Reza Ghiasi

List of Publications by Year in Descending Order

166 papers	1,025 citations	18 h-index	23 g-index
170 ext. papers	1,116 ext. citations	1.4 avg, IF	5.38 L-index

#	Paper	IF	Citations
166	Computational Investigation of Chemisorption of Thiophosgene on Co@B$$_{8}^{-}$$. *Russian Journal of Physical Chemistry A*, **2022**, 96, 267-272	0.7	
165	Exploring of the Solvent Effect on the Electronic Structure and 14N NMR Chemical Shift of Cyclic-N3S3Cl3: A Computational Investigation. *Russian Journal of Physical Chemistry B*, **2021**, 15, S14-S21	1.2	1
164	EDA, CDA and QTAIM Investigations in the (para-C5H4X) Ir(PH3)3 Iridabenzene Complexes. *Russian Journal of Physical Chemistry B*, **2021**, 15, S6-S13	1.2	0
163	SUBSTITUENT EFFECT IN [2+4] DIELS□ALDER CYCLOADDITION REACTIONS OF ANTHRACENE WITH C2X2 (X = H, F, Cl, Me): A COMPUTATIONAL INVESTIGATION. *Journal of Structural Chemistry*, **2021**, 62, 1551-1562	0.9	1
162	Interaction of cisplatin anticancer drug with C20 bowl: DFT investigation. *Main Group Chemistry*, **2021**, 1-12	0.6	0
161	Quantum-chemical calculations on the slippage of cyclopentadienyl and indenyl ligands in the (□-dienyl)Ir(PX3)3; (X = H, F, Cl, Me) complexes. *Journal of the Chinese Chemical Society*, **2021**, 68, 785-792	1.5	
160	The conductor-like polarizable continuum model study of indenyl effect on the ligand substitution reaction in the (□-C9H7)Co(CO)2 complex. *International Journal of Chemical Kinetics*, **2021**, 53, 901-912	1.4	1
159	Cyclometalation in the (□-C5H5)Co(□-C2H2)(PMe3) and (□-C9H7)Co(□-C2H2) (PMe3) complexes: A computational investigation. *Journal of Molecular Liquids*, **2021**, 325, 115097	6	3
158	Structure, electronic properties and slippage of cyclopentadienyl and indenyl ligands in the (□-C5H5) (□-C5H5) W(CO)2 and (□-C9H7) (□-C9H7)W(CO)2 complexes: A C-PCM investigation. *Journal of Molecular Liquids*, **2021**, 329, 115535	6	1
157	Solvent and temperature effects on the tautomerization of a carbonitrile molecule: A conductor-like polarizable continuum model (CPCM) study. *Main Group Chemistry*, **2021**, 20, 59-68	0.6	1
156	Unveiling the influence of solvent polarity on structural, electronic properties, and 31P NMR parameters of rhenabenzyne complex. *Inorganic Chemistry Communication*, **2021**, 127, 108497	3.1	2
155	Interaction between carboplatin with B12P12 and Al12P12 nano-clusters: A computational investigation. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2021**, 196, 751-759	1	1
154	Complex formation of titanocene dichloride anticancer and Al12N12 nano-cluster: A quantum chemical investigation of solvent, temperature and pressure effects. *Main Group Chemistry*, **2021**, 20, 19-32	0.6	2
153	HYDROGEN ADSORPTION AND STORAGE ON PALLADIUM-FUNCTIONALIZED GRAPHYNE AND ITS BORON NITRIDE ANALOGUE. *Journal of Structural Chemistry*, **2021**, 62, 835-844	0.9	0
152	The application of graphyne and its boron nitride analogue in Li-ion batteries. *Computational and Theoretical Chemistry*, **2021**, 1200, 113243	2	2
151	The interaction between carboplatin anticancer drug and B12N12 nano-cluster: A computational investigation. *Main Group Chemistry*, **2021**, 1-10	0.6	3
