Reza Ghiasi

List of Publications by Year
in descending order

169 papers	1,296 citations	489802 18 h-index	651938 25 g-index
170 all docs	170 docs citations	170 times ranked	519 citing authors

#	Article	IF	Citations
1	Interaction of cisplatin anticancer drug with C20 bowl: DFT investigation. Main Group Chemistry, 2022, 21, 43-54.	0.4	8
2	Computational Investigation of Chemisorption of Thiophosgene on Co@B$$_{8}^{ - }$$. Russian Journal of Physical Chemistry A, 2022, 96, 267-272.	0.1	0
3	Quantumâ€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.	0.8	0
4	Computational Investigation of Substituent Effect on the Thermodynamics and Kinetics of Î²-Hydrocarbyl Elimination from a Rhodium(I) Iminyl Complex. Russian Journal of Physical Chemistry A, 2021, 95, 163-171.	0.1	0
5	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.	0.8	5
6	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
7	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.	1.8	4
8	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.	1.0	6
9	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.	2.3	7
10	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.	2.3	6
11	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.	0.4	3
12	Unveiling the influence of solvent polarity on structural, electronic properties, and 31P NMR parameters of rhenabenzyne complex. Inorganic Chemistry Communication, 2021, 127, 108497.	1.8	6
13	Interaction between carboplatin with B12P12 and Al12P12 nano-clusters: A computational investigation. Phosphorus, Sulfur and Silicon and the Related Elements, 2021, 196, 751-759.	0.8	10
14	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.	0.4	4
15	HYDROGEN ADSORPTION AND STORAGE ON PALLADIUM-FUNCTIONALIZEDÂGRAPHYNE AND ITS BORON NITRIDE ANALOGUE. Journal of Structural Chemistry, 2021, 62, 835-844.	0.3	1
16	The application of graphyne and its boron nitride analogue in Li-ion batteries. Computational and Theoretical Chemistry, 2021, 1200, 113243.	1.1	4
17	The interaction between carboplatin anticancer drug and B12N12 nano-cluster: A computational investigation. Main Group Chemistry, 2021, 20, 345-354.	0.4	9
18	Computational investigation of interaction between titanocene dichloride and nanoclusters (B12N12,) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.4	3

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19	Quantumâ€chemical calculations on the slippage of cyclopentadienyl and indenyl ligands in the (Î· 3) Tj ETQq1 1 0.784314 rgBT /Overlo 785-792.	0.8	0
20	SUBSTITUENT EFFECT IN [2+4] DIELSâ€“ALDER CYCLOADDITION REACTIONS OF ANTHRACENE WITH C2X2 (XÂ=ÂH,) Tj ETQq0 0 0 rgBT	0.3	4
21	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.	0.2	6
22	EDA, CDA and QTAIM Investigations in the (para-C5H4X) Ir(PH3)3 Iridabenzene Complexes. Russian Journal of Physical Chemistry B, 2021, 15, S6-S13.	0.2	5
23	Adsorption of Lewisite Warfare Agent on B12N12 Nano-Cluster: A Computational Investigation. Russian Journal of Physical Chemistry A, 2021, 95, 2637-2642.	0.1	2
24	Interaction between Phosgene and B12N12 Nano-Cluster: A Computational Investigation. Russian Journal of Physical Chemistry A, 2021, 95, S323-S330.	0.1	3
25	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.	0.8	8
26	The interaction of 5-fluorouracil with graphene in presence of external electric field: a theoretical investigation. Adsorption, 2020, 26, 905-911.	1.4	10
27	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.	2.3	6
28	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.	0.1	2
29	Computational Investigation of the 14N NQR Parameters of Borazyne. Journal of Applied Spectroscopy, 2020, 87, 538-544.	0.3	0
30	Computational Rationalization of the Interaction of Fe(CO)4 and Substituted Benzyne Ligands. Journal of Structural Chemistry, 2020, 61, 197-206.	0.3	1
31	Quantum Chemical Study of Interaction between Titanocene Dichloride Anticancer Drug and Al12N12 Nano-Cluster. Russian Journal of Inorganic Chemistry, 2020, 65, 1726-1734.	0.3	12
32	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	0
33	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.	0.1	0
34	Exploring the Substituent Đ•ffect on the Structure and Đ•lectronic Đroperties of Si2(para-C6H4X)2 Đœolecules. Russian Journal of Physical Chemistry A, 2020, 94, 2760-2769.	0.1	2
35	Strong chemisorption of E2H2 and E2H4 (Eâ€‰=â€‰C, Si) on B12N12 nano-cage. Journal of Nanostructure in Chemistry, 2020, 10, 179-191.	5.3	27
36	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.	0.1	10

