

Balanced basis sets of split valence, triple zeta valence a for H to Rn: Design and assessment of accuracy

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Citation Report

#	ARTICLE	IF	CITATIONS
581	Hybrid Inorganic~Metalorganic Compounds Containing Copper(II)-Monosubstituted Keggin Polyanions and Polymeric Copper(I) Complexes.. Inorganic Chemistry, 2006, 45, 7748-7757.	1.9	98
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1265	Electron Distribution in Partially Reduced Mixed Metal Oxide Systems: Infrared Spectroscopy of Ce _m V _n O _o Gas-Phase Clusters. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11187-11192.	1.1	42
1266	Structural Elucidation of Biological and Toxicological Complexes: Investigation of Monomeric and Dimeric Complexes of Histidine with Multiply Charged Transition Metal (Zn and Cd) Cations using IR Action Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2011, 115, 12648-12661.	1.2	45
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1271	Cation-Cation \leftrightarrow Attraction \leftrightarrow When London Dispersion Attraction Wins over Coulomb Repulsion. <i>Inorganic Chemistry</i> , 2011, 50, 2619-2628.	1.9	127
1272	A Step beyond the Feltham-Enemark Notation: Spectroscopic and Correlated <i>ab</i> Initio Computational Support for an Antiferromagnetically Coupled M(II)-NO Description of Tp [*] M(NO) (M = Co, Ni). <i>Journal of the American Chemical Society</i> , 2011, 133, 18785-18801.	6.6	89
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1284	Stabilizing carbon-lithium stars. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 12975.	1.3	45
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1288	Geometry optimization using tuned and balanced redistributed charge schemes for combined quantum mechanical and molecular mechanical calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10556.	1.3	20
1289	Reorganization Energy for Internal Electron Transfer in Multicopper Oxidases. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13111-13126.	1.2	55
1290	3-(Hetero)aryl-4-indolylamino-1,4-tetralones by Diastereoselective Internal Redox Cyclization: An α -Azaenamine-Conjugate Addition. <i>Journal of Organic Chemistry</i> , 2011, 76, 5185-5197.	1.7	17
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1310	Exploiting CH- π interactions in supramolecular hydrogels of aromatic carbohydrate amphiphiles. <i>Chemical Science</i> , 2011, 2, 1349.	3.7	84
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1312	Calculation of spin-current densities using gauge-including atomic orbitals. <i>Journal of Chemical Physics</i> , 2011, 134, 054123.	1.2	109
1313	Speciation of uranyl ions in fulvic acid and humic acid: a DFT exploration. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18038.	1.3	35
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1330	DFT Study of Trichloroethene Reaction with Permanganate in Aqueous Solution. <i>Environmental Science & Technology</i> , 2011, 45, 3006-3011.	4.6	29
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1395	Peroxide bond strength of antimalarial drugs containing an endoperoxide cycle. Relation with biological activity. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 4098.	1.5	27
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1401	Perspectives on Basis Sets Beautiful: Seasonal Plantings of Diffuse Basis Functions. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3027-3034.	2.3	566
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1694	Preparation and characterization of ultrathin [Ru(CO) ₃ Cl ₂] ₂ and [BMIM][Tf ₂ N] films on Al ₂ O ₃ /NiAl(110) under UHV conditions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10603.	1.3	15
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1715	Low-Energy States of Manganese-Oxo Corrole and Corrolazine: Multiconfiguration Reference ab Initio Calculations. Inorganic Chemistry, 2012, 51, 4002-4006.	1.9	37
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1739	Intramolecular Aminoalkene Hydroamination Mediated by a Tethered Bis(ureate)zirconium Complex: Computational Perusal of Various Pathways for Aminoalkene Activation. <i>Inorganic Chemistry</i> , 2012, 51, 3786-3795.	1.9	24
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1780	On the electronic spectra and optical properties of [(η^5 -C ₅ H ₅)(L) ₂ M(GaMe ₂)] complexes (M=Fe, Ru, Os; L: Tj ETQq1 1 0.784314 rgBT	0.8	0