150	Computational investigation of interaction between titanocene dichloride and nanoclusters (B12N12, B12P12, Al12N12 and Al12P12). *Main Group Chemistry*, **2021**, 1-10	0.6	2

149	Quantum-chemical investigation of the phosphine ligand effects on the structure and electronic properties of a rhenabenzyne complex. *Journal of the Chinese Chemical Society*, **2021**, 68, 776-784	1.5	
148	Computational Investigation of Substituent Effect on the Thermodynamics and Kinetics of Hydrocarbyl Elimination from a Rhodium(I) Iminyl Complex. *Russian Journal of Physical Chemistry A*, **2021**, 95, 163-171	0.7	
147	Computational investigation of the substituent effect in the [2 + 4] Diels–Alder cycloaddition reactions of HSi?Si(para-C6H4X) with benzene. *Journal of the Chinese Chemical Society*, **2021**, 68, 806-816	1.5	3
146	Computational Investigation of Interaction of Titanocene Dichloride Anti-Cancer Drug with Carbon Nanotube in the Presence of External Electric Field. *Biointerface Research in Applied Chemistry*, **2021**, 11, 12454-12461	2.8	3
145	Theoretical study of the influence of solvent polarity on the 31P and 13C NMR parameters of the Ru(PH3)4(-benzyne) complex. *Inorganic Chemistry Communication*, **2021**, 124, 108412	3.1	2
144	Adsorption of Lewisite Warfare Agent on B12N12 Nano-Cluster: A Computational Investigation. *Russian Journal of Physical Chemistry A*, **2021**, 95, 2637-2642	0.7	0
143	Interaction between Phosgene and B12N12 Nano-Cluster: A Computational Investigation. *Russian Journal of Physical Chemistry A*, **2021**, 95, S323-S330	0.7	0
142	Strong chemisorption of E2H2 and E2H4 (E = C, Si) on B12N12 nano-cage. *Journal of Nanostructure in Chemistry*, **2020**, 10, 179-191	7.6	20
141	Effect of the Solvent Polarity on the Optical Properties in the (OC)5Cr=(OEt)(Ph) Complex: A Quantum Chemical Study. *Russian Journal of Physical Chemistry A*, **2020**, 94, 1047-1052	0.7	6
140	Substituent Effect on the Thermodynamics and Kinetics of Carbyne Complex [(-C5H5)(CO)(COMe)Re?CC6H4X] Isomerization to Carbene Complex [(-C5H5)(CO)2Re=C(Me)(para-C6H4X]: A Theoretical Study. *Russian Journal of Physical Chemistry A*, **2020**, 94, 125-133	0.7	
139	Theoretical understanding the effects of external electric field on the hydrolysis of anticancer drug titanocene dichloride. *Molecular Physics*, **2020**, 118, e1781272	1.7	1
138	Conformational Analysis of 2-Methoxy-2-oxo-1,3,2-dioxaphosphorinane and Its Methylthio and Methylselenyl Analogues. *Russian Journal of Physical Chemistry A*, **2020**, 94, 772-777	0.7	1
137	Hammett and Brown correlations in the structure and electronic properties of H2Si=SiHAr (Ar = p-C6H4X; X = NH2, OH, Me, H, F, Cl, CHO, COOH, CN, NO2) molecules. *Journal of the Chinese Chemical Society*, **2020**, 67, 1348-1355	1.5	1
136	Quantum theory of atoms in molecules, electron localization function, and localized-orbital locator investigations on trans-(NHC)PtI2(para-NC5H4X) complexes. *Journal of Chemical Research*, **2020**, 44, 482-486	0.6	0
135	The Impact of Solvent Polarity on the Stability, Electronic Properties, and 1H NMR Chemical Shift of the Conformers of 2-Chloro-3-Methylcyclohexan-1-One Oxime: a Conceptual DFT Approach. *Journal of Applied Spectroscopy*, **2020**, 86, 1123-1131	0.7	8
