Reza Ghiasi

List of Publications by Year
in descending order

169	1,296	430874	580821
papers	citations	18 h-index	25 g-index

170	170	170	469
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Band Gap Energies and Photocatalytic Properties of CdS and Ag/CdS Nanoparticles for Azo Dye Degradation. Chemical Engineering and Technology, 2016, 39, 149-157.	1.5	61
2	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.	1.5	38
3	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.	1.0	37
4	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.	1.0	35
5	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.	1.3	35
6	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.	0.6	34
7	Strong chemisorption of E2H2 and E2H4 (Eâ€‰=â€‰C, Si) on B12N12 nano-cage. Journal of Nanostructure in Chemistry, 2020, 10, 179-191.	9.1	27
8	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.	1.2	25
9	A theoretical study of the solvent effect on the interaction of C20 and N2H2. Journal of Structural Chemistry, 2017, 58, 30-37.	1.0	23
10	Quantum Mechanical Study of Substituent Dependence on the Structure, Spectroscopic (¹³C, ¹H NMR and UV), NBO, Hyperpolarizability and HOMOï£¿LUMO Analysis of Ru(NHC)₂Cl₂(ï£¾CHâ€‹pâ€C₆H₄X) Complexes. Journal of the Chinese Chemical Society, 2015, 62, 898-905.	1.4	22
11	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.	0.7	21
12	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	21
13	Effect of substitution on the structures, properties, and aromaticity of 1-H-boratabenzene anion. Main Group Chemistry, 2009, 8, 143-150.	0.8	20
14	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.	1.2	20
15	Substituent effect on the structure and properties of dialumene. Russian Journal of Inorganic Chemistry, 2016, 61, 985-992.	1.3	20
16	Computational investigation of solvent effect on the structure, spectroscopic properties (¹³C, ¹H NMR and IR, UV), NLO properties and HOMOâ€“LUMO analysis of Ru(NHC)₂Cl₂(=CH-p-C₆H₅) complex. Physics and Chemistry of Liquids, 2017, 55, 421-431.	1.2	20
17	Solvent effect on the linkage isomerism in [Fe(CO)₄(NCS)]^{â^’}and [Fe(CO)₄(SCN)]^{â^’}anions: A theoretical investigation. Physics and Chemistry of Liquids, 2017, 55, 444-456.	1.2	20
18	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.	1.0	20

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19	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
20	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.	1.2	18
21	Computational study of osmabenzyne: The solvent effects on the structure and spectroscopic properties (IR, NMR). Journal of Structural Chemistry, 2017, 58, 1324-1331.	1.0	18
22	A computational study of the arsabenzenes: Structure, properties and aromaticity. Journal of Organometallic Chemistry, 2005, 690, 4761-4767.	1.8	17
23	Theoretical study of the properties of fluoroborthiin and fluoroboroxine. Computational and Theoretical Chemistry, 2008, 853, 77-81.	1.5	17
24	Metal-stabilized rare tautomers: N4 metalated cytosine (M = Li+, Na+, K+, Rb+ and Cs+), theoretical views. Applied Organometallic Chemistry, 2003, 17, 635-640.	3.5	16
25	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.	0.6	16
26	The Analysis of Osâ‰¡C Bond and Electric Field Influence on the Properties in the Osmium Carbyne Complex OsCl₃ (â‰¡CCH₂ CMe₃)(PH₃)₂ : A Theoretical Insight. Journal of the Chinese Chemical Society, 2017, 64, 651-657.	1.4	16
27	Substituent Effect on the Electronic Properties and Nature of the Wâ‰¡C Bond in transâ€Cl(OC)(H₃P)₃W(â‰¡Câ€paraâ€C₆H₄X) (Xâ€=â€H, F, SiH₃, CN, NO₂, SiMe₃, CMe₃, NH₂): Journal of the Chinese Chemical Society, 2017, 64, 1340-1346.	1.4	16
28	Cytochrome P-450 model reaction: effects of substitution on the rate of aromatic hydroxylation. Journal of Porphyrins and Phthalocyanines, 2000, 04, 285-291.	0.8	15
29	Computational study of substituent effect in para substituted platinabenzene complexes. Russian Journal of Physical Chemistry A, 2013, 87, 973-978.	0.6	15
30	Insight into the solvent effect on the structure, IR-spectrum, and hyperpolarizability of CpMe2Ta(benzyne), a mononuclear Tantalumâ€“benzyne complex. Russian Journal of Inorganic Chemistry, 2017, 62, 1371-1378.	1.3	15
31	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	15
32	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(â‰¡Si-para-C₆H₄X). Journal of the Chinese Chemical Society, 2017, 64, 522-530.	1.4	14
33	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(Si Ph). Journal of Molecular Liquids, 2018, 264, 616-620.	4.9	14
34	Solvent effect on isomerization reaction of [(Î·5-C5H5)(CO)2Re C(C2HB10H10)(C6H5)] carbene complex to [(Î·5-C5H5)(CO)(COC2HB10H10)Re CC6H5] carbyne complex: A computational investigation. Journal of Molecular Liquids, 2018, 265, 164-171.	4.9	14
35	Influence of Solvent and Electric Field on the Structure and IR, 31P NMR Spectroscopic Properties of a Titanoceneâ€“Benzyne Complex. Journal of Applied Spectroscopy, 2018, 85, 526-534.	0.7	14
36	The mono- and di-silanaphthalene: structure, properties, and aromaticity. Computational and Theoretical Chemistry, 2005, 718, 225-233.	1.5	13

