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	Formation and growth mechanisms of polycyclic aromatic hydrocarbons: A mini-review. Chemosphere, 2022, 291, 132793.	8.2	77
2	Optical Study of Solvatochromic Isocyanoaminoanthracene Dyes and 1,5-Diaminoanthracene. International Journal of Molecular Sciences, 2022, 23, 1315.	4.1	5
3	Exploring the Potential to Repurpose Flexible Moulded Polyurethane Foams as Acoustic Insulators. Polymers, 2022, 14, 163.	4.5	8
4	Computational Study of Catalytic Urethane Formation. Polymers, 2022, 14, 8.	4.5	7
5	Comparison of Catalysts with MIRA21 Model in Heterogeneous Catalytic Hydrogenation of Aromatic Nitro Compounds. Catalysts, 2022, 12, 467.	3.5	5
6	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
7	A Theoretical Study on the Phosgenation of 2,4-Toluenediamine (2,4-TDA). Polymers, 2022, 14, 2254.	4.5	6
8	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
9	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
10	Foreseeing the future of green Technology. Molecular dynamic investigation on passive membrane penetration by the products of the CO2 and 1,3-butadiene reaction. Journal of Molecular Liquids, 2022, 361, 119581.	4.9	0
11	Experimental and Theoretical Study of Cyclic Amine Catalysed Urethane Formation. Polymers, 2022, 14, 2859.	4.5	5
12	Carbon nanotube-zeolite composite catalyst - characterization and application. Journal of Dispersion Science and Technology, 2021, 42, 701-706.	2.4	1
13	Application of ion-exchange resin beads to produce magnetic adsorbents. Chemical Papers, 2021, 75, 1187-1195.	2.2	13
14	Kinetics and thermochemistry of cyclohexadienes reactions with hydroxyl radicals. Proceedings of the Combustion Institute, 2021, 38, 947-955.	3.9	4
15	Synthesis of iron oxide nanoparticles for DNA purification. Journal of Dispersion Science and Technology, 2021, 42, 693-700.	2.4	12
16	The Analysis of Human Serum N-Glycosylation in Patients with Primary and Metastatic Brain Tumors. Life, 2021, 11, 29.	2.4	4
17	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
18	Development of Highly Efficient, Glassy Carbon Foam Supported, Palladium Catalysts for Hydrogenation of Nitrobenzene. Nanomaterials, 2021, 11, 1172.	4.1	3

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19	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
20	Preparation of Bamboo-Like Carbon Nanotube Loaded Piezoresistive Polyurethane-Silicone Rubber Composite. Polymers, 2021, 13, 2144.	4.5	6
21	Theoretical investigation of benzo(a)pyrene formation. Chemical Physics Letters, 2021, 772, 138564.	2.6	14
22	Preparation of highly effective carbon black supported Pdâ€“Pt bimetallic catalysts for nitrobenzene hydrogenation. Nanotechnology, 2021, 32, 425701.	2.6	6
23	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
24	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
25	Development of N-doped bamboo-shaped carbon nanotube/magnesium oxide nanocomposites. Journal of Composite Materials, 2020, 54, 857-863.	2.4	0
26	Adsorption capacity of oxidized nitrogen-doped bamboo-like carbon nanotubes. Journal of Dispersion Science and Technology, 2020, 41, 1879-1884.	2.4	3
27	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
28	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
29	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
30	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
31	Membrane Flash Index: Powerful and Perspicuous Help for Efficient Separation System Design. ACS Omega, 2020, 5, 15136-15145.	3.5	11
32	Water enhanced mechanism for CO2 â€“ Methanol conversion. Chemical Physics Letters, 2020, 746, 137298.	2.6	3
33	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
34	Catalytic activity of maghemite supported palladium catalyst in nitrobenzene hydrogenation. Reaction Kinetics, Mechanisms and Catalysis, 2020, 129, 107-116.	1.7	10
35	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
36	Microreactor assisted method for studying isocyanateâ€“alcohol reaction kinetics. Journal of Flow Chemistry, 2019, 9, 199-204.	1.9	9

