ValÃ©rie Brenner

List of Publications by Year
in descending order

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83	2,028	218592	276775
papers	citations	26 h-index	41 g-index

85	85	85	1591
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum Effects in the Threshold Photoionization and Energetics of the Benzeneâ^'H2O and Benzeneâ^'D2O Complexes:â€‰ Experiment and Simulation. Journal of Physical Chemistry A, 1998, 102, 6590-6600.	1.1	127
2	An Experimental and Theoretical Study of Jet-Cooled Complexes of Chiral Molecules:â€‰ The Role of Dispersive Forces in Chiral Discrimination. Journal of Physical Chemistry A, 1998, 102, 128-137.	1.1	91
3	Molecular Dynamics Study of the Hydration of Lanthanum(III) and Europium(III) Including Many-Body Effects. Journal of Physical Chemistry B, 2005, 109, 7614-7616.	1.2	79
4	Ionization, Energetics, and Geometry of the Phenolâ^'S Complexes (S = H2O, CH3OH, and CH3OCH3). Journal of Physical Chemistry A, 1998, 102, 4890-4898.	1.1	78
5	Modeling of Uranyl Cationâ^'Water Clusters. Journal of Physical Chemistry B, 2003, 107, 3051-3060.	1.2	76
6	Dipole binding: An experimental test for small cluster structure calculations. Journal of Chemical Physics, 1995, 102, 4952-4964.	1.2	74
7	Unraveling the Mechanisms of Nonradiative Deactivation in Model Peptides Following Photoexcitation of a Phenylalanine Residue. Journal of the American Chemical Society, 2012, 134, 20340-20351.	6.6	66
8	Site Dependence of the Binding Energy of Water to Indole: Microscopic Approach to the Side Chain Hydration of Tryptophan. Journal of Physical Chemistry A, 1999, 103, 9958-9965.	1.1	62
9	Chirality-Controlled Formation of Î²-Turn Secondary Structures in Short Peptide Chains: Gas-Phase Experiment versus Quantum Chemistry. Angewandte Chemie - International Edition, 2007, 46, 2463-2466.	7.2	56
10	Ion-Neutral Complexes of Protonated Alkylbenzenes: Experimental and Theoretical Studies. The Journal of Physical Chemistry, 1995, 99, 712-720.	2.9	55
11	Energetics of a model NHâ€“Ï€ interaction: the gas phase benzeneâ€“NH3 complex. Physical Chemistry Chemical Physics, 2002, 4, 571-576.	1.3	54
12	Spectroscopy, dynamics and structures of jet formed anthracene clusters. Chemical Physics, 2002, 275, 123-147.	0.9	54
13	Intermolecular interactions: basis set and intramolecular correlation effects on semiempirical methods. Application to (C2H2)2, (C2H2)3 and (C2H4)2. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1994, 30, 327-340.	1.0	52
14	Intramolecular recognition in a jet-cooled short peptide chain: Î³-turn helicity probed by a neighbouring residue. Physical Chemistry Chemical Physics, 2007, 9, 4491.	1.3	52
15	Hydrogen-Bonded Bridges in Complexes of o-Cyanophenol:â€‰ Laser-Induced Fluorescence and IR/UV Double-Resonance Studies. Journal of Physical Chemistry A, 2001, 105, 6841-6850.	1.1	48
16	Spectroscopic Evidence for the Formation of Helical Structures in Gas-Phase Short Peptide Chainsâ€. Journal of Physical Chemistry A, 2007, 111, 7347-7354.	1.1	46
17	[C6H6iso-C3H7+] and [C6H7+C3H6] ion-molecule complexes: theoretical calculations. Journal of the American Chemical Society, 1993, 115, 2505-2507.	6.6	31
18	Experimental and theoretical study of 1-cyanonaphthalene clustered with acetonitrile and water in a supersonic jet. The Journal of Physical Chemistry, 1993, 97, 10570-10579.	2.9	31

