

Ab initio effective core potentials for molecular calculations including the outermost core orbitals

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Citation Report

#	ARTICLE	IF	CITATIONS
221	Ab initio effective core potentials for molecular calculations. Potentials for main group elements Na to Bi. Journal of Chemical Physics, 1985, 82, 284-298.	1.2	9,349
222	Ab initio effective core potentials for molecular calculations. Potentials for the transition metal atoms Sc to Hg. Journal of Chemical Physics, 1985, 82, 270-283.	1.2	12,620
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225	On 3d bonding in the transition metal trimers: The electronic structure of equilateral triangle Ca ₃ , Sc ₃ , Sc ₃ ⁺ , and Ti ₃ . Journal of Chemical Physics, 1985, 83, 5735-5742.	1.2	43
226	An effective core potential investigation of Ni, Pd, and Pt and their monohydrides. Journal of Chemical Physics, 1986, 85, 1447-1455.	1.2	60
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1959	IR spectroelectrochemical study of the binding of carbon monoxide to the active site of <i>Desulfovibrio fructosovorans</i> Ni-Fe hydrogenase. <i>Journal of Biological Inorganic Chemistry</i> , 2002, 7, 318-326.	1.1	78
1960	DFT study of ethene metathesis proceeding on monomeric MoVI centres of MoO ₃ /Al ₂ O ₃ catalyst. <i>Journal of Molecular Catalysis A</i> , 2002, 184, 371-377.	4.8	18
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1969	Theoretical study on the reaction of the ground state Y^+ of YS^+ with oxygen-transfer reagent: $\text{YS}^+ + \text{H}_2\text{O} \rightarrow \text{YO}^+ + \text{H}_2\text{S}$ in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 37-42.	1.5	14
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2008	Preparation, molecular structure, and fundamental vibrational modes of the dinuclear complexes trans- $[\{\text{RhX}(\text{P}i\text{Pr}3)_2\}_2\{\text{I}^{1/4}\text{-1,3-(CN)}_2\text{C}_6\text{H}_4\}]$. <i>Inorganica Chimica Acta</i> , 2002, 334, 355-364.	1.2	8
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2012	Ruthenium d-orbital delocalization in bis(bipyridine)ruthenium derivatives of redox active quinonoid ligands. <i>Coordination Chemistry Reviews</i> , 2002, 230, 97-105.	9.5	95
2013	Quantum chemical study of gas-phase reactions of trimethylaluminium and triethylaluminium with ammonia in III-V nitride semiconductor crystal growth. <i>Journal of Crystal Growth</i> , 2002, 237-239, 936-941.	0.7	24
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4935	Theoretical investigation on possible mechanisms on regioselective formation of (η -3-siloxyallyl)tungsten complexes. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 3456-3461.	0.8	3

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5492	/ > < mml:mrow > < mml:mn > 2 < /mml:mn > < /mml:mrow > < /mml:math > < mml:math <small>xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" > < mml:mrow > < mml:mo</small>		