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1797	The Neat Ternary Solid K ₅ Co ₁ Sn ₉ with Endohedral [Co@Sn ₉] ⁵⁺ Cluster Units: A Precursor for Soluble Intermetalloid [Co ₂ @Sn ₁₇] ⁵⁺ Clusters. Chemistry - A European Journal, 2012, 18, 12000-12007.	1.7	45
1798	Subtle Impact of Atomic Ratio, Charge and Lewis Basicity on Structure Selection and Stability: The Zintl Anion [(La@In ₂ Bi ₁₁)($\frac{1}{4}$ Bi) ₂ (La@In ₂ Bi ₁₁)] ⁶⁻ . Chemistry - A European Journal, 2012, 18, 13589-13595.	1.7	54
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1805	Divalent N(I) Character in 2-(Thiazol-2-yl)guanidine: An Electronic Structure Analysis. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9071-9079.	1.1	31
1806	Design of Neutral Lewis Superacids of Group 13 Elements. <i>Inorganic Chemistry</i> , 2012, 51, 640-646.	1.9	52
1807	CBe ₅ E ⁺ (E = Al, Ga, In, Tl): planar pentacoordinate carbon in heptaatomic clusters. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14764.	1.3	55
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1819	Photodynamics of Free and Solvated Tyrosine. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8762-8770.	1.2	18
1820	Mechanism of "Turn-on" Fluorescent Sensors for Mercury(II) in Solution and Its Implications for Ligand Design. <i>Inorganic Chemistry</i> , 2012, 51, 10904-10915.	1.9	113
1821	Highly selective mercury(II) cations detection in mixed "aqueous media by a ferrocene-based fluorescent receptor. <i>Dalton Transactions</i> , 2012, 41, 4437.	1.6	27
1822	Forming trifluoromethylmetallates: competition between decarboxylation and C-F bond activation of group 11 trifluoroacetate complexes, $[CF_3CO_2ML]^-$. <i>Dalton Transactions</i> , 2012, 41, 3395.	1.6	49
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5218	Benchmark Applications of Variations of Multireference Equation of Motion Coupled-Cluster Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 114-132.	2.3	26

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6645	Ternary Mixed-Valence Organotin Copper Selenide Clusters. <i>Chemistry - A European Journal</i> , 2018, 24, 5840-5848.	1.7	15
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11280	London Dispersion in Alkane Solvents. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 779-786.	7.2	22
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11286	Quantification of Noncovalent Interactions in Azide-Pnictogen, Chalcogen, and Halogen Contacts. <i>Chemistry - A European Journal</i> , 2021, 27, 4627-4639.	1.7	25
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11289	Synthesis, X-ray characterization, Hirshfeld surface analysis and DFT calculations on tetrazolyl-phenol derivatives: H-bonds vs $\text{C}^{\delta+}\text{H}^{\delta-}\cdots\text{N}^{\delta-}\text{N}^{\delta-}\text{N}^{\delta-}\text{N}^{\delta-}$ interactions. <i>Journal of Molecular Structure</i> , 2021, 1227, 129425.	1.8	9
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11348	Fe-chitosan complexes for oxidative degradation of emerging contaminants in water: Structure, activity, and reaction mechanism. <i>Journal of Hazardous Materials</i> , 2021, 408, 124662.	6.5	20
11349	Oxidation Under Reductive Conditions: From Benzylic Ethers to Acetals with Perfect Atom-Economy by Titanocene(III) Catalysis. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 5482-5488.	7.2	20
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11372	Iron-catalysed asymmetric carboazidation of styrenes. <i>Nature Catalysis</i> , 2021, 4, 28-35.	16.1	60
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12232	Computational Mechanistic Study of Brønsted Acid-Catalyzed Unsymmetrical 1,2,4,5-Tetrazines Synthesis. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4715-4726.	1.1	2
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13022	Organotin compounds bearing C ₃ -symmetric Schiff base: Microwave-assisted multicomponent synthesis and their photophysical properties. <i>Journal of Organometallic Chemistry</i> , 2021, 954-955, 122111.	0.8	1
13023	Frustrated Lewis Pairs based on Carbon-Carbon tetrel bonds: A DFT study. Mar a de las Nieves Pi a [a], Antonio Frontera[a], Tiddo. J. Mooibroek[b],* and Antonio Bauz a *[a]. <i>ChemPhysChem</i> , 2021, 22, 2478-2483.	1.0	3
