Reza Ghiasi

List of Publications by Citations

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	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
165	Topological characteristics of the Ring Critical Points and the aromaticity of groups IIIA to VIA hetero-benzenes. *Computational and Theoretical Chemistry*, **2010**, 941, 47-52		35
164	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
163	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
162	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
161	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
160	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
159	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
158	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
157	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
156	Effect of substitution on the structures, properties, and aromaticity of 1-H-boratabenzene anion. *Main Group Chemistry*, **2009**, 8, 143-150	0.6	20
155	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
154	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
153	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
152	Substituent effect on the structure and properties of dialumene. *Russian Journal of Inorganic Chemistry*, **2016**, 61, 985-992	1.5	19
151	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
150	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

149	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
148	Computational investigation of solvent effect on the structure, spectroscopic properties (13C, 1H NMR and IR, UV), NLO properties and HOMO□UMO analysis of Ru(NHC)2Cl2(=CH-p-C6H5) complex. *Physics and Chemistry of Liquids*, **2017**, 55, 421-431	1.5	17
147	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
146	A computational study of the arsabenzenes: Structure, properties and aromaticity. *Journal of Organometallic Chemistry*, **2005**, 690, 4761-4767	2.3	17
145	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
144	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
143	Theoretical study of the properties of fluoroborthiin and fluoroboroxine. *Computational and Theoretical Chemistry*, **2008**, 853, 77-81		16
142	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
141	Insight into the solvent effect on the structure, IR-spectrum, and hyperpolarizability of CpMe2Ta(benzyne), a mononuclear Tantalum□enzyne complex. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 1371-1378	1.5	15
140	Computational study of substituent effect in para substituted platinabenzene complexes. *Russian Journal of Physical Chemistry A*, **2013**, 87, 973-978	0.7	15
139	Metal-stabilized rare tautomers: N4 metalated cytosine (M = Li+, Na+, K+, Rb+ and Cs+), theoretical views. *Applied Organometallic Chemistry*, **2003**, 17, 635-640	3.1	15
138	Cytochrome P-450 model reaction: effects of substitution on the rate of aromatic hydroxylation. *Journal of Porphyrins and Phthalocyanines*, **2000**, 04, 285-291	1.8	15
137	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
136	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
135	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
134	Influence of Solvent and Electric Field on the Structure and IR, 31P NMR Spectroscopic Properties of a Titanocene□enzyne Complex. *Journal of Applied Spectroscopy*, **2018**, 85, 526-534	0.7	13
133	Theoretical study on platinabenzene and mono- and difluorinated platinabenzenes: Structure, properties, and aromaticity. *Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya*, **2011**, 37, 72-76	1.6	13
132	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

131	Theoretical investigation on geometries and aromaticity of heterocyclic platinabenzenes. *Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya*, **2011**, 37, 463-467	1.6	12
130	The mono- and di-silanaphthalene: structure, properties, and aromaticity. *Computational and Theoretical Chemistry*, **2005**, 718, 225-233		12
129	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
128	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
127	Crop protection services by Plant Clinics in Iran: An evaluation through rice farmers'satisfaction. *Crop Protection*, **2017**, 98, 191-197	2.7	8
126	A chromium carbene (OC)5Cr=C(OEt)(□?CEPh): 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
125	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
124	Tautomeric transformations and reactivity of isoindole and sila-indole: A computational study. *Journal of Theoretical and Computational Chemistry*, **2014**, 13, 1450041	1.8	8
123	Theoretical study of borthiin and its derivatives: structure and aromaticity. *Journal of Sulfur Chemistry*, **2007**, 28, 505-511	2.3	8
122	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
121	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	3	6
120	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
119	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
118	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
117	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
116	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
115	The Analysis of Electronic Structures, NBO, EDA, and QTAIM of trans-(H3P)2(□-BH4)W(?C-para-C6H4X)(CO) Complexes. *Journal of the Chinese Chemical Society*, **2017**, 64, 369-378	1.5	5
114	A Theoretical Approach towards Identification of External Electric Field Effect on (□-C5H5)Me2Ta(□-C6H4). *Russian Journal of Physical Chemistry A*, **2019**, 93, 482-487	0.7	5