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
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8327	Guanidine Complexes of Platinum: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5540-5547.	1.1	4
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10178	Automated Quantum Mechanical Predictions of Enantioselectivity in a Rhodium-Catalyzed Asymmetric Hydrogenation. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9101-9105.	7.2	43
10179	Novel pyrrole derivatives bearing sulfonamide groups: Synthesis in vitro cytotoxicity evaluation, molecular docking and DFT study. <i>Journal of Molecular Structure</i> , 2017, 1146, 242-253.	1.8	27
10180	Macrocyclic aza-crown chromogenic reagent to Al ³⁺ and fluorescence sensor for Zn ²⁺ and Al ³⁺ along with live cell application and logic operation. <i>Sensors and Actuators B: Chemical</i> , 2017, 252, 257-267.	4.0	28
10181	Ruthenium(II) Bipyridyl Complexes with Cyclometalated NHC Ligands. <i>Inorganic Chemistry</i> , 2017, 56, 7217-7229.	1.9	33
10182	Photoreactions of Porphyrins Initiated by Deep Ultraviolet Single Photons. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4626-4632.	1.1	6
10183	DFT Studies of Ru-Catalyzed C=O versus C-H Bond Functionalization of Aryl Ethers with Organoboronates. <i>Organometallics</i> , 2017, 36, 2354-2363.	1.1	20
10184	Catalytic Dehydrogenative C-C Coupling by a Pincer-Ligated Iridium Complex. <i>Journal of the American Chemical Society</i> , 2017, 139, 8977-8989.	6.6	35
10185	4,5-Substituted C [∞] C* cyclometalated thiazol-2-ylidene platinum(ii) complexes - synthesis and photophysical properties. <i>Dalton Transactions</i> , 2017, 46, 7800-7812.	1.6	13
10186	The first Re ^I organometallic complex with an organoimido-polyoxometalate ligand. <i>Dalton Transactions</i> , 2017, 46, 8611-8620.	1.6	4
10187	Three Zn(II) complexes with a sexidentate N ₂ O ₄ -donor bis-Schiff base ligand: Synthesis, characterization, DFT studies, in vitro antimicrobial evaluation and molecular docking studies. <i>Inorganica Chimica Acta</i> , 2017, 466, 8-15.	1.2	6
10188	A combination of experimental and computational studies on a new oxamido bridged dinuclear copper(II) complex. <i>Journal of Molecular Structure</i> , 2017, 1146, 43-49.	1.8	0
10189	Reduction of NO to N ₂ O Catalyzed by a Mn-Substituted Keggin-Type Polyoxometalate: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12735-12744.	1.5	12
10190	On the structures, spin states, and optical properties of titanium, platinum, and iron azacalixpyrins: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15903-15913.	1.3	4
10191	Linker Effects in Porphyrin Polymeric Donor Materials for Photovoltaic Devices. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12018-12024.	1.5	6
10192	One Step Toward a New Generation of C-MOS Compatible Oxide P-N Junctions: Structure of the LSMO/ZnO Interface Elucidated by an Experimental and Theoretical Synergic Work. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 20974-20980.	4.0	4
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10194	A benzimidazole-based chemodosimeter for the fluorometric detection of Zn and Cu via 1,5 proton shifts and C-N bond cleavage. <i>Photochemical and Photobiological Sciences</i> , 2017, 16, 1103-1116.	1.6	12

