

George C Shields

List of Publications by Year in descending order

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105
papers

7,480
citations

87723

38
h-index

54797

84
g-index

108
all docs

108
docs citations

108
times ranked

5697
citing authors

#	ARTICLE	IF	CITATIONS
1	Crystal structure of a CAP-DNA complex: the DNA is bent by 90 degrees. <i>Science</i> , 1991, 253, 1001-1007.	6.0	1,189
2	Accurate pKa Calculations for Carboxylic Acids Using Complete Basis Set and Gaussian-n Models Combined with CPCM Continuum Solvation Methods. <i>Journal of the American Chemical Society</i> , 2001, 123, 7314-7319.	6.6	544
3	Absolute pKa Determinations for Substituted Phenols. <i>Journal of the American Chemical Society</i> , 2002, 124, 6421-6427.	6.6	519
4	Structures of Cage, Prism, and Book Isomers of Water Hexamer from Broadband Rotational Spectroscopy. <i>Science</i> , 2012, 336, 897-901.	6.0	377
5	Benchmark Structures and Binding Energies of Small Water Clusters with Anharmonicity Corrections. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12034-12046.	1.1	277
6	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. <i>Science</i> , 2016, 351, 1310-1313.	6.0	256
7	Broadband Fourier transform rotational spectroscopy for structure determination: The water heptamer. <i>Chemical Physics Letters</i> , 2013, 571, 1-15.	1.2	216
8	Accurate Predictions of Water Cluster Formation, $(\text{H}_2\text{O})_n = 2 \times 10^n$. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11725-11737.	1.1	213
9	Experimentation with different thermodynamic cycles used for pKa calculations on carboxylic acids using complete basis set and Gaussian-n models combined with CPCM continuum solvation methods. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 727-741.	1.0	176
10	Molecular Dynamics Simulations of the d(TAA) Triple Helix. <i>Journal of the American Chemical Society</i> , 1997, 119, 7463-7469.	6.6	160
11	Theoretical Calculations of Acid Dissociation Constants: A Review Article. <i>Annual Reports in Computational Chemistry</i> , 2010, , 113-138.	0.9	160
12	Ability of the PM3 quantum-mechanical method to model intermolecular hydrogen bonding between neutral molecules. <i>Journal of Computational Chemistry</i> , 1993, 14, 89-104.	1.5	158
13	Thermodynamics of Forming Water Clusters at Various Temperatures and Pressures by Gaussian-2, Gaussian-3, Complete Basis Set-QB3, and Complete Basis Set-APNO Model Chemistries; Implications for Atmospheric Chemistry. <i>Journal of the American Chemical Society</i> , 2004, 126, 2647-2653.	6.6	155
14	Accurate relative pK _a calculations for carboxylic acids using complete basis set and Gaussian-n models combined with continuum solvation methods. <i>Journal of Chemical Physics</i> , 2001, 114, 4595.	1.2	145
15	Accurate Experimental Values for the Free Energies of Hydration of H ⁺ , OH ⁻ , and H ₃ O ⁺ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 3692-3694.	1.1	135
16	Comparison of CBS-QB3, CBS-APNO, and G3 Predictions of Gas Phase Deprotonation Data. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10483-10487.	1.1	131
17	Quantum Mechanical Study of Sulfuric Acid Hydration: Atmospheric Implications. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2209-2224.	1.1	111
18	Hydrogen Bond Cooperativity and the Three-Dimensional Structures of Water Nonamers and Decamers. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 14368-14372.	7.2	106