13024	Shedding Light on Primary Donors in Photosynthetic Reaction Centers. <i>Frontiers in Microbiology</i> , 2021, 12, 735666.	1.5	19

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13025	Separation of lithium isotopes by crown ether-room temperature ionic liquid-anisole friendly solvent system. <i>Journal of Molecular Liquids</i> , 2021, 340, 117207.	2.3	7
13026	Theoretical exploration of optoelectronic performance of PM6:Y6 series-based organic solar cells. <i>Surfaces and Interfaces</i> , 2021, 26, 101385.	1.5	15
13027	Beauty in chemistry: A self-organized and dual-phase emissive diketopyrrolopyrrole derivative as high-yield fluorescent material. <i>Dyes and Pigments</i> , 2021, 194, 109655.	2.0	4
13028	Crystal structure and optical property of a Cadmium(II) complex based on triphenylamine derivative—Theoretical and experimental investigation. <i>Journal of Luminescence</i> , 2021, 238, 118270.	1.5	2
13029	Improving the performance of palladium-catalysed telomerization of 1,3-butadiene by metallocene-based phosphine ligand. <i>Molecular Catalysis</i> , 2021, 515, 111883.	1.0	2
13030	Adsorption and activation of CO ₂ molecule on subnanometer-sized anionic vanadium carbide clusters V _n C _{4n} (n = 1–6): A theoretical study. <i>Molecular Catalysis</i> , 2021, 515, 111871.	1.0	2
13031	Shapeshifting radicals. <i>Chemical Physics</i> , 2022, 552, 111373.	0.9	1
13032	Pentaphosphaferrocene-mediated synthesis of asymmetric organo-phosphines starting from white phosphorus. <i>Nature Communications</i> , 2021, 12, 5774.	5.8	31
13033	Stereoselective synthesis of (26R)-26-hydroxydiosgenin and its effect on the regulation of rat ovarian function. <i>Bioorganic Chemistry</i> , 2021, 115, 105189.	2.0	2
13034	First-principles characterisation of spectroscopic and bonding properties of cationic bismuth carbide clusters. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113372.	1.1	0
13035	Data for molecular dynamics simulations of Escherichia coli cytochrome bd oxidase with the Amber force field. <i>Data in Brief</i> , 2021, 38, 107401.	0.5	1
13036	Novel synthetic pathway for the production of phosgene. <i>Science Advances</i> , 2021, 7, eabj5186.	4.7	19
13037	Selective copper determination using a sensor based on a vinylferrocene moiety: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113423.	1.1	1
13038	Novel dirhenium(III,III) complexes with bridging diphenylphosphinomethane and dithiocarbamate ligands: A combined experimental and theoretical study. <i>Polyhedron</i> , 2021, 207, 115373.	1.0	2
13039	Novel high-quantum-yield polydiacetylene conjugated AIE micelles for amplified fluorescence signaling and photodynamic therapy. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 419, 113461.	2.0	1
13040	Singlet-to-Triplet Spin Transitions Facilitate Selective 1-Butene Formation during Ethylene Dimerization in Ni(II)-MFU-4l. <i>Journal of Physical Chemistry C</i> , 2021, 125, 22036-22043.	1.5	5
13041	DFT investigation on electronic structure, chemical bonds and optical properties of Cu ₆ (SR) ₆ nanocluster. <i>Chemical Physics Letters</i> , 2021, 780, 138898.	1.2	3
13042	First selective one-stage transformation of A4-to A3B- type Phthalocyanine. <i>Dyes and Pigments</i> , 2021, 194, 109571.	2.0	0

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13043	A cobalt (II)-based semiconductor complex with two-channel slow magnetic relaxation. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 536, 168140.	1.0	10
13044	New heterobimetallic Cu(II)/Mn(II) complexes with trans-1,8-cyclam derivatives: Synthesis, characterization, magnetic properties and crystal structures of (Au ₂ -Chloro)-(dpc)-copper(II)-trichloro-manganese(II) and two polymorphs of (Au ₂ -Chloro)-(dac)-copper(II)-trichloro-manganese(II). <i>Journal of Molecular Structure</i> , 2021, 1241, 130592.	1.8	1
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13047	Adsorption of alkali and alkaline earth ions on nanocages using density functional theory. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113391.	1.1	35
13048	Cationic ruthenium(II)-NHC pincer complexes with hemilabile COD: Solid-state structural characterization and theoretical study of an 1-2-(E,Z)-COD ligand. <i>Journal of Organometallic Chemistry</i> , 2021, 953, 122061.	0.8	7
