

# Vithaya Ruangpornvisuti

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

129  
papers

1,633  
citations

19  
h-index

33  
g-index

132  
ext. papers

1,789  
ext. citations

3.2  
avg, IF

5.01  
L-index

#	Paper	IF	Citations
129	Theoretical and experimental investigations of a gold nanosensor based on rhodamine-modified carbon nanotubes. <i>Journal of Molecular Structure</i> , <b>2022</b> , 1260, 132765	3.4	0
128	A DFT investigation of lithium adsorption on carbonaceous compounds as a potential anode material in lithium-ion batteries. <i>Journal of Molecular Structure</i> , <b>2022</b> , 1265, 133384	3.4	
127	Adsorption of hydrogen molecule on alkali metal-decorated hydrogen boride nanotubes: A DFT study. <i>International Journal of Hydrogen Energy</i> , <b>2021</b> , 46, 39273-39273	6.7	0
126	Hydrogen boride nanotubes and their C, N, O decoration and doping derivatives as materials for hydrogen-containing gases storage and sensing: A SCCDFTB study. <i>Vacuum</i> , <b>2021</b> , 187, 110140	3.7	2
125	Effects of amino proton and denticity of quinoline-pyridine based dyes on Cd <sup>2+</sup> and Zn <sup>2+</sup> fluorescence sensing properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , <b>2021</b> , 415, 113307	4.7	1
124	Adsorption of nitrosamine conformers on the C <sub>24</sub> , B <sub>12</sub> N <sub>12</sub> , Be <sub>12</sub> O <sub>12</sub> and Al <sub>12</sub> P <sub>12</sub> nanocages and their conversion to nitrogen and water molecules: A DFT study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 127, 114506	3	2
123	Adsorption of sulfur-containing gases on B <sub>36</sub> nanocluster: a DFT study. <i>Journal of Sulfur Chemistry</i> , <b>2021</b> , 42, 383-396	2.3	4
122	A DFT calculation on nonenzymatic degradation of isoaspartic residue. <i>Journal of Molecular Modeling</i> , <b>2021</b> , 27, 300	2	
121	Hydrogen adsorption on c-ZrO <sub>2</sub> (111), t-ZrO <sub>2</sub> (101), and m-ZrO <sub>2</sub> (111) surfaces and their oxygen-vacancy defect for hydrogen sensing and storage: A first-principles investigation. <i>Materials Letters</i> , <b>2021</b> , 301, 130243	3.3	3
120	A study of the transition metal doped boron nitride nanosheets as promising candidates for hydrogen and formaldehyde adsorptions. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 134, 114859	3	2
119	Existence of mangostin conformers and effects of aprotic and protic solvents on their equilibria, UV-vis spectra, and chemical descriptors: Density functional theory and time-dependent density functional theory study. <i>Journal of Physical Organic Chemistry</i> , <b>2020</b> , 33, e4080	2.1	
118	8-Hydroxyjulolidine aldimine as a fluorescent sensor for the dual detection of Al <sup>3+</sup> and Mg <sup>2+</sup> . <i>Sensing and Bio-Sensing Research</i> , <b>2020</b> , 29, 100358	3.3	2
117	Masking Phosphate with Rare-Earth Elements Enables Selective Detection of Arsenate by Dipicolylamine-Zn Chemosensor. <i>Scientific Reports</i> , <b>2020</b> , 10, 2656	4.9	2
116	Dipicolylamino quinoline derivative as novel dual fluorescent detecting system for Hg <sup>2+</sup> and Fe <sup>3+</sup> . <i>Sensing and Bio-Sensing Research</i> , <b>2019</b> , 24, 100283	3.3	5
115	UV-vis and theoretical studies on an ensemble of dinuclear Cu(II) complex of anthracene based tripod tetramine with pyrogallol red for cyanide detection and species distribution in aqueous solution. <i>Inorganic Chemistry Communication</i> , <b>2019</b> , 108, 107502	3.1	1
114	Unusual adsorption behavior of hydrogen molecules on Zr doped perfect and oxygen vacancy defective rutile TiO <sub>2</sub> (110) surfaces: Periodic DFT study. <i>International Journal of Hydrogen Energy</i> , <b>2019</b> , 44, 32101-32111	6.7	8
113	A DFT investigation on group 8B transition metal-doped silicon carbide nanotubes for hydrogen storage application. <i>Applied Surface Science</i> , <b>2018</b> , 439, 494-505	6.7	28

