Peeter Burk

List of Publications by Year
in descending order

90	1,942	279798 23	289244 40
papers	citations	h-index	g-index

96	96	96	1989
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Gas-Phase Acidities of Some Neutral BrÃ¸nsted Superacids:Â A DFT and ab Initio Study. Journal of the American Chemical Society, 2000, 122, 5114-5124.	13.7	240
2	Revised and Expanded Scale of Gas-Phase Lithium Cation Basicities. An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 2824-2833.	2.5	131
3	Critical test of performance of B3LYP functional for prediction of gas-phase acidities and basicities. Chemical Physics Letters, 2000, 323, 482-489.	2.6	112
4	Intrinsic Basicities of Phosphorus Imines and Ylides:Â A Theoretical Study. Journal of Physical Chemistry A, 2001, 105, 9575-9586.	2.5	101
5	Generalized Principle of Designing Neutral Superstrong BrÃ¸nsted Acids. Journal of the American Chemical Society, 2002, 124, 5594-5600.	13.7	55
6	Hybrid Quantum Chemical and Density Functional Theory (ONIOM) Study of the Acid Sites in Zeolite ZSM-5. Journal of Physical Chemistry B, 2004, 108, 9893-9899.	2.6	52
7	Theoretical Study of Magnesium Compounds:â€‰ The Schlenk Equilibrium in the Gas Phase and in the Presence of Et2O and THF Molecules. Journal of Physical Chemistry A, 2004, 108, 133-139.	2.5	52
8	Aromaticity of Substituted Cyclopropenes:Â A Theoretical Study. The Journal of Physical Chemistry, 1996, 100, 6992-6997.	2.9	47
9	IEF-PCM Calculations of Absolute pK_a for Substituted Phenols in Dimethyl Sulfoxide and Acetonitrile Solutions. Journal of Physical Chemistry A, 2009, 113, 6206-6212.	2.5	46
10	Cesium cation affinities and basicities. International Journal of Mass Spectrometry, 2007, 267, 7-23.	1.5	45
11	Superacidity of neutral Brï¿½nsted acids in gas phase. Journal of Computational Chemistry, 1996, 17, 30-41.	3.3	43
12	Dihydrogen Generation from Amine/Boranes: Synthesis, FTâ€ICR, and Computational Studies. Chemistry - A European Journal, 2012, 18, 3981-3991.	3.3	38
13	Critical Test of Some Computational Chemistry Methods for Prediction of Gas-Phase Acidities and Basicities. Journal of Chemical Theory and Computation, 2013, 9, 3947-3958.	5.3	38
14	Predicting Cytotoxicity of Metal Oxide Nanoparticles Using Isalos Analytics Platform. Nanomaterials, 2020, 10, 2017.	4.1	34
15	A Quantitative Structureâ^'Property Relationship Study of Lithium Cation Basicities. Journal of Physical Chemistry A, 2004, 108, 4812-4818.	2.5	31
16	Computational Study of Copper-Free Sonogashira Cross-Coupling Reaction. Organometallics, 2011, 30, 5656-5664.	2.3	31
17	Critical test of some computational methods for prediction of NMR 1H and 13C chemical shifts. Journal of Molecular Modeling, 2015, 21, 244.	1.8	30
18	Parametrization of nanoparticles: development of full-particle nanodescriptors. Nanoscale, 2016, 8, 16243-16250.	5.6	30

