Caroline Elizabeth Helen Dessent

List of Publications by Year
in descending order

84 papers	2,491 citations	257450 24 h-index	214800 47 g-index
88 all docs	88 docs citations	88 times ranked	1837 citing authors

#	Article	IF	Citations
1	Performance of M06, M06-2X, and M06-HF Density Functionals for Conformationally Flexible Anionic Clusters: M06 Functionals Perform Better than B3LYP for a Model System with Dispersion and Ionic Hydrogen-Bonding Interactions. Journal of Physical Chemistry A, 2013, 117, 12590-12600.	2.5	549
2	Hydrogen-Bonding and van der Waals Complexes Studied by ZEKE and REMPI Spectroscopy. Chemical Reviews, 2000, 100, 3999-4022.	47.7	198
3	Precursor of the Iaqâ^' chargeâ€transferâ€toâ€solvent (CTTS) band in Iâ^'â‹…(H2O)n clusters. Journal of Chemical Physics, 1996, 105, 7231-7234.	3.0	162
4	Photochemistry of Halide Ionâ^'Molecule Clusters:â€‰ Dipole-Bound Excited States and the Case for Asymmetric Solvation. Accounts of Chemical Research, 1998, 31, 527-534.	15.6	74
5	Dipoleâ€bound excited states of the Iâ^'â‹…CH3CN and Iâ^'â‹…(CH3CN)2 ionâ€"molecule complexes: Evidence for asymmetric solvation. Journal of Chemical Physics, 1995, 103, 2006-2015.	3.0	71
6	Mass analyzed threshold ionization of phenolâ‹…CO: Intermolecular binding energies of a hydrogen-bonded complex. Journal of Chemical Physics, 1999, 111, 1947-1954.	3.0	67
7	Probing the intrinsic features and environmental stabilization of multiply charged anions. Physical Chemistry Chemical Physics, 2006, 8, 5151.	2.8	56
8	Rotational band contour analysis in REMPI and ZEKE spectroscopy: elucidating the structures of phenolÂ·X (X=N2, CO and Ar) complexes. Journal of Electron Spectroscopy and Related Phenomena, 2000, 112, 231-239.	1.7	54
9	Is the phenolÂ·Ar complex van der Waals or hydrogen-bonded? A REMPI and ZEKE spectroscopic study. Journal of Electron Spectroscopy and Related Phenomena, 2000, 108, 1-11.	1.7	50
10	ZEKE Photoelectron Spectroscopy of the cis and trans Isomers of Formanilide. Angewandte Chemie - International Edition, 2002, 41, 166-168.	13.8	45
11	Spectroscopic observation of vibrational Feshbach resonances in near-threshold photoexcitation of X-Â·CH3NO2 (X-=I- and Br-). Faraday Discussions, 2000, 115, 395-406.	3.2	43
12	Observation of the dipoleâ€bound excited state of the Iâ^'â‹…acetone ionâ€molecule complex. Journal of Chemical Physics, 1995, 102, 6335-6338.	3.0	42
13	A PW91 Density Functional Study of Conformational Choice in 2-Phenylethanol,n-Butylbenzene, and Their Cations:Â Problems for Density Functional Theory?. Journal of Physical Chemistry A, 2002, 106, 4623-4631.	2.5	41
14	Experiment and theory confirm that UV laser photodissociation spectroscopy can distinguish protomers formed via electrospray. Physical Chemistry Chemical Physics, 2017, 19, 17434-17440.	2.8	40
15	Observation of Rotational Isomers I:Â A ZEKE and Hole-Burning Spectroscopy Study of 3-Methoxyphenol. Journal of Physical Chemistry A, 2000, 104, 11864-11869.	2.5	36
16	A ZEKE photoelectron spectroscopy and ab initio study of the cis- and trans-isomers of formanilide: Characterizing the cationic amide bond ?. Physical Chemistry Chemical Physics, 2001, 3, 5450-5458.	2.8	35
17	Unravelling the Ketoâ€"Enol Tautomer Dependent Photochemistry and Degradation Pathways of the Protonated UVA Filter Avobenzone. Journal of Physical Chemistry A, 2020, 124, 2919-2930.	2.5	34
