

Associa€ProfªDr Hossein Farrokhpour

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	In situ generated Ligand-Free gold nanoparticles in polyvinylpyrrolidone solution assisted laser in liquid method for green oxidation of cyclohexane to adipic acid with high yield. Applied Surface Science, 2022, 581, 152388.	3.1	2
2	Decomposition of the interaction energy of several flavonoids with Escherichia coli DNA Gyr using the SAPT (DFT) method: The relation between the interaction energy components, ligand structure, and biological activity. Biochimica Et Biophysica Acta - General Subjects, 2022, 1866, 130111.	1.1	2
3	Fast and selective determination of the gasodor S-free using ion mobility spectrometer equipped with corona discharged ionization source: Theoretical study, experimental optimization and field test. Fuel, 2022, 318, 123597.	3.4	1
4	Imine-Linked Covalent Organic Framework with a Naphthalene Moiety as a Sensitive Phosphate Ion Sensing. ACS Applied Materials & Interfaces, 2022, 14, 22398-22406.	4.0	39
5	Water-vapochromic behavior of a mononuclear Pd(II) complex of piroxicam: A DFT and TD-DFT study. Journal of Molecular Graphics and Modelling, 2021, 102, 107773.	1.3	5
6	Electrocatalytic property, anticancer activity, and density functional theory calculation of [NiCl(P [^] N [^] P)]Cl.EtOH. Applied Organometallic Chemistry, 2021, 35, e6092.	1.7	2
7	A TD-DFT study of the excited dissociative electronic states of the DNA nucleobases bound to Li+. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 244, 118862.	2.0	1
8	Sodium salts effect on the time of flight mass spectra of some amino acids in the direct laser desorption ionization and matrix-assisted laser desorption/ionization. Journal of the Chinese Chemical Society, 2021, 68, 1263-1270.	0.8	2
9	Mechanistic insight into the hydrogenation of acetylene on the Pd ₂ /g-C ₃ N ₄ catalyst: effect of Pd clustering on the barrier energy and selectivity. Structural Chemistry, 2021, 32, 2087-2097.	1.0	1
10	Dinuclear Nickel(II) and Copper(II) Complexes of 8-Quinolinecarboxamide: Crystal Structure, Magnetic Properties, and DFT Calculations. European Journal of Inorganic Chemistry, 2021, 2021, 1786-1795.	1.0	4
11	Theoretical study of the vapochromic properties of a mononuclear Pd(II) complex with piroxicam ligands for the detection of the vapor of several solvents. Journal of Molecular Liquids, 2021, 334, 116508.	2.3	1
12	Using surfactants as matrix for the matrix-assisted laser desorption/ionization time of flight mass spectrometry (MALDI-TOF-MS) of amino acids: Sodium dodecyl sulfate (SDS) and sodium octyl sulfate (SOS). Biophysical Chemistry, 2021, 278, 106667.	1.5	0
13	A comparative theoretical study of the chiral discrimination of phenylalanine enantiomers by the cyclic peptides with different sizes as discriminating agents: A DFT study. Journal of Molecular Structure, 2021, 1243, 130904.	1.8	3
14	Li ⁺ and Na ⁺ attachment to some dipeptides via LDI-TOF mass spectrometry: Fragmentation patterns. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 262, 120093.	2.0	1
15	Pd/Cu-Free Cobalt-Catalyzed Suzuki and Heck Using Green Bio-Magnetic Hybrid and DFT-Based Theoretical Study. Catalysis Letters, 2021, 151, 2842-2850.	1.4	5
16	A facile method for sample preparation of ore for quantitative analysis by laser desorption ionization-time of flight mass spectrometry using an internal standard. Journal of Analytical Atomic Spectrometry, 2021, 36, 1576-1581.	1.6	1
17	Interaction of different types of nanocages (Al ₁₂ N ₁₂), Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 112 Td (CfCN: DFT, TD-DFT, OTAIM, and NBO calculations. Molecular Physics, 2020, 118, 1626506.	0.8	29