134	QUANTUM-CHEMICAL INVESTIGATION OF THE COMPLEXATION OF TITANOCENE DICHLORIDE WITH C20 AND M+@C20 (M+ = Li, Na, K) CAGES. *Journal of Structural Chemistry*, **2020**, 61, 1681-1690	0.9	1
133	INVESTIGATING THE EFFECTS OF THE EXTERNAL ELECTRIC FIELD ON OSMABENZYNE IN THE GROUND (S0) AND FIRST EXCITED SINGLET (S1) STATES: INSIGHT INTO STRUCTURES, ENERGY, AND PROPERTIES. *Journal of Structural Chemistry*, **2020**, 61, 1691-1699	0.9	0
132	Effects of External Electric Field on the Hydrolysis of Cisplatin: A Density Functional Theory Approach. *Russian Journal of Inorganic Chemistry*, **2020**, 65, 2053-2061	1.5	0

131	Computational investigation of solvent polarity effect on the structure and properties of a (OC)4Cr-biscarbene complex in the singlet ground state and lowest singlet excited state. *Journal of Molecular Liquids*, **2020**, 300, 112327	6	6
130	Theoretical Analysis of Stereoelectronic Effects in the 2,4,6-Trihalo-1,3,5-trioxane and 2,4,6-Trihalo-1,3,5-trithiane Conformers. *Russian Journal of Physical Chemistry A*, **2020**, 94, 2064-2071	0.7	0
129	Computational Investigation of the 14N NQR Parameters of Borazyne. *Journal of Applied Spectroscopy*, **2020**, 87, 538-544	0.7	
128	Computational Rationalization of the Interaction of Fe(CO)4 and Substituted Benzyne Ligands. *Journal of Structural Chemistry*, **2020**, 61, 197-206	0.9	0
127	Quantum Chemical Study of Interaction between Titanocene Dichloride Anticancer Drug and Al12N12 Nano-Cluster. *Russian Journal of Inorganic Chemistry*, **2020**, 65, 1726-1734	1.5	4
126	Substituent effects on the structure and properties of (para-C5H4X)Ir(PH3)3 complexes in the ground state (S0) and first singlet excited state (S1): DFT and TD-DFT investigations. *Journal of Chemical Research*, **2020**, 174751982094286	0.6	
125	Analysis of Bonding Properties of Osmabenzyne in the Ground State (S0) and Excited Singlet (S1) State: A Quantum-Chemical Calculation. *Russian Journal of Physical Chemistry A*, **2020**, 94, 2594-2600	0.7	
124	Exploring the Substituent Effect on the Structure and Electronic Properties of Si2(para-C6H4X)2 Molecules. *Russian Journal of Physical Chemistry A*, **2020**, 94, 2760-2769	0.7	2
123	Preparation of CoFe2O4/sawdust and NiFe2O4/sawdust magnetic nanocomposites for removal of oil from the water surface. *Journal of the Chinese Chemical Society*, **2020**, 67, 288-297	1.5	3
122	The interaction of 5-fluorouracil with graphene in presence of external electric field: a theoretical investigation. *Adsorption*, **2020**, 26, 905-911	2.6	4
121	Quantum Chemical Study of the Effect of Solvent on Structure, Electronic Properties, and Electronic Spectrum of the Carbyne Complex trans-[ClRu(PH3)4(?C?CH=CMe2)]2+. *Russian Journal of Inorganic Chemistry*, **2020**, 65, 69-75	1.5	2
120	Theoretical Analysis of Solvent Polarity Effect on the Electronic and Spectroscopic Properties (IR and UV) of the Ni(CO)2(NHC)2 Complex (NHC = 1H-Imidazol-2-ylidene). *Russian Journal of Physical Chemistry A*, **2020**, 94, 345-351	0.7	7