13049	Revisiting UF ₆ , NpF ₆ and PuF ₆ for bonding and molecular surface analysis within density functional theory: Comparative study at the different theory levels with the same basis set. <i>Polyhedron</i> , 2021, 209, 115452.	1.0	2
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13052	Gas-liquid interface influencing electronic structure of phenol based on molecular dynamics simulations and theoretical X-ray absorption spectroscopy. <i>Journal of Molecular Liquids</i> , 2021, 341, 117378.	2.3	3
13053	A rotational study of the 1:1 adduct of ethanol and 1,4-dioxane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 261, 120086.	2.0	2
13054	A critical evaluation of [ML(ONO)] ⁺ (M = Fe, Ru, Os) as nitric oxide precursor influenced by spin multiplicity and geometrical parameters (M-O-NO and MO-N-O) for the NO release: A theoretical study. <i>Inorganica Chimica Acta</i> , 2021, 527, 120584.	1.2	2
13055	The influence of intermolecular correlations on the infrared spectrum of liquid dimethyl sulfoxide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 260, 119869.	2.0	9
13056	Configurational isomerism in asymmetrically substituted acylthiourea-based Co(III) complexes; new crystallographic, ⁵⁹ Co NMR, Hirshfeld surface and computational insights. <i>Journal of Molecular Structure</i> , 2021, 1244, 131009.	1.8	4
13057	New mononuclear gold(III) complexes: Synthesis, characterization, kinetic, mechanistic, DNA/BSA/HSA binding, DFT and molecular docking studies. <i>Polyhedron</i> , 2021, 209, 115446.	1.0	6
13058	Predicting both lower and upper flammability limits for fuel mixtures from molecular structures with same descriptors. <i>Chemical Engineering Research and Design</i> , 2021, 155, 177-183.	2.7	4
13059	Correlation between bonding, philicity and substituent effects in cyclopropenylidenes. <i>Computational and Theoretical Chemistry</i> , 2021, 1205, 113437.	1.1	4
13060	Stress degradation mechanism of coal macromolecular structure: Insights from molecular dynamics simulation and quantum chemistry calculations. <i>Fuel</i> , 2021, 303, 121258.	3.4	18

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13061	Assembly of Di-, Tetra- and Hexanuclear Organostannoxanes Using Hemi Labile Intramolecular Nâ†Sn Coordination: Synthesis, Structure, DFT and Antibacterial Studies. <i>Polyhedron</i> , 2021, 209, 115487.	1.0	7
13062	Evaluation of silicon tetrahalide precursors for low-temperature thermal atomic layer deposition of silicon nitride. <i>Applied Surface Science</i> , 2021, 565, 150603.	3.1	13
13063	Experimental and theoretical investigations into the manifestation of the Î³-effect in 2- and	0.8	0
13064	Effective removal of water-soluble methylated arsenic contaminants with phosphorene oxide nanoflakes: A DFT study. <i>Journal of Molecular Liquids</i> , 2021, 341, 117423.	2.3	3
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13068	Influence of the amine donor on hybrid guanidine-stabilized Bis(Î¼-oxido) dicopper(III) complexes and their tyrosinase-like oxygenation activity towards polycyclic aromatic alcohols. <i>Journal of Inorganic Biochemistry</i> , 2021, 224, 111541.	1.5	7
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13070	Ngn (Ng= Ne, Ar, Kr, Xe, and Rn; n=1, 2) encapsulated porphyrin-like porous C24N24 fullerene: A quantum chemical study. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 108, 107986.	1.3	30
13071	A molecular modeling of iodinated organic compounds. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 108, 107985.	1.3	2
13072	Synthesis, spectral characterization, SC-XRD, HSA, DFT and catalytic activity of a dioxidomolybdenum complex with aminosalicyl-hydrazone Schiff base ligand: An experimental and theoretical approach. <i>Polyhedron</i> , 2021, 208, 115428.	1.0	29
13073	Sulphido bridged dinuclear quadruple bond cleavage product from the reaction between Re2(Åu-O2CCH3)4Cl2 and dithiocarbamate: An experimental and theoretical study. <i>Polyhedron</i> , 2021, 208, 115422.	1.0	0
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13075	Highly selective and sensitive optical discrimination of pyrophosphate ion by a Zn(II)-terpyridine complex in aqueous medium at physiological pH. <i>Journal of Molecular Structure</i> , 2021, 1243, 130868.	1.8	4
