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1783	Probing the Properties of Polynuclear Superhalogens without Halogen Ligand via ab Initio Calculations: A Case Study on Double-Bridged [Mg2 (CN)5 ](-1) Anions. <b>2015</b> , 16, 3652-9	24
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1780	Efficient global optimization of reactive force-field parameters. <b>2015</b> , 36, 1550-61	37
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1777	Core Halogenation as a Construction Principle in Tuning the Material Properties of Tetraazaperopyrenes. <b>2015</b> , 21, 17691-700	26
1776	Mechanistic insights on the iodine(III)-mediated Exidation of ketones. <b>2015</b> , 21, 11206-11	57
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1774	Mechanistic Aspects of Aryl-Halide Oxidative Addition, Coordination Chemistry, and Ring-Walking by Palladium. <b>2015</b> , 21, 16113-25	8
1773	Molecular modeling of bioorganometallic compounds: thermodynamic properties of molybdocene-glutathione complexes and mechanism of Peptide hydrolysis. <b>2015</b> , 16, 1646-56	2
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1769	Complementing the characterization of in vivo generated N-glucuronic acid conjugates of stanozolol by collision cross section computation and analysis. <b>2015</b> , 7, 1050-6	12
1768	Monoanionic Dipyrrin <b>B</b> yridine Ligands: Synthesis, Structure and Photophysical Properties. <b>2015</b> , 2015, 5405-5410	12
1767	Determination of the Relative Configuration of EAmino Acid Esters Based on Residual Dipolar Couplings. <b>2015</b> , 2015, 6801-6805	3
1766	Mechanism of proteolysis in matrix metalloproteinase-2 revealed by QM/MM modeling. <b>2015</b> , 36, 1621-30	28

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1764	Highly antiplasmodial non-natural oxidative products of dioncophylline A: synthesis, absolute configuration, and conformational stability. <b>2015</b> , 21, 14507-18	11
1763	Effect of the Metal on Disulfide/Thiolate Interconversion: Manganese versus Cobalt. <b>2015</b> , 21, 18770-8	15
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1753	Going clean: structure and dynamics of peptides in the gas phase and paths to solvation. <b>2015</b> , 27, 493002	26
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1750	Computational study of a model system of enzyme-mediated [4+2] cycloaddition reaction. <b>2015</b> , 10, e0119984	18
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1744	Luminescent copper(I) halide and pseudohalide phenanthroline complexes revisited: simple structures, complicated excited state behavior. <b>2015</b> , 44, 6944-60	37
1743	Mixed-valent, heteroleptic homometallic diketonates as templates for the design of volatile heterometallic precursors. <b>2015</b> , 6, 2835-2842	18
1742	Reactive force fields made simple. <b>2015</b> , 17, 16715-8	20
1741	Dynamic structure elucidation of chemical reactivity by laser pulses and X-ray probes. <b>2015</b> , 44, 6313-9	2
1740	A general non-Abelian density matrix renormalization group algorithm with application to the C2 dimer. <b>2015</b> , 142, 024107	27
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1737	Nitroaminofurazans with Azo and Azoxy Linkages: A Comparative Study of Structural, Electronic, Physicochemical, and Energetic Properties. <b>2015</b> , 119, 12887-12895	84
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1730	X-ray Absorption and Emission Study of Dioxygen Activation by a Small-Molecule Manganese Complex. <b>2015</b> , 54, 6410-22	42

