BÃ©la Viskolcz

List of Publications by Year
in descending order

166 papers	2,169 citations	236925 25 h-index	330143 37 g-index
168 all docs	168 docs citations	168 times ranked	2123 citing authors

#	Article	IF	Citations
1	The thermal unimolecular decomposition rate constants of ethoxy radicals. Physical Chemistry Chemical Physics, 1999, 1, 2935-2944.	2.8	91
2	The Î² Câ€“C bond scission in alkoxy radicals: thermal unimolecular decomposition of t-butoxy radicals. Physical Chemistry Chemical Physics, 2000, 2, 1677-1683.	2.8	82
3	Formation and growth mechanisms of polycyclic aromatic hydrocarbons: A mini-review. Chemosphere, 2022, 291, 132793.	8.2	77
4	Allylic H-Abstraction Mechanism:â€‰ The Potential Energy Surface of the Reaction of Propene with OH Radical. Journal of Chemical Theory and Computation, 2006, 2, 1575-1586.	5.3	66
5	Complete falloff curves for the unimolecular decomposition of i-propoxy radicals between 330 and 408 K. Physical Chemistry Chemical Physics, 1999, 1, 675-681.	2.8	58
6	A detailed experimental and theoretical study on the decomposition of methoxy radicals. Physical Chemistry Chemical Physics, 2001, 3, 2450-2458.	2.8	55
7	A Quantitative Scale for the Extent of Conjugation of the Amide Bond. Amidity Percentage as a Chemical Driving Force. Journal of Physical Chemistry A, 2007, 111, 13245-13254.	2.5	55
8	A Quantitative Scale for the Degree of Aromaticity and Antiaromaticity: A Comparison of Theoretical and Experimental Enthalpies of Hydrogenation. Journal of Physical Chemistry A, 2007, 111, 1123-1132.	2.5	53
9	Addition complex formation vs. direct abstraction in the OH+C2H4 reaction. Physical Chemistry Chemical Physics, 2000, 2, 3591-3596.	2.8	46
10	Application of the Group Additivity Method to Alkyl Radicals:â€‰ An ab Initio Study. Journal of Physical Chemistry A, 2000, 104, 4497-4504.	2.5	39
11	Glycerol carbonate as a fuel additive for a sustainable future. Sustainable Energy and Fuels, 2018, 2, 2171-2178.	4.9	38
12	Hydrogen bondings in deoxynivalenol (DON) conformationsâ€”a density functional study. Computational and Theoretical Chemistry, 2005, 726, 55-59.	1.5	37
13	Activation Mechanism of the Human Histamine H4 Receptor - An Explicit Membrane Molecular Dynamics Simulation Study. Journal of Chemical Information and Modeling, 2008, 48, 1199-1210.	5.4	37
14	Rate Coefficients and Equilibrium Constant for the CH2CHO + O2 Reaction System. Journal of Physical Chemistry A, 2006, 110, 3238-3245.	2.5	34
15	Characterization of the Conformational Probability of N-Acetyl-Phenylalanyl-NH2by RHF, DFT, and MP2 Computation and AIM Analyses, Confirmed by Jet-Cooled Infrared Data. Journal of Physical Chemistry A, 2005, 109, 5289-5302.	2.5	32
16	Conformation-Dependent^{â€¢}OH/H₂O₂Hydrogen Abstraction Reaction Cycles of Gly and Ala Residues: A Comparative Theoretical Study. Journal of Physical Chemistry B, 2012, 116, 1143-1154.	2.6	32
17	High Accuracy ab Initio Calculations on Reactions of OH with 1-Alkenes. The Case of Propene. Journal of Chemical Theory and Computation, 2009, 5, 2313-2321.	5.3	31
18	Mixed Micelles of Sodium Cholate and Sodium Dodecylsulphate 1:1 Binary Mixture at Different Temperatures â€“ Experimental and Theoretical Investigations. PLoS ONE, 2014, 9, e102114.	2.5	31

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19	An experimental and theoretical kinetic study of the reaction of OH radicals with tetrahydrofuran. Proceedings of the Combustion Institute, 2017, 36, 143-150.	3.9	31