119	Theoretical Study of Substituent Effect on the Electronic and Optical Properties of 4-Substituted Ferrocenylethynylbenzenes. *Russian Journal of Physical Chemistry A*, **2019**, 93, 1747-1753	0.7	2
118	Effect of External Electric Field on the Electronic Structure and Aromaticity of Cr(CO)3(?6-C6H6) Complex. *Russian Journal of Inorganic Chemistry*, **2019**, 64, 1035-1040	1.5	2
117	SOLVENT INFLUENCE ON THE STABILITY AND PROPERTIES OF Si4H4 ISOMERS BY COMPUTATIONAL METHODS. *Journal of the Chilean Chemical Society*, **2019**, 64, 4360-4364	2.5	4
116	Quantum Chemical Predictions of Substituent Effect on the Stability, Electronic Structure, and 14N NQR Parameters of a Ruthenium Azirinyl Complex. *Russian Journal of Physical Chemistry A*, **2019**, 93, 880-888	0.7	2
115	Computational Investigation of the Pseudo Jahn–Teller Effect on the Structure and Chemical Properties of Perhaloethene Anions. *Journal of Structural Chemistry*, **2019**, 60, 736-745	0.9	
114	Stability, Electronic, and Structural Features of the Conformers of 2-Methyl-1,3,2-Diheterophosphinane 2-Oxide (Heteroatom = O, S, Se): DFT and NBO Investigations. *Journal of Structural Chemistry*, **2019**, 60, 746-754	0.9	2

113	A Theoretical Approach towards Identification of External Electric Field Effect on (η5-C5H5)Me2Ta(η2-C6H4). *Russian Journal of Physical Chemistry A*, **2019**, 93, 482-487	0.7	5
112	Effect of the External Electric Field on the Electronic Structure and Aromaticity of Iridabenzene: A DFT Study. *Journal of Structural Chemistry*, **2019**, 60, 547-555	0.9	5
111	Assessment of substituent effects on the parameters of 35Cl nuclear quadrupole resonance in para-substituted benzene-sulphenyl chloride via quantum chemical calculations. *Journal of the Chinese Chemical Society*, **2019**, 66, 1577-1582	1.5	
110	Theoretical Study of Substituent Effect on the pKa Values of Cr(CO)3(para-XC6H4COOH) Complexes. *Russian Journal of Physical Chemistry A*, **2019**, 93, 1537-1542	0.7	1
109	Solvent Influence on Structure and Electronic Properties of Si2Me4: A Computational Investigation Using PCM-SCRF Method. *Russian Journal of Physical Chemistry A*, **2019**, 93, 2244-2249	0.7	4
108	Theoretical Approaches to the Conformational Preference of 2,2-Di-tert-Butyl-1,3-Dioxane, 2,2-Di-tert-Butyl-1,3-Dithian, and 2,2-Di-tert-Butyl-1,3-Diselenan. *Russian Journal of Inorganic Chemistry*, **2019**, 64, 1556-1564	1.5	
107	Substituent Effect on the Acidity Strength of para-C6H4XB(OH)2 Boronic Acid: A Theoretical Investigation. *Journal of Structural Chemistry*, **2019**, 60, 1743-1749	0.9	4
106	Thermodynamic and kinetic studies of the retro-Diels-Alder reaction of 1,4-cyclohexadiene, 4H-pyran 4H-thiopyran, 1,4-dioxine, and 1,4-dithiine: a theoretical investigation. *Structural Chemistry*, **2019**, 30, 877-885	1.8	4
105	Pseudo-Jahn□Teller effect in Si4X4 (X = F, Cl, Br, I) molecules: a theoretical investigation. *Molecular Physics*, **2019**, 117, 567-574	1.7	1
104	Substituent Effect on the Stability and 14N NQR Parameters of Linkage Isomers of Nitriles in a Rhodium Half-Sandwich Metallacycle: A Theoretical Study. *Journal of the Chinese Chemical Society*, **2018**, 65, 416-423	1.5	2