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19	Calculated and Experimental Structures of the p-Difluorobenzene-(H2O)n=1-3 Clusters in Their Different Electronic States and Inference for Ionic Nucleophilic Substitution. The Journal of Physical Chemistry, 1995, 99, 5848-5860.	2.9	31
20	Laser induced fluorescence of jet-cooled non-conjugated bichromophores: bis-phenoxymethane and bis-2,6-dimethylphenoxymethane. Chemical Physics, 1996, 208, 243-257.	0.9	31
21	A Model Potential Approach to Charge Resonance Phenomena in Aromatic Cluster Ions. Journal of Physical Chemistry A, 2002, 106, 10326-10341.	1.1	31
22	Secondary Structures in Phe-Containing Isolated Dipeptide Chains: Laser Spectroscopy vs Quantum Chemistry. Journal of Physical Chemistry A, 2015, 119, 5932-5941.	1.1	31
23	Can we understand the different coordinations and structures of closed-shell metal cation-water clusters?. Journal of Computational Chemistry, 2002, 23, 1013-1030.	1.5	29
24	Intrinsic Folding Proclivities in Cyclic Î²â€Peptide Building Blocks: Configuration and Heteroatom Effects Analyzed by Conformerâ€Selective Spectroscopy and Quantum Chemistry. Chemistry - A European Journal, 2015, 21, 16479-16493.	1.7	29
25	Non-radiative relaxation of UV photoexcited phenylalanine residues: probing the role of conical intersections by chemical substitution. Physical Chemistry Chemical Physics, 2014, 16, 2285.	1.3	28
26	Direct Spectroscopic Evidence of Hyperconjugation Unveils the Conformational Landscape of Hydrazides. Angewandte Chemie - International Edition, 2014, 53, 13756-13759.	7.2	27
27	Can we rationalize the structure of small silicon-carbon clusters?. European Physical Journal D, 1998, 1, 197-205.	0.6	25
28	Energetics and Structure of Complexes of Al+with Small Organic Molecules in the Gas Phase. Journal of Physical Chemistry A, 1997, 101, 5885-5894.	1.1	24
29	A simulation of naphthalene matrix isolation: comparison with experiments. Chemical Physics, 2001, 272, 243-258.	0.9	23
30	Far/Mid-Infrared Signatures of Solventâ€“Solute Interactions in a Microhydrated Model Peptide Chain. Journal of Physical Chemistry Letters, 2012, 3, 3307-3311.	2.1	23
31	Infrared spectra of the C[sub 2]H[sub 2]â€“HCl complexes: An experimental and ab initio study. Journal of Chemical Physics, 2000, 113, 4876.	1.2	20
32	Exciplexes or ground state complexes of (dibenzoylmethanato)boron difluoride and benzene derivatives? A study of their optical properties revisited via liquid state investigations and structure calculations. Photochemical and Photobiological Sciences, 2006, 5, 686.	1.6	20
33	New model potentials for sulfurâ€“copper(I) and sulfurâ€“mercury(II) interactions in proteins: Fromab initio to molecular dynamics. Journal of Computational Chemistry, 2006, 27, 837-856.	1.5	20
34	Identification of ion pairs in solution by IR spectroscopy: crucial contributions of gas phase data and simulations. Physical Chemistry Chemical Physics, 2019, 21, 12798-12805.	1.3	20
35	Conformation control through concurrent Nâ€“Hâ‹¯S and Nâ€“Hâ‹¯Oî€C hydrogen bonding and hyperconjugation effects. Chemical Science, 2020, 11, 9191-9197.	3.7	20
36	Local NHâ€“Ï€ interactions involving aromatic residues of proteins: influence of backbone conformation and Ï€Ï€* excitation on the Ï€ H-bond strength, as revealed from studies of isolated model peptides. Physical Chemistry Chemical Physics, 2016, 18, 29969-29978.	1.3	19

