The role of â€˜Excludedâ€™ electronic charge in noncovalent interactions. Molecular Physics, 2019, 117, 2260-2266.	1.7	9
24	Anesthetic activity and the electrostatic potential (revisited). Journal of Molecular Modeling, 2018, 24, 19.	1.8	3
25	Foreword for Festschrift for Peterâ€™s 80th birthday. Journal of Molecular Modeling, 2018, 24, 1.	1.8	13
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.	2.8	8
27	Ïƒâ€holes and Ï€â€holes: Similarities and differences. Journal of Computational Chemistry, 2018, 39, 464-471.	3.3	127
28	In search of the â€˜impenetrableâ€™ volume of a molecule in a noncovalent complex. Molecular Physics, 2018, 116, 570-577.	1.7	8
29	An Occamâ€™s razor approach to chemical hardness: lex parsimoniae. Journal of Molecular Modeling, 2018, 24, 332.	1.8	26
30	The Ïƒâ€Hole Coulombic Interpretation of Trihalide Anion Formation. ChemPhysChem, 2018, 19, 3044-3049.	2.1	42
31	The Hellmann-Feynman theorem: a perspective. Journal of Molecular Modeling, 2018, 24, 266.	1.8	42
32	Electronegativityâ€”a perspective. Journal of Molecular Modeling, 2018, 24, 214.	1.8	43
33	Sensitivities of ionic explosives. Molecular Physics, 2017, 115, 497-509.	1.7	9
34	Computational analysis of polyazoles and their N-oxides. Structural Chemistry, 2017, 28, 1045-1063.	2.0	16
35	Close contacts and noncovalent interactions in crystals. Faraday Discussions, 2017, 203, 113-130.	3.2	62
36	The influence of the metal cations and microhydration on the reaction trajectory of the N3 â†” O2 thymine proton transfer: Quantum mechanical study. Journal of Computational Chemistry, 2017, 38, 2680-2692.	3.3	4

#	Article	IF	Citations
37	Molecular electrostatic potentials and noncovalent interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1326.	14.6	231
38	The Ïƒ-hole revisited. Physical Chemistry Chemical Physics, 2017, 19, 32166-32178.	2.8	319
39	Fluorination promotes chalcogen bonding in crystalline solids. CrystEngComm, 2017, 19, 4955-4959.	2.6	53
40	Ïƒ-Hole Interactions: Perspectives and Misconceptions. Crystals, 2017, 7, 212.	2.2	145
41	Halogen bonding in hypervalent iodine and bromine derivatives: halonium salts. IUCrJ, 2017, 4, 411-419.	2.2	80
42	Electrostatic Potentials, Intralattice Attractive Forces and Crystal Densities of Nitrogen-Rich C,H,N,O Salts. Crystals, 2016, 6, 7.	2.2	24
43	Hydrogen Bonding between Metalâ€Ion Complexes and Noncoordinated Water: Electrostatic Potentials and Interaction Energies. ChemPhysChem, 2016, 17, 2035-2042.	2.1	22
44	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.	2.9	62
45	Perspectives on the crystal densities and packing coefficients of explosive compounds. Structural Chemistry, 2016, 27, 401-408.	2.0	26
46	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
47	Quantitative Analyses of Molecular Surface Electrostatic Potentials in Relation to Hydrogen Bonding and Co-Crystallization. Crystal Growth and Design, 2015, 15, 3767-3774.	3.0	74
48	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.	2.9	83
49	Impact sensitivity and the maximum heat of detonation. Journal of Molecular Modeling, 2015, 21, 262.	1.8	107
50	Correct electrostatic treatment of noncovalent interactions: the importance of polarization. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 169-177.	14.6	97
51	Ïƒ-Hole Interactions of Covalently-Bonded Nitrogen, Phosphorus and Arsenic: A Survey of Crystal Structures. Crystals, 2014, 4, 12-31.	2.2	149
52	Ïƒ-Hole Bonding: A Physical Interpretation. Topics in Current Chemistry, 2014, 358, 19-42.	4.0	133
53	Some Perspectives on Sensitivity to Initiation of Detonation. , 2014, , 45-62.		20
54	Revisiting the seemingly straightforward hydrogen cyanide/hydrogen isocyanide isomerisation. Molecular Physics, 2014, 112, 349-354.	1.7	17