18	On the vibrational fine structure in the nearâ€threshold photofragmentation spectrum of the Iâ^'â‹…CH3I complex: Spectroscopic observation of nonadiabatic effects in electronâ€molecule scattering. Journal of Chemical Physics, 1996, 105, 10416-10423.	3.0	32

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19	Ionic fragmentation versus electron detachment in isolated transition metal complex dianions. Chemical Physics Letters, 2004, 399, 465-470.	2.6	32
20	A density functional theory study of the anthracene anion. Chemical Physics Letters, 2000, 330, 180-187.	2.6	30
21	The PFI-ZEKE photoelectron spectrum of m-fluorophenol and its aqueous complexes: Comparing intermolecular vibrations in rotational isomers. Physical Chemistry Chemical Physics, 2002, 4, 2534-2538.	2.8	30
22	Locating the Proton in Nicotinamide Protomers via Low-Resolution UV Action Spectroscopy of Electrosprayed Solutions. Journal of Physical Chemistry A, 2016, 120, 9209-9216.	2.5	30
23	Photodissociation dynamics of the iodide-uracil (Iâ¯U) complex. Journal of Chemical Physics, 2016, 145, 044319.	3.0	27
24	Stabilization of Excess Charge in Isolated Adenosine 5â€˜-Triphosphate and Adenosine 5â€˜-Diphosphate Multiply and Singly Charged Anions. Journal of Physical Chemistry A, 2005, 109, 9775-9785.	2.5	26
25	UV laser photoactivation of hexachloroplatinate bound to individual nucleobases in vacuo as molecular level probes of a model photopharmaceutical. Physical Chemistry Chemical Physics, 2016, 18, 15143-15152.	2.8	26
26	Photoexcitation of Adenosine 5â€²-Triphosphate Anions in Vacuo: Probing the Influence of Charge State on the UV Photophysics of Adenine. Journal of Physical Chemistry B, 2017, 121, 5553-5561.	2.6	26
27	Protomer-Dependent Electronic Spectroscopy and Photochemistry of the Model Flavin Chromophore Alloxazine. Molecules, 2018, 23, 2036.	3.8	24
28	Mapping the intrinsic absorption properties and photodegradation pathways of the protonated and deprotonated forms of the sunscreen oxybenzone. Physical Chemistry Chemical Physics, 2019, 21, 14311-14321.	2.8	24
29	Solvent evaporation versus proton transfer in nucleobaseâ€“Pt(CN)4,62â¯ dianion clusters: a collisional excitation and electronic laser photodissociation spectroscopy study. Physical Chemistry Chemical Physics, 2014, 16, 15490.	2.8	23
30	Observation of Near-Threshold Resonances in the Flavin Chromophore Anions Alloxazine and Lumichrome. Journal of Physical Chemistry Letters, 2018, 9, 6124-6130.	4.6	23
31	Photoexcitation of iodide ion-pyrimidine clusters above the electron detachment threshold: Intracluster electron transfer versus nucleobase-centred excitations. Journal of Chemical Physics, 2018, 148, 084304.	3.0	22
32	Photoinitiation of Gas-Phase SN2 Reactions through the Evansâ¯Polanyi Excited State Surface. Journal of the American Chemical Society, 1997, 119, 5067-5068.	13.7	21
33	The effect of conformation on the ionization energetics ofn-butylbenzene. II. A zero electron kinetic energy photoelectron spectroscopy study with partial rotational resolution. Journal of Chemical Physics, 2003, 119, 12914-12920.	3.0	20
34	Exploring the microscopic solvation of doubly charged anions: symmetric or asymmetric solvation in the CO2â€“(CH2)4â€“CO22â¯Â·(H2O)2 dicarboxylate dianion cluster?. Chemical Physics Letters, 2003, 370, 52-61.	2.6	19
35	High-energy collision induced dissociation of iridium hexa-halide dianions: Observation of triple electron detachment and other decay pathways. International Journal of Mass Spectrometry, 2005, 244, 60-64.	1.5	19
