Mark A Buntine

List of Publications by Year
in descending order

81 papers	1,669 citations	257450 24 h-index	330143 37 g-index
84 all docs	84 docs citations	84 times ranked	1557 citing authors

#	Article	IF	Citations
1	Influence of Crystal Packing on Molecular Geometry:â€‰ A Crystallographic and Theoretical Investigation of Selected Diorganotin Systems. Journal of Physical Chemistry A, 1998, 102, 2472-2482.	2.5	106
2	Production of Acrylic Acid through Nickel-Mediated Coupling of Ethylene and Carbon Dioxideâ€”A DFT Study. Organometallics, 2007, 26, 6784-6792.	2.3	95
3	Quantitative determination of H2, HD, and D2 internalâ€state distributions by (2+1) resonanceâ€enhanced multiphoton ionization. Journal of Chemical Physics, 1991, 95, 214-225.	3.0	77
4	Photodissociation of acetylene: Determination of D00 (HCCâ€“H) by photofragment imaging. Journal of Chemical Physics, 1990, 93, 6578-6584.	3.0	71
5	A twoâ€color laserâ€induced grating technique for gasâ€phase excitedâ€state spectroscopy. Journal of Chemical Physics, 1992, 97, 707-710.	3.0	69
6	Photoreduction Kinetics of Sodium Tetrachloroaurate under Synchrotron Soft X-ray Exposure. Langmuir, 2011, 27, 8099-8104.	3.5	63
7	Application of ion imaging to the atomâ€“molecule exchange reaction: H+HIâ†'H2+I. Journal of Chemical Physics, 1991, 94, 4672-4675.	3.0	51
8	Reaction Pathways of Singlet Silylene and Singlet Germylene with Water, Methanol, Ethanol, Dimethyl Ether, and Trifluoromethanol:Â An ab Initio Molecular Orbital Study. Journal of Physical Chemistry A, 2001, 105, 1185-1196.	2.5	51
9	Supramolecular Snâ‹¯Cl associations in diorganotin dichlorides and their influence on molecular geometry as studied by ab initio molecular orbital calculations. CrystEngComm, 2003, 5, 331-336.	2.6	47
10	Regioselective control of the nickel-mediated coupling of acetylene and carbon dioxide â€“ A DFT study. Journal of Organometallic Chemistry, 2008, 693, 2703-2710.	1.8	43
11	Structural Variation in Diorganotin Dimethylxanthates, R2Sn(S2COMe)2:Â A Combined Crystallographic and Theoretical Investigationâ€. Organometallics, 2000, 19, 5410-5415.	2.3	40
12	Neutral Tantalumâ^'Carbide Clusters:â€‰ A Multiphoton Ionization and Density Functional Theory Study. Journal of Physical Chemistry A, 2000, 104, 3308-3316.	2.5	35
13	Photodissociation dynamics of doubly excited Rydberg states of molecular hydrogen. Journal of Chemical Physics, 1992, 96, 5843-5856.	3.0	34
14	Examination of the effect of crystal packing forces on geometric parameters: a combined crystallographic and theoretical study of 2,2'-bipyridyl adducts of R2SnCl2. Zeitschrift Fur Kristallographie - Crystalline Materials, 2000, 215, .	0.8	33
15	Influence of Cationic Surfactants on the Formation and Surface Oxidation States of Gold Nanoparticles Produced via Laser Ablation. Langmuir, 2013, 29, 12452-12462.	3.5	32
16	Detection of vibrationalâ€overtone excitation in water via laserâ€induced grating spectroscopy. Journal of Chemical Physics, 1995, 102, 2718-2726.	3.0	31
17	Aspects of Electrokinetic Charging in Liquid Microjets. Journal of Physical Chemistry B, 1999, 103, 3035-3042.	2.6	31
18	Advancing Chemistry by Enhancing Learning in the Laboratory (ACELL): a model for providing professional and personal development and facilitating improved student laboratory learning outcomes. Chemistry Education Research and Practice, 2007, 8, 232-254.	2.5	31