20	Serum N-Glycosylation in Parkinsonâ€™s Disease: A Novel Approach for Potential Alterations. Molecules, 2019, 24, 2220.	3.8	30
21	Competition between alkyl radical addition to carbonyl bonds and H-atom abstraction reactions. Physical Chemistry Chemical Physics, 2002, 4, 4663-4668.	2.8	29
22	First Principle Computational Study on the Full Conformational Space ofl-Proline Diamides. Journal of Physical Chemistry A, 2005, 109, 2660-2679.	2.5	29
23	Formation Mechanism of Benzo(a)pyrene: One of the Most Carcinogenic Polycyclic Aromatic Hydrocarbons (PAH). Molecules, 2019, 24, 1040.	3.8	28
24	Absorption Spectrum and Absolute Absorption Cross Sections of CH₃O₂ Radicals and CH₃I Molecules in the Wavelength Range 7473â€“7497 cm^{â€“1}. Journal of Physical Chemistry A, 2013, 117, 12802-12811.	2.5	27
25	Rate and Equilibrium Constant of the Reaction of 1-Methylvinoxy Radicals with O2:Â CH3COCH2+ O2â†” CH3COCH2O2â€. Journal of Physical Chemistry A, 2006, 110, 6667-6672.	2.5	26
26	Allylic hydrogen abstraction II. H-abstraction from 1,4 type polyalkenes as a model for free radical trapping by polyunsaturated fatty acids (PUFAs). Physical Chemistry Chemical Physics, 2007, 9, 1931.	2.8	26
27	Measurement of Absolute Absorption Cross Sections for Nitrous Acid (HONO) in the Near-Infrared Region by the Continuous Wave Cavity Ring-Down Spectroscopy (cw-CRDS) Technique Coupled to Laser Photolysis. Journal of Physical Chemistry A, 2011, 115, 10720-10728.	2.5	26
28	Antioxidant Potential of Glutathione: A Theoretical Study. Journal of Physical Chemistry B, 2011, 115, 11269-11277.	2.6	26
29	Experimental determination of the rate constant of the reaction between C 2 H 5 O 2 and OH radicals. Chemical Physics Letters, 2015, 619, 196-200.	2.6	26
30	Quantitative Scale for the Extent of Conjugation of Carbonyl Groups: â€œCarbonylicityâ€•Percentage as a Chemical Driving Force. Journal of Physical Chemistry A, 2008, 112, 9153-9165.	2.5	25
31	Penicillin's catalytic mechanism revealed by inelastic neutrons and quantum chemical theory. Physical Chemistry Chemical Physics, 2013, 15, 20447-20455.	2.8	24
32	Glutathione â€“ Hydroxyl Radical Interaction: A Theoretical Study on Radical Recognition Process. PLoS ONE, 2013, 8, e73652.	2.5	24
33	Enthalpy of formation of selected carbonyl radicals from theory and comparison with experiment. Physical Chemistry Chemical Physics, 2000, 2, 5430-5436.	2.8	22
34	Direct Kinetic Study of Reactions of Hydroxyl Radicals with Alkyl Formates. Zeitschrift Fur Physikalische Chemie, 2004, 218, 479-492.	2.8	19
35	Can Four-Membered Heterophosphete Structures Exist? The Contribution of Phosphorus d Orbitals to Antiaromaticity. European Journal of Organic Chemistry, 2007, 2007, 1759-1767.	2.4	19
36	Quantum Chemical Analysis of the Unfolding of a Penta-alanyl 310-Helix Initiated by HOâ€¢, HO2â€¢and O2â€“â€¢. Journal of Physical Chemistry B, 2011, 115, 8014-8023.	2.6	19

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37	Pyrolysis of Ethyl Iodide as Hydrogen Atom Source: Kinetics and Mechanism in the Temperature Range 950â€“1200 K. Zeitschrift Fur Physikalische Chemie, 2011, 225, 1117-1128.	2.8	19
38	Urethane Formation with an Excess of Isocyanate or Alcohol: Experimental and Ab Initio Study. Polymers, 2019, 11, 1543.	4.5	16
39	Quantifying the Intrinsic Effects of Two Point Mutation Models of Prolineâ^'Proline Diamino Acid Diamide: A First-Principle Computational Study. Journal of Physical Chemistry B, 2007, 111, 11592-11602.	2.6	15
