Arvi Rauk

List of Publications by Year
in descending order

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86	5,335	201674	88630
papers	citations	27 h-index	70 g-index

91	91	91	5145
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	On the calculation of bonding energies by the Hartree Fock Slater method. Theoretica Chimica Acta, 1977, 46, 1-10.	0.8	2,151
2	On the calculation of multiplet energies by the hartree-fock-slater method. Theoretica Chimica Acta, 1977, 43, 261-271.	0.8	912
3	The chemistry of Alzheimerâ€™s disease. Chemical Society Reviews, 2009, 38, 2698.	38.1	391
4	Why is the amyloid beta peptide of Alzheimer's disease neurotoxic?. Dalton Transactions, 2008, , 1273.	3.3	122
5	Entropies in Solution from Entropies in the Gas Phase. Journal of Physical Chemistry A, 2004, 108, 2720-2725.	2.5	98
6	Is Oxidative Damage by Î²-Amyloid and Prion Peptides Mediated by Hydrogen Atom Transfer from Glycine Î±-Carbon to Methionine Sulfur within Î²-Sheets?. Journal of the American Chemical Society, 2000, 122, 9761-9767.	13.7	89
7	Molecular Dynamics Study of the Beta Amyloid Peptide of Alzheimer's Disease and Its Divalent Copper Complexes. Journal of Physical Chemistry B, 2007, 111, 3789-3799.	2.6	77
8	Computational studies of Cu(II)[peptide] binding motifs: Cu[HGGG] and Cu[HG] as models for Cu(II) binding to the prion protein octarepeat region. Journal of Biological Inorganic Chemistry, 2003, 8, 53-65.	2.6	65
9	Mechanism of Hydrogen Peroxide Production by Copper-Bound Amyloid Beta Peptide: A Theoretical Study. Journal of Physical Chemistry B, 2009, 113, 1202-1209.	2.6	64
10	Mechanism of Dioxirane Oxidation of CH Bonds:Â Application to Homo- and Heterosubstituted Alkanes as a Model of the Oxidation of Peptides. Journal of Organic Chemistry, 1998, 63, 5413-5422.	3.2	59
11	Alkoxy radicals in the gaseous phase: Î²-scission reactions and formation by radical addition to carbonyl compounds. Canadian Journal of Chemistry, 2003, 81, 431-442.	1.1	58
12	On the calculation of bonding energies by the Hartree Fock Slater method. Theoretica Chimica Acta, 1977, 46, 1-10.	0.8	55
13	Influence of Î²-Sheet Structure on the Susceptibility of Proteins to Backbone Oxidative Damage:â€‰ Preference for Î±C-Centered Radical Formation at Glycine Residues of Antiparallel Î²-Sheets. Journal of the American Chemical Society, 2000, 122, 4185-4192.	13.7	54
14	Ab initio model studies of copper binding to peptides containing a Hisâ€“His sequence: relevance to the Î²-amyloid peptide of Alzheimerâ€™s disease. Journal of Biological Inorganic Chemistry, 2005, 10, 887-902.	2.6	54
15	A Computational Investigation of the Stereoisomerism in Heteroatom-Substituted Amides. Journal of Organic Chemistry, 1996, 61, 2337-2345.	3.2	52
16	Ab initio modelling of the structure and redox behaviour of copper(I) bound to a Hisâ€“His model peptide: relevance to the Î²-amyloid peptide of Alzheimerâ€™s disease. Journal of Biological Inorganic Chemistry, 2007, 12, 147-164.	2.6	48
17	Rearrangement of Protonated Propene Oxide to Protonated Propanal. Journal of the American Chemical Society, 1997, 119, 4712-4718.	13.7	47
18	Conformational Stereochemistry of the HERON Amide,N-Methoxy-N-dimethylaminoformamide:Â A Theoretical Study. Journal of Organic Chemistry, 1999, 64, 2340-2345.	3.2	46