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37	Substituent Effect on the Thermodynamics and Kinetics of Carbyne Complex [(Î·5-C5H5)(CO)(COMe)Reâ‰¡CC6H4X] Isomerization to Carbene Complex		

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55	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.	0.3	5
56	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.	0.1	6
57	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.	0.3	10
58	Assessment of substituent effects on the parameters of 35 Cl nuclear quadrupole resonance in para â€substituted benzeneâ€sulphenyl chloride via quantum chemical calculations. Journal of the Chinese Chemical Society, 2019, 66, 1577-1582.	0.8	1
59	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.	0.3	0
60	Substituent Effect on the Acidity Strength of para-C6H4XB(OH)2 Boronic Acid: A Theoretical Investigation. Journal of Structural Chemistry, 2019, 60, 1743-1749.	0.3	5
61	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.	1.0	6
62	Pseudo-Jahnâ€“Teller effect in Si4X4 (Xâ€‰=â€‰F, Cl, Br, I) molecules: a theoretical investigation. Molecular Physics, 2019, 117, 567-574.	0.8	1
63	Computational study of substituent effect on the electronic properties of ferrocylidene acetophenones complexes. Eurasian Chemical Communications, 2019, 1, 411-418.	1.1	1
64	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.	0.8	2
65	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.	0.3	20
66	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.	1.0	6
67	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.	0.1	1
68	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.	0.3	5
69	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.	0.3	4
70	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.	0.9	7
71	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.	0.3	3
72	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.	0.3	3

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73	Theoretical Study of NO Linkage Isomers in a Rhenacarborane Nitrosyl Complex. Russian Journal of Physical Chemistry A, 2018, 92, 2518-2523.	0.1	0
74	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.	0.3	7
75	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.	0.1	10
76	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.	1.0	5
77	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.	2.3	14
78	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.	2.3	14
79	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.	0.3	14
80	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.	0.5	3
81	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.	0.3	6
82	Borepine: A Density Functional Approach toward Structural Features and Properties. Russian Journal of Inorganic Chemistry, 2018, 63, 800-808.	0.3	1
83	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.	0.3	1
84	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.	0.3	6
85	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.	0.3	19
86	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
87	Crop protection services by Plant Clinics in Iran: An evaluation through rice farmers' satisfaction. Crop Protection, 2017, 98, 191-197.	1.0	13
88	Solvent Effects on Stability, Electronic Structure, and 14N NQR Parameters of Fe(CO)4py Isomers. Journal of Applied Spectroscopy, 2017, 84, 148-155.	0.3	21
89	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.	0.8	16
90	Theoretical study of solvent effect on the ligand field parameter in [M(CO)6] n complexes (M = Vâ€", Cr,) Tj ETQq0 0 0 rgBT /Overlock 1	0.1	5

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91	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.	0.8	4
92	A theoretical study of the solvent effect on the interaction of C20 and N2H2. Journal of Structural Chemistry, 2017, 58, 30-37.	0.3	23
93	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.	0.8	14
94	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.	0.8	3
95	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.	0.7	16
96	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.	0.3	15
97	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.	0.4	20
98	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.	0.4	20
99	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.	0.3	3
100	Computational study of osmabenzyne: The solvent effects on the structure and spectroscopic properties (IR, NMR). Journal of Structural Chemistry, 2017, 58, 1324-1331.	0.3	18
101	THEORETICAL STUDY OF THE PH3-ASSISTED MIGRATION OF A COORDINATED ARYL GROUP TO A COORDINATED CO IN THE COMPLEXES RhCpI(CO)(p-XC6H4). Journal of the Chilean Chemical Society, 2017, 62, 3454-3461.	0.5	0
102	Substituent Effect in para Substituted Osmabenzene Complexes. Journal of the Mexican Chemical Society, 2017, 57, .	0.2	2
103	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.	0.5	20
104	Band Gap Energies and Photocatalytic Properties of CdS and Ag/CdS Nanoparticles for Azo Dye Degradation. Chemical Engineering and Technology, 2016, 39, 149-157.	0.9	61
105	Substituent effect on the structure and properties of dialumene. Russian Journal of Inorganic Chemistry, 2016, 61, 985-992.	0.3	20
106	DFT and TD-DFT study of benzene and borazines containing chromophores for DSSC materials. Russian Journal of Inorganic Chemistry, 2016, 61, 1267-1273.	0.3	6
107	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.	0.1	16
108	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.	0.3	35