40	First-Principle Computational Study on the Full Conformational Space of l-Threonine Diamide, the Energetic Stability of Cis and Trans Isomers. Journal of Physical Chemistry A, 2006, 110, 11527-11536.	2.5	14
41	Quantifying the Intrinsic Effects of Two Point Mutation Models of Pro-Pro-Pro Triamino Acid Diamide. A First-Principle Computational Study. Journal of Physical Chemistry B, 2007, 111, 13135-13142.	2.6	14
42	Chemical evolution of biomolecule building blocks. Can thermodynamics explain the accumulation of glycine in the prebiotic ocean?. Physical Chemistry Chemical Physics, 2011, 13, 7449.	2.8	14
43	Molecular Surgery Concept from Bench to Bedside: A Focus on TRPV1+ Pain-Sensing Neurons. Frontiers in Physiology, 2017, 8, 378.	2.8	14
44	Theoretical investigation of benzo(a)pyrene formation. Chemical Physics Letters, 2021, 772, 138564.	2.6	14
45	Flexibility of â€œPolyunsaturated Fatty Acid Chainsâ€•and Peptide Backbones:â€‰ A Comparative ab Initio Study. Journal of Physical Chemistry A, 2005, 109, 520-533.	2.5	13
46	Thermodynamic Functions of Conformational Changes. 2. Conformational Entropy as a Measure of Information Accumulation. Journal of Physical Chemistry A, 2006, 110, 3808-3813.	2.5	13
47	High efficiency two-photon uncaging coupled by the correction of spontaneous hydrolysis. Organic and Biomolecular Chemistry, 2018, 16, 1958-1970.	2.8	13
48	Application of ion-exchange resin beads to produce magnetic adsorbents. Chemical Papers, 2021, 75, 1187-1195.	2.2	13
49	Mechanism of the 1-C4H9 + O reaction and the kinetics of the intermediate 1-C4H9O radical. Physical Chemistry Chemical Physics, 2001, 3, 2365-2371.	2.8	12
50	Formation of acetamide in interstellar medium. Molecular Astrophysics, 2018, 13, 1-5.	1.6	12
51	Renewable energy and raw materials â€“ The thermodynamic support. Journal of Cleaner Production, 2019, 241, 118221.	9.3	12
52	Synthesis of iron oxide nanoparticles for DNA purification. Journal of Dispersion Science and Technology, 2021, 42, 693-700.	2.4	12
53	Sonochemical Combined Synthesis of Nickel Ferrite and Cobalt Ferrite Magnetic Nanoparticles and Their Application in Glycan Analysis. International Journal of Molecular Sciences, 2022, 23, 5081.	4.1	12
54	The influence of exocyclic phosphorous substituents on the intrinsic stability of four-membered heterophosphetes: a theoretical study. Tetrahedron, 2008, 64, 1868-1878.	1.9	11

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55	Thermodynamic Role of Glutathione Oxidation by Peroxide and Peroxybicarbonate in the Prevention of Alzheimerâ€™s Disease and Cancer. Journal of Physical Chemistry A, 2009, 113, 9138-9149.	2.5	11
56	Critical evaluation of the potential energy surface of the CH3 + HO2reaction system. Journal of Chemical Physics, 2015, 142, 054308.	3.0	11
57	Fine-tuning the catalytic activity by applying nitrogen-doped carbon nanotubes as catalyst supports for the hydrogenation of olefins. Reaction Kinetics, Mechanisms and Catalysis, 2020, 129, 95-106.	1.7	11
58	Membrane Flash Index: Powerful and Perspicuous Help for Efficient Separation System Design. ACS Omega, 2020, 5, 15136-15145.	3.5	11
59	Folded and Unfolded Conformations of the Ï‰-3 Polyunsaturated Fatty Acid Family:Â CH3CH2[CHCHCH2]B[CH2]MCOOH. First Principles Study. Journal of Physical Chemistry A, 2006, 110, 6100-6111.	2.5	10
60	Glutathione as a Prebiotic Answer to Î±-Peptide Based Life. Journal of Physical Chemistry B, 2015, 119, 3940-3947.	2.6	10