113	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
112	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
111	Dibromidobis(pyridine-3-carbonitrile-κN)zinc(II). *Acta Crystallographica Section E: Structure Reports Online*, **2010**, 67, m101		5
110	A Theoretical Study of Metal-Stabilised Rare Tautomers Stability: N4 Metalated Cytosine (M=Be2+, Mg2+, Ca2+, Sr2+ and Ba2+) in Gas Phase and Different Solvents. *Journal of Chemical Research*, **2004**, 2004, 11-18	0.6	5
109	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
108	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
107	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
106	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
105	Theoretical study of classical isomers tropylium, azatropylium, phosphatropylium, and arsatropylium cations: structure, properties and aromaticity. *Main Group Chemistry*, **2008**, 7, 147-154	0.6	4
104	Theoretical Studies on the Structure and Aromaticity of 1H-Indene and Mono-sila-1H-Indene. *Journal of the Korean Chemical Society*, **2006**, 50, 281-290		4
103	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
102	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
101	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
100	The interaction of 5-fluorouracil with graphene in presence of external electric field: a theoretical investigation. *Adsorption*, **2020**, 26, 905-911	2.6	4
99	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
98	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
97	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
96	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

95	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
94	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
93	A Computational Understanding of Solvent Effect on the Structure, Electronic, Thermochemical, and Spectroscopic Properties of Ni(η2-C6H4)(H2PCH2CH2PH2) Complex. *Journal of the Chinese Chemical Society*, **2017**, 64, 925-933	1.5	3
92	Computational Insights on the Structure and Properties of C24, C18B3N3, C12B6N6 and Their Endohedral Complexes with Alkaline and Earth Alkaline Metals. *Fullerenes Nanotubes and Carbon Nanostructures*, **2013**, 21, 644-652	1.8	3
91	Theoretical investigation of the structure and properties of H2B=NH2...Mn+, HB?NH...Mn+, and Borazine...Mn+ complexes (M = Alkaline and Earth Alkaline Metals). *Russian Journal of Physical Chemistry A*, **2011**, 85, 2148-2155	0.7	3
90	Theoretical studies on the structures, properties, and aromaticity of germatropylium cations. *Main Group Chemistry*, **2006**, 5, 203-214	0.6	3
89	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
88	Cyclometalation in the (η5-C5H5)Co(η2-C2H2)(PMe3) and (η5-C9H7)Co(η2-C2H2) (PMe3) complexes: A computational investigation. *Journal of Molecular Liquids*, **2021**, 325, 115097	6	3
87	The interaction between carboplatin anticancer drug and B12N12 nano-cluster: A computational investigation. *Main Group Chemistry*, **2021**, 1-10	0.6	3
86	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
85	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
84	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
83	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
82	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
81	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
80	Effect of External Electric Field on the Electronic Structure and Aromaticity of Cr(CO)3(η6-C6H6) Complex. *Russian Journal of Inorganic Chemistry*, **2019**, 64, 1035-1040	1.5	2
79	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
78	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