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37	Urethane Formation with an Excess of Isocyanate or Alcohol: Experimental and Ab Initio Study. Polymers, 2019, 11, 1543.	4.5	16
38	Beyond Chelation: EDTA Tightly Binds Taq DNA Polymerase, MutT and dUTPase and Directly Inhibits dNTPase Activity. Biomolecules, 2019, 9, 621.	4.0	6
39	Purification of Fluorescently Derivatized N-Glycans by Magnetic Iron Nanoparticles. Nanomaterials, 2019, 9, 1480.	4.1	5
40	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
41	Renewable energy and raw materials â€“ The thermodynamic support. Journal of Cleaner Production, 2019, 241, 118221.	9.3	12
42	Serum N-Glycosylation in Parkinsonâ€™s Disease: A Novel Approach for Potential Alterations. Molecules, 2019, 24, 2220.	3.8	30
43	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
44	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
45	Formation Mechanism of Benzo(a)pyrene: One of the Most Carcinogenic Polycyclic Aromatic Hydrocarbons (PAH). Molecules, 2019, 24, 1040.	3.8	28
46	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
47	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
48	Synthesis Optimization and Characterization of Nitrogen-Doped Bamboo-Shaped Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2019, 19, 429-435.	0.9	10
49	Chlorate Elimination by Catalytically Hydrogenation, Catalyst Development and Characterization. Catalysis Letters, 2019, 149, 196-202.	2.6	3
50	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
51	High efficiency two-photon uncaging coupled by the correction of spontaneous hydrolysis. Organic and Biomolecular Chemistry, 2018, 16, 1958-1970.	2.8	13
52	Reactivity of Ala-Gly dipeptide with Î²-turn secondary structure. Chemical Physics Letters, 2018, 692, 402-406.	2.6	6
53	Industrial application of molecular computations on the dimerization of methylene diphenyl diisocyanate. Reaction Kinetics, Mechanisms and Catalysis, 2018, 124, 1-14.	1.7	4
54	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

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55	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
56	Ligand binding constants of the cucurbit[7]uril predicted with molecular docking: a theoretical study. Turkish Journal of Chemistry, 2018, 42, .	1.2	1
57	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
58	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
59	Formation of acetamide in interstellar medium. Molecular Astrophysics, 2018, 13, 1-5.	1.6	12
60	A prelude to building mathematical models for polypeptide folding: analysis on the conformational potential energy hypersurface cross-sections of N-acetyl-glycyl-glycine-Nâ€²-methylamide. Canadian Journal of Chemistry, 2018, 96, 912-921.	1.1	0
61	Glycerol carbonate as a fuel additive for a sustainable future. Sustainable Energy and Fuels, 2018, 2, 2171-2178.	4.9	38
62	A theoretical study on the phosgenation of methylene diphenyl diamine (MDA). Chemical Physics Letters, 2018, 706, 568-576.	2.6	8
63	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
64	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
65	A high temperature kinetic study for the thermal unimolecular decomposition of diethyl carbonate. Chemical Physics Letters, 2017, 684, 390-396.	2.6	6
66	Molecular Surgery Concept from Bench to Bedside: A Focus on TRPV1+ Pain-Sensing Neurons. Frontiers in Physiology, 2017, 8, 378.	2.8	14
67	Protein Stability and Unfolding Following Glycine Radical Formation. Molecules, 2017, 22, 655.	3.8	7
68	Ortho-Methoxy Group as a Mild Inhibitor of the Reactions Between Carboxylic Acid and Phenols. Croatica Chemica Acta, 2017, 90, .	0.4	0
69	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
70	Reply to comment on â€œRadicalicity: A scale to compare reactivities of radicalsâ€• Chemical Physics Letters, 2016, 654, 141.	2.6	0
71	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
72	Critical evaluation of the potential energy surface of the CH3 + HO2reaction system. Journal of Chemical Physics, 2015, 142, 054308.	3.0	11

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73	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
74	Glutathione as a Prebiotic Answer to Îł-Peptide Based Life. Journal of Physical Chemistry B, 2015, 119, 3940-3947.	2.6	10
75	Big data reduction by fitting mathematical functions. Chemical Physics Letters, 2015, 625, 91-97.	2.6	8
76	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
77	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
78	Radicalicity: A scale to compare reactivities of radicals. Chemical Physics Letters, 2015, 618, 99-101.	2.6	1
79	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
80	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
81	Molecular ageing: Free radical initiated epimerization of thymopentin â€“ A case study. Journal of Chemical Physics, 2014, 140, 205102.	3.0	4
82	Quantum Chemical Calculations on Small Protein Models. , 2014, , 5-50.		2
83	Global optimization of cholic acid aggregates. Journal of Chemical Physics, 2014, 140, 144302.	3.0	7
84	The effect of oxidative stress on the bursopentin peptide structure: a theoretical study. Physical Chemistry Chemical Physics, 2014, 16, 9602-9609.	2.8	5
85	Impairment of a model peptide by oxidative stress: Thermodynamic stabilities of asparagine diamide CÎą-radical foldamers. Chemical Physics Letters, 2014, 593, 104-108.	2.6	2
86	Fourier type potential energy function for conformational change of selected organic functional groups. Chemical Physics Letters, 2014, 599, 169-174.	2.6	6
87	A theoretical study of the stability of disulfide bridges in various Îą-sheet structures of protein segment models. Chemical Physics Letters, 2014, 593, 48-54.	2.6	4
88	Atropisomerism of the Asn Îą Radicals Revealed by Ramachandran Surface Topology. Journal of Physical Chemistry B, 2013, 117, 12402-12409.	2.6	6
89	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
90	Helix compactness and stability: Electron structure calculations of conformer dependent thermodynamic functions. Chemical Physics Letters, 2013, 563, 80-87.	2.6	2