61	Application of carbon nanotube coated aluminosilicate beads as â€œsupport on supportâ€•catalyst for hydrogenation of nitrobenzene. Journal of Industrial and Engineering Chemistry, 2019, 79, 307-313.	5.8	10
62	Synthesis Optimization and Characterization of Nitrogen-Doped Bamboo-Shaped Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2019, 19, 429-435.	0.9	10
63	Catalytic activity of maghemite supported palladium catalyst in nitrobenzene hydrogenation. Reaction Kinetics, Mechanisms and Catalysis, 2020, 129, 107-116.	1.7	10
64	Theoretical Study on Reactions of HO₂ Radical with Photodissociation Products of Cl₂SO (ClSO and SO). Journal of Physical Chemistry A, 2009, 113, 9981-9987.	2.5	9
65	A Quantitative Scale for the Extent of Conjugation of Substituted Olefines. Journal of Physical Chemistry A, 2009, 113, 7953-7962.	2.5	9
66	The effect of a Pro28Thr point mutation on the local structure and stability of human galactokinase enzymeâ€”a theoretical study. Journal of Molecular Modeling, 2011, 17, 2639-2649.	1.8	9
67	A computational study of glutathione and its fragments: N-acetylcisteinylglycine and Î³-glutamylmethylamide. Chemical Physics Letters, 2011, 507, 168-173.	2.6	9
68	Development and Application of Carbonâ€Layerâ€Stabilized, Nitrogenâ€Doped, Bambooâ€Like Carbon Nanotube Catalysts in CO₂ Hydrogenation. ChemistryOpen, 2018, 7, 789-796.	1.9	9
69	Microreactor assisted method for studying isocyanateâ€“alcohol reaction kinetics. Journal of Flow Chemistry, 2019, 9, 199-204.	1.9	9
70	Application of nitrogen doped bamboo-like carbon nanotube for development of electrically conductive lubricants. Journal of Materials Research and Technology, 2019, 8, 3244-3250.	5.8	9
71	Application of carbonized ion exchange resin beads as catalyst support for gas phase hydrogenation processes. Reaction Kinetics, Mechanisms and Catalysis, 2020, 129, 85-94.	1.7	9
72	Ultrasonic cavitation assisted deposition of catalytically active metals on nitrogen-doped and non-doped carbon nanotubes â€” A comparative study. Journal of Materials Research and Technology, 2020, 9, 4283-4291.	5.8	9

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73	The fitting and functional analysis of a double rotor potential energy surface for the R and S enantiomers of 1-chloro-3-fluoro-isobutane. Computational and Theoretical Chemistry, 2003, 666-667, 79-87.	1.5	8
74	The reactions of the branched alkyl radicals iso-butyl and neo-pentyl with oxygen atomsâ€”an experimental and theoretical study. Proceedings of the Combustion Institute, 2005, 30, 1005-1013.	3.9	8
75	Thermodynamic Functions of Conformational Changes: Conformational Network of Glycine Diamide Folding, Entropy Lowering, and Informational Accumulation. Journal of Physical Chemistry A, 2006, 110, 13325-13331.	2.5	8
76	Nonenzymatic Pathway of PUFA Oxidation. A First-Principles Study of the Reactions of OH Radical with 1,4-Pentadiene and Arachidonic Acid. Journal of Chemical Theory and Computation, 2008, 4, 1472-1479.	5.3	8
77	Molecular Dynamics Simulation at High Sodium Chloride Concentration: Toward the Inactive Conformation of the Human Adenosine A2A Receptor. Journal of Physical Chemistry Letters, 2010, 1, 1008-1013.	4.6	8
78	Big data reduction by fitting mathematical functions. Chemical Physics Letters, 2015, 625, 91-97.	2.6	8
79	A Hidden Active Site in the Potential Drug Target Mycobacterium tuberculosis dUTPase Is Accessible through Small Amplitude Protein Conformational Changes. Journal of Biological Chemistry, 2016, 291, 26320-26331.	3.4	8