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19	Molecular Dynamics Simulation of a PNA-DNA-PNA Triple Helix in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1998, 120, 5895-5904.	6.6	99
20	Prediction of Accurate Anharmonic Experimental Vibrational Frequencies for Water Clusters, (H ₂ O) _n , n = 2-5. <i>Journal of Physical Chemistry A</i> , 2006, 110, 303-309.	1.1	99
21	Do Hydroxyl Radical-Water Clusters, OH(H ₂ O) _n , n = 1-5, Exist in the Atmosphere?. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13283-13289.	1.1	93
22	Computational Study of the Hydration of Sulfuric Acid Dimers: Implications for Acid Dissociation and Aerosol Formation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9745-9758.	1.1	91
23	Global Search for Minimum Energy (H ₂ O) _n Clusters, n = 3-5. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6773-6778.	1.1	89
24	The Role of Anharmonicity in Hydrogen-Bonded Systems: The Case of Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2804-2817.	2.3	87
25	Computational estimation of pK _a values. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2015, 5, 290-297.	6.2	85
26	Hydration of the Bisulfate Ion: Atmospheric Implications. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5151-5163.	1.1	65
27	Comparison of CBS-QB3, CBS-APNO, G2, and G3 thermochemical predictions with experiment for formation of ionic clusters of hydronium and hydroxide ions complexed with water. <i>Journal of Chemical Physics</i> , 2005, 122, 024302.	1.2	57
28	Comparison of Model Chemistry and Density Functional Theory Thermochemical Predictions with Experiment for Formation of Ionic Clusters of the Ammonium Cation Complexed with Water and Ammonia; Atmospheric Implications. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4905-4910.	1.1	54
29	Effect of Mixing Ammonia and Alkylamines on Sulfate Aerosol Formation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1612-1622.	1.1	54
30	Hydration of the Sulfuric Acid-Methylamine Complex and Implications for Aerosol Formation. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7430-7441.	1.1	53
31	First-principle studies of intermolecular and intramolecular catalysis of protonated cocaine. <i>Journal of Computational Chemistry</i> , 2005, 26, 980-986.	1.5	50
32	Ortho Effect in the Bergman Cyclization: Electronic and Steric Effects in Hydrogen Abstraction by 1-Substituted Naphthalene 5,8-Diradicals. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2517-2526.	1.1	48
33	ArbAlign: A Tool for Optimal Alignment of Arbitrarily Ordered Isomers Using the Kuhn-Munkres Algorithm. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1045-1054.	2.5	48
34	Capturing the Elusive Water Trimer from the Stepwise Growth of Water on the Surface of the Polycyclic Aromatic Hydrocarbon Acenaphthene. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5744-5750.	2.1	48
35	The Limitations of Certain Density Functionals in Modeling Neutral Water Clusters. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 2008, 38, 32-39.	0.6	45
36	Crystallization of Escherichia coli catabolite gene activator protein with its DNA binding site. <i>Journal of Molecular Biology</i> , 1990, 213, 159-166.	2.0	44

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37	Comparison of density functional theory predictions of gas-phase deprotonation data. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 580-587.	1.0	43
38	Atmospheric Implications for Formation of Clusters of Ammonium and $1\text{--}10$ Water Molecules. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4266-4271.	1.1	41
39	Exploration of the Potential Energy Surfaces, Prediction of Atmospheric Concentrations, and Prediction of Vibrational Spectra for the $\text{HO}_2\text{--}(\text{H}_2\text{O})_n$ ($n = 1\text{--}2$) Hydrogen Bonded Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3686-3691.	1.1	39
40	Corannulene and its complex with water: a tiny cup of water. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14214-14223.	1.3	39
41	Pople's Gaussian-3 model chemistry applied to an investigation of $(\text{H}_2\text{O})_8$ water clusters. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 565-572.	1.0	38
42	Ramachandran-type plots for glycosidic linkages: Examples from molecular dynamic simulations using the Glycam06 force field. <i>Journal of Computational Chemistry</i> , 2009, 30, 910-921.	1.5	38
43	Modeling of magic water clusters $(\text{H}_2\text{O})_{20}$ and $(\text{H}_2\text{O})_{21}\text{H}^+$ with the PM3 quantum-mechanical method. <i>Journal of Computational Chemistry</i> , 1993, 14, 1326-1332.	1.5	35
44	The ability of the Gaussian-2, Gaussian-3, Complete Basis Set-QB3, and Complete Basis Set-APNO model chemistries to model the geometries of small water clusters. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 1065-1070.	1.0	33
45	Thermodynamics of the Hydroxyl Radical Addition to Isoprene. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7064-7071.	1.1	31
46	Particle formation and surface processes on atmospheric aerosols: A review of applied quantum chemical calculations. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26350.	1.0	30
47	Quantum-Mechanical investigation of large water clusters. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 349-360.	1.0	29
48	CCSD(T), W1, and other model chemistry predictions for gas-phase deprotonation reactions. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3122-3128.	1.0	29
49	Comparison of Experimental and Theoretical Structures of a Transition State Analogue Used for the Induction of Anti-Cocaine Catalytic Antibodies. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8526-8529.	1.1	28
50	Hydration of OCS with One to Four Water Molecules in Atmospheric and Laboratory Conditions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4490-4495.	1.1	27
51	Computational Design and Experimental Discovery of an Antiestrogenic Peptide Derived from E^{\pm} -Fetoprotein. <i>Journal of the American Chemical Society</i> , 2007, 129, 6263-6268.	6.6	26
52	Importance and Reliability of Small Basis Set CCSD(T) Corrections to MP2 Binding and Relative Energies of Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1439-1448.	2.3	25
53	Experimental and Theoretical Study of the OH Vibrational Spectra and Overtone Chemistry of Gas-Phase Vinylacetic Acid. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10226-10235.	1.1	24
54	Hydrogen bonding of nucleotide base pairs: Application of the PM3 method. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 95-107.	1.0	23