13076	Heteroleptic complexes of Ni(II) with 2,2'-bipyridine and benzoato ligands. Magnetic properties of [Ni(bpy)(Bz)2]. <i>Inorganica Chimica Acta</i> , 2021, 527, 120588.	1.2	9
13077	Experimental and theoretical studies of new dioxomolybdenum complex: Synthesis, characterization and application as an efficient homogeneous catalyst for the selective sulfoxidation. <i>Inorganica Chimica Acta</i> , 2021, 527, 120568.	1.2	28
13078	Oxygen-mediated oxidation of ferrous nitrosylated nitrobindins. <i>Journal of Inorganic Biochemistry</i> , 2021, 224, 111579.	1.5	10

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13080	p-Block Heterobenzenes: Recurring Features in Structural, Vibrational, Electronic and Topological Properties. <i>Journal of Molecular Structure</i> , 2021, 1245, 131258.	1.8	1
13081	Synthesis, characterization, molecular structure, and computational studies on 4(1H)-pyran-4-one and its derivatives. <i>Journal of Molecular Structure</i> , 2021, 1245, 131077.	1.8	2
13082	Influence of progressive halogenation of Zn(II)-tetraarylporphyrins and their free bases on the structure and spectral-fluorescence properties of tetrapyrrolic macrocycle. <i>Inorganica Chimica Acta</i> , 2021, 528, 120620.	1.2	1
13083	Revisiting exo \rightarrow endo isomerization of transition metal half-sandwich η^3 -allyl complexes. <i>Journal of Organometallic Chemistry</i> , 2021, 954-955, 122076.	0.8	1
13084	Metal organic frameworks as sacrificial templates for preparation of hierarchical covalent organic frameworks enabling ultrafast sample treatment in nontargeted food safety analysis. <i>Chemical Engineering Journal</i> , 2021, 425, 130673.	6.6	4
13085	Chirality, structure and hydrogen bonding in dithiols: Rotational spectrum of the chiral and meso 2,3-butanedithiol. <i>Journal of Molecular Structure</i> , 2021, 1246, 131221.	1.8	1
13086	Quantification and understanding of non-covalent interactions in molecular and ionic systems: Dispersion interactions and hydrogen bonding analysed by thermodynamic methods. <i>Journal of Molecular Liquids</i> , 2021, 343, 117547.	2.3	13
13087	Synthesis, spectra (FT-IR, NMR) investigations, DFT, FMO, MEP, NBO analysis and catalytic activity of MoO ₂ (VI) complex with ONO tridentate hydrazone Schiff base ligand. <i>Journal of Molecular Structure</i> , 2021, 1245, 131259.	1.8	34
13088	Synthesis of [(CO) ₅ MS=CFcCH ₃] and exploration of the nature of M-S vs. M-O bonds in [(CO) ₅ ME=CFcCH ₃]; (M=Cr, Mo, W and E=O, S) complexes. <i>Journal of Organometallic Chemistry</i> , 2021, 954-955, 122080.	0.8	0
13089	Hydride- and boron-free solid hypergolic H ₂ O ₂ -ignitophores. <i>Chemical Engineering Journal</i> , 2021, 426, 131806.	6.6	13
13090	Adsorption of diatomic molecules on nitrogenated holey graphene: Theoretical insights. <i>Surfaces and Interfaces</i> , 2021, 27, 101446.	1.5	1
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13092	Palladium determination with a new dye PNBTAN: Structural, UV-VIS, and DFT study. <i>Journal of Molecular Structure</i> , 2021, 1246, 131150.	1.8	4
13093	Boosting Photo-Fenton reactions by amidoxime chelated ferrous iron (Fe(III)) catalyst for highly efficient pollutant control. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120574.	10.8	11
13094	Improved NH ₃ -N conversion efficiency to N ₂ activated by BDD substrate on NiCu electrocatalysis process. <i>Separation and Purification Technology</i> , 2021, 276, 119350.	3.9	12
13095	Towards a symmetric reversible single-molecule switch: Amino-imino-cyclo-n-enes. <i>Chemical Physics Impact</i> , 2021, 3, 100035.	1.7	1
13096	Metalloid Chalcogen \rightarrow pnictogen σ -hole bonding competition in stibanyl telluranes. <i>Journal of Organometallic Chemistry</i> , 2021, 954-955, 122092.	0.8	5

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13097	Reticular chemistry approach to explore the catalytic CO ₂ -epoxide cycloaddition reaction over tetrahedral coordination Lewis acidic sites in a Rutile-type Zinc-phosphonocarboxylate framework. <i>Chemical Engineering Journal</i> , 2022, 427, 131759.	6.6	20
13098	Ru(III) single site solid micellar catalyst for selective aqueous phase hydrogenation of carbonyl groups in biomass-derived compounds. <i>Applied Catalysis B: Environmental</i> , 2022, 300, 120730.	10.8	12