80	Hydrogenation of nitrobenzene over a composite catalyst based on zeolite supported N-doped carbon nanotubes decorated with palladium. Reaction Kinetics, Mechanisms and Catalysis, 2018, 125, 583-593.	1.7	8
81	A theoretical study on the phosgenation of methylene diphenyl diamine (MDA). Chemical Physics Letters, 2018, 706, 568-576.	2.6	8
82	Exploring the Potential to Repurpose Flexible Moulded Polyurethane Foams as Acoustic Insulators. Polymers, 2022, 14, 163.	4.5	8
83	Development of High-Efficiency, Magnetically Separable Palladium-Decorated Manganese-Ferrite Catalyst for Nitrobenzene Hydrogenation. International Journal of Molecular Sciences, 2022, 23, 6535.	4.1	8
84	Polymerization dependence of the entropy of homo-oligomer peptides. Chemical Physics Letters, 2010, 501, 30-32.	2.6	7
85	Quantum chemical analysis of the unfolding of a penta-glycyl 310-helix initiated by HOâ€¢, HO2â€¢, and O2â^'â€¢. Journal of Chemical Physics, 2011, 135, 035101.	3.0	7
86	Global optimization of cholic acid aggregates. Journal of Chemical Physics, 2014, 140, 144302.	3.0	7
87	An experimental and theoretical study on the kinetic isotope effect of C2H6 and C2D6 reaction with OH. Chemical Physics Letters, 2015, 641, 158-162.	2.6	7
88	Protein Stability and Unfolding Following Glycine Radical Formation. Molecules, 2017, 22, 655.	3.8	7
89	Molecular Dynamics and Metadynamics Insights of 1,4-Dioxane-Induced Structural Changes of Biomembrane Models. Journal of Physical Chemistry B, 2019, 123, 7869-7884.	2.6	7
90	An Ab Initio Investigation of the 4,4â€²-Methlylene Diphenyl Diamine (4,4â€²-MDA) Formation from the Reaction of Aniline with Formaldehyde. Polymers, 2019, 11, 398.	4.5	7

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91	Sonochemical Deposition of Palladium Nanoparticles Onto the Surface of N-Doped Carbon Nanotubes: A Simplified One-Step Catalyst Production Method. Catalysis Letters, 2020, 150, 505-513.	2.6	7
92	Computational Study of Catalytic Urethane Formation. Polymers, 2022, 14, 8.	4.5	7
93	An exploratory ab initio study on the entropy of various backbone conformers for the HCO-Gly-Gly-Gly-NH2 tripeptide motif. Computational and Theoretical Chemistry, 2003, 666-667, 89-94.	1.5	6
94	Transition State Infrared Spectra for the Transâ†'Cis Isomerization of a Simple Peptide Model. Journal of Physical Chemistry A, 2007, 111, 8384-8389.	2.5	6
95	Information accumulation in helical oligopeptide structures. Chemical Physics Letters, 2007, 450, 123-126.	2.6	6
96	Thermodynamics of competing oxidation reactions of allyl methyl disulfide by hydrogen peroxide: a first principle molecular computational study on the conformations of allyl methyl disulfide and its oxidized products. Journal of Physical Organic Chemistry, 2008, 21, 1048-1058.	1.9	6
97	Atropisomerism of the Asn Î± Radicals Revealed by Ramachandran Surface Topology. Journal of Physical Chemistry B, 2013, 117, 12402-12409.	2.6	6
98	Fourier type potential energy function for conformational change of selected organic functional groups. Chemical Physics Letters, 2014, 599, 169-174.	2.6	6
99	A high temperature kinetic study for the thermal unimolecular decomposition of diethyl carbonate. Chemical Physics Letters, 2017, 684, 390-396.	2.6	6
100	Reactivity of Ala-Gly dipeptide with Î²-turn secondary structure. Chemical Physics Letters, 2018, 692, 402-406.	2.6	6