#	Article	IF	Citations
55	Some interesting aspects of N-oxides. Molecular Physics, 2014, 112, 719-725.	1.7	27
56	Factors affecting the strengths of Ïƒ-hole electrostatic potentials. Journal of Computational Science, 2014, 5, 590-596.	2.9	76
57	Density functional theory study of Te(CN)2, Te(CN)(NC), and Te(NC)2 and their isomerizations. Structural Chemistry, 2013, 24, 2047-2057.	2.0	7
58	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.	1.8	219
59	Enthalpy and entropy factors in gas phase halogen bonding: compensation and competition. CrystEngComm, 2013, 15, 3145.	2.6	42
60	Halogen Bonding: An Interim Discussion. ChemPhysChem, 2013, 14, 278-294.	2.1	620
61	Directional Noncovalent Interactions: Repulsion and Dispersion. Journal of Chemical Theory and Computation, 2013, 9, 2264-2275.	5.3	64
62	Halogen bonding and other Ïƒ-hole interactions: a perspective. Physical Chemistry Chemical Physics, 2013, 15, 11178.	2.8	1,401
63	Computational analysis of relative stabilities of polyazine N-oxides. Structural Chemistry, 2013, 24, 1965-1974.	2.0	37
64	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.	1.8	190
65	Perspectives on halogen bonding and other Ïƒ-hole interactions: Lex parsimoniae (Occamâ€™s Razor). Computational and Theoretical Chemistry, 2012, 998, 2-8.	2.5	333
66	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.	1.4	102
67	Ïƒ-Holes, Ï€-holes and electrostatically-driven interactions. Journal of Molecular Modeling, 2012, 18, 541-548.	1.8	545
68	Fluorine-Centered Halogen Bonding: A Factor in Recognition Phenomena and Reactivity. Crystal Growth and Design, 2011, 11, 4238-4246.	3.0	225
69	The fluorine atom as a halogen bond donor, viz. a positive site. CrystEngComm, 2011, 13, 6593.	2.6	217
70	Average Local Ionization Energies as a Route to Intrinsic Atomic Electronegativities. Journal of Chemical Theory and Computation, 2011, 7, 377-384.	5.3	55
71	The electrostatic potential: an overview. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 153-163.	14.6	1,049
72	Molecular surface electrostatic potentials as guides to Si-O-N angle contraction: tunable Ïƒ-holes. Journal of Molecular Modeling, 2011, 17, 2151-2157.	1.8	27

#	Article	IF	Citations
73	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.	1.8	374
74	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.	1.4	30
75	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
76	The unique role of the nitro group in intramolecular interactions: chloronitromethanes. Structural Chemistry, 2010, 21, 139-146.	2.0	37
77	Directional tendencies of halogen and hydrogen bonds. International Journal of Quantum Chemistry, 2010, 110, 2823-2832.	2.0	243
78	Identification of pseudodiatomic behavior in polyatomic bond dissociation: Reaction force analysis. Journal of Chemical Physics, 2010, 132, 154308.	3.0	9
79	Directional Weak Intermolecular Interactions: Ïƒ-Hole Bonding. Australian Journal of Chemistry, 2010, 63, 1598.	0.9	235
80	Halogen bonding: an electrostatically-driven highly directional noncovalent interaction. Physical Chemistry Chemical Physics, 2010, 12, 7748.	2.8	1,389
81	An electrostatic correction for improved crystal density predictions of energetic ionic compounds. Molecular Physics, 2010, 108, 1391-1396.	1.7	75
82	Expansion of the Ïƒ-hole concept. Journal of Molecular Modeling, 2009, 15, 723-729.	1.8	669
83	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.	1.8	30
84	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.	1.4	29
85	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.	2.0	24
86	Computational determination of effects of electric fields upon â€œtrigger linkagesâ€•of prototypical energetic molecules. International Journal of Quantum Chemistry, 2009, 109, 534-539.	2.0	31