13099	N-substituted sumanene and cation- π interactions towards Li cations: A theoretical study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 135, 114949.	1.3	7
13100	Mechanochemical bromination of unburned carbon in fly ash and its mercury removal mechanism: DFT study. <i>Journal of Hazardous Materials</i> , 2022, 423, 127198.	6.5	19
13101	Controllable synthesis of uniform large-sized spherical covalent organic frameworks for facile sample pretreatment and as naked-eye indicator. <i>Talanta</i> , 2022, 236, 122829.	2.9	15
13102	The construction and application of asphalt molecular model based on the quantum chemistry calculation. <i>Fuel</i> , 2022, 308, 122037.	3.4	26
13103	Unravelling the effects of complexation of transition metal ions on the hydroxylation of catechol over the whole pH region. <i>Journal of Environmental Sciences</i> , 2022, 115, 392-402.	3.2	7
13104	Structural elucidation of the antitubercular benzothiazinone BTZ043: A combined X-ray, variable temperature NMR and DFT study. <i>Journal of Molecular Structure</i> , 2022, 1248, 131419.	1.8	3
13105	Molecular dynamics study of droplet electrocoalescence in the oil phase and the gas phase. <i>Separation and Purification Technology</i> , 2021, 278, 119622.	3.9	17
13106	Balanced lipase interactions for degradation-controlled paclitaxel release from lipid cubic phase formulations. <i>Journal of Colloid and Interface Science</i> , 2022, 607, 978-991.	5.0	4
13107	Innovative computationally designed-spectrofluorimetric method for determination of modafinil in tablets and human plasma. <i>Talanta</i> , 2022, 236, 122890.	2.9	3
13108	Strongly polarized light from highly aligned electrospun luminescent natural rubber fibers. <i>Journal of Luminescence</i> , 2022, 241, 118498.	1.5	3
13109	Theoretical research on mercury-laden halogenated activated carbon adsorbent bonding nature. <i>Chemical Engineering Journal</i> , 2022, 428, 131076.	6.6	8
13110	Synthesis, physicochemical properties, crystal molecular structure and DFT investigation of an organobismuth(III) bis(dimethyldithiocarbamate) and its organolithium precursor. <i>Journal of Molecular Structure</i> , 2022, 1247, 131335.	1.8	1
13111	Probing reactions between imipramine and hydroxyl radical with the photolysis of iron(III) oxalate: Implications for the indirect photooxidation of tricyclic antidepressants in waters. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 422, 113559.	2.0	5
13112	N-Donor stabilized tin(II) cations as efficient ROP catalysts for the synthesis of linear and star-shaped PLAs via the activated monomer mechanism. <i>Dalton Transactions</i> , 2021, 50, 16039-16052.	1.6	5
13113	<i>peri</i> -Acenoacene molecules: tuning of the singlet and triplet excitation energies by modifying their radical character. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24016-24028.	1.3	5
13114	Chemistry of group 5 metallaboranes with heterocyclic thiol ligands: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2021, 50, 4036-4044.	1.6	4

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13116	Boron–noble gas covalent bonds in borenium and boronium compounds. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6896-6902.	1.3	7
13117	Accurate correlation energy functional for uniform electron gas from an interpolation ansatz without fitting parameters. <i>Physical Review B</i> , 2021, 103, .	1.1	2
13118	Computational predictions of metal–macrocycle stability constants require accurate treatments of local solvent and pH effects. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9189-9197.	1.3	4
13119	Dual emissive dinuclear Pt(II) complexes and application to singlet oxygen generation. <i>Journal of Materials Chemistry C</i> , 2021, 9, 5808-5818.	2.7	10
13120	Furil-based ionic small molecules for green-emitting non-doped LECs with improved color purity. <i>New Journal of Chemistry</i> , 2021, 45, 12576-12584.	1.4	4
13121	Quinol-containing ligands enable high superoxide dismutase activity by modulating coordination number, charge, oxidation states and stability of manganese complexes throughout redox cycling. <i>Chemical Science</i> , 2021, 12, 10483-10500.	3.7	15
13122	Titanium complexes of pyrrolylaldimine ligands and their exploitation for the ring-opening polymerization of cyclic esters. <i>Dalton Transactions</i> , 2021, 50, 10964-10981.	1.6	7