77	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
76	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
75	Chemical bonding and properties in [Ni(N-heterocylic carbene)(NO)(R)] (R = H, Me, HC=CH2, and C?CH) complexes: Theoretical insights. *Journal of Structural Chemistry*, **2012**, 53, 377-382	0.9	2
74	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
73	A quantum chemistry study of ruthenabenzene complexes. *Russian Journal of Physical Chemistry A*, **2013**, 87, 1506-1514	0.7	2
72	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
71	Benzene-1,3-diammonium bis-(pyridine-2,6-dicarboxyl-ato-□O,N,O)cobaltate(II) penta-hydrate. *Acta Crystallographica Section E: Structure Reports Online*, **2011**, 67, m507-8		2
70	Substitute Effect on the Structure, Stability of Valence Isomers and Aromaticity of 1-H-Boratabenzene. *Journal of the Chinese Chemical Society*, **2008**, 55, 1308-1312	1.5	2
69	Arsacyclopentadienyl anions: Structure, properties and aromaticity. *Main Group Chemistry*, **2006**, 5, 153-166	0.6	2
68	Theoretical study of Borazanaphthalene and itsmono-Fluorinated derivatives: structure and properties. *Main Group Chemistry*, **2007**, 6, 43-51	0.6	2
67	Substituent Effect in para Substituted Osmabenzene Complexes **2017**, 57,		2
66	Exploring the Substituent □ffect on the Structure and □lectronic □roperties of Si2(para-C6H4X)2 □olecules. *Russian Journal of Physical Chemistry A*, **2020**, 94, 2760-2769	0.7	2
65	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
64	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
63	The application of graphyne and its boron nitride analogue in Li-ion batteries. *Computational and Theoretical Chemistry*, **2021**, 1200, 113243	2	2
62	Computational investigation of interaction between titanocene dichloride and nanoclusters (B12N12, B12P12, Al12N12 and Al12P12). *Main Group Chemistry*, **2021**, 1-10	0.6	2
61	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
60	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

59	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
58	Theoretical understanding the effects of external electric field on the hydrolysis of anticancer drug titanocene dichloride. *Molecular Physics*, **2020**, 118, e1781272	1.7	1
57	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
56	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
55	Borepine: A Density Functional Approach toward Structural Features and Properties. *Russian Journal of Inorganic Chemistry*, **2018**, 63, 800-808	1.5	1
54	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
53	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
52	Quantum chemical predictions of structural, bonding and spectroscopic properties of ruthenanaphthalenes and ring-fused BN ruthenabenzenes. *Journal of Theoretical and Computational Chemistry*, **2014**, 13, 1450011	1.8	1
51	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
50	DFT studies and AIM analysis of AlN-polycycles. *Russian Journal of Physical Chemistry A*, **2012**, 86, 402-407	0.7	1
49	Molecular interaction of H2 and H2O with borthiin: a theoretical study. *Russian Chemical Bulletin*, **2012**, 61, 248-252	1.7	1
48	A quantum chemical study of Cr(CO)3(B3N3H6 −n F n) (n = 1–3) complexes. *Russian Journal of Physical Chemistry A*, **2012**, 86, 1542-1548	0.7	1
47	MOLECULAR STRUCTURE, NATURAL BOND ORBITAL, SUBSTITUENT EFFECT AND CHEMICAL REACTIVITY ANALYSIS OF TERMINAL BORYLENE RUTHENIUM COMPLEXES: Ru(PH3)2HCl(BC6H4X). *Journal of Theoretical and Computational Chemistry*, **2013**, 12, 1350071	1.8	1
46	Theoretical insights into the properties of the borazine–X- complexes (X- = H, F, Cl, CN, NC or NCO). *Journal of the Serbian Chemical Society*, **2009**, 74, 1105-1111	0.9	1
45	Dibromidobis(pyridine-3-carbonitrile-κN)mercury(II). *Acta Crystallographica Section E: Structure Reports Online*, **2011**, 67, m595		1
44	Theoretical insights into the properties of the XY?YX...Mn+ complexes (X = H, F, Cl; Y = C, Si; M = alkaline and alkaline earth metals). *Journal of Structural Chemistry*, **2010**, 51, 204-210	0.9	1
43	Theoretical studies on the structures, properties, and aromaticities of fluorinated arsabenzenes. *Journal of Structural Chemistry*, **2008**, 49, 600-605	0.9	1
42	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

41	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
40	SUBSTITUENT EFFECT IN [2+4] DIELSÂLDER 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
39	Structure and Bonding of Ni(C6H4-nFn)(CO)2(C6H4=benzyne, n=1-4) Complexes. *Journal of the Korean Chemical Society*, **2011**, 55, 183-188		1
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