18	A naphthylamide based fluorescent probe for detection of Al ³⁺ , Fe ³⁺ , and CN ⁻ with high sensitivity and selectivity. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117753.	2.0	14

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19	Theoretical study of the desorption of neutral and ionic alkali metal atoms from the excited Li + (H ₂) Tj ETQq1 1 0.784314 rgBT /Overlo Journal of Quantum Chemistry, 2020, 120, e26104.	1.0	3
20	Surface modification of alumina with P ₂ O ₅ and its application in 2-octanol dehydration. Reaction Kinetics, Mechanisms and Catalysis, 2020, 129, 265-282.	0.8	3
21	Electron affinities of X ₁₂ O ₁₂ (X = Be, Mg, and Ca), X ₁₂ N ₁₂ (X = B, Al, and Ga), and X ₁₂ P ₁₂ (X = B, Al, and) Tj ETQq1 1 0.784314 rgBT /Overlo 2020, 135, 1.	1.2	3
22	SBA-15-Supported Imidazolium Ionic Liquid through Different Linkers as a Sustainable Catalyst for the Synthesis of Cyclic Carbonates: A Kinetic Study and Theoretical DFT Calculations. Industrial & Engineering Chemistry Research, 2020, 59, 12632-12644.	1.8	42
23	Excitation of hydrated Li ⁺ and Na ⁺ to their dissociative states: The effect of hydrogen bond on the dissociation of Li O and Na O bonds and the comparison of the TD-DFT and SAC-CI excited dissociative states. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 234, 118273.	2.0	3
24	Mechanism of lithiation of amino acids in aqueous solutions: A laser desorption/ionization-time-of-flight mass spectrometry and theoretical study. International Journal of Mass Spectrometry, 2020, 455, 116389.	0.7	1
25	Effect of sacrificial agents on the photoelectrochemical properties of titanium dioxide co-doped with tungsten and manganese as new visible light active. Journal of the Iranian Chemical Society, 2020, 17, 3317-3326.	1.2	4
26	Theoretical insights into the electron affinity of manganese superhalogen compounds; NBO, QTAIM and energy decomposition analysis. Molecular Physics, 2020, 118, e1718791.	0.8	1
27	Adenine dimer on the pure and bimetallic nanosurfaces of Au and Ag metals: Hydrogen bonding on metal nanosurfaces. Computational Materials Science, 2020, 175, 109609.	1.4	2
28	Ionization of adenine in the presence of Na ⁺ in the gas phase and water. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 392, 112404.	2.0	0
29	The Role of Delocalization Energy on Superhalogen Property: The Electron Affinity of , , and (X=O, S,) Tj ETQq1 1 0.784314 rgBT /Overlo 0.7	0.7	1
30	Extended light absorption and enhanced photoelectrochemical activity of palladium-decorated hematite nanotubes prepared by photodeposition method. Applied Organometallic Chemistry, 2019, 33, e5087.	1.7	3
31	Humidity Effect on the Drift Times of the Reactant Ions in Ion Mobility Spectrometry. Analytical Chemistry, 2019, 91, 15932-15940.	3.2	20
32	The adsorption of small size Pd clusters on a g-C ₃ N ₄ quantum dot: DFT and TD-DFT study. Materials Research Express, 2019, 6, 105079.	0.8	10
33	Fabrication of Pd/WO ₃ colloidal nanoparticles by laser ablation in liquid of tungsten for optical hydrogen detection. Journal of Laser Applications, 2019, 31, .	0.8	7
34	Fabrication of tungsten-iron-doped TiO ₂ nanotubes via anodization: new photoelectrodes for photoelectrochemical cathodic protection under visible light. SN Applied Sciences, 2019, 1, 1.	1.5	21
35	Theoretical Spectroscopic Study on the Au, Ag, Au/Ag, and Ag/Au Nanosurfaces and Their Cytosine/Nanosurface Complexes: UV, IR, and Charge-Transfer SERS Spectra. Journal of Physical Chemistry C, 2019, 123, 16345-16358.	1.5	5
36	A comparative study of the counterion effect on the perrhenate-catalyzed deoxydehydration reaction. Molecular Catalysis, 2019, 471, 27-37.	1.0	8