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55	A Semiempirical Transition State Structure for the First Step in the Alkaline Hydrolysis of Cocaine. Comparison between the Transition State Structure, the Phosphonate Monoester Transition State Analog, and a Newly Designed Thiophosphonate Transition State Analog. <i>Journal of Molecular Modeling</i> , 1996, 2, 62-69.	0.8	23
56	Doubly-charged gas phase cations. <i>Theoretica Chimica Acta</i> , 1986, 69, 147-159.	0.9	22
57	Calculating Reliable Gibbs Free Energies for Formation of Gas-Phase Clusters that Are Critical for Atmospheric Chemistry: (H ₂ SO ₄) ₃ . <i>Journal of Physical Chemistry A</i> , 2021, 125, 3169-3176.	1.1	22
58	Charge transfer reactions of organic ions containing oxygen: Correlation between reaction energetics and cross sections. <i>Organic Mass Spectrometry</i> , 1987, 22, 64-69.	1.3	21
59	Use of the Supermolecule Approach To Model the Syn and Anti Conformations of Solvated Cyclic 3',5'-Adenosine Monophosphate. <i>The Journal of Physical Chemistry</i> , 1996, 100, 3293-3298.	2.9	21
60	In search of CS ₂ (H ₂ O) _{n=1-4} clusters. <i>Journal of Chemical Physics</i> , 2007, 126, 154320.	1.2	20
61	Exploring the Rich Potential Energy Surface of (H ₂ O) ₁₁ and Its Physical Implications. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1141-1153.	2.3	20
62	Water induces the same crown shapes as Li ⁺ or Na ⁺ in 15-crown-5 ether: a broadband rotational study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2875-2881.	1.3	20
63	Twenty years of exceptional success: The molecular education and research consortium in undergraduate computational chemistry (MERCURY). <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26274.	1.0	19
64	Hydrogen-Bond Topology Is More Important Than Acid/Base Strength in Atmospheric Prenucleation Clusters. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1718-1728.	1.1	19
65	Efficient and Accurate Characterization of the Bergman Cyclization for Several Eneidyne Including an Expanded Substructure of Esperamicin A1. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16917-16934.	1.2	18
66	Investigation of the potential energy surface for the first step in the alkaline hydrolysis of methyl acetate. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 83-93.	1.0	17
67	Ligand-to-Metal Charge-Transfer Photophysics and Photochemistry of Emissive d ⁰ Titanocenes: A Spectroscopic and Computational Investigation. <i>Inorganic Chemistry</i> , 2021, 60, 14399-14409.	1.9	17
68	Water-Mediated Peptide Bond Formation in the Gas Phase: A Model Prebiotic Reaction. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4150-4159.	1.1	16
69	Structures, energetics and fragmentation pathways of C _n H ₂₂ ⁺ carbocations. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1985, 64, 315-333.	1.9	15
70	Further Quantum Mechanical Evidence that Difluorotoluene Does Not Hydrogen Bond. <i>Journal of Physical Chemistry B</i> , 2001, 105, 8445-8451.	1.2	15
71	Structural Analysis of Î±-Fetoprotein (AFP)-like Peptides with Anti-Breast-Cancer Properties. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4514-4526.	1.2	15
72	Single- and double-electron transfer reactions of ground and metastable state Ar ²⁺ ions. <i>Journal of Physics B: Atomic and Molecular Physics</i> , 1983, 16, 3591-3607.	1.6	14