101	Beyond Chelation: EDTA Tightly Binds Taq DNA Polymerase, MutT and dUTPase and Directly Inhibits dNTPase Activity. Biomolecules, 2019, 9, 621.	4.0	6
102	Preparation of Bamboo-Like Carbon Nanotube Loaded Piezoresistive Polyurethane-Silicone Rubber Composite. Polymers, 2021, 13, 2144.	4.5	6
103	Preparation of highly effective carbon black supported Pdâ€“Pt bimetallic catalysts for nitrobenzene hydrogenation. Nanotechnology, 2021, 32, 425701.	2.6	6
104	Combustion method combined with sonochemical step for synthesis of maghemite-supported catalysts for the hydrogenation of 2,4-dinitrotoluene. Catalysis Communications, 2021, 159, 106342.	3.3	6
105	A Theoretical Study on the Phosgenation of 2,4-Toluenediamine (2,4-TDA). Polymers, 2022, 14, 2254.	4.5	6
106	Palladium Decorated N-Doped Carbon Foam as a Highly Active and Selective Catalyst for Nitrobenzene Hydrogenation. International Journal of Molecular Sciences, 2022, 23, 6423.	4.1	6
107	Molecular orbital computations on lipids: an ab initio exploratory study on the conformations of glycerol and its fluorine congeners. Computational and Theoretical Chemistry, 2005, 722, 79-96.	1.5	5
108	Thermodynamic functions of conformational changes I. A comparative first principles study of 1,2-disubstituted ethanes. Molecular Physics, 2006, 104, 795-803.	1.7	5

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109	3D QSAR models for Î±2a-adrenoceptor agonistsâ˜†. Neurochemistry International, 2007, 51, 268-276.	3.8	5
110	Ab initio study on alkyl radical decomposition and alkyl radical addition to olefins. Reaction Kinetics and Catalysis Letters, 2009, 96, 245-262.	0.6	5
111	The Effect of Newly Developed OPLS-AA Alanyl Radical Parameters on Peptide Secondary Structure. Journal of Chemical Theory and Computation, 2012, 8, 2569-2580.	5.3	5
112	The effect of oxidative stress on the bursopentin peptide structure: a theoretical study. Physical Chemistry Chemical Physics, 2014, 16, 9602-9609.	2.8	5
113	Nitrogen-doped bamboo-shaped carbon nanotube supported catalysts for heterogeneous hydrogenation. The effect of surface polarity. Reaction Kinetics, Mechanisms and Catalysis, 2018, 125, 37-46.	1.7	5
114	Purification of Fluorescently Derivatized N-Glycans by Magnetic Iron Nanoparticles. Nanomaterials, 2019, 9, 1480.	4.1	5
115	Development of Nickel- and Magnetite-Promoted Carbonized Cellulose Bead-Supported Bimetallic Pdâ€“Pt Catalysts for Hydrogenation of Chlorate Ions in Aqueous Solution. International Journal of Molecular Sciences, 2021, 22, 11846.	4.1	5
116	Optical Study of Solvatochromic Isocyanoaminoanthracene Dyes and 1,5-Diaminoanthracene. International Journal of Molecular Sciences, 2022, 23, 1315.	4.1	5
117	Comparison of Catalysts with MIRA21 Model in Heterogeneous Catalytic Hydrogenation of Aromatic Nitro Compounds. Catalysts, 2022, 12, 467.	3.5	5
118	Experimental and Theoretical Study of Cyclic Amine Catalysed Urethane Formation. Polymers, 2022, 14, 2859.	4.5	5
119	Conformational analysis of oxidized vitamin-C. Computational and Theoretical Chemistry, 2003, 666-667, 397-400.	1.5	4
120	Reaction profiling of the MAO-B catalyzed oxidative deamination of amines in Alzheimer's disease. Computational and Theoretical Chemistry, 2003, 666-667, 527-536.	1.5	4
121	Theoretical studies of carbon dioxide catalysis of peroxynitrite isomerizations. Computational and Theoretical Chemistry, 2005, 731, 57-60.	1.5	4