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19	The basicity of substituted N,Nâ€dimethylanilines in solution and in the gas phase. Journal of Physical Organic Chemistry, 2013, 26, 171-181.	1.9	29
20	QSPR analysis for infinite dilution activity coefficients of organic compounds. Journal of Molecular Modeling, 2006, 12, 417-421.	1.8	28
21	Calculation of the properties of acid sites of the zeolite ZSM-5 using ONIOM method. Computational and Theoretical Chemistry, 2002, 589-590, 281-290.	1.5	27
22	Critical test of PM3 calculated gas-phase acidities. Theoretica Chimica Acta, 1993, 86, 417-427.	0.8	25
23	Can Oâ^'H Acid be More Acidic Than Its Sâ^'H Analog? A G2 Study of Fluoromethanols and Fluoromethanethiols. Journal of Physical Chemistry A, 2000, 104, 1602-1607.	2.5	25
24	Fe-Doped ZnO nanoparticle toxicity: assessment by a new generation of nanodescriptors. Nanoscale, 2018, 10, 21985-21993.	5.6	23
25	Quantum chemical calculations of geometries and gas-phase deprotonation energies of linear polyyne chains. International Journal of Quantum Chemistry, 2001, 82, 73-85.	2.0	21
26	Solvent effects in the Grignard reaction with alkynes. Journal of Physical Organic Chemistry, 2002, 15, 701-705.	1.9	21
27	Why are carboxylic acids stronger acids than alcohols? The electrostatic theory of Siggelâ€“Thomas revisited. Computational and Theoretical Chemistry, 2000, 505, 161-167.	1.5	20
28	Computational Study of Cesium Cation Interactions with Neutral and Anionic Compounds Related to Soil Organic Matter. Journal of Physical Chemistry A, 2009, 113, 10734-10744.	2.5	19
29	Gas-Phase Basicities Around and Below Water Revisited. Journal of Physical Chemistry A, 2010, 114, 10694-10699.	2.5	19
30	Supramolecular chirogenesis in zinc porphyrins by enantiopure hemicucurbit[n]urils (n) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	4.1	19
31	Gas-phase basicities and proton affinities of alkali metal oxides and hydroxides. A theoretical study. Computational and Theoretical Chemistry, 2001, 543, 223-231.	1.5	18
32	Stereoelectronic, Strain, and Medium Effects on the Protonation of Cubylamine, a Janus-like Base. Angewandte Chemie - International Edition, 2003, 42, 2281-2285.	13.8	18
33	Gas-Phase Lithium Cation Basicity: Revisiting the High Basicity Range by Experiment and Theory. Journal of the American Society for Mass Spectrometry, 2014, 25, 1962-1973.	2.8	18
34	NMR and DFT Study of the Copper(I)â€Catalyzed Cycloaddition Reaction: H/D Scrambling of Alkynes and Variable Reaction Order of the Catalyst. ChemCatChem, 2016, 8, 1804-1808.	3.7	18
35	Protonation of Cubane in the Gas Phase: A High-Level Ab Initio and DFT Study. Angewandte Chemie - International Edition, 2003, 42, 1044-1046.	13.8	17
36	Acidity of Anilines: Calculations vs Experiment. Journal of Physical Chemistry A, 2011, 115, 10335-10344.	2.5	17

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37	Critical test ofPM3-calculated proton affinities. International Journal of Quantum Chemistry, 1993, 48, 633-641.	2.0	16
38	1,10-Phenanthroline and Its Complexes with Magnesium Compounds. Disproportionation Equilibria. Journal of Physical Chemistry A, 2001, 105, 8554-8561.	2.5	16
39	Quantum chemical calculations of linear cumulene chains. Computational and Theoretical Chemistry, 2004, 712, 81-89.	1.5	16
40	Computational study of vibrational frequencies of bridging hydroxyl groups in zeolite ZSM-5. Chemical Physics Letters, 2004, 393, 285-289.	2.6	16
41	Investigations of cluster ions formed between cesium cations and benzoic, salicylic and phthalic acids by electrospray mass spectrometry and density-functional theory calculations. Toward a modeling of the interaction of Cs+ with humic substances. Rapid Communications in Mass Spectrometry, 2005, 19, 568-573.	1.5	16
42	Computational study of the Sonogashira cross-coupling reaction in the gas phase and in dichloromethane solution. Journal of Molecular Modeling, 2012, 18, 3025-3033.	1.8	16
43	Theoretical Calculation of Intrinsic Acidity and Basicity of FOH. The Journal of Physical Chemistry, 1995, 99, 1432-1435.	2.9	15
44	Interaction of the cesium cation with mono-, di-, and tricarboxylic acids in the gas phase. A Cs+ affinity scale for cesium carboxylates ion pairs. Journal of the American Society for Mass Spectrometry, 2009, 20, 1912-1924.	2.8	15
45	Theoretical study of structure and basicity of some alkali metal oxides, hydroxides, and amides. International Journal of Quantum Chemistry, 1994, 51, 313-318.	2.0	13
46	Computational Study on the Reactivity of Tetrazines toward Organometallic Reagents. Journal of Organic Chemistry, 2010, 75, 6196-6200.	3.2	13
47	Evaluation of Alkali Metal Cation Affinities and Basicities Using Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2014, 118, 1906-1917.	2.5	13
48	Theoretical Study of Dimethyl Sulfoxideâ^'Anion Clusters. The Journal of Physical Chemistry, 1996, 100, 16137-16140.	2.9	12
49	A study of the cesium cation bonding to carboxylate anions by the kinetic method and quantum chemical calculations. Journal of Mass Spectrometry, 2010, 45, 520-527.	1.6	12
50	A theoretical study of gas-phase basicities and proton affinities of alkali metal oxides and hydroxides. Computational and Theoretical Chemistry, 2003, 638, 119-128.	1.5	11
51	Bonding energetics in clusters formed by cesium salts: a study by collision-induced dissociation and density functional theory. Rapid Communications in Mass Spectrometry, 2006, 20, 2057-2062.	1.5	11
52	Theoretical modeling of sensitivity factors of Bayard-Alpert ionization gauges. International Journal of Mass Spectrometry, 2013, 341-342, 52-58.	1.5	11
53	Proton transfer reactions of hydrazine-boranes. Journal of Physical Organic Chemistry, 2015, 28, 244-249.	1.9	11
54	Photoelectron spectra of molecules. Part 12. Vinyl, allyl, and phenyl ethers and sulphides. Computational and Theoretical Chemistry, 2002, 579, 205-220.	1.5	10