36	On the Stability of IrCl63- and Other Triply Charged Anions:â€‰ Solvent Stabilization versus Ionic Fragmentation and Electron Detachment for the IrCl63-Â·(H2O)n n = 0â¯10 Microsolvated Clusters. Journal of Physical Chemistry A, 2005, 109, 5836-5845.	2.5	19

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37	The effect of conformation on the ionization energetics of n-butylbenzene. I. A threshold ionization study. Journal of Chemical Physics, 2003, 119, 12908-12913.	3.0	18
38	Collision-Induced Dissociation of Halide Ionâ€“Arginine Complexes: Evidence for Anion-Induced Zwitterion Formation in Gas-Phase Arginine. Journal of Physical Chemistry A, 2012, 116, 801-809.	2.5	18
39	Observation of Hydrogen-Bonded Rotational Isomers of the ResorcinolÂ·Water Complex. Journal of Physical Chemistry A, 1999, 103, 7186-7191.	2.5	17
40	Mapping the UV Photophysics of Platinum Metal Complexes Bound to Nucleobases: Laser Spectroscopy of Isolated UracilÂ·Pt(CN)42â€“ and UracilÂ·Pt(CN)62â€“ Complexes. Journal of Physical Chemistry Letters, 2014, 5, 3281-3285.	4.6	15
41	Effect of Noncovalent Interactions on Conformers of the n-Butylbenzene Monomer Studied by Mass Analyzed Threshold Ionization Spectroscopy and Basis-set Convergent ab initio Computations. Journal of Physical Chemistry A, 2008, 112, 5866-5871.	2.5	14
42	Effect of Cation Complexation on the Structure of a Conformationally Flexible Multiply Charged Anion: Stabilization of Excess Charge in the Na+Â·Adenosine 5â€²-Triphosphate Dianion Ion-Pair Complex. Journal of Physical Chemistry A, 2009, 113, 2683-2692.	2.5	14
43	Direct Observation of Photochemical Free Radical Production from the Sunscreen 2â€Phenylbenzimidazoleâ€5â€Sulfonic Acid via Laserâ€Interfaced Mass Spectrometry. ChemPhotoChem, 2019, 3, 1231-1237.	3.0	14
44	Hydration of a cationic amide group: a ZEKE spectroscopic study of trans-formanilideâ€“H2OElectronic supplementary information (ESI) available: Ab initio CASSCF/cc-pVDZ geometry parameters of t-FAâ€“H2ONH in the S0, S1 and D0 states (Table S1), CASSCF/cc-pVDZ charges of t-FAâ€“H2ONH in the S0, S1 and D0 states (Table S2), CASSCF/cc-pVDZ harmonic frequencies for the S0, S1 and D0 of t-FAâ€“H2ONH up to 1000 cmâ€“1 (Table S3). See http://www.rsc.org/suppdata/cp/b2/b200125j/. Physical Chemistry Chemical Physics, 2002, 4, 2897-2903.	2.8	13
45	Decolonizing the Undergraduate Chemistry Curriculum: An Account of How to Start. Journal of Chemical Education, 2022, 99, 5-9.	2.3	13
46	Observation of Rotational Isomers II:Â A ZEKE and Hole-Burning Spectroscopy Study of Hydrogen-Bonded 3-MethoxyphenolÂ·Water Clusters. Journal of Physical Chemistry A, 2000, 104, 11870-11876.	2.5	12
47	Characterizing the intrinsic stability of gas-phase clusters of transition metal complex dianions with alkali metal counterions: Counterion perturbation of multiply charged anions. Journal of Chemical Physics, 2007, 126, 064308.	3.0	12
48	Observation of Enhanced Dissociative Photochemistry in the Non-Native Nucleobase 2-Thiouracil. Molecules, 2020, 25, 3157.	3.8	12
49	Linking Electronic Relaxation Dynamics and Ionic Photofragmentation Patterns for the Deprotonated UV Filter Benzophenone-4. Journal of Physical Chemistry Letters, 2021, 12, 2831-2836.	4.6	12
50	ZEKE and Hole-Burning Spectroscopy of the Rotational Isomers of ResorcinolÂ·CO. Journal of Physical Chemistry A, 1999, 103, 9687-9692.	2.5	11