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37	<i>In situ</i> synthesis of carbon nanotube-encapsulated cobalt nanoparticles by a novel and simple chemical treatment process: efficient and green catalysts for the Heck reaction. <i>New Journal of Chemistry</i> , 2019, 43, 8215-8219.	1.4	16
38	Facile and green synthesis of copper nanoparticles loaded on the amorphous carbon nitride for the oxidation of cyclohexane. <i>Chemical Engineering Journal</i> , 2019, 370, 1310-1321.	6.6	76
39	Theoretical Evaluation of One-Pot Synthesis of Aliphatic PNP Pincer Ligands. <i>Journal of Structural Chemistry</i> , 2019, 60, 1735-1742.	0.3	1
40	Study of the structural ligand effects on the fragmentation pattern of some Schiff base complexes of V (IV), Cu(II) and Ni (II) against the IR laser radiation using Matrix-free LDI-TOF technique. <i>International Journal of Mass Spectrometry</i> , 2019, 436, 33-41.	0.7	7
41	Directional affinity of a spherical Gold nanoparticle for the adsorption of DNA bases. <i>Colloids and Surfaces B: Biointerfaces</i> , 2019, 173, 493-503.	2.5	7
42	Diastereomeric discrimination by achiral substances: the effect of diverse ions in the stability of amphi-ionophore cystine-based cyclopeptide stereoisomers. <i>Molecular Physics</i> , 2019, 117, 557-566.	0.8	0
43	The effect of the diameter of cyclic peptide nanotube on its chirality discrimination. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 691-701.	2.0	10
44	Immobilization of gold nanoparticles on folate-conjugated dendritic mesoporous silica-coated reduced graphene oxide nanosheets: a new nanoplatform for curcumin pH-controlled and targeted delivery. <i>Soft Matter</i> , 2018, 14, 2400-2410.	1.2	64
45	Energy decomposition analysis of the intermolecular interaction energy between different gas molecules (H ₂ , O ₂ , H ₂ O, N ₂ , CO ₂ , H ₂ S, and CO) and selected Li ⁺ -doped graphitic molecules: DF-SAPT (DFT) calculations. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	1
46	Stabilization of DOPA Zwitterions on Laser-Generated Gold Nanoparticles: ONIOM Computational Study of the Charge-Dependent Structural and Electronic Changes of DOPA Adsorbed on the Gold Nanosurface. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8680-8692.	1.5	4
47	A Comparison of Catalytic Effect of Nano-Mn ₃ O ₄ derived from Mn ₂ O ₄ .2H ₂ O and Mn(acac) ₃ on Thermal Decomposition of Ammonium Perchlorate. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2018, 644, 241-252.	0.6	2
48	Ionization of the Conformers of <i>cis</i> Nanotubular Cyclic Peptides in the Gas Phase: Effect of Size and Conformation on Ionization. <i>Journal of the Chinese Chemical Society</i> , 2018, 65, 405-415.	0.8	1
49	Alkali halides based on nano-alumina as positive and negative ion source for ion mobility and mass spectrometry. <i>Journal of the Iranian Chemical Society</i> , 2018, 15, 863-870.	1.2	1
50	Cyclic peptide nanocapsule as ion carrier for halides: a theoretical survey. <i>Structural Chemistry</i> , 2018, 29, 1351-1357.	1.0	3
51	Urea changes oocyte competence and gene expression in resultant bovine embryo <i>in vitro</i> . <i>Zygote</i> , 2018, 26, 207-219.	0.5	12
52	Investigation of simultaneous formation of nano-sized CuO and ZnO on the thermal decomposition of ammonium perchlorate for composite solid propellants. <i>Journal of Thermal Analysis and Calorimetry</i> , 2018, 132, 879-893.	2.0	24
53	Theoretical studies on the potentials of some nanocages (Al ₁₂ N ₁₂ , Al ₁₂ P ₁₂ , B ₁₂ N ₁₂ , Be ₁₂ O ₁₂ , C ₁₂ Si ₁₂), <i>Tj ETQq1 1 0.784314 rgB</i> of <i>Molecular Liquids</i> , 2018, 260, 138-148.	2.3	58