103	Solvent Effects on the Structure And Spectroscopic Properties of the Second-Generation Anticancer Drug Carboplatin: A Theoretical Insight. *Journal of Structural Chemistry*, **2018**, 59, 245-251	0.9	18
102	Theoretical exploring of the substituent effect on the NQR and NMR parameters in a platinum-based anticancer drug, trans-(NHC) PtI2 (para-NC5H4X) complex. *Structural Chemistry*, **2018**, 29, 435-440	1.8	5
101	Influence of Solvent and Electric Field on the Structure and IR, 31P NMR Spectroscopic Properties of a Titanocene□Benzyne Complex. *Journal of Applied Spectroscopy*, **2018**, 85, 526-534	0.7	13
100	ONE-POT SYNTHESIS OF 2-ACYLAMINOBENZIMIDAZOLES FROM THE REACTION BETWEEN TRICHLOROACETYL ISOCYANATE AND 1,2-PHENYLENEDIAMINE DERIVATIVES AND THEORETICAL STUDY OF STRUCTURE AND PROPERTIES OF SYNTHESIZED 2-ACYLAMINOBENZIMIDAZOLES. *Journal of the Chilean Chemical Society*, **2018**, 63, 3968-3973	2.5	2
99	Theoretical Study of Tautomerization in 1,5-Dimethyl-6-Thioxo-1,3,5-Triazinane-2,4-Dione. *Journal of Structural Chemistry*, **2018**, 59, 541-549	0.9	6
98	Borepine: A Density Functional Approach toward Structural Features and Properties. *Russian Journal of Inorganic Chemistry*, **2018**, 63, 800-808	1.5	1
97	Theoretical Study of Substituent Effect in Aryl Group Migration in (para-C6H4X)Mn(CO)5 Complexes. *Russian Journal of Inorganic Chemistry*, **2018**, 63, 906-910	1.5	1
96	Theoretical Study of Solvent Effect on the Kinetics and Thermochemistry of the Reaction of a (NHC)Cu(boryl) Complex with Ethylene. *Russian Journal of Physical Chemistry A*, **2018**, 92, 2628-2633	0.7	

95	Exploration of Solvent Effects on the Spectroscopic Properties (Ir and 13C NMR) in the OsCl3(?CCH2CMe3)(PH3)2 Carbyne Complex. *Journal of Structural Chemistry*, **2018**, 59, 1052-1057	0.9	2
94	A Computational Approach for Hydrolysis of the Third-Generation Anticancer Drug: Trans-Platinum(Ii) Complex of 3-Aminoflavone. *Journal of Structural Chemistry*, **2018**, 59, 1791-1796	0.9	3
93	Influences of the substituents on the Cr=C bond in [(OC)5Cr=C(OEt)-para-C6H4X] complexes: quantum Theory of Atoms in Molecules, Energy Decomposition Analysis, and Interacting Quantum Atoms. *Monatshefte F□ Chemie*, **2018**, 149, 2167-2174	1.4	6
92	Theoretical Study of the Arene Ligand Effect on the Structure and Properties of Cr(CO)3(Arene) Complexes (Arene = Benzene, Biphenyl, Triphenly, Tetraphenyl). *Journal of Structural Chemistry*, **2018**, 59, 1784-1790	0.9	3
91	Theoretical Study of the Solvent Effect on the Electronic and Vibrational Properties of [CpFe(CO)2(NCS)] and [CpFe(CO)2(SCN)] Linkage Isomers. *Journal of Structural Chemistry*, **2018**, 59, 1058-1066	0.9	1
90	Theoretical Study of NO Linkage Isomers in a Rhenacarborane Nitrosyl Complex. *Russian Journal of Physical Chemistry A*, **2018**, 92, 2518-2523	0.7	
89	Analysis of the Interaction Between the C20 Cage and cis-Ptcl2(NH3)2: A DFT Investigation of the Solvent Effect, Structures, Properties, and Topologies. *Journal of Structural Chemistry*, **2018**, 59, 1044-1051	0.9	4
88	Theoretical Studies of Solvent Effect on the Structure, □nding, and Spectroscopic □operties (IR, NMR) in the cis-[Pt(PH3)2(NCS)2] and [Pt(PH3)2(SCN)2] Linkage Isomers. *Russian Journal of Physical Chemistry A*, **2018**, 92, 1748-1756	0.7	9