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10196	Structure and spin state of nonheme Fe ^{IV} O complexes depending on temperature: predictive insights from DFT calculations and experiments. <i>Chemical Science</i> , 2017, 8, 5460-5467.	3.7	25
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10201	Hypervalent-Iodine-Mediated Formation of Epoxides from Carbon(sp ²)-Carbon(sp ³) Single Bonds. <i>Journal of Organic Chemistry</i> , 2017, 82, 11691-11702.	1.7	15
10202	The Origins of Dramatic Differences in Five-Membered vs Six-Membered Chelation of Pd(II) on Efficiency of C(sp ³)-H Bond Activation. <i>Journal of the American Chemical Society</i> , 2017, 139, 8514-8521.	6.6	96
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10206	Sonochemical synthesis and DFT studies of nano novel Schiff base cadmium complexes: Green, efficient, recyclable catalysts and precursors of Cd NPs. <i>Journal of Molecular Structure</i> , 2017, 1146, 644-659.	1.8	14
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10210	Synthesis, characterization, DFT calculations and antibacterial activity of palladium(II) cyanide complexes with thioamides. <i>Journal of Molecular Structure</i> , 2017, 1141, 204-212.	1.8	11
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10238	Studies on hydrolysis mechanism of anticancer ruthenium drug ImH[trans-Ru(Im) ₂ Cl ₄] via ABEEM's polarizable force field combined with QM and MD-FEP. <i>Chemical Research in Chinese Universities</i> , 2017, 33, 239-247.	1.3	3
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10240	Effect of ionâ€“ligand binding on ion pairing dynamics studied by two-dimensional infrared spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10889-10897.	1.3	7
10241	Mechanistic investigation of Rh(i)-catalyzed alkyneâ€“isatin decarbonylative coupling. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1304-1312.	2.3	10
10242	A DFT study of Cu nanoparticles adsorbed on defective graphene. <i>Applied Surface Science</i> , 2017, 412, 146-151.	3.1	20
10243	Synthesis and biological studies of ruthenium, rhodium and iridium metal complexes with pyrazole-based ligands displaying unpredicted bonding modes. <i>Inorganica Chimica Acta</i> , 2017, 462, 223-235.	1.2	13
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10256	Efficient deep red electroluminescence of iridium complexes with 2,3-diphenylquinoxaline derivatives and tetraphenylimidodiphosphinate. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3714-3724.	2.7	37
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10259	Metallapentalenofurans and Lactone-Fused Metallapentalynes. <i>Chemistry - A European Journal</i> , 2017, 23, 6426-6431.	1.7	39
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10265	Ruthenium(II) DMSO complexes with C [†] C* cyclometalated phenylimidazol NHC ligands. <i>Journal of Organometallic Chemistry</i> , 2017, 829, 101-107.	0.8	12
10266	Diastereoselective Synthesis of Highly Substituted Tetrahydrofurans by Pd-Catalyzed Tandem Oxidative Cyclization-Redox Relay Reactions Controlled by Intramolecular Hydrogen Bonding. <i>Journal of Organic Chemistry</i> , 2017, 82, 57-75.	1.7	11

