Alireza Fattahi

List of Publications by Year
in descending order

68	866	623574	580701
papers	citations	14 h-index	25 g-index

69	69	69	884
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational insight into networking Hâ€bonds in open and cyclic forms of glucose. Journal of Physical Organic Chemistry, 2022, 35, e4285.	0.9	1
2	Computational insight into networking H-bonds in open and cyclic forms of galactose. Journal of Molecular Structure, 2022, 1255, 132432.	1.8	0
3	Acidity enhancement of Î±â€carbon of beta diketones via hydroxyl substituents: A density functional theory study. Journal of Physical Organic Chemistry, 2021, 34, e4157.	0.9	1
4	Hydrogen bonding effects on acidity enhancement of barbiturates and their metabolites in gas and solution phase, a DFT study. Computational and Theoretical Chemistry, 2021, 1196, 113112.	1.1	1
5	Gold at crossroads of radical generation and scavenging at density functional theory level: Nitrogen and oxygen free radicals versus their precursors in the face of nanogold. Journal of Physical Organic Chemistry, 2021, 34, .	0.9	1
6	Design of carboxylate-based ionic liquids (ILs) containing OH and CF3 groups; influence of intramolecular hydrogen bonds and inductive effect on the binding energy between the cation and anion of ILs, a DFT study. New Journal of Chemistry, 2021, 45, 4710-4723.	1.4	2
7	Theoretical investigation of the effect of hydrogen bonding on the stereoselectivity of the Dielsâ€“Alder reaction. New Journal of Chemistry, 2021, 45, 16760-16772.	1.4	3
8	New pathways of stability for NHCs derived from azole, di-azole, n-tetrazole, and ab-tetrazole, by DFT. Journal of Molecular Modeling, 2020, 26, 324.	0.8	2
9	Influence of Hâ€bonds on acidity of deoxyâ€hexose sugars. Journal of Physical Organic Chemistry, 2020, 33, e4094.	0.9	4
10	Comparison of acidity and metal ion affinity of D-Glucosamine and N-acetyl-D-glucosamine, a DFT study. Journal of Molecular Graphics and Modelling, 2020, 98, 107612.	1.3	12
11	Influence of remote intramolecular hydrogen bonding on the acidity of hydroxyâ€1,4â€benzoquinonederivatives: A DFT study. Journal of Physical Organic Chemistry, 2019, 32, e3919.	0.9	17
12	Ionic liquid based on 6â€aminoâ€6â€deoxy hexopyranose cation and BF₄^{Â¯}, PF₆^{Â¯}, and ClO₄^{Â¯} as anions: A DFT study on the structural and electronic properties. Journal of Physical Organic Chemistry, 2018, 31, e3798.	0.9	2
13	The free radical scavenging activity of lespedezacoumestan toward Ë™OH radical: A quantum chemical and computational kinetics study. Journal of Physical Organic Chemistry, 2018, 31, e3755.	0.9	6
14	Does gold cluster promote or scavenge radicals? A controversy at <scp>DFT</scp>. Journal of Physical Organic Chemistry, 2018, 31, e3776.	0.9	3
15	A quantum chemical study on the OH radical quenching by natural antioxidant fisetin. Journal of Physical Organic Chemistry, 2017, 30, e3692.	0.9	5
16	Theoretical aspects of the enhancement of metal binding affinity by intramolecular hydrogen bonding and modulating pK_avalues. New Journal of Chemistry, 2017, 41, 15110-15119.	1.4	8
17	Phenylcyclopropane Energetics and Characterization of Its Conjugate Base: Phenyl Substituent Effects and the Câ€“H Bond Dissociation Energy of Cyclopropane. Journal of Organic Chemistry, 2016, 81, 9175-9179.	1.7	2
18	Power of a Remote Hydrogen Bond Donor: Anion Recognition and Structural Consequences Revealed by IR Spectroscopy. Journal of Organic Chemistry, 2015, 80, 1130-1135.	1.7	11