112	DFT investigation on adsorption of diatomic and tetraatomic gases on Sc-doped ZnO sodalite like cage for gas sensing purpose. <i>Materials Chemistry and Physics</i> , <b>2018</b> , 217, 63-73	4.4	3
111	Adsorption of hydrogen and hydrogen-containing gases on Pd and Ag single atoms doped on anatase TiO <sub>2</sub> (1 0 1) surfaces and their sensing performance. <i>Applied Surface Science</i> , <b>2018</b> , 450, 112-121	6.7	4
110	Adsorption of propane and propylene in zeolitic imidazolate framework ZIF-8 pore: periodic SCC-DFTB method. <i>Adsorption</i> , <b>2018</b> , 24, 691-701	2.6	3
109	Self-assembly of Gd/SDS/HEPES complex and curcumin entrapment for enhanced stability, fluorescence image in cellular system. <i>Colloids and Surfaces B: Biointerfaces</i> , <b>2017</b> , 156, 254-261	6	5
108	Acemannan increases NF- $\kappa$ B/DNA binding and IL-6/-8 expression by selectively binding Toll-like receptor-5 in human gingival fibroblasts. <i>Carbohydrate Polymers</i> , <b>2017</b> , 161, 149-157	10.3	18
107	Adsorption of hydrogen molecule on noble metal doped on oxygen-vacancy defect of anatase TiO <sub>2</sub> (101) surface: Periodic DFT study. <i>International Journal of Hydrogen Energy</i> , <b>2017</b> , 42, 19106-19113	6.7	19
106	Simultaneous removal of Ag(I), Cd(II), Cr(III), Ni(II), Pb(II), and Zn(II) from wastewater using humic acid-coated aminopropyl silica gel. <i>Desalination and Water Treatment</i> , <b>2016</b> , 57, 17411-17420		8
105	DFT investigation on molecular structures of metal and nonmetal-doped ZnO sodalite-like cage and their electronic properties. <i>Structural Chemistry</i> , <b>2016</b> , 27, 773-784	1.8	5
104	Hydrogen adsorption on Pt-decorated closed-end armchair (3,3), (4,4) and (5,5) single-walled carbon nanotubes. <i>Molecular Physics</i> , <b>2016</b> , 114, 3508-3517	1.7	3
103	Substituent effect on the proton-related phenomena and chelation behavior of hydroxypicolinic compounds: a DFT investigation. <i>Structural Chemistry</i> , <b>2016</b> , 27, 505-524	1.8	3
102	Arsenite and arsenate removal from wastewater using cationic polymer-modified waste tyre rubber. <i>Journal of Environmental Management</i> , <b>2016</b> , 166, 574-8	7.9	16
101	DFT investigation on molecular structure of zirconia nanoparticle and its adsorption structures with elementary gases. <i>Journal of Molecular Structure</i> , <b>2016</b> , 1108, 187-194	3.4	4
100	Chelation behavior of various flavonols and transfer of flavonol-chelated zinc(II) to alanyl aspartic dipeptide: A PCM/DFT investigation. <i>Journal of Molecular Structure</i> , <b>2016</b> , 1107, 278-290	3.4	7
99	Tautomeric transformation of temozolomide, their proton affinities and chemical reactivities: A theoretical approach. <i>Journal of Molecular Graphics and Modelling</i> , <b>2016</b> , 66, 76-84	2.8	
98	Deacetylation affects the physical properties and bioactivity of acemannan, an extracted polysaccharide from Aloe vera. <i>Carbohydrate Polymers</i> , <b>2015</b> , 133, 556-66	10.3	84
97	Highly promising discrimination of various catecholamines using ratiometric fluorescence probes with intermolecular self-association of two sensing elements. <i>RSC Advances</i> , <b>2015</b> , 5, 78468-78475	3.7	3
96	Ferrocenyl derivative of 1,8-naphthalimide as a new turn-on fluorescent sensor for Au(III) ion. <i>Dyes and Pigments</i> , <b>2015</b> , 112, 236-238	4.6	36
95	Syntheses of amide based anion receptors and investigation of their associations with anions and their molecular structures using proton NMR titration and DFT methods. <i>Journal of Molecular Structure</i> , <b>2014</b> , 1061, 32-40	3.4	2