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19	Threshold Photoionization and Density Functional Theory Studies of the Niobium Carbide Clusters Nb₃C_n (n = 1â^'4) and Nb₄C_n (n = 1â^'6). Journal of Physical Chemistry A, 2008, 112, 5582-5592.	2.5	31
20	Photoinitiation of the Oâ^' + H2Oâ†'OHâ^'+OH ionâ€"molecule reaction within the Oâ^'2Â·H2O binary complex. Chemical Physics Letters, 1993, 216, 471-478.	2.6	28
21	Ionization Potentials of Tantalumâ^'Carbide Clusters:â€‰ An Experimental and Density Functional Theory Study. Journal of Physical Chemistry A, 2005, 109, 11180-11190.	2.5	27
22	Development, Evaluation and Use of a Student Experience Survey in Undergraduate Science Laboratories: The Advancing Science by Enhancing Learning in the Laboratory Student Laboratory Learning Experience Survey. International Journal of Science Education, 2015, 37, 1795-1814.	1.9	27
23	Photoionization of Nb3CO and Nb3(CO)2:Â Is CO Molecularly or Dissociatively Adsorbed on Niobium?. Journal of Physical Chemistry A, 2004, 108, 964-970.	2.5	26
24	Laser-Based Formation and Properties of Gold Nanoparticles in Aqueous Solution: Formation Kinetics and Surfactant-Modified Particle Size Distributions. Journal of Physical Chemistry C, 2010, 114, 15931-15940.	3.1	26
25	Diastereomeric 1,4,7,10-Tetrakis((S)-2-hydroxypropyl)- 1,4,7,10-tetraazacyclododecane and Its Alkali Metal Complex Ions. A Nuclear Magnetic Resonance, Potentiometric Titration, and Molecular Orbital Study. Journal of the American Chemical Society, 1997, 119, 6126-6134.	13.7	23
26	Metal Ion Dependent Molecular Inclusion Chemistry:Â Inclusion ofp-Toluenesulfonate andp-Nitrophenolate within the Structure of Coordinated 1,4,7,10-Tetrakis((S)-2-hydroxy-3-phenoxypropyl)-1,4,7,10-tetraazacyclododecane. Inorganic Chemistry, 1999, 38, 4986-4992.	4.0	23
27	Observation of the Aâ€‰2Îuâ†Xâ€‰2Îg dissociative transition in isolated O2â^' using massâ€selected photofragmentation spectroscopy. Journal of Chemical Physics, 1993, 99, 5910-5916.	3.0	22
28	Structural Aspects of the Coordination of Triethylphosphinegold(I) to 2-Thiouracil:â€‰ A Comparison between Theory and Experiment. Journal of Physical Chemistry A, 1997, 101, 5368-5373.	2.5	19
29	Diastereomeric Î"-1,4,7,10-Tetrakis((R)-2-hydroxy-2-phenylethyl)- 1,4,7,10-tetraazacyclododecane and Its Alkali-Metal Complex Ions. A Potentiometric Titration, Nuclear Magnetic Resonance, and Molecular Orbital Study. Journal of the American Chemical Society, 1998, 120, 2862-2869.	13.7	19
30	The (n, 3s) Rydberg State in Deuterated Aldehydes: Jet-Cooled MPI Spectra of the Propanal Isotopomeric Series. Journal of Molecular Spectroscopy, 1994, 165, 32-56.	1.2	18
31	On the structure of the monohydrated superoxide molecular anion, O2-Â·(H2O). An ab initio molecular orbital study. Physical Chemistry Chemical Physics, 1999, 1, 3961-3966.	2.8	17
32	Cyclodextrin and modified cyclodextrin complexes of E-4-tert-butylphenyl-4â€²-oxyazobenzene: UV-visible,1H NMR and ab initio studies. Organic and Biomolecular Chemistry, 2005, 3, 1481-1488.	2.8	16
33	Collisional electrochemistry of laser-ablated gold nanoparticles by electrocatalytic oxidation of glucose. Electrochemistry Communications, 2017, 77, 24-27.	4.7	16
34	Effect of indistinguishable nuclei on product rotational distributions: D+DIâ†'D2+I. Chemical Physics Letters, 1990, 169, 365-371.	2.6	15
35	Product internalâ€state distribution for the reaction H+HIâ†'H2+I. Journal of Chemical Physics, 1991, 95, 1663-1670.	3.0	15
36	Excess Energy-Dependent Photodissociation Probabilities for O2- in Water Clusters: O2-.cntdot.(H2O)n, 1 .ltoreq. n .ltoreq. 33. The Journal of Physical Chemistry, 1995, 99, 8453-8457.	2.9	15