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55	Adsorption of carbon monoxide on Li-ZSM-5: theoretical study of complexation of Li+ cation with two CO molecules. Physical Chemistry Chemical Physics, 2007, 9, 824.	2.8	10
56	Feasibility of the spontaneous gasâ€phase proton transfer equilibria between neutral BrÃ¸nsted acids and BrÃ¸nsted bases. Journal of Physical Organic Chemistry, 2008, 21, 571-574.	1.9	10
57	An AM1 and PM3 study of hexafluoroacetylacetone. Computational and Theoretical Chemistry, 1993, 282, 277-282.	1.5	8
58	Photoelectron spectra of molecules. II. Carboxylic acids and their esters. International Journal of Quantum Chemistry, 1997, 62, 303-314.	2.0	8
59	Acidity of saturated hydrocarbons. Computational and Theoretical Chemistry, 2001, 535, 49-59.	1.5	8
60	Bonding between the cesium cation and substituted benzoic acids or benzoate anions in the gas phase: A density functional theory and mass spectrometric study. Collection of Czechoslovak Chemical Communications, 2009, 74, 167-188.	1.0	8
61	Comparative calculations of alkali metal cation basicities of some Lewis bases; 107-121. Proceedings of the Estonian Academy of Sciences: Chemistry, 2007, 56, 107.	0.3	8
62	Interaction between the Cesium Cation and Cesium Carboxylates: An Extended Cs⁺ Basicity Scale. ChemPlusChem, 2013, 78, 1195-1204.	2.8	7
63	Effect of strain on gas-phase basicity of (E)-1-methyl-2-(1-methyl-2-adamantylidene)adamantane. Journal of Physical Organic Chemistry, 2015, 28, 447-451.	1.9	7
64	Conformational analysis of 1-acetyl-2-methylhydrazine. Computational and Theoretical Chemistry, 2001, 546, 119-125.	1.5	6
65	Computational study of the Grignard reaction with alkynes. Computational and Theoretical Chemistry, 2004, 674, 233-239.	1.5	6
66	The enormous apparent gas-phase acidity of cubylamine. Chemical Physics Letters, 2004, 398, 560-563.	2.6	6
67	An Integrated Data-Driven Strategy for Safe-by-Design Nanoparticles: The FP7 MODERN Project. Advances in Experimental Medicine and Biology, 2017, 947, 257-301.	1.6	6
68	Complexes between divalent metals and carboxylic acids: Semiempirical study. International Journal of Quantum Chemistry, 1997, 62, 653-658.	2.0	5
69	Computational study of the copper-free Sonogashira cross-coupling reaction: shortcuts in the mechanism. Proceedings of the Estonian Academy of Sciences, 2013, 62, 133.	1.5	5
70	Catalytic Effect of Cesium Cation Adduct Formation on the Decarboxylation of Carboxylate Ions in the Gas Phase. Chemistry - A European Journal, 2014, 20, 815-823.	3.3	5
71	Reaction kinetics and solubility in water-organic binary solutions are governed by similar solvation equilibria. Journal of Physical Organic Chemistry, 2016, 29, 118-126.	1.9	5
72	Computational modeling of strained alkenes: Choosing the right computational model. International Journal of Quantum Chemistry, 2017, 117, e25439.	2.0	5