94	Substituent effect on quantum efficiency in 4-aryloxy-N-(2,6-diisopropylphenyl)-1,8-naphthalimides: Experimental and computational investigations. <i>Dyes and Pigments</i> , <b>2014</b> , 109, 175-180	4.6	6
93	Discriminate sensing of pyrophosphate using a new tripodal tetramine-based dinuclear Zn(II) complex under an indicator displacement assay approach. <i>Dalton Transactions</i> , <b>2014</b> , 43, 14701-9	4.3	10
92	First-principles investigation of ZnO sodalite-like cage binding onto TiO <sub>2</sub> (001) surface and its ability for CO oxidation to CO <sub>2</sub> . <i>Journal of Materials Science</i> , <b>2014</b> , 49, 7620-7624	4.3	
91	Exploring molecular structures, orbital interactions, intramolecular proton-transfer reaction kinetics, electronic transitions and complexation of 3-hydroxycoumarin species using DFT methods. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 51, 13-26	2.8	6
90	Density functional studies of small gases adsorbed on the ZnO sodalite-like cage and its adsorption abilities. <i>Computational and Theoretical Chemistry</i> , <b>2013</b> , 1020, 100-107	2	13
89	Fundamental insights into conformational stability and orbital interactions of antioxidant (+)-catechin species and complexation of (+)-catechin with zinc(II) and oxovanadium(IV). <i>Journal of Molecular Structure</i> , <b>2013</b> , 1047, 344-357	3.4	11
88	A density functional theory study on peptide bond cleavage at aspartic residues: direct vs cyclic intermediate hydrolysis. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 5501-13	2	26
87	Density functional investigation of CO adsorption on Ni-doped single-walled armchair (5,5) boron nitride nanotubes. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 239-45	2	23
86	Theoretical study on isomerization and peptide bond cleavage at aspartic residue. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 3627-36	2	7
85	Theoretical investigation of CO <sub>2</sub> and NO <sub>2</sub> adsorption onto Co-, Rh- and Ir-doped (5,5) single-walled carbon nanotubes. <i>Materials Chemistry and Physics</i> , <b>2013</b> , 138, 709-715	4.4	14
84	Density functional theory investigation of the VIII B transition metal atoms deposited on (5,5) single-walled carbon nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2013</b> , 49, 61-67 <sup>3</sup>		3 <sup>1</sup>
83	Synthesis of chromium(III) complex with 1-hydroxy-2-pyridinone-6-carboxylic acid as insulin-mimetic agent and its spectroscopic and computational studies. <i>Journal of Molecular Structure</i> , <b>2013</b> , 1031, 144-154		9
82	Co-adsorptions of CO/N <sub>2</sub> O, NO/NH <sub>3</sub> , CO <sub>2</sub> /N <sub>2</sub> and conversion of CO/N <sub>2</sub> O to CO <sub>2</sub> /N <sub>2</sub> on ZnO graphene-like nanosheet. <i>Journal of Molecular Structure</i> , <b>2012</b> , 1012, 50-55	3.4	11
81	Quantum chemical investigation on structures of pyrrolic amides functionalized (5,5) single-walled carbon nanotube and their binding with halide ions. <i>Structural Chemistry</i> , <b>2012</b> , 23, 7-15	1.8	12
80	Theoretical Investigation of Ethanol Conversion to Ethylene over H <sub>2</sub> SM <sub>5</sub> and Transition Metals Exchanged ZSM <sub>5</sub> . <i>Catalysis Letters</i> , <b>2012</b> , 142, 143-149	2.8	9
79	Gas adsorption on the Zn-, Pd- and Os-doped armchair (5,5) single-walled carbon nanotubes. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 351-8	2	18
78	Density functional investigation of hydrogen gas adsorption on Fe-doped pristine and Stone-Wales defected single-walled carbon nanotubes. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 3941-9	2	30
77	Discrimination of nucleotides by single fluorescence sensor under solvent-dependent recognition patterns. <i>Sensors and Actuators B: Chemical</i> , <b>2012</b> , 171-172, 969-975	8.5	15