1729	54, 6245-56	43
1728	Synthesis and spectroscopic characterization of diorganotin(IV) complexes of N?-(4-hydroxypent-3-en-2-ylidene)isonicotinohydrazide: chemotherapeutic potential validation by in vitro interaction studies with DNA/HSA, DFT, molecular docking and cytotoxic activity. <b>2015</b> , 5, 50673-5069	56 <b>0</b>
1727	From Chiral Islands to Smectic Layers: A Computational Journey Across Sexithiophene Morphologies on C60. <b>2015</b> , 25, 1985-1995	28
1726	Electronic Structures of Ilow-ValentINeutral Complexes [NiL2]0 (S = 0; L = bpy, phen, tpy) IAn Experimental and DFT Computational Study. <b>2015</b> , 2015, 1511-1523	24
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1724	On Predicting the Excited-State Properties of Thermally Activated Delayed Fluorescence Emitters. <b>2015</b> , 119, 13535-13544	125
1723	Hydrogen bond donation to the heme distal ligand of Staphylococcus aureus IsdG tunes the electronic structure. <b>2015</b> , 20, 757-70	11
1722	Understanding natural semiquinone radicalsmultifrequency EPR and relativistic DFT studies of the structure of Hg(II) complexes. <b>2015</b> , 119, 479-484	10
1721	Iron Complexes of a Macrocyclic N-Heterocyclic Carbene/Pyridine Hybrid Ligand. 2015, 34, 2819-2825	39
1720	Exploration of the active site of <code>AGalT7</code> : modifications of the aglycon of aromatic xylosides. <b>2015</b> , 13, 3351-62	22
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1717	A mononuclear Ni(ii) complex: a field induced single-molecule magnet showing two slow relaxation processes. <b>2015</b> , 44, 12484-7	104
1716	Anomalous orbital admixture in ammine complexes. <b>2015</b> , 792, 6-12	5
1715	Managing Complexity in Distributed Data Life Cycles Enhancing Scientific Discovery. 2015,	8
1714	The FeW Cofactor of Vanadium Nitrogenase Contains an Interstitial Carbon Atom. <b>2015</b> , 127, 13447-13450	8
1713	The Fe-V Cofactor of Vanadium Nitrogenase Contains an Interstitial Carbon Atom. <b>2015</b> , 54, 13249-52	62
1712	Liponitroxides: EPR study and their efficacy as antioxidants in lipid membranes. <b>2015</b> , 5, 98955-98966	9

1711	Experimental and theoretical studies on extraction behavior of di-n-alkyl phosphine oxides towards actinides. <b>2015</b> , 5, 107421-107429	19
1710	Theoretical insights into structure, bonding, reactivity and importance of ion-pair interactions in Kirby's tetrafluoroboric acid salts of twisted amides. <b>2015</b> , 5, 105668-105677	2
1709	Time-Dependent Density Functional Theory Study of Low-Lying Absorption and Fluorescence Band Shapes for Phenylene-Containing Oligoacenes. <b>2015</b> , 119, 12706-14	8
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1703	Four-Component Relativistic Density Functional Theory Calculations of EPR g- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spin-Orbit Effects. <b>2015</b> , 119, 12892-905	38
1702	Strategy for Enhancement of (13)C-Photo-CIDNP NMR Spectra by Exploiting Fractional (13)C-Labeling of Tryptophan. <b>2015</b> , 119, 13934-43	3
1701	Structure, Bonding, and Stability of Mercury Complexes with Thiolate and Thioether Ligands from High-Resolution XANES Spectroscopy and First-Principles Calculations. <b>2015</b> , 54, 11776-91	40
1700	Illustrating Concepts in Physical Organic Chemistry with 3D Printed Orbitals. <b>2015</b> , 92, 2113-2116	44
1699	Surface site coordination dependent responses resolved in free clusters: applications for neutral sub-nanometer cluster studies. <b>2015</b> , 17, 7012-22	8
1698	Dispersion-Corrected Relativistic Density Functional Theory (DFT) Calculations of Structure and (119)Sn MBsbauer Parameters for M?SnR Bonding in Filippou's Stannylidyne Complexes of Molybdenum and Tungsten. <b>2015</b> , 54, 10849-54	2
1697	Fluorination-dependent molecular orbital occupancy in ring-shaped perfluorocarbons. <b>2015</b> , 17, 18337-43	5
1696	Optimization and prediction of the electron-nuclear dipolar and scalar interaction in H and C liquid state dynamic nuclear polarization. <b>2015</b> , 6, 6482-6495	21
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1694	New massively parallel linear-response coupled-cluster module in ACES III: application to static polarisabilities of closed-shell molecules and oligomers and of open-shell radicals. <b>2015</b> , 1-15	1