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19	One-Electron Oxidation of Methionine in Peptide Environments:Â The Effect of Three-Electron Bonding on the Reduction Potential of the Radical Cation. Journal of Physical Chemistry A, 2004, 108, 11032-11041.	2.5	46
20	Vibrational circular dichroism intensities: Ab initio vibronic coupling theory using the distributed origin gauge. Journal of Chemical Physics, 1992, 97, 6517-6534.	3.0	43
21	Tertiary cyclohexyl cations. Definitive evidence for the existence of isomeric structures (hyperconjomers). Perkin Transactions II RSC, 2001, , 869-874.	1.1	38
22	Binding Affinities for Models of Biologically Available Potential Cu(II) Ligands Relevant to Alzheimer's Disease:â€‰ An ab Initio Study. Journal of Physical Chemistry A, 2005, 109, 8361-8370.	2.5	36
23	H-atom abstraction by thiyl radicals from peptides and cyclic dipeptides. A theoretical study of reaction rates. Physical Chemistry Chemical Physics, 2003, 5, 3994-3999.	2.8	34
24	Alzheimerâ€™s disease and the â€˜ABSENTâ€™ hypothesis: mechanism for amyloid Î² endothelial and neuronal toxicity. Medical Hypotheses, 2005, 65, 123-137.	1.5	33
25	H-atom abstraction from thiols by C-centered radicals. A theoretical and experimental study of reaction rates. Physical Chemistry Chemical Physics, 2002, 4, 2965-2974.	2.8	32
26	Reactions of One-Electron-Oxidized Methionine with Oxygen:Â An ab Initio Study. Journal of Physical Chemistry A, 2004, 108, 6222-6230.	2.5	32
27	Structures, barriers for rotation and inversion, vibrational frequencies, and thermodynamic functions of ethyl, Î±â€fluoroethyl, and Î±,Î±â€difluoroethyl radicals: An ab inito study. Journal of Chemical Physics, 1990, 93, 1187-1195.	3.0	28
28	Structures, barriers for internal rotation, vibrational frequencies, and thermodynamic functions of CH2FCH2, CHF2CH2, and CF3CH2radicals: Anabinitiostudy. Journal of Chemical Physics, 1990, 93, 6620-6629.	3.0	27
29	Structures and Stabilities of Fe2+/3+Complexes Relevant to Alzheimerâ€™s Disease: An ab Initio Study. Journal of Physical Chemistry A, 2011, 115, 12523-12530.	2.5	27
30	Testing synthetic amyloid-Î² aggregation inhibitor using single molecule atomic force spectroscopy. Biosensors and Bioelectronics, 2014, 54, 492-498.	10.1	26
31	The radical model of Alzheimer's disease: Specific recognition of Gly29 and Gly33 by Met35 in a Î²-sheet model of AÎ²: An ONIOM study. Journal of Alzheimer's Disease, 2002, 4, 283-289.	2.6	25
32	A computational investigation of the structure of the novel anomeric amide N-azido-N-methoxyformamide and its concerted decomposition to methyl formate and nitrogen. Perkin Transactions II RSC, 2002, , 1740-1746.	1.1	24
33	One-electron oxidation of methionine peptides â€” Stability of the three-electron Sâ€”N(amide) bond. Canadian Journal of Chemistry, 2006, 84, 893-904.	1.1	24
34	Vibrational circular dichroism intensities by ab initio secondâ€order Mo/llerâ€“Plesset vibronic coupling theory. Journal of Chemical Physics, 1994, 100, 7995-8002.	3.0	22
35	Regioselective Preparation of 2,4-, 3,4-, and 2,3,4-Substituted Furan Rings. 2.1Regioselective Lithiation of 2-Silylated-3-substituted Furan Rings. Journal of Organic Chemistry, 1997, 62, 8750-8759.	3.2	22
36	Can copper binding to the prion protein generate a misfolded form of the protein?. BioMetals, 2009, 22, 159-175.	4.1	21