76	A periodic DFT study on binding of Pd, Pt and Au on the anatase TiO <sub>2</sub> (0 0 1) surface and adsorption of CO on the TiO <sub>2</sub> surface-supported Pd, Pt and Au. <i>Applied Surface Science</i> , <b>2012</b> , 258, 3298-3301	6.7	37
75	First-principles investigation of adsorption of N <sub>2</sub> O on the anatase TiO <sub>2</sub> (101) and the CO pre-adsorbed TiO <sub>2</sub> surfaces. <i>Computational Materials Science</i> , <b>2012</b> , 58, 24-30	3.2	21
74	Geometries and stabilities of transition metals doped perfect and Stone-Wales defective armchair (5,5) boron nitride nanotubes. <i>Structural Chemistry</i> , <b>2012</b> , 23, 1819-1830	1.8	16
73	An ONIOM investigation of reaction mechanisms of propylene glycol dehydration over H-ZSM-5 and H-MOR catalysts. <i>Journal of Molecular Catalysis A</i> , <b>2012</b> , 363-364, 171-177		5
72	First principles investigation of oxygen adsorptions on hydrogen-terminated ZnO graphene-like nanosheets. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 1447-54	2	9
71	An ONIOM investigation on anion recognition of alkali-metal complexes with diurea calix[4]arene receptor. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 2613-20	2	
70	Adsorption CO <sub>2</sub> on the perfect and oxygen vacancy defect surfaces of anatase TiO <sub>2</sub> and its photocatalytic mechanism of conversion to CO. <i>Applied Surface Science</i> , <b>2011</b> , 257, 10322-10328	6.7	87
69	Structures and conformations of acridinium mono- and polymethine cyanine dyes and their UV-Vis absorption spectra in protic solvents: A PCM/TD-DFT study. <i>Journal of Molecular Structure</i> , <b>2011</b> , 1006, 635-641	3.4	5
68	A theoretical investigation on structures of tripodal thiourea derivatives and their anion recognition. <i>Structural Chemistry</i> , <b>2011</b> , 22, 839-847	1.8	5
67	Theoretical study on the adsorption behaviors of H <sub>2</sub> O and NH <sub>3</sub> on hydrogen-terminated ZnO nanoclusters and ZnO graphene-like nanosheets. <i>Journal of Molecular Structure</i> , <b>2011</b> , 994, 276-282	3.4	4
66	A DFT study of structures of dipicolyl urea isomers and their recognition with carboxylic acids and their carboxylate anions. <i>Journal of Physical Organic Chemistry</i> , <b>2011</b> , 24, 92-100	2.1	0
65	IR spectroscopic and DFT investigations on molecular conformations of thio-free oxo technetium (V) benzamidoxime complexes. <i>Journal of Molecular Structure</i> , <b>2011</b> , 990, 152-157	3.4	2
64	First principles theoretical study of the hole-assisted conversion of CO to CO <sub>2</sub> on the anatase TiO <sub>2</sub> (101) surface. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 104701	3.9	34
63	Cation recognition of thiacalix[2]thianthrene and p-tert-butylthiacalix[2]thianthrene and their conformers and complexes with Zn(II), Cd(II) and Hg(II): a theoretical investigation. <i>Journal of Molecular Modeling</i> , <b>2010</b> , 16, 243-53	2	5
62	Molecular modeling of dissociative and non-dissociative chemisorption of nitrosamine on close-ended and open-ended pristine and Stone-Wales defective (5,5) armchair single-walled carbon nanotubes. <i>Journal of Molecular Modeling</i> , <b>2010</b> , 16, 1127-38	2	14
61	Molecular structures and electronic properties of helical thiophene carbon-sulfur oligomers, H <sub>2</sub> (C <sub>2</sub> S) <sub>n</sub> C <sub>2</sub> H <sub>2</sub> (n = 1-20). <i>Structural Chemistry</i> , <b>2010</b> , 21, 715-725	1.8	2
60	Adsorption of CO, H <sub>2</sub> , N <sub>2</sub> O, NH <sub>3</sub> and CH <sub>4</sub> on the anatase TiO <sub>2</sub> (001) and (101) surfaces and their competitive adsorption predicted by periodic DFT calculations. <i>Materials Chemistry and Physics</i> , <b>2010</b> , 124, 720-725	4.4	59
59	A steroid-based receptor for unprotected amino acids: the enantioselective recognition of l-tryptophan. <i>Tetrahedron</i> , <b>2010</b> , 66, 7423-7428	2.4	12