51	Investigating the mapping of chromophore excitations onto the electron detachment spectrum: photodissociation spectroscopy of iodide ionâ€“thiouracil clusters. Physical Chemistry Chemical Physics, 2021, 23, 1021-1030.	2.8	11
52	Counter-ion perturbation of the fragmentation pathways of multiply charged anions: Evidence for exit channel complexes on the fragmentation potential energy surfaces. Journal of Chemical Physics, 2006, 125, 021105.	3.0	10
53	Complexation of carboxylate anions with the arginine gas-phase amino acid: Effects of chain length on the geometry of extended ion binding. Chemical Physics Letters, 2013, 577, 1-5.	2.6	10
54	Electron Transfer and Charge Separation in Clusters. Advances in Chemical Physics, 2007, , 265-302.	0.3	9

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55	Structural characterization of negatively charged glycosaminoglycans using high-energy (50â€“150keV) collisional activation. International Journal of Mass Spectrometry, 2009, 285, 70-77.	1.5	9
56	Complexation of anions to gas-phase amino acids: Conformation is critical in determining if the global minimum is canonical or zwitterionic. Chemical Physics Letters, 2013, 588, 43-46.	2.6	9
57	Electron Detachment as a Probe of Intrinsic Nucleobase Dynamics in Dianion-Nucleobase Clusters: Photoelectron Spectroscopy of the Platinum II Cyanide Dianion Bound to Uracil, Thymine, Cytosine, and Adenine. Journal of Physical Chemistry B, 2015, 119, 11626-11631.	2.6	9
58	Near-threshold electron transfer in anion-nucleobase clusters: does the identity of the anion matter?. Molecular Physics, 2019, 117, 3001-3010.	1.7	9
59	Sodium cationization can disrupt the intramolecular hydrogen bond that mediates the sunscreen activity of oxybenzone. Physical Chemistry Chemical Physics, 2020, 22, 19522-19531.	2.8	9
60	Intermolecular vibration and internal rotation of a methyl group in acetanilideÂ·Ar: a ZEKE photoelectron spectroscopy study. Physical Chemistry Chemical Physics, 2002, 4, 3578-3582.	2.8	8
61	A REMPI and ZEKE spectroscopic study of the trans-formanilideÂ·Ar van der Waals cluster. Chemical Physics Letters, 2002, 351, 121-127.	2.6	8
62	Microsolvation of the chlorine oxide anion and chlorine oxide radical: Structures and energetics of the ClOâ¯Â·(H2O)n and ClOÂ·(H2O)nn=1â€“4 clusters. Chemical Physics Letters, 2006, 429, 32-37.	2.6	8
63	Photoelectron spectroscopy of hexachloroplatinate-nucleobase complexes: Nucleobase excited state decay observed via delayed electron emission. Journal of Chemical Physics, 2015, 143, 184307.	3.0	8
64	Direct Measurement of the Visible to UV Photodissociation Processes for the PhotoCORM TryptoCORM. Chemistry - A European Journal, 2020, 26, 10297-10306.	3.3	8
65	Emerging contaminant exposure to aquatic systems in the Southern African Development Community. Environmental Toxicology and Chemistry, 2022, 41, 382-395.	4.3	8
66	Illuminating the Effect of the Local Environment on the Performance of Organic Sunscreens: Insights From Laser Spectroscopy of Isolated Molecules and Complexes. Frontiers in Chemistry, 2021, 9, 812098.	3.6	8
67	On the intrinsic stability of the isolated dichromate dianion: Collision activated dissociation of a multiply charged anion via electron detachment. International Journal of Mass Spectrometry, 2008, 276, 31-36.	1.5	7