87	Electrostatically driven complexes of SiF₄ with amines. International Journal of Quantum Chemistry, 2009, 109, 3773-3780.	2.0	43
88	An electrostatic interaction correction for improved crystal density prediction. Molecular Physics, 2009, 107, 2095-2101.	1.7	365
89	Links between surface electrostatic potentials of energetic molecules, impact sensitivities and Câ€“NO₂/Nâ€“NO₂bond dissociation energies. Molecular Physics, 2009, 107, 89-97.	1.7	280
90	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.	5.3	303

#	Article	IF	Citations
91	Intra- and intermolecular electrostatic interactions and their significance for the structure, acidity, and tautomerization behavior of trinitromethane. Journal of Chemical Physics, 2009, 130, 104304.	3.0	17
92	Why are dimethyl sulfoxide and dimethyl sulfone such good solvents?. Journal of Molecular Modeling, 2008, 14, 689-697.	1.8	159
93	Ïƒ-hole bonding between like atoms; a fallacy of atomic charges. Journal of Molecular Modeling, 2008, 14, 659-665.	1.8	368
94	Blue shifts vs red shifts in Ïƒ-hole bonding. Journal of Molecular Modeling, 2008, 14, 699-704.	1.8	231
95	Computational characterization of the hydroxylamino (ï£¿NHï£¿OH) group. Journal of Physical Organic Chemistry, 2008, 21, 155-162.	1.9	9
96	Simultaneous Ïƒâ€hole and hydrogen bonding by sulfurâ€•and seleniumâ€containing heterocycles. International Journal of Quantum Chemistry, 2008, 108, 2770-2781.	2.0	172
97	Molecular Electrostatic Potentials and Chemical Reactivity. Reviews in Computational Chemistry, 2007, , 273-312.	1.5	153
98	An Operational Definition of Relative Hardness. Collection of Czechoslovak Chemical Communications, 2007, 72, 51-63.	1.0	12
99	A predicted new type of directional noncovalent interaction. International Journal of Quantum Chemistry, 2007, 107, 2286-2292.	2.0	341
100	A noteworthy feature of bond dissociation/formation reactions. International Journal of Quantum Chemistry, 2007, 107, 2153-2157.	2.0	30
101	Ïƒ-Hole bonding and hydrogen bonding: Competitive interactions. International Journal of Quantum Chemistry, 2007, 107, 3046-3052.	2.0	305
102	Halogen bonding: the Ïƒ-hole. Journal of Molecular Modeling, 2007, 13, 291-296.	1.8	2,004
103	An overview of halogen bonding. Journal of Molecular Modeling, 2007, 13, 305-311.	1.8	1,284
104	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.	1.8	342
105	Ïƒ-hole bonding: molecules containing group VI atoms. Journal of Molecular Modeling, 2007, 13, 1033-1038.	1.8	475
106	Computational determination of the relative polarizabilities of molecular components. International Journal of Quantum Chemistry, 2006, 106, 2347-2355.	2.0	12
107	Electrostatic potential as a measure of gas phase carbocation stability. International Journal of Quantum Chemistry, 2006, 106, 2904-2909.	2.0	15
108	The Use of the Molecular Electrostatic Potential in Medicinal Chemistry. Methods and Principles in Medicinal Chemistry, 2005, , 233-254.	0.3	5

#	Article	IF	Citations
109	The reaction force: Three key points along an intrinsic reaction coordinate. Journal of Chemical Sciences, 2005, 117, 467-472.	1.5	122
110	Relationships between aqueous acidities and computed surface-electrostatic potentials and local ionization energies of substituted phenols and benzoic acids. Journal of Molecular Modeling, 2004, 10, 235.	1.8	33
111	Local ionization energy and local polarizability. International Journal of Quantum Chemistry, 2004, 96, 394-401.	2.0	43
112	Density Functional Tight-Binding Studies of Carbon Nanotube Structures. Structural Chemistry, 2003, 14, 431-443.	2.0	44
113	Computational prediction of relative group polarizabilities. International Journal of Quantum Chemistry, 2003, 95, 632-637.	2.0	19
114	THE FUNDAMENTAL SIGNIFICANCE OF ELECTROSTATIC POTENTIALS AT NUCLEI. , 2002, , 63-84.		3