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19	DFT investigations for â€œFischerâ€•esterification mechanism over silica-propyl-SO3H catalyst: Is the reaction reversible?. Computational and Theoretical Chemistry, 2015, 1071, 27-32.	1.1	15
20	Stereoelectronic effects: a simple yet powerful tool to manipulate anion affinity. Organic and Biomolecular Chemistry, 2015, 13, 2170-2176.	1.5	5
21	Interaction of ionic liquids with the surface of silica gel using nanocluster approach: a combined density functional theory and experimental study. Journal of Physical Organic Chemistry, 2014, 27, 163-167.	0.9	13
22	The intramolecular cationâ€“Ï€ interaction of some aryl amines and its drastic influence on the basicity of them: AIM and NBO analysis. Computational and Theoretical Chemistry, 2014, 1036, 51-60.	1.1	8
23	Excellent response of the DFT study to the calculations of accurate relative pKa value of different benzo-substituted quinuclidines. Computational and Theoretical Chemistry, 2014, 1027, 191-196.	1.1	10
24	A study on the catalytic activity and theoretical modeling of a novel dual acidic mesoporous silica. RSC Advances, 2014, 4, 16647.	1.7	10
25	Calculating The Acidity of Silica Supported Alkyl Sulfonic Acids Considering the Matrix Effect: A Dft Study. Phosphorus, Sulfur and Silicon and the Related Elements, 2014, 189, 849-857.	0.8	10
26	Cooperativity effects of intramolecular OHâ€¦O interactions on pK _a values of polyolalkyl sulfonic acids in the gas phase and solution: a density functional theory study. Journal of Physical Organic Chemistry, 2014, 27, 604-612.	0.9	13
27	DFT study on Thiotepa and Tepa interactions with their DNA receptor. Structural Chemistry, 2013, 24, 1-11.	1.0	10
28	Investigation of the scavenging mechanism of tyrosyl radical by hydroxybenzohydroxamic acid derivatives: A DFT study. Computational and Theoretical Chemistry, 2013, 1018, 35-44.	1.1	8
29	Conformational aspects of glutathione tripeptide: electron density topological & natural bond orbital analyses. Structural Chemistry, 2013, 24, 147-158.	1.0	5
30	Computational investigation of thermochemical properties of non-natural C-nucloebases: different hydrogen-bonding preferences for non-natural Watsonâ€“Crick base pairs. Structural Chemistry, 2013, 24, 1015-1025.	1.0	5
31	Comparison of gas phase intrinsic properties of cytosine and thymine nucleobases with their O-alkyl adducts: different hydrogen bonding preferences for thymine versus O-alkyl thymine. Journal of Molecular Modeling, 2013, 19, 2993-3005.	0.8	4
32	INFLUENCE OF CATION-HETEROATOM (Li+, Na+, AND K+) INTERACTION ON THE STRUCTURAL AND THERMOCHEMICAL PROPERTIES OF 2â€²-DEOXYTHYMIDINE NUCLEOSIDE: QTAIM AND NBO ANALYZES. Journal of Theoretical and Computational Chemistry, 2013, 12, 1250113.	1.8	2
33	DRASTIC INFLUENCE OF BORON ATOM ON THE ACIDITY OF ALCOHOL IN BOTH GAS PHASE AND SOLUTION PHASE, A DFT STUDY. Journal of Theoretical and Computational Chemistry, 2013, 12, 1250103.	1.8	7
34	Interactions of coinage metal clusters with histidine and their effects on histidine acidity; theoretical investigation. Organic and Biomolecular Chemistry, 2012, 10, 9373.	1.5	9
35	Mechanisms and kinetics of thiotepa and tepa hydrolysis: DFT study. Journal of Molecular Modeling, 2012, 18, 3563-3576.	0.8	10
36	Theoretical descriptors response to the calculations of the relative pKa values of some boronic acids in aqueous solution: A DFT study. Computational and Theoretical Chemistry, 2012, 1000, 1-5.	1.1	23

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37	Can anion interaction accelerate transformation of cytosine tautomers? Detailed view form QTAIM analysis. Structural Chemistry, 2012, 23, 1843-1855.	1.0	2
38	Experimental and Computational Bridgehead Câ€“H Bond Dissociation Enthalpies. Journal of Organic Chemistry, 2012, 77, 1909-1914.	1.7	9
39	EFFECT OF CATION RADICAL FORMATION ON REACTIVITY AND ACIDITY ENHANCEMENT OF CYTOSINE NUCLEOBASE: NATURAL BOND ORBITAL AND ATOM IN MOLECULE ANALYSIS. Journal of Theoretical and Computational Chemistry, 2012, 11, 313-327.	1.8	11
40	Ionic Liquid Based on Î±-Amino Acid Anion and N7,N9-Dimethylguaninium Cation ([dMG][AA]): Theoretical Study on the Structure and Electronic Properties. Journal of Physical Chemistry A, 2012, 116, 5436-5444.	1.1	30
41	Interaction of cations with 2â€²â€deoxythymidine nucleoside and analysis of the nature and strength of cation bonds. Journal of Physical Organic Chemistry, 2012, 25, 153-161.	0.9	9
42	What roles do boron substitutions play in structural, tautomeric, base pairing and electronic properties of uracil? NBO & AIM analysis. Journal of Physical Organic Chemistry, 2012, 25, 787-796.	0.9	4
43	Influence of the hydrogen bonding on the basicity of selected macrocyclic amines. Journal of Physical Organic Chemistry, 2012, 25, 803-810.	0.9	19
44	How hydrogenâ€bonded MnO₄^{â€} can influence oxidation of olefins in both gas phase and solution?. Journal of Physical Organic Chemistry, 2012, 25, 1198-1209.	0.9	4
45	Thermochemical properties of some vinyl chloride-induced DNA lesions: detailed view from NBO & AIM analysis. Structural Chemistry, 2012, 23, 1987-2001.	1.0	3
46	Effect of Hydrogen Bonds on pK_a Values: Importance of Networking. Journal of the American Chemical Society, 2012, 134, 10646-10650.	6.6	82
47	Molecular structure and character of bonding of mono and divalent metal cations (Li+, Na+, K+,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 613-626.	1.0	12
48	Influence of the water molecules (nÂ=Â1â€“6) on the interaction between Li+, Na+, K+ cations and indole molecule as tryptophan amino acid residue. Structural Chemistry, 2012, 23, 857-865.	1.0	8
49	Structural behavior of sugar radicals formed by proton transfer reaction of deoxycytidine cation radical: detailed view from NBO analysis. Structural Chemistry, 2012, 23, 1185-1192.	1.0	2
50	Theoretical investigation on the structural and electronic properties of complexes formed by thymine and 2â€²-deoxythymidine with different anions. Structural Chemistry, 2012, 23, 17-28.	1.0	11
51	Structures, stabilities & conformational behaviors of hydrogen-atom abstractions of cytosine nucleosides: AIM & NBO analysis. Computational and Theoretical Chemistry, 2011, 971, 19-29.	1.1	7
52	DFT STUDY ON CONFORMATIONAL BEHAVIOR OF HYDROGEN ION ABSTRACTIONS OF CYTOSINE NUCLEOSIDES: AIM AND NBO ANALYSIS. Journal of Theoretical and Computational Chemistry, 2011, 10, 803-817.	1.8	3
53	Conformational behavior and potential energy profile of gaseous histidine. Computational and Theoretical Chemistry, 2010, 960, 73-85.	1.5	20
54	DFT STUDY ON METAL CATIONIZATION AND O6-PROTONATION ON 2â€²-DEOXYGUANOSINE CONFIGURATION: CHANGES ON SUGAR PUCKERING AND STRENGTH OF THE N-GLYCOSIDIC BOND. Journal of Theoretical and Computational Chemistry, 2010, 09, 585-609.	1.8	5