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37	Theoretical study on platinabenzene and mono- and difluorinated platinabenzenes: Structure, properties, and aromaticity. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2011, 37, 72-76.	1.0	13
38	Theoretical investigation on geometries and aromaticity of heterocyclic platinabenzenes. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2011, 37, 463-467.	1.0	13
39	Crop protection services by Plant Clinics in Iran: An evaluation through rice farmers' satisfaction. Crop Protection, 2017, 98, 191-197.	2.1	13
40	Quantum Chemical Study of Interaction between Titanocene Dichloride Anticancer Drug and Al12N12 Nano-Cluster. Russian Journal of Inorganic Chemistry, 2020, 65, 1726-1734.	1.3	12
41	Quantum mechanical study of the structure, natural bond analysis, HOMOâ€“LUMO analysis, substituents effect, and aromaticity on iridanaphthalene. Structural Chemistry, 2014, 25, 829-838.	2.0	11
42	Theoretical study of borthiin and its derivatives: structure and aromaticity. Journal of Sulfur Chemistry, 2007, 28, 505-511.	2.0	10
43	Tautomeric transformations and reactivity of isoindole and sila-indole: A computational study. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450041.	1.8	10
44	Theoretical Studies of Solvent Effect on the Structure, Đ’onding, and Spectroscopic Đroperties (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.	0.6	10
45	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.	1.0	10
46	The interaction of 5-fluorouracil with graphene in presence of external electric field: a theoretical investigation. Adsorption, 2020, 26, 905-911.	3.0	10
47	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.	0.6	10
48	Interaction between carboplatin with B12P12 and Al12P12 nano-clusters: A computational investigation. Phosphorus, Sulfur and Silicon and the Related Elements, 2021, 196, 751-759.	1.6	10
49	The interaction between carboplatin anticancer drug and B12N12 nano-cluster: A computational investigation. Main Group Chemistry, 2021, 20, 345-354.	0.8	9
50	A chromium carbene (OC)5Cr=C(OEt)(â€“Câ‰¡Câ€“Ph): Quantum mechanical study of molecular structure, HOMOâ€“LUMO analysis, IR spectroscopy, natural bond orbital analysis. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550022.	1.8	8
51	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.	1.4	8
52	Theoretical Analysis of Solvent Polarity Effect on the Electronic and Spectroscopic Properties (IR and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf A, 2020, 94, 345-351.	0.6	8
53	Interaction of cisplatin anticancer drug with C20 bowl: DFT investigation. Main Group Chemistry, 2022, 21, 43-54.	0.8	8
54	A Theoretical Study of Metal-Stabilised Rare Tautomers Stability: N4 Metalated Cytosine (M=Be2+,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 2004, 11-18.	1.3	7

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55	Theoretical view on structure, chemical reactivity, aromaticity and 14N NQR parameters of iridapyridine isomers. Journal of Structural Chemistry, 2015, 56, 1458-1467.	1.0	7
56	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.	2.7	7
57	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 FÃ¼r Chemie, 2018, 149, 2167-2174.	1.8	7
58	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.	1.0	7
59	Cyclometalation in the (Î·3-C5H5)Co(Î·2-C2H2)(PMe3) and (Î·3-C9H7)Co(Î·2-C2H2) (PMe3) complexes: A computational investigation. Journal of Molecular Liquids, 2021, 325, 115097.	4.9	7
60	Theoretical study of classical isomers tropylium, azatropylium, phosphatropylium, and arsatropylium cations: structure, properties and aromaticity. Main Group Chemistry, 2008, 7, 147-154.	0.8	6
61	DFT and TD-DFT study of benzene and borazines containing chromophores for DSSC materials. Russian Journal of Inorganic Chemistry, 2016, 61, 1267-1273.	1.3	6
62	The Analysis of Electronic Structures, <scp>NBO</scp>, <scp>EDA,</scp> and <scp>QTAIM</scp> of transâ€{<scp>H₃P</scp>)₂(Î·²â€<scp>BH₄</scp>)W(â‰¡Câ€paraâ€ Complexes. Journal of the Chinese Chemical Society, 2017, 64, 369-378.		6
63	Evolution of the interaction between C₂₀cage and Cr(CO)₅: A solvent effect, QTAIM and EDA investigation. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750007.	1.8	6
64	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.	2.0	6
65	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.	1.0	6
66	A Theoretical Approach towards Identification of External Electric Field Effect on (Î·5-C5H5)Me2Ta(Î·2-C6H4). Russian Journal of Physical Chemistry A, 2019, 93, 482-487.	0.6	6
67	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.	2.0	6
68	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.	4.9	6
69	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.	1.3	6
70	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.	1.0	6
71	The conductorâ€like polarizable continuum model study of indenyl effect on the ligand substitution reaction in the (Î·⁵â€C₉H₇)Co(CO)₂ complex. International Journal of Chemical Kinetics, 2021, 53, 901-912.	1.6	6
72	Structure, electronic properties and slippage of cyclopentadienyl and indenyl ligands in the (Î·5-C5H5) (Î·3-C5H5) W(CO)2 and (Î·5-C9H7) (Î·3-C9H7)W(CO)2 complexes: A C-PCM investigation. Journal of Molecular Liquids, 2021, 329, 115535.	4.9	6