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37	Ab initio calculations of stationary points on the benzeneâ€“Ar and p-difluorobenzeneâ€“Ar potential energy surfaces: barriers to bound orbiting states. Journal of Chemical Physics, 2004, 121, 4635-4641.	3.0	15
38	UVâ€“Vis and fluorimetric Al3+, Zn2+, Cd2+ and Pb2+ complexation studies of two 3-hydroxyflavones and a 3-hydroxythioflavone. Inorganica Chimica Acta, 2007, 360, 3380-3386.	2.4	15
39	The (n, 3s) Rydberg State in Deuterated Aldehydes: Jet-Cooled MPI Spectra of the sym and asym Rotamers of CHD2CHO and CDH2CHO. Journal of Molecular Spectroscopy, 1994, 165, 12-31.	1.2	14
40	Crystal structure of anhydrous potassium O-n-propyldithiocarbonate. Theoretical calculations of O-alkyl dithiocarbonates. Zeitschrift Fur Kristallographie - Crystalline Materials, 2003, 218, .	0.8	14
41	Anionâ˜Ï€ Interactions of Hexaaryl[3]radialenes. Journal of Physical Chemistry A, 2012, 116, 8001-8007.	2.5	14
42	The dynamics of evaporation from a liquid surface. Chemical Physics Letters, 2011, 513, 1-11.	2.6	13
43	Facile Decarboxylation of Propiolic Acid on a Ruthenium Center and Related Chemistry. Organometallics, 2012, 31, 5262-5273.	2.3	13
44	Some ruthenium complexes containing cyanocarbon ligands: syntheses, structures and extent of electronic communication in binuclear systems. Journal of Organometallic Chemistry, 2004, 689, 3308-3326.	1.8	12
45	The lowest-lying excited singlet and triplet electronic states of propanal: an ab initio molecular orbital investigation of the potential energy surfaces. Physical Chemistry Chemical Physics, 2004, 6, 688.	2.8	12
46	Associative versus dissociative binding of CO to 4d transition metal trimers: A density functional study. Journal of Computational Chemistry, 2008, 29, 1497-1506.	3.3	12
47	Surface movement in water of splendipherin, the aquatic male sex pheromone of the tree frog Litoriaâ€ splendida. FEBS Journal, 2008, 275, 3362-3374.	4.7	12
48	Onset of carbonâ€“carbon bonding in the Nb₅C_y (y = 0â€“6) clusters: a threshold photo-ionisation and density functional theory study. Physical Chemistry Chemical Physics, 2009, 11, 1060-1068.	2.8	12
49	Benzene Internal Energy Distributions Following Spontaneous Evaporation from a Waterâ˜Ethanol Solution. Journal of Physical Chemistry C, 2009, 113, 637-643.	3.1	11
50	Time-of-flight mass spectrometric detection of mono- and di-substituted benzenes at parts per million concentrations by way of liquid microjet injection and laser ionisation. International Journal of Mass Spectrometry, 2001, 207, 1-12.	1.5	10
51	Title is missing!. Australian Journal of Chemistry, 2001, 54, 185.	0.9	10
52	Gas phase ion formation from a liquid beam of arginine in aqueous solution by IR multiphoton excitation. Chemical Physics Letters, 2006, 420, 18-23.	2.6	10
53	A disconnect between staff and student perceptions of learning: an ACELL educational analysis of the first year undergraduate chemistry experiment â€˜investigating sugar using a home made polarimeterâ€™. Chemistry Education Research and Practice, 2011, 12, 469-477.	2.5	10
54	Competitive charge-remote and anion-induced fragmentations of the non-8-enoate anion. A charge-remote reaction which co-occurs with hydrogen scrambling. Journal of the Chemical Society Perkin Transactions II, 1997, , 695-702.	0.9	9