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55	DFT STUDY OF BOND ENERGIES AND ATTACHMENT SITES OF SAMPLE DIVALENT CATIONS (Mg²⁺, Ca²⁺, Zn²⁺) TO HISTIDINE IN THE GAS PHASE. Journal of Theoretical and Computational Chemistry, 2009, 08, 347-371.	1.8	8
56	DFT STUDY ON GAS-PHASE INTERACTION BETWEEN HISTIDINE AND ALKALI METAL IONS (Li⁺, Na⁺, K⁺); AND INFLUENCE OF THESE IONS ON HISTIDINE ACIDITY. Journal of Theoretical and Computational Chemistry, 2009, 08, 475-490.	1.8	6
57	Comparison of thermochemistry of aspartame (artificial sweetener) and glucose. Carbohydrate Research, 2009, 344, 127-133.	1.1	12
58	Interaction of Mg2+, Ca2+, Zn2+ and Cu+ with cytosine nucleosides: Influence of metal on sugar puckering and stability of N-Glycosidic bond, a DFT study. Computational and Theoretical Chemistry, 2009, 913, 117-125.	1.5	22
59	Anion interactions of cytosine nucleobase and its nucleosides: Detailed view from DFT study. Computational and Theoretical Chemistry, 2009, 913, 277-283.	1.5	7
60	DFT study of the interaction of cytidine and 2â€²-deoxycytidine with Li+, Na+, and K+: effects of metal cationization on sugar puckering and stability of the N-glycosidic bond. Carbohydrate Research, 2009, 344, 771-778.	1.1	17
61	Single-Centered Hydrogen-Bonded Enhanced Acidity (SHEA) Acids: A New Class of BrÃ¸nsted Acids. Journal of the American Chemical Society, 2009, 131, 16984-16988.	6.6	70
62	Conversion of a weak organic acid to a super acid in the gas phase. Journal of Physical Organic Chemistry, 2008, 21, 112-118.	0.9	17
63	The Heat of Formation of Cyclobutadiene. Angewandte Chemie - International Edition, 2006, 45, 4984-4988.	7.2	56
64	The Enthalpies of Formation of o-, m-, and p-Benzoquinone:â€‰ Gas-Phase Ion Energetics, Combustion Calorimetry, and Quantum Chemical Computations Combined. Journal of the American Chemical Society, 2005, 127, 6116-6122.	6.6	72
65	Experimental Determination of the Heat of Hydrogenation of Phenylcyclobutadiene. Journal of the American Chemical Society, 2005, 127, 13065-13069.	6.6	12
66	Correlating Acidities, Electron Affinities, and Bond Dissociation Energies. Measure One, Get All Three!. Journal of Organic Chemistry, 2004, 69, 9176-9183.	1.7	18
67	Why Does Cyclopropene Have the Acidity of an Acetylene but the Bond Energy of Methane?. Journal of the American Chemical Society, 2003, 125, 11746-11750.	6.6	50
68	In silico design of novel anticancer drugs with amino acid and carbohydrate building blocks to inhibit PIM kinases. Molecular Simulation, 0, , 1-15.	0.9	0