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91	Penicillin's catalytic mechanism revealed by inelastic neutrons and quantum chemical theory. Physical Chemistry Chemical Physics, 2013, 15, 20447-20455.	2.8	24
92	Controlled antioxidative steps of the cell. The concept of chalcogenicity. Chemical Physics Letters, 2013, 590, 83-86.	2.6	1
93	Glutathione â€“ Hydroxyl Radical Interaction: A Theoretical Study on Radical Recognition Process. PLoS ONE, 2013, 8, e73652.	2.5	24
94	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
95	Disulfidicity: A scale to characterize the disulfide bond strength via the hydrogenation thermodynamics. Chemical Physics Letters, 2012, 539-540, 11-14.	2.6	4
96	Homology Modeling and Validation of the Human M1 Muscarinic Acetylcholine Receptor. Molecular Informatics, 2012, 31, 635-638.	2.5	3
97	Water treatment by membrane technology. , 2012, , .		0
98	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
99	Conformational and thermodynamic analysis of the COXIB scaffold using quantum chemical calculations. International Journal of Quantum Chemistry, 2012, 112, 922-936.	2.0	1
100	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
101	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
102	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
103	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
104	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
105	Antioxidant Potential of Glutathione: A Theoretical Study. Journal of Physical Chemistry B, 2011, 115, 11269-11277.	2.6	26
106	Theoretical investigation of the conformational intricacies and thermodynamic functions of noradrenaline. Canadian Journal of Chemistry, 2011, 89, 1010-1020.	1.1	1
107	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
108	A computational study of glutathione and its fragments: N-acetylcisteinylglycine and Î³-glutamylmethylamide. Chemical Physics Letters, 2011, 507, 168-173.	2.6	9

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109	Polymerization dependence of the entropy of homo-oligomer peptides. Chemical Physics Letters, 2010, 501, 30-32.	2.6	7
110	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
111	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
112	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
113	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
114	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
115	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
116	A Quantitative Scale for the Extent of Conjugation of Substituted Olefines. Journal of Physical Chemistry A, 2009, 113, 7953-7962.	2.5	9
117	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
118	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
119	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
120	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
121	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
122	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
123	3D QSAR models for Î±2a-adrenoceptor agonistsâ^†. Neurochemistry International, 2007, 51, 268-276.	3.8	5
124	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
125	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
126	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

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127	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
128	Quantifying the Intrinsic Effects of Two Point Mutation Models of Prolineâˆ'Proline Diamino Acid Diamide: A First-Principle Computational Study. Journal of Physical Chemistry B, 2007, 111, 11592-11602.	2.6	15
129	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
130	Information accumulation in helical oligopeptide structures. Chemical Physics Letters, 2007, 450, 123-126.	2.6	6
131	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
132	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
133	Rate Coefficients and Equilibrium Constant for the CH2CHO + O2 Reaction System. Journal of Physical Chemistry A, 2006, 110, 3238-3245.	2.5	34
134	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
135	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
136	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
137	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
138	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
139	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
140	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
141	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
142	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
143	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
144	Theoretical studies of carbon dioxide catalysis of peroxynitrite isomerizations. Computational and Theoretical Chemistry, 2005, 731, 57-60.	1.5	4

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145	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
146	Hydrogen bondings in deoxynivalenol (DON) conformationsâ€"a density functional study. Computational and Theoretical Chemistry, 2005, 726, 55-59.	1.5	37
147	First Principle Computational Study on the Full Conformational Space ofl-Proline Diamides. Journal of Physical Chemistry A, 2005, 109, 2660-2679.	2.5	29
148	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
149	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
150	Direct Kinetic Study of Reactions of Hydroxyl Radicals with Alkyl Formates. Zeitschrift Fur Physikalische Chemie, 2004, 218, 479-492.	2.8	19
151	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
152	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
153	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
154	Conformational analysis of oxidized vitamin-C. Computational and Theoretical Chemistry, 2003, 666-667, 397-400.	1.5	4
155	Molecular orbital computations on lipids: modular numbering. Computational and Theoretical Chemistry, 2003, 666-667, 445-449.	1.5	0
156	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
157	Competition between alkyl radical addition to carbonyl bonds and H-atom abstraction reactions. Physical Chemistry Chemical Physics, 2002, 4, 4663-4668.	2.8	29
158	A detailed experimental and theoretical study on the decomposition of methoxy radicals. Physical Chemistry Chemical Physics, 2001, 3, 2450-2458.	2.8	55
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