54	DFT and TD-DFT study of the adsorption and detection of sulfur mustard chemical warfare agent by the C ₂₄ , C ₁₂ Si ₁₂ , Al ₁₂ N ₁₂ , Al ₁₂ P ₁₂ , Be ₁₂ O ₁₂ , B ₁₂ N ₁₂ and Mg ₁₂ O ₁₂ nanocages. <i>Journal of Molecular Structure</i> , 2018, 1164, 227-238.	1.8	52

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55	Theoretical studies on the thermodynamics and kinetics of one-pot synthesis of aromatic PCP and PNP pincer ligands. <i>Structural Chemistry</i> , 2018, 29, 81-88.	1.0	3
56	Synthesis and spectroscopic characterization study of new palladium complexes containing bioactive O,O-chelated ligands: evaluation of the DNA/protein BSA interaction, <i>in vitro</i> antitumoural activity and molecular docking. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 3324-3340.	2.0	33
57	The effect of the hydrogen fluoride chain on the aromaticity of C ₆ H ₆ in the C ₆ H ₆ ·(HF) _n complexes. <i>Molecular Physics</i> , 2018, 116, 313-322.	0.8	1
58	A generalised perturbation-based equation of state for thermodynamic modelling of fluids over a wide range of density. <i>Physics and Chemistry of Liquids</i> , 2018, 56, 730-750.	0.4	2
59	Au-Pd@g-C ₃ N ₄ as an Efficient Photocatalyst for Visible-Light Oxidation of Benzene to Phenol: Experimental and Mechanistic Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27477-27485.	1.5	58
60	ONIOM DFT study of the adsorption of cytosine on the Au/Ag and Ag/Au bimetallic nanosurfaces: The effect of sublayer. <i>Applied Surface Science</i> , 2018, 457, 712-725.	3.1	12
61	Utilization of CO ₂ as a carbon source for production of CO and syngas using a ruthenium(II) electrocatalyst. <i>Journal of CO₂ Utilization</i> , 2018, 26, 612-622.	3.3	7
62	The effect of curvature of Li-doped polycyclic hydrocarbon on its interaction energy with H ₂ and H ₂ O: DF-SAPT (DFT) calculation. <i>Structural Chemistry</i> , 2018, 29, 1745-1751.	1.0	1
63	Thermochemistry of the Reaction of Solvated Sodium Ion Clusters with Thymine in the Gas Phase: An Example of the Reaction in Microcosmic Environment. <i>Journal of Cluster Science</i> , 2018, 29, 521-531.	1.7	2
64	A highly selective fluorescence turn-on chemosensor for Zn ²⁺ , and its application in live cell imaging, and as a colorimetric sensor for Co ²⁺ : experimental and TD-DFT calculations. <i>New Journal of Chemistry</i> , 2018, 42, 12595-12606.	1.4	42
65	A Comparative Study between Co and CoFe ₂ O ₄ NPs Catalytic Activities in Synthesis of Flavone Derivatives; Study of Their Interactions with Estrogen Receptor by Molecular Docking. <i>ChemistrySelect</i> , 2018, 3, 6279-6285.	0.7	5
66	An experimental and theoretical study on the interaction of DNA and BSA with novel Ni ²⁺ , Cu ²⁺ and VO ²⁺ complexes derived from vanillin bidentate Schiff base ligand. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 180, 144-153.	2.0	20
67	Adsorption modes of 1,3-thiazol-2-amine on the TiO ₂ (001) and (101) anatase surfaces. <i>Structural Chemistry</i> , 2017, 28, 1151-1162.	1.0	4
68	Evaluation of one-dimensional potential energy surfaces for prediction of spectroscopic properties of hydrogen bonds in linear bonded complexes. <i>Journal of Molecular Modeling</i> , 2017, 23, 157.	0.8	3
69	Combined Experimental and Computational Study of the In Situ Adsorption of Piroxicam Anions on the Laser-Generated Gold Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8589-8600.	1.5	8
70	A single chemosensor with combined ionophore/fluorophore moieties acting as a fluorescent α -Off-On-Zn ²⁺ sensor and a colorimetric sensor for Cu ²⁺ : Experimental, logic gate behavior and TD-DFT calculations. <i>Sensors and Actuators B: Chemical</i> , 2017, 250, 647-658.	4.0	36