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1693	Single-stage synthesis of 3-hydroxy- and 3-alkoxy-5-arylimidazolidine-2,4-diones by reaction of arylglyoxal hydrates with N-hydroxy- and N-alkoxyureas. <b>2015</b> , 51, 553-559	4
1692	The Nonlocal Correlation Density Functional VV10. <b>2015</b> , 11, 37-102	17
1691	Spectroscopic Evidence for Through-Space Arene-Sulfur-Arene Bonding Interaction in m-Terphenyl Thioether Radical Cations. <b>2015</b> , 119, 12990-8	5
1690	Structural and Optical Properties of Point Defects in ∃SiO 2 Cluster. <b>2015</b> , 64, 244-248	6
1689	Theoretical Investigation of the Reaction Paths of the Aluminum Cluster Cation with Water Molecule in the Gas Phase: A Facile Route for Dihydrogen Release. <b>2015</b> , 119, 8683-91	8
1688	Aggregation of photosensitizers: the role of dispersion and solvation on dimer formation energetics. <b>2015</b> , 134, 1	11
1687	Structural, magnetic, thermal and visible light-driven water oxidation studies of heterometallic Mn/V complexes. <b>2015</b> , 88, 81-89	13
1686	Theoretical rationalization of the singlet-triplet gap in OLEDs materials: impact of charge-transfer character. <b>2015</b> , 11, 168-77	86
1685	Molecular origin of enhanced proton conductivity in anhydrous ionic systems. <b>2015</b> , 137, 1157-64	37
1684	Mapping the HO3 ground state potential energy surface with DFT: Can we reproduce the MRCI+Q/CBS data?. <b>2015</b> , 620, 61-66	4
1683	A nickel phosphine complex as a fast and efficient hydrogen production catalyst. <b>2015</b> , 137, 1109-15	116
1682	Integrated Ugi-based assembly of functionally, skeletally, and stereochemically diverse 1,4-benzodiazepin-2-ones. <b>2015</b> , 80, 1533-49	31
1681	Theoretical study on the reaction of . <b>2015</b> , 620, 82-87	1
1680	NTChem: A high-performance software package for quantum molecular simulation. <b>2015</b> , 115, 349-359	45
1679	Hydrogen bond network between amino acid radical intermediates on the proton-coupled electron transfer pathway of E. coli ♣ ribonucleotide reductase. <b>2015</b> , 137, 289-98	56
1678	New ruthenium nitrosyl pincer complexes bearing an O2 ligand. Mono-oxygen transfer. <b>2015</b> , 54, 2253-63	10
1677	Synthesis and photophysical properties of a "face-to-face" stacked tetracene dimer. <b>2015</b> , 17, 6523-31	43
1676	MBius-Hākel topology switching in an expanded porphyrin cation radical as studied by EPR and ENDOR spectroscopy. <b>2015</b> , 17, 6644-52	17

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1674	The Association of Two BrustratedLewis Pairs by State-of-the-Art Quantum Chemical Methods. <b>2015</b> , 55, 235-242	20
1673	Prato and Bingel-Hirsch cycloaddition to heptagon-containing LaSc2N@C(s)(hept)-C80: importance of pentalene units. <b>2015</b> , 51, 5637-40	8
1672	Rational design of long-wavelength absorbing and emitting carbostyrils aided by time-dependent density functional calculations. <b>2015</b> , 1055, 25-32	3
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1668	Multinuclear diffusion NMR spectroscopy and DFT modeling: a powerful combination for unraveling the mechanism of phosphoester bond hydrolysis catalyzed by metal-substituted polyoxometalates. <b>2015</b> , 21, 4428-39	39
1667	Identification of a second GTP-bound magnesium ion in archaeal initiation factor 2. <b>2015</b> , 43, 2946-57	18
1666	Relationship between coupling constants in Heisenberg exchange Hamiltonian and Ising model. <b>2015</b> , 621, 102-108	10
1665	Accurate Treatment of Large Supramolecular Complexes by Double-Hybrid Density Functionals Coupled with Nonlocal van der Waals Corrections. <b>2015</b> , 11, 932-9	38
1664	Counterion Effect in the Reaction Mechanism of NHC Gold(I)-Catalyzed Alkoxylation of Alkynes: Computational Insight into Experiment. <b>2015</b> , 5, 803-814	86
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1661	Ultrafast Photoinduced Electron Transfer from Peroxide Dianion. <b>2015</b> , 119, 7422-9	10
1660	EPR and Quantum Chemical Investigation of a Bioinspired Hydrogenase Model with a Redox-Active Ligand in the First Coordination Sphere. <b>2015</b> , 34, 995-1000	12
1659	Synthesis, Spectroscopic and Theoretical Studies of Ruthenafuran and Osmafuran Prepared by Activation of Ynone in Alcohol. <b>2015</b> , 34, 1005-1012	26
1658	Unusual Mechanism for the Reaction of a Niobocene Hydride Complex with Activated Alkynes. Experimental and DFT Studies. <b>2015</b> , 34, 2695-2698	6