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109	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.	0.3	21
110	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.	0.8	22
111	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.	0.5	25
112	Theoretical view on structure, chemical reactivity, aromaticity and 14N NQR parameters of iridapyridine isomers. Journal of Structural Chemistry, 2015, 56, 1458-1467.	0.3	7
113	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.	0.3	35
114	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.	0.3	37
115	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.	0.1	34
116	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.	1.3	7
117	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
118	Tautomeric transformations and reactivity of isoindole and sila-indole: A computational study. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450041.	1.8	10
119	Quantum mechanical study of the structure, natural bond analysis, HOMOâ€“LUMO analysis, substituents effect, and aromaticity on iridanaphthalene. Structural Chemistry, 2014, 25, 829-838.	1.0	11
120	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
121	Spectroscopic studies and molecular orbital analysis on platinanaphthalenes and ring-fused B-N platinanaphthalenes. Russian Journal of Physical Chemistry A, 2014, 88, 616-624.	0.1	2
122	Borazine-based conjugated derivatives: Structural, electronic, and optical properties. Russian Journal of Physical Chemistry A, 2014, 88, 984-994.	0.1	0
123	A density functional approach toward structural features and properties of C20â€¦N2X2 (X = H, F, Cl,) Tj ETQq1 1 0.784314 rgBT /Ov	1.8	5
124	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.	0.5	3
125	Theoretical study of structure, bonding, and aromaticity of borazyne and B-substituted borazynes. Russian Journal of Physical Chemistry A, 2013, 87, 2231-2238.	0.1	2
126	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.	0.6	18

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127	Theoretical investigations on electronics structure and chemical bonding on iridathiabenzene and iridaoxabenzene. Russian Journal of Physical Chemistry A, 2013, 87, 1684-1691.	0.1	4
128	A quantum chemistry study of ruthenabenzene complexes. Russian Journal of Physical Chemistry A, 2013, 87, 1506-1514.	0.1	2
129	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.	1.0	3
130	Computational study of substituent effect in para substituted platinabenzene complexes. Russian Journal of Physical Chemistry A, 2013, 87, 973-978.	0.1	15
131	MOLECULAR STRUCTURE, NATURAL BOND ORBITAL, SUBSTITUENT EFFECT AND CHEMICAL REACTIVITY ANALYSIS OF TERMINAL BORYLENE RUTHENIUM COMPLEXES: Ru(PH₃)₂HCl(BC₆H<sub> Journal of Theoretical and Computational Chemistry, 2013, 12, 1350071.	1.8	1
132	Structure and bonding of Cu bis-dithiolenes complexes: a theoretical study. Journal of Sulfur Chemistry, 2012, 33, 93-100.	1.0	0
133	Molecular interaction of H2 and H2O with borthiin: a theoretical study. Russian Chemical Bulletin, 2012, 61, 248-252.	0.4	2
134	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.	0.1	3
135	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.	0.3	2
136	DFT studies and AIM analysis of AlN-polycycles. Russian Journal of Physical Chemistry A, 2012, 86, 402-407.	0.1	1
137	A theoretical study of the interaction between [HBâ‰¡CH]â^', [H2B=CH2]â^', and boratabenzene anions with alkali and alkaline earth metals: properties and structures. Journal of Structural Chemistry, 2011, 52, 683-689.	0.3	0
138	Theoretical study on platinabenzene and mono- and difluorinated platinabenzenes: Structure, properties, and aromaticity. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2011, 37, 72-76.	0.3	13
139	Theoretical investigation on geometries and aromaticity of heterocyclic platinabenzenes. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2011, 37, 463-467.	0.3	13
140	Structure and bonding of three-coordinate N-heterocyclic carbene nickel nitrosyl complexes: Theoretical study. Russian Journal of Physical Chemistry A, 2011, 85, 1174-1178.	0.1	0
141	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.	0.1	3
142	Dibromidobis(pyridine-3-carbonitrile-ÎºN1)mercury(II). Acta Crystallographica Section E: Structure Reports Online, 2011, 67, m595-m595.	0.2	1
143	Dibromidobis(pyridine-3-carbonitrile-ÎºN1)zinc(II). Acta Crystallographica Section E: Structure Reports Online, 2011, 67, m101-m101.	0.2	5
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