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73	Unveiling the influence of solvent polarity on structural, electronic properties, and 31P NMR parameters of rhenabenzyne complex. Inorganic Chemistry Communication, 2021, 127, 108497.	3.9	6
74	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.	1.3	6
75	Dibromidobis(pyridine-3-carbonitrile-Î¹N1)zinc(II). Acta Crystallographica Section E: Structure Reports Online, 2011, 67, m101-m101.	0.2	5
76	A density functional approach toward structural features and properties of C20â€¦N2X2 (X = H, F, Cl,) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.8	5
77	Theoretical study of solvent effect on the ligand field parameter in [M(CO)6] n complexes (M = Vâ€“, Cr,) Tj ETQq1 1 0.784314 rgBT /O	0.6	5
78	Exploration of Solvent Effects on the Spectroscopic Properties (Ir and 13C NMR) in the OsCl3(â‰¡CCH2CMe3)(PH3)2 Carbyne Complex. Journal of Structural Chemistry, 2018, 59, 1052-1057.	1.0	5
79	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.	2.0	5
80	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.	1.0	5
81	Substituent Effect on the Acidity Strength of para-C6H4XB(OH)2 Boronic Acid: A Theoretical Investigation. Journal of Structural Chemistry, 2019, 60, 1743-1749.	1.0	5
82	Computational investigation of the substituent effect in the [2â€‰+â€‰4] Dielsâ€“Alder cycloaddition reactions of <scp>HSi</scp>â‰¡Si(<scp>paraâ€C₆H₄X</scp>) with benzene. Journal of the Chinese Chemical Society, 2021, 68, 806-816.	1.4	5
83	EDA, CDA and QTAIM Investigations in the (para-C5H4X) Ir(PH3)3 Iridabenzene Complexes. Russian Journal of Physical Chemistry B, 2021, 15, S6-S13.	1.3	5
84	Theoretical investigations on electronics structure and chemical bonding on iridathiabenzene and iridaoxabenzene. Russian Journal of Physical Chemistry A, 2013, 87, 1684-1691.	0.6	4
85	A Computational Approach to the Effects of Solvent on the Structural, Electronic, Spectroscopic (¹⁹⁵ Pt 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.	1.4	4
86	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.	1.0	4
87	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.	0.6	4
88	SOLVENT INFLUENCE ON THE STABILITY AND PROPERTIES OF Si4H4 ISOMERS BY COMPUTATIONAL METHODS. Journal of the Chilean Chemical Society, 2019, 64, 4360-4364.	1.2	4
89	Theoretical understanding the effects of external electric field on the hydrolysis of anticancer drug titanocene dichloride. Molecular Physics, 2020, 118, .	1.7	4
90	Quantum Chemical Study of the Effect of Solvent on Structure, Electronic Properties, and Electronic Spectrum of the Carbyne Complex trans-[ClRu(PH3)4(â‰¡Câ€“CH=CMe2)]2+. Russian Journal of Inorganic Chemistry, 2020, 65, 69-75.	1.3	4