122	Selenocysteine derivatives I. Sidechain conformational potential energy surface of N-acetyl-l-selenocysteine-N-methylamide (MeCO-l-Sec-NH-Me) in its Î²l backbone conformation. Computational and Theoretical Chemistry, 2005, 725, 111-125.	1.5	4
123	Disulfidicity: A scale to characterize the disulfide bond strength via the hydrogenation thermodynamics. Chemical Physics Letters, 2012, 539-540, 11-14.	2.6	4
124	Molecular ageing: Free radical initiated epimerization of thymopentin â€“ A case study. Journal of Chemical Physics, 2014, 140, 205102.	3.0	4
125	A theoretical study of the stability of disulfide bridges in various Î²-sheet structures of protein segment models. Chemical Physics Letters, 2014, 593, 48-54.	2.6	4
126	Industrial application of molecular computations on the dimerization of methylene diphenyl diisocyanate. Reaction Kinetics, Mechanisms and Catalysis, 2018, 124, 1-14.	1.7	4

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127	Kinetics and thermochemistry of cyclohexadienes reactions with hydroxyl radicals. Proceedings of the Combustion Institute, 2021, 38, 947-955.	3.9	4
128	The Analysis of Human Serum N-Glycosylation in Patients with Primary and Metastatic Brain Tumors. Life, 2021, 11, 29.	2.4	4
129	Transmembrane penetration mechanism of cyclic pollutants inspected by molecular dynamics and metadynamics: the case of morpholine, phenol, 1,4-dioxane and oxane. Physical Chemistry Chemical Physics, 2021, 23, 15338-15351.	2.8	4
130	Thermodynamic functions of conformational changes, part IV: Functional analysis of conformational entropy of substituted ethane and methanol. International Journal of Quantum Chemistry, 2007, 107, 1826-1834.	2.0	3
131	Network of hydrogen bonds in Pro-Ala-Pro and Pro-Phe-Pro diamides: A first principles study of Alaâ†'Phe point mutation in proline environment. Journal of Chemical Physics, 2009, 131, 035105.	3.0	3
132	Homology Modeling and Validation of the Human M1 Muscarinic Acetylcholine Receptor. Molecular Informatics, 2012, 31, 635-638.	2.5	3
133	Radical Formation Initiates Solvent-Dependent Unfolding and Î²-sheet Formation in a Model Helical Peptide. Journal of Physical Chemistry B, 2016, 120, 4878-4889.	2.6	3
134	Multiscale Modeling of Interfacial Oxidation Mechanism at Air/Organic Interface: Reactions of CH₂â•CH-Terminated Self-Assembled Monolayer with OH^{â€¢}, O₃, and HO₂^{â€¢}. Journal of Physical Chemistry C, 2018, 122, 9886-9898.	3.1	3
135	Development of nitrogen-doped bamboo-like carbon nanotubes coated zeolite beads as â€œsupport on supportâ€•catalyst for the catalytic hydrogenation of olefins. Reaction Kinetics, Mechanisms and Catalysis, 2019, 127, 705-714.	1.7	3
136	Chlorate Elimination by Catalytically Hydrogenation, Catalyst Development and Characterization. Catalysis Letters, 2019, 149, 196-202.	2.6	3
137	Adsorption capacity of oxidized nitrogen-doped bamboo-like carbon nanotubes. Journal of Dispersion Science and Technology, 2020, 41, 1879-1884.	2.4	3
138	Hydrogenation of chlorate ions by commercial carbon supported palladium catalystsâ€"a comparative study. Reaction Kinetics, Mechanisms and Catalysis, 2020, 131, 129-137.	1.7	3
139	Water enhanced mechanism for CO2 â€“ Methanol conversion. Chemical Physics Letters, 2020, 746, 137298.	2.6	3
140	Development of Highly Efficient, Glassy Carbon Foam Supported, Palladium Catalysts for Hydrogenation of Nitrobenzene. Nanomaterials, 2021, 11, 1172.	4.1	3
141	Precious-Metal-Decorated Chromium(IV) Oxide Nanowires as Efficient Catalysts for 2,4-Toluenediamine Synthesis. International Journal of Molecular Sciences, 2021, 22, 5945.	4.1	3