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55	Diastereomeric discrimination in 1,4,7-tris((Sâ€Š)-2-hydroxypropyl)-1,4,7-triazacyclononane and its lithium(I), sodium(I) and zinc(II) complexes. Dalton Transactions RSC, 2001, , 2157-2163.	2.3	9
56	Infrared Laser Desorption of Hydroquinone from a Waterâ^'Ethanol Liquid Beam. Journal of Physical Chemistry A, 2003, 107, 6130-6135.	2.5	9
57	Synthesis and coordination chemistry of 1,4,7,10,13-pentakis(2-hydroxyethyl)-1,4,7,10,13-pentaazacyclopentadecane: a five armed pendant donor macrocycle. Dalton Transactions RSC, 2002, , 3571-3577.	2.3	8
58	DFT Calculations on Group 5 Mixed Metal Tetramers: TaxNbyVz (x + y + z = 4). Australian Journal of Chemistry, 2004, 57, 1197.	0.9	8
59	BFW:Â A Density Functional for Transition Metal Clusters. Journal of Physical Chemistry A, 2007, 111, 2625-2628.	2.5	8
60	The degenerate Payne rearrangement of the 2,3-epoxypropoxide anion in the gas phase. A joint theoretical and experimental study. Journal of the Chemical Society Perkin Transactions II, 1997, , 1991-1997.	0.9	7
61	Study of the Isomers of Isoelectronic C₄, (C₃B)^{â^'}, and (C₃N)⁺: Rearrangements through Cyclic Isomers. Journal of Physical Chemistry A, 2009, 113, 12952-12960.	2.5	7
62	A Comparison between Crystallographic and Theoretical Structures for Three Hypervalent RSnCl3 Compounds. Phosphorus, Sulfur and Silicon and the Related Elements, 1999, 150, 261-270.	1.6	6
63	Jet-Cooled Multiphoton Ionization Spectroscopy of the iso-Butanal 3sâ†n Rydberg Transition. Journal of Molecular Spectroscopy, 2001, 206, 73-82.	1.2	6
64	Rotational Energy Distributions of Benzene Liberated from Aqueous Liquid Microjets: A Comparison between Evaporation and Infrared Desorption. Australian Journal of Chemistry, 2006, 59, 104.	0.9	6
65	Metal ion-activated molecular receptors for aromatic anions with receptor cavities formed from 1- or 2-naphthyloxy moieties appended to cyclen. Dalton Transactions, 2003, , 3028.	3.3	5
66	Ultraviolet Laser Irradiation of Low Concentration Liquid Microjets: Solute Evaporation and Solvent Initiated Reactivity. Australian Journal of Chemistry, 2003, 56, 481.	0.9	5
67	Photoionization efficiency spectroscopy and density functional theory investigations of RhHo2On (n=0â€“2) clusters. Journal of Chemical Physics, 2009, 130, 164311.	3.0	5
68	The timing of an experiment in the laboratory program is crucial for the student laboratory experience: acylation of ferrocene as a case study. Chemistry Education Research and Practice, 2013, 14, 476-484.	2.5	4
69	Enantiomerization of Pendant-Arm Triaza Macrocyclic Lithium(I) and Sodium(I) Complex Ions. Australian Journal of Chemistry, 1997, 50, 853.	0.9	4
70	The gas phase Payne rearrangement. Part 2. Methyl substitution: a joint ab initio and experimental study. International Journal of Mass Spectrometry and Ion Processes, 1997, 165-166, 139-153.	1.8	3
71	Influence of Surfactant Concentration on Laser-Based Gold Nanoparticle Formation and Stability. Australian Journal of Chemistry, 2012, 65, 97.	0.9	3
72	What Makes a Good Laboratory Learning Exercise? Student Feedback from the ACELL Project. , 2009, , 363-376.		3

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73	Diastereomeric preference in 1,4,7-tris((S)-2-hydroxy-3-phenylpropyl)-1,4,7-triazacyclononanelithium(I) and its sodium(I) analogue. Inorganica Chimica Acta, 2002, 331, 340-344.	2.4	2
74	Measuring the internal energy content of molecules transported across the liquid-gas interface. Journal of Physics: Conference Series, 2009, 185, 012027.	0.4	2
75	Laser-Based Formation of Copper Nanoparticles in Aqueous Solution: Optical Properties, Particle Size Distributions, and Formation Kinetics. Australian Journal of Chemistry, 2017, 70, 1212.	0.9	2
76	Structure of the Molecular Receptor 1,4,7,10-Tetrakis[(S)-2-hydroxy-2-phenylethyl]-1,4,7,10-tetraazacyclododecane: A Combined X-Ray Crystallographic and Theoretical Study Producing an Assessment of the Crystal Packing Energy. Australian Journal of Chemistry, 2006, 59, 123.	0.9	1
77	Production of metal atoms, clusters and complexes in pulsed discharge-excited jets : Studies via mass-resolved laser multiphoton ionization. Organic Mass Spectrometry, 1991, 26, 195-200.	1.3	0
78	The mechanism of methanol loss from the (M ? H)? ions of cis- and trans-4-methoxycyclohexanol. The application of experiment and theory in concert. Journal of the Chemical Society Perkin Transactions II, 1996, , 2489.	0.9	0
79	DFT Calculations on Group 5 Mixed Metal Tetramers: TaxNbyVz (x + y + z = 4).. ChemInform, 2005, 36, no.	0.0	0
80	Translational and rotational energy content of benzene molecules IR-desorbed from an in vacuo liquid surface. Physical Chemistry Chemical Physics, 2012, 14, 9185.	2.8	0
81	Perceptions and Misconceptions about the Undergraduate Laboratory from Chemistry, Physics and Biology Academics. International Journal of Innovation in Science and Mathematics Education, 2020, 28, .	0.2	0