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37	On the turn-inducing properties of asparagine: the structuring role of the amide side chain, from isolated model peptides to crystallized proteins. Physical Chemistry Chemical Physics, 2018, 20, 3411-3423.	1.3	19
38	Photoinduced electron transfer in isolated, jet-cooled molecular systems. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 3277-3287.	1.7	18
39	Evidencing Intermolecular Effects with Core-Level Photoelectron Spectroscopy via the Accurate Density Functional Calculation of Coreâ^'Electron Binding Energies on Model Systems: Î³-APS as a Test. Journal of Physical Chemistry B, 1997, 101, 10254-10261.	1.2	18
40	Methanol-acetonitrile complexes trapped in argon and nitrogen matrices: Infrared induced isomerization and theoretical calculations. Journal of Chemical Physics, 1999, 110, 10046-10057.	1.2	17
41	Methanolâ€“pyridine complexes trapped in argon and nitrogen matrices: Infrared induced isomerization and theoretical calculations. Journal of Chemical Physics, 2000, 113, 8059-8069.	1.2	16
42	Binding Energies and Structures of Naâ^'(CH3CN)n=1-9 Clusters: Theoretical Study of the Contact Ion Pair versus the Solvent-Separated Ion Pair Structures in a Molecular Cluster. Journal of Physical Chemistry A, 2000, 104, 5204-5212.	1.1	16
43	Rationalizing the diversity of amideâ€“amide H-bonding in peptides using the natural bond orbital method. Physical Chemistry Chemical Physics, 2019, 21, 24601-24619.	1.3	16
44	Monte Carlo growth method: application to molecular clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 39, 239.	1.0	16
45	Existence of two internal energy distributions in jet-formed van der Waals heteroclusters: example of the anthraceneâ€“argon system. Chemical Physics, 1998, 239, 151-175.	0.9	15
46	Infrared spectra of C2H4â€“HCl complex. Journal of Chemical Physics, 2002, 117, 1522-1528.	1.2	14
47	A new method for deriving atomic charges and dipoles forn, -alkanes: investigation of transferability and geometry dependence. Molecular Physics, 1999, 97, 1117-1128.	0.8	13
48	Electrostatic interactions and hydrogen bond in clusters. Theoretical approach. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1995, 92, 428-444.	0.2	13
49	Nâ€“Hâ‹¯X interactions stabilize intra-residue C5 hydrogen bonded conformations in heterocyclic Î±-amino acid derivatives. Chemical Science, 2021, 12, 14826-14832.	3.7	13
50	Characterization of Photoinduced Electron Transfer in Jet-Formed Acceptorâ^'Donor Complexes. 1. Isomeric Forms of Complexes of Anthracene with Aniline Derivatives. Journal of Physical Chemistry A, 1998, 102, 2798-2807.	1.1	12
51	Ab initio anharmonic intermolecular potential of the C2H2â€“HCl hydrogen bonded complex. Chemical Physics Letters, 2001, 336, 335-342.	1.2	12
52	On the near UV photophysics of a phenylalanine residue: conformation-dependent Ï€Ï€* state deactivation revealed by laser spectroscopy of isolated neutral dipeptides. Physical Chemistry Chemical Physics, 2014, 16, 22192-22200.	1.3	12
53	Gas-Phase Spectroscopic Signatures of Carboxylateâ€“Li⁺ Contact Ion Pairs: New Benchmarks For Characterizing Ion Pairing in Solution. Journal of Physical Chemistry Letters, 2016, 7, 1192-1197.	2.1	12
54	Unimolecular and Bimolecular Reactions of the .beta.-Distonic Ion CH3CH2OH+CH2CH2.bul.: An Experimental and Theoretical Study. The Journal of Physical Chemistry, 1995, 99, 10837-10846.	2.9	11