68	Communication: Evidence for dipole-bound excited states in gas-phase Iâ¯ â‹… MI (M = Na, K, Cs) anionic salt microclusters. Journal of Chemical Physics, 2015, 143, 101103.	3.0	7
69	UV laser spectroscopy of mass-selected ionic liquid building blocks in the gas-phase. Chemical Physics Letters, 2015, 634, 216-220.	2.6	7
70	Photodegradation of Riboflavin under Alkaline Conditions: What Can Gas-Phase Photolysis Tell Us about What Happens in Solution?. Molecules, 2021, 26, 6009.	3.8	7
71	On the propensity for electron transfer in high-energy collisions of iridium complex anions with cesium atoms. Chemical Physics Letters, 2007, 442, 201-205.	2.6	6
72	Communication: Photoactivation of nucleobase bound platinumIImetal complexes: Probing the influence of the nucleobase. Journal of Chemical Physics, 2014, 141, 241101.	3.0	6

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73	What Makes a Professional Chemist? Embedding Equality, Diversity, and Inclusion into Chemistry Skills Training for Undergraduates. Journal of Chemical Education, 2022, 99, 480-486.	2.3	6
74	A â€œone potâ€•mass spectrometry technique for characterizing solution- and gas-phase photochemical reactions by electrospray mass spectrometry. RSC Advances, 2021, 11, 19500-19507.	3.6	5
75	Measurement of the Population of Electrosprayed Deprotomers of Coumaric Acids Using UVâ€“Vis Laser Photodissociation Spectroscopy. Journal of Physical Chemistry A, 2021, 125, 6703-6714.	2.5	5
76	Noncovalent Interactions in the Gas-Phase Conformers of Anionic Iduronate (methyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 632 Td (2-O- Prototypical Anionic Monosaccharide Studied Using Computational Methods. Journal of Physical Chemistry A, 2010, 114, 11153-11160.	2.5	4
77	Evidence for hydrogen bond network formation in microsolvated clusters of Pt(CN)42â^': collision induced dissociation studies of Pt(CN)42â^'Â·(H2O)nn = 1â€“4, and Pt(CN)42â^'Â·(MeCN)mm = 1, 2 cluster ions. Physical Chemistry Chemical Physics, 2011, 13, 18379.	2.8	4
78	Electron detachment dynamics of the iodide-guanine cluster: does ionization occur from the iodide or from guanine?. Molecular Physics, 2020, 118, e1662128.	1.7	4
79	Photoproducts of the Photodynamic Therapy Agent Verteporfin Identified via Laser Interfaced Mass Spectrometry. Molecules, 2020, 25, 5280.	3.8	4
80	Photoinitiation of the anionic condensation reaction in 2-chloroacrylonitrile via the charge-transfer bands of the Clâ^'Â·(2-chloroacrylonitrile)1,2 clusters. Chemical Physics Letters, 1995, 244, 127-132.	2.6	3
81	New insights into dianionâ€“cation contact ion-pairs: understanding the effect of cation complexation on the electron detachment and ionic fragmentation pathways of multiply charged anions. Physica Scripta, 2007, 76, C56-C62.	2.5	3
82	Photostability of the deprotonated forms of the UV filters homosalate and octyl salicylate: molecular dissociation versus electron detachment following UV excitation. Physical Chemistry Chemical Physics, 2022, 24, 17068-17076.	2.8	3
83	Multidimensional Franck-Condon simulations of photodetachment spectra for the formate-water cluster anion: Investigating H atom transfer along the HCOOH+OH reaction coordinate. Journal of Chemical Physics, 2007, 127, 234308.	3.0	2
84	Probing the gas-phase stability of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Re</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:r (X = Cl, Br) and <mml:math xmlns:mml="http://www.w3.org/1. Chemical Physics Letters, 2009, 479, 184-188.	2.6	2