71	Correlation of isothermal compressibility coefficient and reduced bulk modulus of dense fluids using perturbed linear Yukawa isotherm regularity. <i>Physics and Chemistry of Liquids</i> , 2017, 55, 637-649.	0.4	6
72	van der Waals DFT ONIOM study of the adsorption of DNA bases on the Cu(111) nanosurface. <i>Applied Surface Science</i> , 2017, 422, 372-387.	3.1	10

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73	Modeling the $p \sim v \sim T$ behavior of furfural compounds using perturbed linear Yukawa isotherm regularity. <i>Journal of Molecular Liquids</i> , 2017, 236, 18-26.	2.3	4
74	Description of adenine and cytosine on Au(111) nano surface using different DFT functionals (PW91PW91, wB97XD, M06-2X, M06-L and CAM-B3LYP) in the framework of ONIOM scheme: Non-periodic calculations. <i>Chemical Physics</i> , 2017, 488-489, 1-10.	0.9	36
75	Transport Behavior of the Enantiomers of Lactic Acid through the Cyclic Peptide Nanotube: Enantiomer Discrimination. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8165-8176.	1.5	8
76	Electrocatalytic reduction of CO ₂ to CO in the presence of a mononuclear polypyridyl ruthenium(II) complex. <i>Journal of CO₂ Utilization</i> , 2017, 17, 80-89.	3.3	16
77	Ionization of vitamin B6 in the gas phase and water: Theoretical study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 336, 77-88.	2.0	11
78	Absorption spectra of small helium Nano clusters (4He ; n= 2-29) and characterization of their low-lying excited states. <i>Journal of Molecular Liquids</i> , 2017, 230, 190-199.	2.3	4
79	Perrhenate-Catalyzed Deoxydehydration of a Vicinal Diol: A Comparative Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8688-8696.	1.1	11
80	Stabilized gold nanoparticles by laser ablation in ferric chloride solutions. <i>Applied Physics A: Materials Science and Processing</i> , 2017, 123, 1.	1.1	5
81	Constants of explosive limits. <i>Chemical Engineering Science</i> , 2017, 173, 384-389.	1.9	13
82	Effect of helium nanoclusters on the spectroscopic properties of embedded SF ₆ : Ionization, excitation and vibration. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 173, 772-782.	2.0	2
83	Synthesis, structure, DNA/protein binding, and cytotoxic activity of a rhodium(III) complex with 2,6-bis(2-benzimidazolyl)pyridine. <i>European Journal of Medicinal Chemistry</i> , 2017, 127, 958-971.	2.6	46
84	Average drift time and average mobility in ion mobility spectrometry. <i>International Journal of Mass Spectrometry</i> , 2017, 412, 20-25.	0.7	7
85	Quantum mechanical/molecular mechanical and docking study of the novel analogues based on hybridization of common pharmacophores as potential anti-breast cancer agents. <i>Research in Pharmaceutical Sciences</i> , 2017, 12, 233.	0.6	11
86	Investigation of the in situ generation of oxide-free copper nanoparticles using pulsed-laser ablation of bulk copper in aqueous solutions of DNA bases. <i>RSC Advances</i> , 2016, 6, 109885-109896.	1.7	8
87	A comparative MP2 study between water- and acid-assisted proton transfer: allophanic acid as a case of study. <i>Structural Chemistry</i> , 2016, 27, 1345-1362.	1.0	7
88	Kinetics, mechanism and thermodynamics of reactions of hydrazine with CH ₃ and OOH radicals. <i>Research on Chemical Intermediates</i> , 2016, 42, 1181-1194.	1.3	2
89	Towards new thermodynamic regularities for dense fluids based on the effective attraction pair potential via the perturbation theory. <i>Journal of Molecular Liquids</i> , 2016, 220, 623-630.	2.3	4
90	Ionization of vitamin C in gas phase: Theoretical study. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2016, 160, 11-17.	1.7	13