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13124	A new bis-pyrazolylpyridine ruthenium(III) complex as a potential anticancer drug: in vitro and in vivo activity in murine colon cancer. <i>Dalton Transactions</i> , 2021, 50, 7686-7704.	1.6	6
13125	Synthesis, crystal structure, magnetic, spectroscopic, and theoretical investigations of two new nitronyl-nitroxide complexes. <i>Journal of Coordination Chemistry</i> , 2021, 74, 279-293.	0.8	5
13126	Synthesis, structural characterization, and bonding analysis of two-coordinate copper(I) and silver(I) complexes of pyrrole-based bis(phosphinimine): new metal–pyrrole ring π -interactions. <i>Dalton Transactions</i> , 2021, 50, 8036-8044.	1.6	6
13127	Thermo- and photoinduced spin state switching in an iron(II) 2D coordination network associated with large light-induced thermal hysteresis and tuning of dimensionality via ligand modulation. <i>Dalton Transactions</i> , 2021, 50, 7725-7735.	1.6	12
13128	$\text{O}^{\cdot-}$ -Semiquinone radical anion isolated as an amorphous porous solid. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17408-17419.	1.3	5
13129	Impact of Solvent Polarity on the Ligand Configuration in Tetravalent Thorium N-Donor Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 1092-1098.	1.9	2
13130	Random-Phase Approximation in Many-Body Noncovalent Systems: Methane in a Dodecahedral Water Cage. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 804-817.	2.3	6
13131	Delivery of Electrons by Proton-Hole Transfer in Ice at 10 K: Role of Surface OH Radicals. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 704-710.	2.1	6
13132	Selenium chalcogen bonds are involved in protein–carbohydrate recognition: a combined PDB and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17656-17662.	1.3	14

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13134	The influence mechanism of the molecular structure on the peak current and peak potential in electrochemical detection of typical quinolone antibiotics. Physical Chemistry Chemical Physics, 2021, 23, 13873-13877.	1.3	7
13135	A quinone based single-molecule switch as building block for molecular electronics. Physical Chemistry Chemical Physics, 2021, 23, 1811-1814.	1.3	3
13136	Bi- and trinuclear coinage metal complexes of a PNNP ligand featuring metallophilic interactions and an unusual charge separation. Dalton Transactions, 2021, 50, 13412-13420.	1.6	14
13137	Computational Investigation of Adsorptive Removal of Pb ²⁺ from Water by the UiO-66 Metal-Organic Framework: Comparison of Adsorption Sites on Defects and Functionalised Linkers. Australian Journal of Chemistry, 2021, , .	0.5	1
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13139	Manganese(II) bromo- and iodo-complexes with phosphoramidate and phosphonate ligands: synthesis, characterization and photoluminescence. New Journal of Chemistry, 2021, 45, 12871-12878.	1.4	16
13140	Computational study on the reactivity of imidazolium-functionalized manganese bipyridyl tricarbonyl electrocatalysts [Mn(bpyMe(lm-R))(CO) ₃ Br] ⁺ (R = Me, Me ₂) and Tj ETQq1 1.0.784314 rgBT / Ov Chemistry Chemical Physics, 2021, 23, 14940-14951.	1.3	6
13141	Unmasking the elusive 1,4-diazabutatrienes: the stabilizing role of the N-substituents. Physical Chemistry Chemical Physics, 2021, 23, 6091-6097.	1.3	3
13142	Investigating the effect of Î±-pinene on the ROMP of Î±-pinene. Polymer Chemistry, 2021, 12, 5048-5058.	1.9	7
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13146	Substituted aromatic pentaphosphole ligands " a journey across the p-block. Chemical Science, 2021, 12, 13037-13044.	3.7	10
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13148	Quantifying Uncertainties in Solvation Procedures for Modeling Aqueous Phase Reaction Mechanisms. Journal of Physical Chemistry A, 2021, 125, 154-164.	1.1	24
13149	Organic Mixed-Valence Compounds and the Overhauser Effect in Insulating Solids. Journal of Physical Chemistry A, 2021, 125, 867-874.	1.1	11
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13152	Diethylammonium iodide as catalyst for the metal-free synthesis of 5-aryl-2-oxazolidinones from aziridines and carbon dioxide. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 4152-4161.	1.5	12
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