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91	Theoretical study of the influence of solvent polarity on the 31P and 13C NMR parameters of the Ru(PH3)4(Î·2-benzyne) complex. Inorganic Chemistry Communication, 2021, 124, 108412.	3.9	4
92	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.	0.8	4
93	The application of graphyne and its boron nitride analogue in Li-ion batteries. Computational and Theoretical Chemistry, 2021, 1200, 113243.	2.5	4
94	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.	0.2	4
95	Effects of External Electric Field on the Hydrolysis of Cisplatin: A Density Functional Theory Approach. Russian Journal of Inorganic Chemistry, 2020, 65, 2053-2061.	1.3	4
96	SUBSTITUENT EFFECT IN [2+4] DIELSâ€“ALDER CYCLOADDITION REACTIONS OF ANTHRACENE WITH C2X2 (XÂ=ÂH,) Tj ETQq0 0 0 rgBT	1.0	4
97	Arsacyclopentadienyl anions: Structure, properties and aromaticity. Main Group Chemistry, 2006, 5, 153-161.	0.8	3
98	Theoretical studies on the structures, properties, and aromaticity of germatropylium cations. Main Group Chemistry, 2006, 5, 203-214.	0.8	3
99	Theoretical study of Borazanaphthalene and itsmono-Fluorinated derivatives: structure and properties. Main Group Chemistry, 2007, 6, 43-51.	0.8	3
100	Substitute Effect on the Structure, Stability of Valence Isomers and Aromaticity of 1â€Hâ€Boratabenzene. Journal of the Chinese Chemical Society, 2008, 55, 1308-1312.	1.4	3
101	Theoretical insights into the properties of the borazineâ€¦ X- complexes (X- = H, F, Cl, CN, NC or NCO). Journal of the Serbian Chemical Society, 2009, 74, 1105-1111.	0.8	3
102	Theoretical investigation of the structure and properties of H2B=NH2...M n+, HBâ‰¡NH...M n+, and Borazine...M n+ complexes (M = Alkaline and Earth Alkaline Metals). Russian Journal of Physical Chemistry A, 2011, 85, 2148-2155.	0.6	3
103	A quantum chemical study of Cr(CO)3(B3N3H6 â^' n F n) (n = 1â€“3) complexes. Russian Journal of Physical Chemistry A, 2012, 86, 1542-1548.	0.6	3
104	Computational Insights on the Structure and Properties of C₂₄, C₁₈B₃N₃, C₁₂B₆N₆and Their Endohedral Complexes with Alkaline and Earth Alkaline Metals. Fullerenes Nanotubes and Carbon Nanostructures, 2013, 21, 644-652.	2.1	3
105	A Computational Understanding of Solvent Effect on the Structure, Electronic, Thermochemical, and Spectroscopic Properties of Ni(Î·2-C6H4)(H2PCH2CH2PH2) Complex. Journal of the Chinese Chemical Society, 2017, 64, 925-933.	1.4	3
106	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.	1.0	3
107	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.	1.0	3
108	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.	1.0	3

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109	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.	1.2	3
110	Effect of External Electric Field on the Electronic Structure and Aromaticity of Cr(CO)3(Î·6-C6H6) Complex. Russian Journal of Inorganic Chemistry, 2019, 64, 1035-1040.	1.3	3
111	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.	0.6	3
112	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.	0.8	3
113	Computational investigation of interaction between titanocene dichloride and nanoclusters (B12N12,) Tj ETQq1 1 0.784314 rgBT /Over	0.8	3
114	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.	1.0	3
115	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.	1.2	3
116	Interaction between Phosgene and B12N12 Nano-Cluster: A Computational Investigation. Russian Journal of Physical Chemistry A, 2021, 95, S323-S330.	0.6	3
117	Benzene-1,3-diammonium bis(pyridine-2,6-dicarboxylato-Î¹³O²,N,O⁶)cobaltate(II) pentahydrate. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, m507-m508.	0.2	2
118	Molecular interaction of H2 and H2O with borthiin: a theoretical study. Russian Chemical Bulletin, 2012, 61, 248-252.	1.5	2
119	Chemical bonding and properties in [Ni(N-heterocylic carbene)(NO)(R)] (R = H, Me, HC=CH2, and Câ‰¡CH) complexes: Theoretical insights. Journal of Structural Chemistry, 2012, 53, 377-382.	1.0	2
120	Theoretical study of structure, bonding, and aromaticity of borazyne and B-substituted borazynes. Russian Journal of Physical Chemistry A, 2013, 87, 2231-2238.	0.6	2
121	A quantum chemistry study of ruthenabenzene complexes. Russian Journal of Physical Chemistry A, 2013, 87, 1506-1514.	0.6	2
122	Quantum chemical predictions of structural, bonding and spectroscopic properties of ruthenanaphthalenes and ring-fused Bâ€“N ruthenabenzenes. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450011.	1.8	2
123	Spectroscopic studies and molecular orbital analysis on platinanaphthalenes and ring-fused B-N platinanaphthalenes. Russian Journal of Physical Chemistry A, 2014, 88, 616-624.	0.6	2
124	Substituent Effect on the Stability and ¹⁴N NQR Parameters of Linkage Isomers of Nitriles in a Rhodium Halfâ€Sandwich Metallacycle: A Theoretical Study. Journal of the Chinese Chemical Society, 2018, 65, 416-423.	1.4	2
125	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.	0.6	2
126	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.	0.6	2

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