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91	In situ generation of the gold nanoparticles-“bovine serum albumin (AuNPs-BSA) bioconjugated system using pulsed-laser ablation (PLA). <i>Materials Chemistry and Physics</i> , 2016, 177, 360-370.	2.0	34
92	Electrocatalytic reduction of CO ₂ to CO by a mononuclear ruthenium(II) complex. <i>New Journal of Chemistry</i> , 2016, 40, 6347-6357.	1.4	17
93	Molecular thermodynamic modeling of ionic liquids using the perturbation-based linear Yukawa isotherm regularity. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 235101.	0.7	8
94	Experimental and ONIOM computational evaluation of DNA- and BSA-binding and cytotoxic activity of a mononuclear Pd(II) complex with piroxicam. <i>Inorganica Chimica Acta</i> , 2016, 453, 415-429.	1.2	15
95	A new force field for the adsorption of H ₂ , O ₂ , N ₂ , CO, H ₂ O, and H ₂ S gases on alkali doped carbon nanotubes. <i>Molecular Physics</i> , 2016, 114, 3375-3387.	0.8	6
96	Theoretical Modeling of the Chirality Discrimination of Enantiomers by Nanotubular Cyclic Peptides using Gas-Phase Photoelectron Spectroscopy: An ONIOM Spectroscopic Calculations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6780-6791.	1.1	5
97	Regioselective Heck reaction catalyzed by Pd nanoparticles immobilized on DNA-modified MWCNTs. <i>RSC Advances</i> , 2016, 6, 59124-59130.	1.7	26
98	Enantiomeric discrimination of leucine enantiomers by nanotubular cyclic peptides: DFT and ONIOM calculation of the absorption spectra of guested enantiomers. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2016, 85, 329-339.	0.9	5
99	The effect of deformation and intermolecular interaction on the absorption spectrum of 5-aminotetrazole and hydrazine: A computational molecular spectroscopy study on hydrazinium 5-aminotetrazolate. <i>Journal of Molecular Structure</i> , 2016, 1107, 121-136.	1.8	2
100	Sodium affinity of caffeine and adenine: the effect of microsolvation and electrostatic field of solvent on the sodium affinity. <i>Molecular Physics</i> , 2016, 114, 730-740.	0.8	3
101	An experimental and quantum chemical study on the non-covalent interactions of a cyclometallated Rh(III) complex with DNA and BSA. <i>RSC Advances</i> , 2016, 6, 23913-23929.	1.7	16
102	Ionization energies, electron affinities, and binding energies of Li-doped gold nanoclusters. <i>Research on Chemical Intermediates</i> , 2016, 42, 4921-4936.	1.3	7
103	Linear Yukawa Isotherm Regularity for dense fluids derived based on the perturbation theory. <i>Fluid Phase Equilibria</i> , 2016, 409, 105-112.	1.4	11
104	Selective Complexation of Cationic Block Cations with Nanotubular Silk Type Cyclopeptides: A DFT Study. <i>Journal of the Chinese Chemical Society</i> , 2015, 62, 1105-1113.	0.8	2
105	Experimental and theoretical spectroscopic study and structural determination of nickel(II) tridentate Schiff base complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 220-229.	2.0	29
106	Adsorption of small gas molecules on B36 nanocluster. <i>Journal of Chemical Sciences</i> , 2015, 127, 2029-2038.	0.7	44
107	Green, efficient and large-scale synthesis of benzimidazoles, benzoxazoles and benzothiazoles derivatives using ligand-free cobalt-nanoparticles: as potential anti-estrogen breast cancer agents, and study of their interactions with estrogen receptor by molecular docking. <i>RSC Advances</i> , 2015, 5, 107822-107828.	1.7	33
108	Ab initio intermolecular potential energy surface of Ne-NCN van der Waals complex: effect of the place of midbond function on the interaction. <i>Molecular Physics</i> , 2015, 113, 3303-3311.	0.8	5