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10270	Tuning the dipolar second-order nonlinear optical properties of 5- <i>π</i> -delocalized-donor-1,3-di(2-pyridyl)benzenes, related cyclometallated platinum(II) complexes and methylated salts. <i>Dalton Transactions</i> , 2017, 46, 1179-1185.	1.6	10
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10276	Push-pull pyropheophorbides for nonlinear optical imaging. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 947-956.	1.5	28
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10278	Quinoline appended pyrazoline based Ni sensor and its application towards live cell imaging and environmental monitoring. <i>Sensors and Actuators B: Chemical</i> , 2017, 243, 549-556.	4.0	31
10279	Transient photocyclization in ruthenium(II) polypyridine complexes of indolamines. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2140-2147.	1.3	7
10280	The mechanism of selective catalytic reduction of NO _x on Cu-SSZ-13: a computational study. <i>Dalton Transactions</i> , 2017, 46, 369-377.	1.6	6
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#	ARTICLE	IF	CITATIONS
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10952	Crystal structure, Hirshfeld surface analysis, spectroscopic and biological studies on sulfamethazine and sulfaquinoxaline ternary complexes with 2,2'-biquinoline. <i>New Journal of Chemistry</i> , 2018, 42, 891-901.	1.4	9
10953	Synthesis of stable polymetalated aromatic complexes through metal- π -macrocycle capsule-triggered cyclization. <i>Chemical Science</i> , 2018, 9, 1481-1487.	3.7	24
10954	Analysis of the conformational properties of amine ligands at the gold/water interface with QM, MM and QM/MM simulations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3349-3362.	1.3	15
10955	Exploring the mechanism of the Pd-catalyzed spirocyclization reaction: a combined DFT and experimental study. <i>Chemical Science</i> , 2018, 9, 1496-1509.	3.7	62
10956	Computational Studies on the Mechanism of Rh-Catalyzed Decarbonylative [5+2] Reaction between Isatins and Alkynes: High Selectivity by Directing Group. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 806-814.	1.2	8
10957	Mechanistic insight into the C7-selective C-H functionalization of <i>N</i> -acyl indole catalyzed by a rhodium complex: a theoretical study. <i>Organic Chemistry Frontiers</i> , 2018, 5, 725-733.	2.3	25
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10959	Syntheses, crystal structures, DNA binding, DNA cleavage, molecular docking and DFT study of Cu(II) complexes involving N ₂ O ₄ donor azo Schiff base ligands. <i>New Journal of Chemistry</i> , 2018, 42, 246-259.	1.4	33
10960	Examining the effects of variations in ligand framework and pnictogen substitution on the geometry and electronic structure of metal complexes of N-heterocyclic phosphido ligands incorporated into a diphosphine pincer ligand framework. <i>Polyhedron</i> , 2018, 143, 215-222.	1.0	6
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10962	Recognition dynamics of trinuclear copper cluster and associated histidine residues through conserved or semi-conserved water molecules in human Ceruloplasmin: The involvement of aspartic and glutamic acid gates. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 3829-3842.	2.0	10
10963	Mechanistic study on the Rh(III)-catalyzed synthesis of indolines via selective O-atom transfer of aryl nitrones: Origins of the regioselectivity and the improved yield with pivalic acid additive. <i>Journal of Organometallic Chemistry</i> , 2018, 854, 15-26.	0.8	7
10964	Structure-performance relationship on the asymmetric methoxy substituents of spiro-OMeTAD for perovskite solar cells. <i>Solar Energy Materials and Solar Cells</i> , 2018, 176, 318-323.	3.0	18
10965	Design and synthesis of new thiobarbituric acid metal complexes as potent protease inhibitors: spectral characterization, thermal analysis and DFT calculations. <i>Journal of the Iranian Chemical Society</i> , 2018, 15, 269-280.	1.2	8
10966	Inclusion complexes between cisplatin and oxidized carbon nanostructures: A theoretical approach. <i>Journal of Inorganic Biochemistry</i> , 2018, 178, 134-143.	1.5	16
10967	Photochemical properties of a Re(I) polymer containing dppz in its structure. An interplay between dark and bright states of dppz. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 353, 86-100.	2.0	4
10968	δ^+ -Acidity of benzene in [(benzene)RuII(N-N)Cl] ⁺ . Crystal structures, nuclear magnetic resonance spectra and nucleus independent chemical shifts. <i>Inorganica Chimica Acta</i> , 2018, 471, 228-233.	1.2	6

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10972	Combined plane wave and localized orbital electronic structure calculation: Adsorption energy of hydrogen on Pd(111). <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25452.	1.0	5
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10975	Quantum-Chemical Study of the Adsorption of Bi ³⁺ Ions on Au(111). <i>Russian Journal of Electrochemistry</i> , 2018, 54, 1201-1208.	0.3	1
10976	Trapping of an Heterometallic Unsaturated Hydride: Structure and Properties of the Ammonia Complex [MoMnCp(η^5 -H)(η^5 -PPh ₂)(CO) ₅ (NH ₃)]. <i>Inorganics</i> , 2018, 6, 125.	1.2	2
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10978	Interaction between Thallium and the Au(111) Surface. Quantum-Chemical Analysis. <i>Russian Journal of Electrochemistry</i> , 2018, 54, 912-921.	0.3	0
10979	Synthesis and characterization of Cu(I) isocyanide complexes exhibiting reversible luminescence. <i>Japanese Journal of Applied Physics</i> , 2018, 57, 081601.	0.8	2
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10981	Cyclometallation of a germylene ligand by concerted metalation-deprotonation of a methyl group. <i>Dalton Transactions</i> , 2018, 47, 15835-15844.	1.6	13
10982	Mechanism and origins of chemo- and regioselectivities of (NHC)NiH-catalyzed cross-hydroalkenylation of vinyl ethers with E -olefins: a computational study. <i>Organic Chemistry Frontiers</i> , 2018, 5, 3410-3420.	2.3	8
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10984	The conformational behavior of multivalent tris(imidazolium)cyclophanes in the hybrids with metal (pseudo)halides or polyoxometalates. <i>CrystEngComm</i> , 2018, 20, 7184-7194.	1.3	16
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10986	Asymmetric abstraction of two chemically-equivalent methylene hydrogens: significant enantioselectivity of endoperoxide presented by fumitremorgin B endoperoxidase. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26500-26505.	1.3	13