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73	Theoretical study of prototropic tautomerism and acidity of tris(fluorosulfonyl)methane. Computational and Theoretical Chemistry, 1994, 315, 191-196.	1.5	4
74	Gas phase acidities of N-substituted amine-boranes. Journal of Molecular Modeling, 2013, 19, 5089-5095.	1.8	4
75	Kinetic sonication effects in light of molecular dynamics simulation of the reaction medium. Ultrasonics Sonochemistry, 2013, 20, 703-707.	8.2	4
76	P-substituted phosphineâ€“boranes: Gas phase acidities, basicities and dihydrogen release. A comparison to amineâ€“boranes. Computational and Theoretical Chemistry, 2014, 1032, 12-19.	2.5	4
77	Relative stability and proton transfer reactions of unsaturated isocyanides and cyanides. Journal of Physical Organic Chemistry, 2016, 29, 452-459.	1.9	4
78	Bromine formation in solid NaBr/KNO3 mixture and assay of this reaction via bromination of activated aromatics. Chemical Papers, 2018, 72, 2893-2898.	2.2	4
79	Stereoelectronic, Strain, and Medium Effects on the Protonation of Cubylamine, a Janus-like Base. Angewandte Chemie, 2003, 115, 2383-2387.	2.0	3
80	Quantitative description of acidity of XOH compounds in the gas phase and dimethyl sulphoxide with use of HOMO energies of XO? anions. Journal of Physical Organic Chemistry, 1995, 8, 364-370.	1.9	2
81	UV-VIS SPECTRUM OF THE 1,10-PHENANTHROLINE-ETHYLMAGNESIUM BROMIDE COMPLEX. AN EXPERIMENTAL AND COMPUTATIONAL STUDY. Main Group Metal Chemistry, 2000, 23, .	1.6	2
82	Alkali Metal Cations Bonding to Carboxylate Anions: Studies using Mass Spectrometry and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2020, 124, 4390-4399.	2.5	2
83	A Kinetic View of the Mechanism of the Grignard Reaction with Alkoxysilanes. Phosphorus, Sulfur and Silicon and the Related Elements, 2015, 190, 509-519.	1.6	1
84	Synthesis of Unprotected CH2-Skipped Piperazine-Pyridine Alternating Cycles with Azide End-Group. Heterocycles, 2015, 90, 625.	0.7	1
85	Theoretical Modeling of HPV: QSAR and Novodesign with Fragment Approach. Current Computer-Aided Drug Design, 2015, 10, 303-314.	1.2	1
86	Robust Modeling and Scaffold Hopping: Case Study Based on HIV Reverse Transcriptase Inhibitors Type-1 Data. Medicinal Chemistry, 2016, 12, 513-526.	1.5	1
87	Structure and superacidity of neutral Bronsted acids. AIP Conference Proceedings, 1995, , .	0.4	0
88	Relativistic effects on acidities and basicities of BrÃ¸nsted acids and bases containing gold. Physical Chemistry Chemical Physics, 2013, 15, 17971.	2.8	0
89	Strain criteria for alkenes: Two different manifestations. Computational and Theoretical Chemistry, 2020, 1178, 112764.	2.5	0
90	Energetics and Structures of Adducts of JohnPhos(Au+), PPh3(Au+), and IPr(Au+) with Organic Substrates: A Mass Spectrometry and DFT Study. Organometallics, 2021, 40, 1642-1653.	2.3	0