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109	Protein-ligand interaction study of signal transducer smoothed protein with different drugs: molecular docking and QM/MM calculations. RSC Advances, 2015, 5, 68829-68838.	1.7	10
110	Structures and Photoelectron Spectra of Helium Nano Clusters. Journal of Physical Chemistry C, 2015, 119, 18641-18649.	1.5	5
111	Design of novel potential aromatase inhibitors via hybrid pharmacophore approach: docking improvement using the QM/MM method. RSC Advances, 2015, 5, 58055-58064.	1.7	21
112	Direct Fabrication of Au/Pd(II) Colloidal Core-Shell Nanoparticles by Pulsed Laser Ablation of Gold in PdCl ₂ Solution. Journal of Physical Chemistry C, 2015, 119, 9534-9542.	1.5	28
113	Photoreduction of CO ₂ to CO by a mononuclear Re(^{sc}) complex and DFT evaluation of the photocatalytic mechanism. RSC Advances, 2015, 5, 41125-41134.	1.7	30
114	A DFT-D study on the interaction between lactic acid and single-wall carbon nanotubes. RSC Advances, 2015, 5, 97724-97733.	1.7	9
115	Ab initio study of the Ar-CS ₂ (V1B2) intermolecular potential surface: effect of van der Waals interaction on the emission of CS ₂ molecule. Molecular Physics, 2015, 113, 483-491.	0.8	1
116	Kinetics, mechanism and thermodynamics of reactions of CH ₃ NHNH ₂ with OOH. Molecular Physics, 2015, 113, 577-583.	0.8	2
117	Selective complexation of alkaline earth metal ions with nanotubular cyclopeptides: DFT theoretical study. RSC Advances, 2015, 5, 2305-2317.	1.7	23
118	Immobilization of cobalt(III) Schiff base complexes onto Montmorillonite-K10: Synthesis, experimental and theoretical structural determination. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1582-1592.	2.0	16
119	Simple and water-assisted tautomerism in succinimide. Structural Chemistry, 2015, 26, 539-545.	1.0	9
120	Theoretical study on the mechanism and kinetics of atmospheric reactions C _n H _{2n} +2 + NH ₂ (n=3). Structural Chemistry, 2015, 26, 383-391.	1.0	6
121	A Simple Method for Estimating the Absolute Solvation Free Energy of Monovalent Ions in Different Solvents. Journal of Physical Chemistry A, 2015, 119, 160-171.	1.1	5
122	A Differential Pulse Voltammetric Sensor for Determination of Glutathione in Real Samples Using a Trichloro(terpyridine)ruthenium(III)/Multiwall Carbon Nanotubes Modified Paste Electrode. IEEE Sensors Journal, 2015, 15, 483-490.	2.4	16
123	Corona discharge ionization of paracetamol molecule: Peak assignment. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 646-651.	2.0	4
124	Gas phase ionization energies of some important unsaturated steroids. Structural Chemistry, 2015, 26, 71-86.	1.0	8
125	Ab initio intermolecular potential energy surfaces for the Ar-NCCN van der Waals complexes. Molecular Physics, 2014, 112, 2924-2932.	0.8	9
126	Reply to comments on Valence ionization of l-proline amino acid: Experimental and theoretical study. Chemical Physics Letters, 2014, 601, 188-193.	1.2	2

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127	Ag/Pd core-shell nanoparticles by a successive method: Pulsed laser ablation of Ag in water and reduction reaction of PdCl ₂ . <i>Applied Surface Science</i> , 2014, 292, 892-897.	3.1	38
128	DFT and MP2 Study of Intermolecular Interaction of 5-Aminotetrazole and Hydrazine: Enthalpy of Formation of Hydrasinium 5-Aminotetrazolate in the Gas Phase. <i>Propellants, Explosives, Pyrotechnics</i> , 2014, 39, 496-503.	1.0	5
129	Effect of hydration on the stability and tautomerisms of different isomers of uracil. <i>RSC Advances</i> , 2014, 4, 61643-61651.	1.7	11
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