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55	Diffusion and clustering of N2O molecules in argon clusters: A theoretical approach by molecular dynamics simulations. Journal of Chemical Physics, 1997, 106, 9155-9171.	1.2	11
56	Theoretical interpretation of the stability of â€œanomalouslyâ€•small doubly charged paradifluorobenzene clusters. Chemical Physics, 1992, 162, 303-320.	0.9	10
57	Characterization of Photoinduced Electron Transfer in Jet-Formed Acceptor Donor Complexes. 2. Photoinduced Electron Transfer:Â Rates and Mechanisms. Journal of Physical Chemistry A, 1998, 102, 2808-2816.	1.1	10
58	Are lithium hydride clusters purely ionic? Study using model potentials and density-functional theory. Journal of Chemical Physics, 2001, 115, 4070-4079.	1.2	10
59	Assessment of time-dependent density functional theory for predicting excitation energies of bichromophoric peptides: case of tryptophan-phenylalanine. Theoretical Chemistry Accounts, 2008, 121, 307-312.	0.5	10
60	Assessment of density functional theory for bonds formed between rare gases and open-shell atoms: a computational study of small molecules containing He, Ar, Kr and Xe. Physical Chemistry Chemical Physics, 2012, 14, 553-561.	1.3	10
61	Conformation dependence of electron transfer in jet-cooled anthracene complexes with aniline derivatives. Journal of Photochemistry and Photobiology A: Chemistry, 1994, 80, 95-101.	2.0	9
62	Influence of covalence and anion symmetry on the structure of small metal hydroxide clusters: Sodium versus silver hydroxide. European Physical Journal D, 2000, 11, 387-394.	0.6	9
63	Theoretical Investigation of Small Alkali Cationâ^'Molecule Clusters:â€‰ A Model Potential Approach. Journal of Physical Chemistry B, 2004, 108, 1497-1506.	1.2	9
64	Electronic Stark Effect in Isolated Ion Pairs. Journal of Physical Chemistry Letters, 2019, 10, 7458-7462.	2.1	9
65	Intrinsic folding of the cysteine residue: competition between folded and extended forms mediated by the â€“SH group. Physical Chemistry Chemical Physics, 2020, 22, 20284-20294.	1.3	9
66	Pumpâ€“probe dissociative ionization of NaI and CsI aggregated with CH3CN. Journal of Chemical Physics, 2002, 116, 10753-10759.	1.2	7
67	Non-Coulombic states of N24+and O24+ions probed by laser-induced multi-ionization of N2and O2. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, L145-L151.	0.6	6
68	Collision-Induced Dissociation by Helium:Â A Piecewise Construction of the Cross Section. Journal of Physical Chemistry A, 2002, 106, 1714-1726.	1.1	6
69	Ion Pair Supramolecular Structure Identified by ATRâ€FTIR Spectroscopy and Simulations in Explicit Solvent**. ChemPhysChem, 2021, 22, 2442-2455.	1.0	6
70	Low-lying excited states of model proteins: Performances of the CC2 method versus multireference methods. Journal of Chemical Physics, 2018, 148, 184105.	1.2	5
71	Effects of complexation with sulfuric acid on the photodissociation of protonated Cinchona alkaloids in the gas phase. Physical Chemistry Chemical Physics, 2019, 21, 15439-15451.	1.3	5
72	CC2 Benchmark for Models of Phenylalanine Protein Chains: 0â€“0 Transition Energies and IR Signatures of the Ï€Ï€* Excited State. Journal of Chemical Theory and Computation, 2020, 16, 601-611.	2.3	5

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73	An intraresidue H-bonding motif in selenocysteine and cysteine, revealed by gas phase laser spectroscopy and quantum chemistry calculations. Physical Chemistry Chemical Physics, 2020, 22, 20409-20420.	1.3	5
74	A theoretical and experimental case study of the hydrogen bonding predilection of S-methylcysteine. Amino Acids, 2021, 53, 621-633.	1.2	4
75	Characterization of Asx Turn Types and Their Connate Relationship with Î²â€Turns. Chemistry - A European Journal, 2022, , .	1.7	4
76	Stepwise dissociation of ion pairs by water molecules: cation-dependent separation mechanisms between carboxylate and alkali-earth metal ions. Physical Chemistry Chemical Physics, 2022, 24, 12121-12125.	1.3	4
77	Selenium in Proteins: Conformational Changes Induced by Se Substitution on Methionine, as Studied in Isolated Model Peptides by Optical Spectroscopy and Quantum Chemistry. Molecules, 2022, 27, 3163.	1.7	4
78	Excited States Computation of Models of Phenylalanine Protein Chains: TD-DFT and Composite CC2/TD-DFT Protocols. International Journal of Molecular Sciences, 2022, 23, 621.	1.8	3
79	Rovibrational laser jet-cooled spectroscopy of SF₆â€“rare gas complexes in the Î½₃ region of SF₆. Physical Chemistry Chemical Physics, 2018, 20, 28105-28113.	1.3	2
80	Infrared study on hydrogen chloride complexed with allene. Journal of Chemical Physics, 2010, 132, 164306.	1.2	1
81	Conformational analysis by UV spectroscopy: the decisive contribution of environment-induced electronic Stark effects. Chemical Science, 2021, 12, 2803-2815.	3.7	1
82	Model protein excited states: MRCI calculations with large active spaces vs CC2 method. Journal of Chemical Physics, 2021, 154, 214105.	1.2	1
83	Characterization of Asx Turn Types and Their Connate Relationship with Î²â€Turns. Chemistry - A European Journal, 2022, , e202200969.	1.7	0