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37	Ring Opening of Bicyclo[n.1.0]alkanones to 2-Cycloalkanone-1,3-diyls. Why Does Oxyallyl Diradical Formation Require Less Energy from Bicyclo[3.1.0]hexan-6-ones than from Bicyclo[1.1.0]butan-2-ones?. Journal of the American Chemical Society, 1996, 118, 4159-4166.	13.7	20
38	Computational Studies of Cu(II)/Met and Cu(I)/Met Binding Motifs Relevant for the Chemistry of Alzheimer's Disease. Journal of Physical Chemistry A, 2005, 109, 5498-5508.	2.5	20
39	Effect of Side Chains on Competing Pathways for Î²-Scission Reactions of Peptide-Backbone Alkoxyl Radicals. Journal of Physical Chemistry A, 2006, 110, 10316-10323.	2.5	19
40	On the Involvement of Copper Binding to the N-Terminus of the Amyloid Beta Peptide of Alzheimer's Disease: A Computational Study on Model Systems. International Journal of Alzheimer's Disease, 2011, 2011, 1-15.	2.0	18
41	Structure and reactions of the peroxy radicals of glycine and alanine in peptides: anab initiostudy. Journal of Physical Organic Chemistry, 2004, 17, 777-786.	1.9	17
42	New Orbital Symmetry-Allowed Route for Cycloreversion of Silacyclobutane and Its Methyl Derivatives. Journal of Physical Chemistry A, 2019, 123, 1749-1757.	2.5	17
43	The electronic structure and optical activity of conjugated dienes: 1,3-Butadiene and ?- and ?-phellandrene. Journal of Computational Chemistry, 1980, 1, 240-256.	3.3	16
44	Structures, barriers for internal rotation and inversion, vibrational frequencies, and thermodynamic functions of CH2FCHF, CHF2CHF, and CF3CHF radicals: An ab initio study. Journal of Chemical Physics, 1991, 94, 7299-7310.	3.0	16
45	Structures, barriers for internal rotation and inversion, vibrational frequencies, and thermodynamic functions of CH2FCF2, CHF2CF2, and CF3CF2 radicals: An ab initio study. Journal of Chemical Physics, 1991, 95, 2774-2786.	3.0	15
46	The Structures and Stabilities of the Complexes of Biologically Available Ligands with Fe(III)â˜Porphine: An Ab Initio Study. Journal of Physical Chemistry B, 2011, 115, 569-579.	2.6	15
47	H-Atom abstraction by C-centered radicals from cyclic and acyclic dipeptides. A theoretical and experimental study of reaction rates. Physical Chemistry Chemical Physics, 2003, 5, 3278-3288.	2.8	14
48	Exploring Amyloid-Î² Dimer Structure Using Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2019, 123, 4658-4670.	2.5	13
49	Î²-N-Methylamino-l-alanine (BMAA) Not Involved in Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2018, 122, 4472-4480.	2.6	12
50	Pseudopeptide Amyloid Aggregation Inhibitors: In Silico, Single Molecule and Cell Viability Studies. International Journal of Molecular Sciences, 2021, 22, 1051.	4.1	12
51	Magnetic dipole moment integrals over Slater orbitals. Journal of Chemical Physics, 1973, 59, 5720-5724.	3.0	10
52	The Binding of Fe(II)â€“Heme to the Amyloid Beta Peptide of Alzheimerâ€™s Disease: QM/MM Investigations. Journal of Chemical Theory and Computation, 2012, 8, 5150-5158.	5.3	10
53	Copper(I) Chelators for Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2017, 121, 11304-11310.	2.6	10
54	The lifetimes of gas phase CO2?? and N2O?? calculated from the transition probability of the autodetachment processA? ?A +e?. International Journal of Chemical Kinetics, 1994, 26, 7-24.	1.6	9