87	Theoretical investigation of vinylogous anomeric effect on 4-halo-4-H-pyran and 4-halo-4-H-thiopyran molecules. *Journal of Sulfur Chemistry*, **2018**, 39, 665-673	2.3	4
86	A quantum chemical investigation of the influence of solvent polarity on the structural, electronic, spectroscopic properties and hyperpolarizability in Molybdenum Silylidyne complex CpMo(CO)2(SiPh). *Journal of Molecular Liquids*, **2018**, 264, 616-620	6	14
85	Solvent effect on isomerization reaction of [(□5-C5H5)(CO)2Re C(C2HB10H10)(C6H5)] carbene complex to [(□5-C5H5)(CO)(COC2HB10H10)Re CC6H5] carbyne complex: A computational investigation. *Journal of Molecular Liquids*, **2018**, 265, 164-171	6	14
84	The Analysis of Electronic Structures, NBO, EDA, and QTAIM of trans-(H3P)2(□2-BH4)W(?C-para-C6H4X)(CO) Complexes. *Journal of the Chinese Chemical Society*, **2017**, 64, 369-378	1.5	5
83	Quantum Chemical Study of the Solvent Effect on the Anticancer Active Molecule of Iproplatin: Structural, Electronic, and Spectroscopic Properties (IR, 1H NMR, UV). *Journal of Applied Spectroscopy*, **2017**, 83, 909-916	0.7	19
82	Evolution of the interaction between C20 cage and Cr(CO)5: A solvent effect, QTAIM and EDA investigation. *Journal of Theoretical and Computational Chemistry*, **2017**, 16, 1750007	1.8	3
81	Crop protection services by Plant Clinics in Iran: An evaluation through rice farmers□satisfaction. *Crop Protection*, **2017**, 98, 191-197	2.7	8
80	Solvent Effects on Stability, Electronic Structure, and 14N NQR Parameters of Fe(CO)4py Isomers. *Journal of Applied Spectroscopy*, **2017**, 84, 148-155	0.7	19
79	The Analysis of Os?C Bond and Electric Field Influence on the Properties in the Osmium Carbyne Complex OsCl3 (?CCH2CMe3)(PH3)2: A Theoretical Insight. *Journal of the Chinese Chemical Society*, **2017**, 64, 651-657	1.5	16
78	Theoretical study of solvent effect on the ligand field parameter in [M(CO)6]n complexes (M = V□ Cr, Mn+, Fe2+). *Russian Journal of Physical Chemistry A*, **2017**, 91, 1026-1036	0.7	4

77	A Computational Approach to the Effects of Solvent on the Structural, Electronic, Spectroscopic (195Pt NMR and IR), and Thermochemical Properties of a Third-Generation Anticancer Drug: Trans-Platinum(II) Complex of 3-Aminoflavone. *Journal of the Chinese Chemical Society*, **2017**, 64, 934-939	1.5	3
76	A theoretical study of the solvent effect on the interaction of C20 and N2H2. *Journal of Structural Chemistry*, **2017**, 58, 30-37	0.9	19
75	Theoretical Study of Substituent Effects on Geometric and Spectroscopic Parameters (IR, 13C, 29Si NMR) and Energy Decomposition Analysis of the Bonding in Molybdenum Silylidyne Complexes CpMo(CO)2(?Si-para-C6H4X). *Journal of the Chinese Chemical Society*, **2017**, 64, 522-530	1.5	14
74	A Computational Understanding of Solvent Effect on the Structure, Electronic, Thermochemical, and Spectroscopic Properties of Ni(?2-C6H4)(H2PCH2CH2PH2) Complex. *Journal of the Chinese Chemical Society*, **2017**, 64, 925-933	1.5	3