58	Adsorption of di-, tri- and polyatomic gases on the anatase TiO <sub>2</sub> (0 0 1) and (1 0 1) surfaces and their adsorption abilities. <i>Computational and Theoretical Chemistry</i> , <b>2010</b> , 952, 103-108		35
57	A DFT investigation of dissociation of nitrous acid, transformation of its monomeric isomers, their dimeric isomers, and dimerization. <i>International Journal of Quantum Chemistry</i> , <b>2010</b> , 110, 1019-1029	2.1	1
56	A density functional investigation of 1,3-bis(4-nitrophenyl)urea as anion receptor. <i>Computational and Theoretical Chemistry</i> , <b>2009</b> , 902, 33-40		6
55	Isomeric structures of benzimidazole, benzoxazole, and benzothiazole derivatives, their electronic properties and transformations. <i>Structural Chemistry</i> , <b>2009</b> , 20, 619-631	1.8	13
54	Molecular structures of 8,8?-dithioureido-2,2?-binaphthalene derivatives and their anions recognition: an ONIOM investigation. <i>Structural Chemistry</i> , <b>2009</b> , 20, 767-780	1.8	4
53	A DFT study of transformation of nitrosothiol isomers and their decomposition to nitric oxide in gas phase. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 109, 275-284	2.1	12
52	Structural and conformational investigations of chiral bis(phenylamido)ferrocenes by X-ray crystallography and density functional calculations. <i>Journal of Molecular Structure</i> , <b>2009</b> , 938, 117-124	3.4	
51	Non-rigid bis-(2,5-diamidopyrrole) receptor, its deprotonated species and their complexes with fluoride, chloride and hydroxide ions. <i>Computational and Theoretical Chemistry</i> , <b>2009</b> , 907, 131-134		3
50	Inter- and intra-molecular OH stretching modes of bicarbonate in aqueous solution. <i>Computational and Theoretical Chemistry</i> , <b>2009</b> , 913, 236-239		9
49	Tryptophan receptors containing acridine-based thiourea. <i>Supramolecular Chemistry</i> , <b>2009</b> , 21, 486-494	1.8	5
48	A-D-A sensors based on naphthoimidazoledione and boronic acid as turn-on cyanide probes in water. <i>Journal of Organic Chemistry</i> , <b>2009</b> , 74, 3919-22	4.2	100
47	Molecular modeling of nitrosamines adsorbed on H-ZSM-5 zeolite: an ONIOM study. <i>Journal of Molecular Modeling</i> , <b>2008</b> , 14, 1035-41	2	18
46	Isomers of various species of 1-hydroxy-2-pyridinone-6-carboxylic acid, their proton dissociation and complexes with Cr(III) and Zn(II). <i>Journal of Molecular Structure</i> , <b>2008</b> , 891, 1-10	3.4	4
45	Conformational analysis of alkali metal complexes of anionic species of aspartic acid, their interconversion and deprotonation: a DFT investigation. <i>Journal of Molecular Graphics and Modelling</i> , <b>2008</b> , 26, 982-90	2.8	6
44	Theoretical study of adsorption of C <sub>11</sub> B <sub>3</sub> alkoxides on various cap-ended and open-ended armchair (5,5) single-walled carbon nanotubes. <i>Carbon</i> , <b>2008</b> , 46, 12-18	10.4	7
43	Anion binding of 3,4-dichloro-2,5-diamidopyrrole and anionic self-assembly dimerization of its deprotonated species. <i>Computational and Theoretical Chemistry</i> , <b>2008</b> , 864, 26-30		5
42	A DFT study of chloride and hydroxide anions effects on deprotonations of 3,4-dichloro-2,5-diamido-substituted pyrrole derivatives. <i>Computational and Theoretical Chemistry</i> , <b>2007</b> , 806, 145-153		7
41	Addition of diazomethane to armchair single-walled carbon nanotubes and their reaction sequences: A computational study. <i>Chemical Physics Letters</i> , <b>2007</b> , 436, 218-223	2.5	17