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10988	Electron-poor hemilabile dicationic palladium NHC complexes – synthesis, structure and catalytic activity. <i>Dalton Transactions</i> , 2018, 47, 16638-16650.	1.6	12
10989	Base-free glucose dehydration catalysed by NHC-stabilised heterohalo cyclopentadienyl Cr(III) complexes. <i>New Journal of Chemistry</i> , 2018, 42, 19193-19204.	1.4	13
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10991	Interaction of a gold(I) dicarbene anticancer drug with human telomeric DNA G-quadruplex: solution and computationally aided X-ray diffraction analysis. <i>Dalton Transactions</i> , 2018, 47, 16132-16138.	1.6	35
10992	Substrate switchable Suzuki–Miyaura coupling for benzyl ester vs. benzyl halide. <i>RSC Advances</i> , 2018, 8, 35056-35061.	1.7	9
10993	New heterobimetallic Au–Pt polyynes achieving a good trade-off between transparency and optical power limiting performance. <i>Journal of Materials Chemistry C</i> , 2018, 6, 11416-11426.	2.7	17
10994	A simple strategy to achieve remarkable mechanochromism of cationic Ir(III) phosphors through subtle ligand modification. <i>Journal of Materials Chemistry C</i> , 2018, 6, 11686-11693.	2.7	28
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11001	Polarizable Charge Equilibration Model for Transition-Metal Elements. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9350-9358.	1.1	9
11002	Temperature Dependent Micro-Structure of KAlF_4 from Solid to Molten States. <i>Materials</i> , 2018, 11, 1846.	1.3	4
11003	Mechanisms of Bisphosphine Iron-Catalyzed $\text{C}(\text{SP}^2)\text{-C}(\text{SP}^3)$ Cross-Coupling Reactions: Inner-Sphere or Outer-Sphere Arylation?. <i>Comments on Inorganic Chemistry</i> , 2018, 38, 210-237.	3.0	8
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11010	DFT Calculations of Structure and Optical Properties in Wide Band-Gap Semiconductor Clusters for Dye-Sensitized Solar Cells. , 2018, , .		0
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11013	Cobalt(I) Complexes of 5-Aryl-2-iminopyrrolyl Ligands: Synthesis, Spin Isomerism, and Application in Catalytic Hydroboration. <i>Inorganic Chemistry</i> , 2018, 57, 14671-14685.	1.9	28
11014	Computation Revealed Mechanistic Complexity of Low-Valent Cobalt-Catalyzed Markovnikov Hydrosilylation. <i>Journal of Organic Chemistry</i> , 2018, 83, 14646-14657.	1.7	8
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11018	Raman and Computational Study on the Adsorption of Xanthine on Silver Nanocolloids. <i>ACS Omega</i> , 2018, 3, 13530-13537.	1.6	16
11019	Synthesis, Characterization and Electronic Structure of Dirhenadehydro[12]annulene Complexes. <i>ChemPlusChem</i> , 2019, 84, 85-91.	1.3	7
11020	Theoretical investigation of auxiliary electronic acceptors in modifying D-D-Î€-A sensitizers for dye-sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2018, 24, 339.	0.8	1
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11024	Adsorption of Hydrophobic and Hydrophilic Ionic Liquids at the Au(111) Surface. ACS Omega, 2018, 3, 18039-18051.	1.6	37
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11044	Structure and dynamics of <i>Helicobacter pylori</i> nickel-chaperone HypA: an integrated approach using NMR spectroscopy, functional assays and computational tools. <i>Journal of Biological Inorganic Chemistry</i> , 2018, 23, 1309-1330.	1.1	20
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11047	Computational study of Rh(I)-Catalyzed Cycloaddition-Fragmentation of N-cyclopropylacrylamides. <i>Tetrahedron</i> , 2018, 74, 6475-6483.	1.0	2
11048	Cooperative Metal-Ligand Hydroamination Catalysis Supported by C-H Activation in Cyclam Zr(IV) Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 13034-13045.	1.9	12
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11057	Electronic structure and photoelectron spectroscopy of manganese dihalides from quantum chemical methods and Dyson orbitals. <i>Chemical Physics</i> , 2018, 515, 513-520.	0.9	2
11058	Iron-catalyzed olefin synthesis by direct coupling of alkenes with alcohols: A DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2018, 1143, 36-42.	1.1	0