115	Atomic polarizability, volume and ionization energy. Journal of Chemical Physics, 2002, 117, 8197-8202.	3.0	82
116	The fundamental nature and role of the electrostatic potential in atoms and molecules. Theoretical Chemistry Accounts, 2002, 108, 134-142.	1.4	965
117	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.	2.0	166
118	Computational prediction of condensed phase properties from statistical characterization of molecular surface electrostatic potentials. Fluid Phase Equilibria, 2001, 185, 129-137.	2.5	89
119	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.	2.0	16
120	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.	2.0	50
121	Molecular surface electrostatic potentials in relation to noncovalent interactions in biological systems. International Journal of Quantum Chemistry, 2001, 85, 676-684.	2.0	217
122	Prediction of solvation free energies from computed properties of solute molecular surfaces. International Journal of Quantum Chemistry, 2000, 76, 643-647.	2.0	17
123	Density functional study of dimers of dimethylnitramine. International Journal of Quantum Chemistry, 2000, 80, 184-192.	2.0	62
124	Computed molecular surface electrostatic potentials of the nonionic and zwitterionic forms of glycine, histidine, and tetracycline. International Journal of Quantum Chemistry, 2000, 80, 1216-1223.	2.0	28
125	Two potential energetic compounds: Ammonium superoxide and ammonium ozonide. Journal of Energetic Materials, 2000, 18, 89-95.	2.0	1
126	Conformational dependence of molecular surface electrostatic potentials. International Journal of Quantum Chemistry, 1999, 75, 267-273.	2.0	29

#	Article	IF	Citations
127	Prediction of Aqueous Solvation Free Energies from Properties of Solute Molecular Surface Electrostatic Potentials. Journal of Physical Chemistry A, 1999, 103, 1853-1856.	2.5	64
128	Statistical analysis of the molecular surface electrostatic potential: an approach to describing noncovalent interactions in condensed phases. Computational and Theoretical Chemistry, 1998, 425, 107-114.	1.5	255
129	Comparison of density functional and Hartree-Fock average local ionization energies on molecular surfaces. International Journal of Quantum Chemistry, 1998, 69, 607-613.	2.0	152
130	Molecular surface electrostatic potentials of anticonvulsant drugs. International Journal of Quantum Chemistry, 1998, 70, 1137-1143.	2.0	17
131	Câ^'H and Câ^'NO2 Dissociation Energies in Some Azines and Nitroazines. Journal of Physical Chemistry A, 1998, 102, 6697-6701.	2.5	19
132	Relationships between Lattice Energies and Surface Electrostatic Potentials and Areas of Anions. Journal of Physical Chemistry A, 1998, 102, 1018-1020.	2.5	47
133	Molecular electrostatic potentials as indicators of covalent radii. Journal of Chemical Physics, 1996, 104, 5109-5111.	3.0	32
134	Relationship between Measured Diffusion Coefficients and Calculated Molecular Surface Properties. The Journal of Physical Chemistry, 1996, 100, 5538-5540.	2.9	30
135	Structures and molecular surface electrostatic potentials of high-density C, N, H systems. Structural Chemistry, 1996, 7, 273-280.	2.0	9
136	Computational Determination of Heats of Formation of Energetic Compounds. Materials Research Society Symposia Proceedings, 1995, 418, 55.	0.1	12
137	Nonlocal density functional calculation of gas phase heats of formation. Journal of Computational Chemistry, 1995, 16, 654-658.	3.3	59
138	Analytical Representation and Prediction of Macroscopic Properties. ACS Symposium Series, 1995, , 109-118.	0.5	6
139	Relationships between impact sensitivities and molecular surface electrostatic potentials of nitroaromatic and nitroheterocyclic molecules. Molecular Physics, 1995, 85, 1-8.	1.7	157