40	Adsorptions of proton, hydroxide on various cap-ended and open-ended armchair (5,5) single-walled carbon nanotubes. <i>Chemical Physics Letters</i> , <b>2007</b> , 441, 127-131	2.5	8
39	Conformational analysis of alkali metal complexes of aspartate dianion and their interactions in gas phase. <i>Journal of Molecular Graphics and Modelling</i> , <b>2007</b> , 26, 342-51	2.8	3
38	Determination of aqueous acid-dissociation constants of aspartic acid using PCM/DFT method. <i>International Journal of Quantum Chemistry</i> , <b>2007</b> , 108, 1181-1188	2.1	81
37	Tautomerizations of 2-, 3-, and 4-formylpyridine semicarbazone conformers in gas and aqueous phases. <i>Structural Chemistry</i> , <b>2007</b> , 18, 555-561	1.8	3
36	A DFT study of molecular structures and tautomerizations of 2-benzoylpyridine semicarbazone and picolinaldehyde N-oxide thiosemicarbazone and their complexations with Ni(II), Cu(II), and Zn(II). <i>Structural Chemistry</i> , <b>2007</b> , 18, 977-984	1.8	5
35	Molecular structures of 3,6-di(hexylthioureido)acridine conformers, their protonation, 1H NMR and IR analyses: Theoretical and experimental studies. <i>Journal of Molecular Structure</i> , <b>2007</b> , 832, 16-25	3.4	1
34	Molecular model for host-guest interaction of tetraamino-tert-butylthiacalix[4]arene and tetraamino-tert-butylcalix[4]arene receptors with carboxylate and dicarboxylate guests: an ONIOM study. <i>Journal of Molecular Modeling</i> , <b>2007</b> , 13, 65-77	2	11
33	An investigation of molecular structures of sulfonylcalix[4]arene, mercaptosulfonylcalix[4]arene and aminosulfonylcalix[4]arene, their proton affinities and complexation with zinc(II). <i>Journal of Molecular Structure</i> , <b>2006</b> , 787, 76-89	3.4	6
32	Conformational study of cationic, zwitterionic, anionic species of aspartic acid, water-added forms and their protonation. A DFT method. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 758, 181-187		13
31	DFT investigation of structures of nitrosamine isomers and their transformations in gas phase. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 766, 159-164		11
30	Molecular structures of 3,4-dichloro-2,5-diamido-substituted pyrrole anion dimers, their deprotonation reactions in systems with and without fluoride ion. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 772, 23-30		8
29	Structures of gas-phase nitrosamine-dimer isomers, their interconversions and energetics: A DFT study. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 775, 113-120		8
28	A DFT investigation on molecular structures of semicarbazone complexes with Co(II), Ni(II) and Zn(II) and reaction energies of their complexation. <i>Structural Chemistry</i> , <b>2006</b> , 17, 27-34	1.8	7
27	Conformational investigation of N,N'-propylene bis(benzohydroxamamide), its oxotechnetium(v) and oxorhenium(v) complexes and determination of their reaction energies. <i>Computational and Theoretical Chemistry</i> , <b>2005</b> , 755, 45-53		6
26	Tautomeric and rotameric transformations of 4-methyl-3,6-pyridazinedione isomers. <i>Chemical Physics Letters</i> , <b>2005</b> , 415, 176-182	2.5	12
25	A density functional study of propylene glycol conversion to propanal and propanone of various acid-catalyzed reaction models: a water-addition effect. <i>Journal of Computational Chemistry</i> , <b>2005</b> , 26, 1592-9	3.5	12
24	Theoretical study of conversion reactions of ketone to hydroxyalkylene in cluster models of zeolite H-ZSM-5. <i>Journal of Molecular Catalysis A</i> , <b>2005</b> , 239, 68-75		19
23	A DFT investigation of conformational geometries and interconversion equilibria of phenylthiosemicarbazone and its complexation with zinc. <i>Journal of Molecular Modeling</i> , <b>2004</b> , 10, 418-26		14