73	Substituent Effect on the Electronic Properties and Nature of the W?C Bond in trans-Cl(OC)(H3P)3W(?C-para-C6H4X) (X = H, F, SiH3, CN, NO2, SiMe3, CMe3, NH2, NMe2) Complexes: A Computational Quantum Chemistry Study. *Journal of the Chinese Chemical Society*, **2017**, 64, 1340-1346	1.5	16
72	Insight into the solvent effect on the structure, IR-spectrum, and hyperpolarizability of CpMe2Ta(benzyne), a mononuclear Tantalum–benzyne complex. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 1371-1378	1.5	15
71	Computational investigation of solvent effect on the structure, spectroscopic properties (13C, 1H NMR and IR, UV), NLO properties and HOMO–LUMO analysis of Ru(NHC)2Cl2(=CH-p-C6H5) complex. *Physics and Chemistry of Liquids*, **2017**, 55, 421-431	1.5	17
70	Solvent effect on the linkage isomerism in [Fe(CO)4(NCS)]− and [Fe(CO)4(SCN)]− anions: A theoretical investigation. *Physics and Chemistry of Liquids*, **2017**, 55, 444-456	1.5	20
69	Theoretical approach to the molecular structure, chemical reactivity, molecular orbital analysis, spectroscopic properties (IR, UV, NMR), and NBO analysis of deferiprone. *Journal of Structural Chemistry*, **2017**, 58, 1307-1317	0.9	2
68	Computational study of osmabenzyne: The solvent effects on the structure and spectroscopic properties (IR, NMR). *Journal of Structural Chemistry*, **2017**, 58, 1324-1331	0.9	17
67	Substituent Effect in para Substituted Osmabenzene Complexes **2017**, 57,		2
66	DFT and TD-DFT study of benzene and borazines containing chromophores for DSSC materials. *Russian Journal of Inorganic Chemistry*, **2016**, 61, 1267-1273	1.5	3
65	Solvent effect on the stability and properties of platinum-substituted borirene and boryl isomers: The polarizable continuum model. *Russian Journal of Physical Chemistry A*, **2016**, 90, 2211-2216	0.7	15
64	Solvent and substitution effects on the structure and properties of a half-sandwich complex of vanadium with a terminal borylene ligand: Theoretical study. *Russian Journal of Inorganic Chemistry*, **2016**, 61, 327-333	1.5	33
63	A highly efficient CuI nanoparticles-catalyzed synthesis of tetrahydrochromenediones and dihydropyrano[c]chromenediones under grinding. *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **2016**, 71, 777-782	1	12
62	SOLVENT EFFECT ON THE STRUCTURAL, ELECTRONIC, SPECTRA PROPERTIES AND FIRST HYPERPOLARIZABILITY OF W(CO)5L, L=(4-PYRIDYLMETHYLENE)MALONONITRILE. *Journal of the Chilean Chemical Society*, **2016**, 61, 2921-2928	2.5	18
61	Band Gap Energies and Photocatalytic Properties of CdS and Ag/CdS Nanoparticles for Azo Dye Degradation. *Chemical Engineering and Technology*, **2016**, 39, 149-157	2	42
60	Substituent effect on the structure and properties of dialumene. *Russian Journal of Inorganic Chemistry*, **2016**, 61, 985-992	1.5	19

59	Structural, energetic and electrical properties of encapsulation of penicillamine drug into the CNTs based on vdW-DF perspective. *Physica E: Low-Dimensional Systems and Nanostructures*, **2015**, 72, 120-127	?	6
58	A chromium carbene (OC)5Cr=C(OEt)(C?CPh): Quantum mechanical study of molecular structure, HOMO–LUMO analysis, IR spectroscopy, natural bond orbital analysis. *Journal of Theoretical and Computational Chemistry*, **2015**, 14, 1550022	1.8	8