142	Role of Aromacity, Ring Strain, and Stereochemistry of Selected Disulfides and Their Congeners in the Oxidative Linkage of DNA Strands at the Major Groove. A Computational Study. Journal of Chemical Information and Modeling, 2006, 46, 2527-2536.	5.4	2
143	Thermodynamic Functions of Molecular Conformations of (2-Fluoro-2-phenyl-1-ethyl)ammonium Ion and (2-Hydroxy-2-phenyl-1-ethyl)ammonium Ion as Models for Protonated Noradrenaline and Adrenaline: First-Principles Computational Study of Conformations and Thermodynamic Functions for the Noradrenaline and Adrenaline Models. Journal of Physical Chemistry A, 2009, 113, 2507-2515.	2.5	2
144	Energy Managements in the Chemical and Biochemical World, as It may be Understood from the Systems Chemistry Point of View. , 0, , .		2

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145	Helix compactness and stability: Electron structure calculations of conformer dependent thermodynamic functions. Chemical Physics Letters, 2013, 563, 80-87.	2.6	2
146	Quantum Chemical Calculations on Small Protein Models. , 2014, , 5-50.		2
147	Impairment of a model peptide by oxidative stress: Thermodynamic stabilities of asparagine diamide Cî±-radical foldamers. Chemical Physics Letters, 2014, 593, 104-108.	2.6	2
148	Dimension reduction in conformational analysis: a two-rotor mathematical model of amino acid diamide conformational potential energy surface. Canadian Journal of Chemistry, 2017, 95, 830-836.	1.1	2
149	An improved two-rotor function for conformational potential energy surfaces of 20 amino acid diamides. Canadian Journal of Chemistry, 2018, 96, 58-71.	1.1	2
150	Oxidatively-mediated in silico epimerization of a highly amyloidogenic segment in the human calcitonin hormone (hCT15-19). Computational Biology and Chemistry, 2019, 80, 259-269.	2.3	2
151	Conformation analysis of 1,4-pentadien-3-yl radicals by ab initio and DFT methods. Computational and Theoretical Chemistry, 2003, 666-667, 153-158.	1.5	1
152	Theoretical investigation of the conformational intricacies and thermodynamic functions of noradrenaline. Canadian Journal of Chemistry, 2011, 89, 1010-1020.	1.1	1
153	Conformational and thermodynamic analysis of the COXIB scaffold using quantum chemical calculations. International Journal of Quantum Chemistry, 2012, 112, 922-936.	2.0	1
154	Controlled antioxidative steps of the cell. The concept of chalcogenicity. Chemical Physics Letters, 2013, 590, 83-86.	2.6	1
155	The Effect of Hydroxyl Moieties and Their Oxosubstitution on Bile Acid Association Studied in Floating Monolayers. Scientific World Journal, The, 2014, 2014, 1-10.	2.1	1
156	Radicalicity: A scale to compare reactivities of radicals. Chemical Physics Letters, 2015, 618, 99-101.	2.6	1
157	Ligand binding constants of the cucurbit[7]uril predicted with molecular docking: a theoretical study. Turkish Journal of Chemistry, 2018, 42, .	1.2	1
158	Carbon nanotube-zeolite composite catalyst - characterization and application. Journal of Dispersion Science and Technology, 2021, 42, 701-706.	2.4	1
159	Molecular orbital computations on lipids: modular numbering. Computational and Theoretical Chemistry, 2003, 666-667, 445-449.	1.5	0
160	Water treatment by membrane technology. , 2012, , .		0
161	Conformation change of opiorphin derivates. A theoretical study of the radical initiated epimerization of opiorphin. Chemical Physics Letters, 2015, 626, 29-38.	2.6	0
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