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55	Molecular dynamics study of the monomers and dimers of N-AcAÎ²(13â€“23)NH2: on the effect of pH on the aggregation of the amyloid beta peptide of Alzheimerâ€™s disease. Canadian Journal of Chemistry, 2016, 94, 273-281.	1.1	9
56	d-Amino Acid Pseudopeptides as Potential Amyloid-Beta Aggregation Inhibitors. Molecules, 2018, 23, 2387.	3.8	9
57	Measurement of the interaction of aqueous copper(II) with a model amyloid-Î² protein fragmentÂâ€” Interference from buffers. Canadian Journal of Chemistry, 2011, 89, 1429-1444.	1.1	8
58	Fe(III)â€“Heme Complexes with the Amyloid Beta Peptide of Alzheimerâ€™s Disease: QM/MM Investigations of Binding and Redox Properties of Heme Bound to the His Residues of AÎ²(1â€“42). Journal of Chemical Theory and Computation, 2013, 9, 4233-4242.	5.3	7
59	Modeling Î²-Scission Reactions of Peptide Backbone Alkoxy Radicals:Â Backbone Câ^'C Bond Fission. Journal of Chemical Theory and Computation, 2005, 1, 889-899.	5.3	6
60	Molecular dynamics studies of a Î²-sheet blocking peptide with the full-length amyloid beta peptide of Alzheimerâ€™s disease. Canadian Journal of Chemistry, 2016, 94, 833-841.	1.1	6
61	Molecular dynamics study of the interaction of AÎ²(13-23) with Î²-sheet inhibitors. Arkivoc, 2009, 2009, 116-134.	0.5	6
62	Concerning the conformational preferences of the 2-cyano derivatives of oxane, thiane, and selenane. Canadian Journal of Chemistry, 2010, 88, 831-838.	1.1	5
63	Interaction of the N-AcAÎ²(13â€“23)NH2 segment of the beta amyloid peptide with beta-sheet-blocking peptides: site and edge specificity. Canadian Journal of Chemistry, 2016, 94, 583-592.	1.1	5
64	Cheletropic Decomposition of Cyclic Nitrosoamines Revisited:â€‰ The Nature of the Transition States and a Critical Role of the Ring Strain. Journal of Organic Chemistry, 2000, 65, 3612-3619.	3.2	4
65	The a Priori Calculation of Vibrational Circular Dichroism Intensities. Reviews in Computational Chemistry, 2007, , 261-301.	1.5	4
66	Implementation and applications of Gaussian 82 on a CDC Cyber 205. Journal of Computational Chemistry, 1987, 8, 324-332.	3.3	3
67	The transition probability of electron loss from anions in the gas phase: The lifetime of O2â€‰â‹…â^'. Journal of Chemical Physics, 1992, 97, 5522-5531.	3.0	3
68	Pseudopeptide Designed to Inhibit Oligomerization and Redox Chemistry in Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2019, 123, 5206-5215.	2.6	3
69	Dialkyl sulphur radical cations: competition between proton and methyl cation transfers to sulphur nucleophiles: anab initiostudy. Molecular Physics, 2005, 103, 1201-1209.	1.7	2
70	Appendix B: Exercises. , 0, , 247-312.		0
71	References and Notes. , 0, , 313-324.		0
72	Nucleophilic Substitution Reactions. , 0, , 129-136.		0

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73	Appendix A: Derivation of Hartreeâ€“Fock Theory. , 0, , 218-246.		0
74	Symmetry and Stereochemistry. , 0, , 1-19.		0
75	Molecular Orbital Theory. , 0, , 20-33.		0
76	Orbital Interaction Theory. , 0, , 34-71.		0
77	Sigma Bonds and Orbital Interaction Theory. , 0, , 72-85.		0
78	Simple HÃ¼ckel Molecular Orbital Theory. , 0, , 86-97.		0
79	Reactions and Properties of Ï€ Bonds. , 0, , 98-104.		0
80	Reactive Intermediates. , 0, , 105-120.		0
81	Carbonyl Compounds. , 0, , 121-128.		0
82	Aromatic Compounds. , 0, , 150-160.		0
83	Pericyclic Reactions. , 0, , 161-174.		0
84	Organometallic Compounds. , 0, , 175-195.		0
85	Orbital and State Correlation Diagrams. , 0, , 196-208.		0
86	Bonds to Hydrogen. , 0, , 137-149.		0