140	C-NO2dissociation energies and surface electrostatic potential maxima in relation to the impact sensitivities of some nitroheterocyclic molecules. Molecular Physics, 1995, 86, 251-255.	1.7	79
141	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
142	Does antiaromaticity imply net destabilization?. International Journal of Quantum Chemistry, 1994, 49, 575-579.	2.0	31
143	Antiaromaticity in relation to 1,3,5,7-cyclooctatetraene structures. International Journal of Quantum Chemistry, 1994, 50, 273-277.	2.0	15
144	X-NO2 rotational energy barriers: Local density functional calculations. International Journal of Quantum Chemistry, 1993, 45, 15-20.	2.0	19

#	Article	IF	Citations
145	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
146	Polarizability and volume. Journal of Chemical Physics, 1993, 98, 4305-4306.	3.0	216
147	C?H Bond dissociation of acetylene: Local density functional calculations. International Journal of Quantum Chemistry, 1992, 42, 267-272.	2.0	11
148	An analysis of molecular electrostatic potentials obtained by a local density functional approach. International Journal of Quantum Chemistry, 1992, 44, 113-122.	2.0	28
149	Surface electrostatic potentials of halogenated methanes as indicators of directional intermolecular interactions. International Journal of Quantum Chemistry, 1992, 44, 57-64.	2.0	370
150	Quantitative determination of the total local polarity (charge separation) in molecules. Molecular Physics, 1992, 76, 609-617.	1.7	118
151	Electronegativity and the concept of charge capacity. Computational and Theoretical Chemistry, 1992, 259, 99-120.	1.5	91
152	Correlations between the solvent hydrogen bond acceptor parameter .beta. and the calculated molecular electrostatic potential. Journal of Organic Chemistry, 1991, 56, 3734-3737.	3.2	122
153	Correlations between the solvent hydrogen-bond-donating parameter .alpha. and the calculated molecular surface electrostatic potential. Journal of Organic Chemistry, 1991, 56, 6715-6717.	3.2	133
154	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
155	Effects of the simultaneous presence of nitro and amine substituents in cubane and some azacubanes. Structural Chemistry, 1991, 2, 153-166.	2.0	25
156	A computational analysis of some diaryl ureas in relation to their observed crystalline hydrogen bonding patterns. Molecular Engineering, 1991, 1, 75-87.	0.2	14
157	Radial behavior of the average local ionization energies of atoms. Journal of Chemical Physics, 1991, 95, 6699-6704.	3.0	88
158	A comparative analysis of the electrostatic potentials of some structural analogues of 2,3,7,8-tetrachlorodibenzo-p-dioxin and of related aromatic systems. International Journal of Quantum Chemistry, 1990, 37, 271-289.	2.0	29
159	A computational analysis of the electrostatic potentials and relative bond strengths of hydrazine and some of its 1,1-dimethyl derivatives. International Journal of Quantum Chemistry, 1990, 37, 611-629.	2.0	12
160	Average local ionization energies computed on the surfaces of some strained molecules. International Journal of Quantum Chemistry, 1990, 38, 645-653.	2.0	126
161	Evaluation of a finite multipole expansion technique for the computation of electrostatic potentials of dibenzo-p-dioxins and related systems. Journal of Computational Chemistry, 1990, 11, 112-120.	3.3	9
162	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

#	Article	IF	Citations
163	A computational study of some isomerization equilibria and their possible relation to vinyl chloride carcinogenicity. International Journal of Quantum Chemistry, 1987, 31, 569-579.	2.0	1
164	General and theoretical aspects of theï£¿OH,ï£¿Oï£¿ andï£¿Oï£¿Oï£¿ groups: Integration of theory and experiment. , 0, , 1-39.		1
165	General and Theoretical Aspects of the Cï£¿X Bonds (X = F, Cl, Br, I): Integration of Theory and Experiment. , 0, , 1-30.		2