22	Conformational investigation of benzyhydroxamamide, its oxotechnetium(V) complexes and determination of their reaction energies. <i>Computational and Theoretical Chemistry</i> , <b>2004</b> , 676, 65-71		17
21	Theoretical investigation of geometrical conformation, protonation of tetraamino-p-tert-butylthiacalix[4]arene and complexation with zinc: a comparative theoretical method. <i>Computational and Theoretical Chemistry</i> , <b>2004</b> , 685, 57-71		6
20	Conformational structures, proton affinity of p-tert-butylthiacalix[4]arene and its zinc complex. <i>Computational and Theoretical Chemistry</i> , <b>2004</b> , 683, 103-113		11
19	Recognition of carboxylate and dicarboxylates by azophenolthiourea derivatives: a theoretical host-guest investigation. <i>Computational and Theoretical Chemistry</i> , <b>2004</b> , 686, 47-55		20
18	Structure and physico-chemical properties of hexadentate Schiff base zinc complexes derived from salicylaldehydes and triethylenetetramine. <i>Journal of Molecular Structure</i> , <b>2004</b> , 701, 93-103	3-4	42
17	Protonation and Energetical Investigations of Calix[4]-cyclen-benzo-crown-6 and Its Complexes with Zinc and Copper. <i>Bulletin of the Korean Chemical Society</i> , <b>2004</b> , 25, 819-822	1.2	3
16	Conformational and energetical structures of sulfonylcalix[4]arene, p-tert-butylsulfonylcalix[4]arene and their zinc complexes. <i>Computational and Theoretical Chemistry</i> , <b>2003</b> , 629, 137-150		19
15	. <i>ScienceAsia</i> , <b>2003</b> , 29, 45	1.4	2
14	Synthesis of tripodal aza crown ether calix[4]arenes and their supramolecular chemistry with transition-, alkali metal ions and anions. <i>Tetrahedron</i> , <b>2002</b> , 58, 10277-10285	2.4	67
13	. <i>ScienceAsia</i> , <b>2002</b> , 28, 25	1.4	2
12	Conformational Investigations of HMPAO Isomers and Their Zinc(II) Complexes. <i>Bulletin of the Korean Chemical Society</i> , <b>2002</b> , 23, 555-562	1.2	5
11	Synthesis of stilbene crown ether p-tert-butylcalix[4]arenes. <i>Tetrahedron Letters</i> , <b>2001</b> , 42, 5291-5293	2	17
10	Aza crown ether calix[4]arenes containing cation and anion binding sites: effects of metal ions towards anion binding ability. <i>Tetrahedron Letters</i> , <b>2001</b> , 42, 5541-5544	2	36
9	Recognition Studies of a Pyridine-Pendant Calix[4]arene with Neutral Molecules: Effects of Non-covalent Interactions on Supramolecular Structures and Stabilities. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , <b>2001</b> , 39, 47-53		5
8	Synthesis of 1,3-alternate calix[4]-cyclen-benzo-crown-6 as a hard-soft receptor. <i>Tetrahedron Letters</i> , <b>2000</b> , 41, 9167-9171	2	11
7	p-tert-Butylcalix[4]arene Derivatives Containing Azathiol Receptors and Their Recognition towards Hg(II). <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , <b>2000</b> , 38, 113-122		13
6	Synthesis of the tripodal-amine capped benzo crown p-tert-butylcalix[4]arene and its host-guest chemistry. <i>Tetrahedron Letters</i> , <b>1997</b> , 38, 3985-3988	2	12
5	Magnesium and lithium complexation by 1,4,7,10-tetraazacyclododecane. <i>Inorganica Chimica Acta</i> , <b>1988</b> , 144, 21-23	2.7	7



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| 4 | A Monte Carlo Study on a Magnesium Cyclen Complex. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , <b>1988</b> , 43, 797-800                                 | 1.4 |   |
| 3 | The Interaction of Magnesium Cyclen Complex with Water. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , <b>1987</b> , 42, 871-874                            | 1.4 | 2 |
| 2 | A Monte Carlo study on the hydration of a macrocyclic magnesium complex. <i>Inorganica Chimica Acta</i> , <b>1987</b> , 134, 297-302  | 2.7 | 1 |
| 1 | On the additivity of intermolecular potential functions in ion/neutral-molecule interactions. <i>International Journal of Mass Spectrometry and Ion Processes</i> , <b>1986</b> , 71, 283-286 |     | 2 |