57	Quantum Mechanical Study of Substituent Dependence on the Structure, Spectroscopic (13C, 1H NMR and UV), NBO, Hyperpolarizability and HOMO?LUMO Analysis of Ru(NHC)2Cl2(?CH-p-C6H4X) Complexes. *Journal of the Chinese Chemical Society*, **2015**, 62, 898-905	1.5	21
56	UNDERSTANDING THE STRUCTURE, SUBSTITUENT EFFECT, NATURAL BOND ANALYSIS AND AROMATICITY OF OSMABENZYNE: A DFT STUDY. *Journal of the Chilean Chemical Society*, **2015**, 60, 2740-2746	2.5	25
55	Theoretical view on structure, chemical reactivity, aromaticity and 14N NQR parameters of iridapyridine isomers. *Journal of Structural Chemistry*, **2015**, 56, 1458-1467	0.9	6
54	Theoretical study of solvent and substituent effects on the structure, 14N NQR and electronic spectra of [Cr(CO)5py]. *Journal of Structural Chemistry*, **2015**, 56, 1474-1482	0.9	33
53	Substituent and solvent effects on geometric and electronic structure of C5H5Ir(PH3)3 iridabenzene: A theoretical insight. *Journal of Structural Chemistry*, **2015**, 56, 1483-1494	0.9	33
52	Theoretical study of the solvent and substitution effects on the structure and properties of iridatropylium cations: [C7H6Ir(PX3)3]+; X = H, Me, F. *Russian Journal of Physical Chemistry A*, **2015**, 89, 250-255	0.7	34
51	Quantum mechanical study of the structure, natural bond analysis, HOMO–LUMO analysis, substituents effect, and aromaticity on iridanaphthalene. *Structural Chemistry*, **2014**, 25, 829-838	1.8	9
50	Quantum chemical predictions of structural, bonding and spectroscopic properties of ruthenanaphthalenes and ring-fused B–N ruthenabenzenes. *Journal of Theoretical and Computational Chemistry*, **2014**, 13, 1450011	1.8	1
49	Spectroscopic studies and molecular orbital analysis on platinanaphthalenes and ring-fused B-N platinanaphthalenes. *Russian Journal of Physical Chemistry A*, **2014**, 88, 616-624	0.7	1
48	Borazine-based conjugated derivatives: Structural, electronic, and optical properties. *Russian Journal of Physical Chemistry A*, **2014**, 88, 984-994	0.7	
47	A density functional approach toward structural features and properties of C20N2X2 (X = H, F, Cl, Br, Me) molecules. *Journal of Theoretical and Computational Chemistry*, **2014**, 13, 1450023	1.8	4
46	Tautomeric transformations and reactivity of isoindole and sila-indole: A computational study. *Journal of Theoretical and Computational Chemistry*, **2014**, 13, 1450041	1.8	8
45	A DENSITY FUNCTIONAL THEORY STUDY ON STRUCTURE AND PROPERTIES OF BENZENE AND BORAZINE-BASED CHROMOPHORES. *Journal of the Chilean Chemical Society*, **2014**, 59, 2666-2673	2.5	3
44	Theoretical study of structure, bonding, and aromaticity of borazyne and B-substituted borazynes. *Russian Journal of Physical Chemistry A*, **2013**, 87, 2231-2238	0.7	2
43	Theoretical Study of Solvent Effects on the Cis-to-Trans Isomerization of [Pd(C6Cl2F3)I(PH3)2]. *Journal of Solution Chemistry*, **2013**, 42, 1902-1911	1.8	18
42	Theoretical investigations on electronics structure and chemical bonding on iridathiabenzene and iridaoxabenzene. *Russian Journal of Physical Chemistry A*, **2013**, 87, 1684-1691	0.7	3

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