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11060	Analysis of the Raman Spectrum of Kinked Carbon Chains Taking into Account the Model of Various End Groups. <i>Journal of Surface Investigation</i> , 2018, 12, 564-569.	0.1	2
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11068	Building polynitrogen clusters with metal—metal multiple bonds. <i>Polyhedron</i> , 2018, 156, 54-57.	1.0	5
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11072	Rhodium(III) and Iridium(III) Complexes of a NHC-Based Macrocyclic: Persistent Weak Agostic Interactions and Reactions with Dihydrogen. <i>Organometallics</i> , 2018, 37, 3963-3971.	1.1	28
11073	Push—Pull <i>N,N'</i> -Diphenylhydrazones Bearing Bithiophene or Thienothiophene Spacers as Nonlinear Optical Second Harmonic Generators and as Photosensitizers for Nanocrystalline TiO_2 Dye-Sensitized Solar Cells. <i>ACS Omega</i> , 2018, 3, 12893-12904.	1.6	25
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11076	Ligand Design for <i>N,N'</i> - or <i>N,N'</i> -Pyrazolone-Based Hydrazones Ruthenium(II)-Arene Complexes and Investigation of Their Anticancer Activity. <i>Inorganic Chemistry</i> , 2018, 57, 14123-14133.	1.9	47

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11078	Adsorption of CO ₂ on sodium iodide (NaI) _n (n = 1-10) clusters: A density functional theory investigation. <i>Computational and Theoretical Chemistry</i> , 2018, 1145, 37-43.	1.1	3
11079	Impact of Ligand Substitutions on Multielectron Redox Properties of Fe Complexes Supported by Nitrogenous Chelates. <i>ACS Omega</i> , 2018, 3, 14766-14778.	1.6	10
11080	Cyclometalated Ir(III) Complexes Involving Functionalized Terpyridine-Based Ligands Exhibiting Aggregation-Induced Emission and Their Potential Applications in CO ₂ Detection. <i>Organometallics</i> , 2018, 37, 3827-3838.	1.1	12
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11082	Which Amino Acids are Capable of Nucleating Fluorescent Silver Clusters in Proteins?. <i>Journal of Physical Chemistry C</i> , 2018, 122, 26275-26280.	1.5	13
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11096	Synthesis and Characterization of (pyNO ⁺) ₂ GaCl: A Redox-Active Gallium Complex. <i>Inorganics</i> , 2018, 6, 50.	1.2	3
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11112	Mechanistic insight into the Rh(III)-catalyzed cascade annulation of \hat{N} -ethynylanilines with diazo compounds towards Benzo[a]carbazoles. <i>Journal of Organometallic Chemistry</i> , 2018, 876, 17-25.	0.8	2