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73	Sensitivity of charge transfer reactions to hydrocarbon ion structures. <i>Organic Mass Spectrometry</i> , 1986, 21, 137-149.	1.3	14
74	A computationally efficient procedure for modeling the first step in the alkaline hydrolysis of esters. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 103-112.	1.0	14
75	Antiestrogenic and anticancer activities of peptides derived from the active site of alpha-fetoprotein. <i>Journal of Peptide Science</i> , 2009, 15, 319-325.	0.8	14
76	Computation of Atmospheric Concentrations of Molecular Clusters from H_2O and H_2O_2 . <i>Journal of Visualized Experiments</i> , 2020, , .	0.2	14
77	Molecular charge-transfer cross sections and their correlation with reactant ion structures. <i>The Journal of Physical Chemistry</i> , 1985, 89, 4027-4031.	2.9	13
78	Structure and thermodynamics of $\text{H}_3\text{O}^+(\text{H}_2\text{O})_8$ clusters: A combined molecular dynamics and quantum mechanics approach. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 240-248.	1.1	13
79	AM1 and PM3 calculations of the potential energy surfaces for hydroxymethyl radical reactions with nitric oxide and nitrogen dioxide. <i>The Journal of Physical Chemistry</i> , 1991, 95, 5085-5089.	2.9	12
80	The search for low energy conformational families of small peptides: Searching for active conformations of small peptides in the absence of a known receptor. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3001-3012.	1.0	12
81	The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 16894-16899.	7.2	12
82	Monomers of Glycine and Serine Have a Limited Ability to Hydrate in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8454-8467.	1.1	12
83	Evidence for long-lived excited states of $[\text{C}_n\text{H}_2]^{2+}$ carbocations. <i>Organic Mass Spectrometry</i> , 1986, 21, 69-75.	1.3	11
84	Catalytic activity of water molecules in gas-phase glycine dimerization. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26469.	1.0	11
85	Doubly-charged ethane ions: Solution to the dilemma of stability predicted by theory and instability observed in experiment. <i>Organic Mass Spectrometry</i> , 1986, 21, 479-483.	1.3	10
86	An ONIOM study of the Bergman reaction: a computationally efficient and accurate method for modeling the enediyne anticancer antibiotics. <i>Chemical Physics Letters</i> , 2001, 347, 505-511.	1.2	10
87	The Molecular Education and Research Consortium in Undergraduate Computational Chemistry (MERCURY): Twenty Years of Exceptional Success Supporting Undergraduate Research and Inclusive Excellence. <i>Scholarship and Practice of Undergraduate Research</i> , 2020, 3, 5-15.	0.2	10
88	Quantum mechanical investigation of cyclic $3',5'$ -adenosine monophosphate, the second hormonal messenger. <i>Computational and Theoretical Chemistry</i> , 1996, 362, 297-304.	1.5	9
89	Photochemistry and Photophysics of Charge-Transfer Excited States in Emissive $\text{Ti}(\text{Cp})_2$ Heterobimetallic Titanocene Tweezer Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 10986-10998.	1.9	9
90	A Departmental Focus on High Impact Undergraduate Research Experiences. <i>ACS Symposium Series</i> , 2013, , 5-22.	0.5	8

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91	The Physical Chemistry Sequence at Liberal Arts Colleges: The Lake Forest College Approach. <i>Journal of Chemical Education</i> , 1994, 71, 951.	1.1	7
92	Experiment in quantization: Atomic line spectra. <i>Journal of Chemical Education</i> , 1992, 69, 329.	1.1	6
93	Computational approaches for the design of peptides with anti-breast cancer properties. <i>Future Medicinal Chemistry</i> , 2009, 1, 201-212.	1.1	6
94	A Roadmap to Successful Collaborations between Primarily Undergraduate Institutions and Research Institutions. <i>ACS Symposium Series</i> , 2018, , 105-127.	0.5	6
95	Doubly charged ion mass spectra of alkyl-substituted furans and pyrroles. <i>Organic Mass Spectrometry</i> , 1987, 22, 389-399.	1.3	5
96	Insights into the charge-transfer character of electronic transitions in $R^2Cp^2Ti(C_2Fc)_2$ complexes using solvatochromism, resonance Raman spectroscopy, and TDDFT. <i>Dalton Transactions</i> , 2021, 50, 2233-2242.	1.6	5
97	Double electron transfer reactions of CO_2^+ ions. <i>Chemical Physics Letters</i> , 1983, 101, 287-290.	1.2	4
98	Maintaining a high degree of research productivity at a predominately undergraduate institution as your career advances. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26370.	1.0	4
99	Competition between single and double electron transfer in collisions of doubly charged molecular pyrrole ions with neutral pyrrole molecules. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1987, 79, 127-140.	1.9	3
100	Using the Franck-Hertz Experiment To Illustrate Quantization: Energy States of the Neon Atom by Electron Impact. <i>Journal of Chemical Education</i> , 1994, 71, 466.	1.1	3
101	Semiempirical study of the bergman reaction: Towards a computationally efficient and accurate method for modeling the enediyne anticancer antibiotics. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 51-59.	1.0	2
102	Using Early Introduction to Research To Increase STEM Majors: A Tale of Two Colleges, One Small Highly Selective Private and One Non-Selective Regional Public. <i>ACS Symposium Series</i> , 2017, , 107-119.	0.5	2
103	Polarizabilities of organic ions. <i>Organic Mass Spectrometry</i> , 1986, 21, 449-450.	1.3	1
104	Formation of deprotonated 2-imidazoline-4(5)-one product ions in the collision-induced dissociation of some serine-containing dipeptides. <i>International Journal of Mass Spectrometry</i> , 2015, 381-382, 25-32.	0.7	1
105	The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. <i>Angewandte Chemie</i> , 2021, 133, 17031-17036.	1.6	0