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11126	Theoretical design of metal-phthalocyanine dye-sensitized solar cells with improved efficiency. <i>Journal of Molecular Modeling</i> , 2018, 24, 279.	0.8	8
11127	The structural and electronic properties of TiO ₂ polymorphs towards water splitting reaction. <i>Journal of Materials Science: Materials in Electronics</i> , 2018, 29, 18282-18289.	1.1	1
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11129	Di-niobium gold clusters: Multiply-bonded Nb ₂ dimer coordinated equatorially by Au atoms. <i>International Journal of Mass Spectrometry</i> , 2018, 434, 7-16.	0.7	3
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11136	Surface enhancement Raman spectroscopy and density functional theory study of silver nanoparticles synthesized with d-glucose. <i>Journal of Raman Spectroscopy</i> , 2018, 49, 1756-1764.	1.2	10
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11150	Structural and Electronic Properties in Titanium-Doped Stannum Clusters: Comparison with Their Anions and Cations. <i>Journal of Cluster Science</i> , 2018, 29, 909-919.	1.7	7
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11163	Optically Active CdSe-Dot/CdS-Rod Nanocrystals with Induced Chirality and Circularly Polarized Luminescence. <i>ACS Nano</i> , 2018, 12, 5341-5350.	7.3	102
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11165	Lewis acidity of benzene in half-sandwich ruthenium arene complex. A computational study. <i>Computational and Theoretical Chemistry</i> , 2018, 1136-1137, 34-48.	1.1	7
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11171	The Crystalline Structure of Tensile Strained SrRuO ₃ : A First-Principles Investigation. <i>Crystal Growth and Design</i> , 2018, 18, 3397-3403.	1.4	4
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11454	Bis-tridentate Ir ^{III} Phosphors Bearing Two Fused Five-Six-Membered Metallacycles: A Strategy to Improved Photostability of Blue Emitters. <i>Chemistry - A European Journal</i> , 2019, 25, 15375-15386.	1.7	27

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11560	Molecular design and synthesis of D–A structured porphyrin dyes with various acceptor units for dye-sensitized solar cells. <i>Journal of Materials Chemistry C</i> , 2019, 7, 2843-2852.	2.7	73
11561	Nonlinear optical response of endohedral all-metal electride cages 2e ⁻ Mg ₂ (M@E12)2 ⁺ Ca ₂ (M = Ni, Tj) <i>ETQq1_2,7</i> 0.784314 rgBT 16		
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11566	Synthesis, catalysis, and DFT study of a ruthenium carbene complex bearing a 1,2-dicarbododecaborane (12)-1,2-dithiolate ligand. <i>Dalton Transactions</i> , 2019, 48, 2646-2656.	1.6	4
11567	An ES IPT based chromogenic and fluorescent ratiometric probe for Zn ²⁺ with imaging in live cells and tissues. <i>New Journal of Chemistry</i> , 2019, 43, 1857-1863.	1.4	17
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12306	Reactivity and Selectivity Controlling Factors in the Pd/Dialkylbiarylphosphine-Catalyzed C-C Cleavage/Cross-Coupling of an N-Fused Bicyclo[1.1.0]butane-2-Hydroxy-1 ² -Lactam. Journal of the American Chemical Society, 2020, 142, 21140-21152.	6.6	20
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12324	Molecular Bismuth Cations: Assessment of Soft Lewis Acidity. <i>Chemistry - A European Journal</i> , 2020, 26, 10250-10258.	1.7	52
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12650	Metal-carbon bonding in perfluoroethylene and perfluorobenzene transition metal complexes. Some underappreciated <i>f</i> - and <i>l</i> -acceptor components. , 2021, , 343-364.		0
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12698	Silver-catalyzed desulfurizative annulation of 1,2-benzisothiazoles with ynamides to construct multi-substituted isoquinolines. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5446-5453.	2.3	3
12699	Theoretical calculation of regioselectivity and solvation effects on α -H activation of <i>O</i> -carborane guided by directing group. <i>Dalton Transactions</i> , 2021, 50, 10291-10298.	1.6	2
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12706	An enantiomeric pair of alkaline-earth metal based coordination polymers showing room temperature phosphorescence and circularly polarized luminescence. <i>Journal of Materials Chemistry C</i> , 2021, 9, 5544-5553.	2.7	10
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