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1656	Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the CBS-QB3 composite method and their consequences in DFT benchmark studies. <b>2015</b> , 36, 622-32	92
1655	Stable bis(trifluoromethyl)nickel(III) complexes. <b>2015</b> , 51, 3113-6	31
1654	Synthesis, Structure, and Reactivity of Pentamethylcyclopentadienyl 2,4,6-Triphenylphosphinine Iron Complexes. <b>2015</b> , 34, 622-635	11
1653	High-frequency and -field electron paramagnetic resonance of vanadium(IV, III, and II) complexes. <b>2015</b> , 301-302, 123-133	42
1652	Modeling of catalytically active metal complex species and intermediates in reactions of organic halides electroreduction. <b>2015</b> , 17, 5594-605	1
1651	Unprecedented ring-ring interconversion of N,P,C-cage ligands. <b>2015</b> , 21, 3727-35	15
1650	Spin Filter Circuit Design Based on a Finite Single-Walled Carbon Nanotube of the Zigzag Type. <b>2015</b> , 119, 3740-3745	1
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1648	Soft-landing electrospray ion beam deposition of sensitive oligoynes on surfaces in vacuum. <b>2015</b> , 377, 228-234	15
1647	Natural abundance 15N NMR by dynamic nuclear polarization: fast analysis of binding sites of a novel amine-carboxyl-linked immobilized dirhodium catalyst. <b>2015</b> , 21, 3798-805	52
1646	The origin of the absorption spectra of porphyrin N- and dithiaporphyrin S-oxides in their neutral and protonated states. <b>2015</b> , 17, 3560-9	9
1645	Metal oxidation states in biological water splitting. <b>2015</b> , 6, 1676-1695	225
1644	Experimental benchmark data and systematic evaluation of two a posteriori, polarizable-continuum corrections for vertical excitation energies in solution. <b>2015</b> , 119, 5446-64	97
1643	Ring opening of donor-acceptor cyclopropanes with the azide ion: a tool for construction of N-heterocycles. <b>2015</b> , 21, 4975-87	114
1642	An iridium N-heterocyclic carbene complex [IrCl(CO)2(NHC)] as a carbon monoxide-releasing molecule (CORM). <b>2015</b> , 782, 116-123	12
1641	Estimating orientation factors in the FRET theory of fluorescent proteins: the TagRFP-KFP pair and beyond. <b>2015</b> , 108, 126-32	19
1640	Tyrosine-glycine revisited: Resolving the discrepancy between theory and experiment. <b>2015</b> , 621, 124-128	6

1639	Syntheses, structural, magnetic, and electron paramagnetic resonance studies of monobridged cyanide and azide dinuclear copper(II) complexes: antiferromagnetic superexchange interactions. <b>2015</b> , 54, 1487-500	22
1638	Photophysical and quantum chemical studies on the interactions of oxazine-1 dye with cucurbituril macrocycles. <b>2015</b> , 119, 3046-57	26
1637	Carbide clusterfullerenes with odd number of carbon atoms: molecular and electronic structures of Sc4C@C80, Sc4C@C82, and Sc4C3@C80. <b>2015</b> , 134, 1	6
1636	Naphtho[4,3,2,1-lmn][2,9]phenanthrolines: Synthesis, flaracterization, optical properties and light-induced electron transfer in composites with the semiconducting polymer MEH-PPV. <b>2015</b> , 201, 43-48	8
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1634	Energetic salts with Estacking and hydrogen-bonding interactions lead the way to future energetic materials. <b>2015</b> , 137, 1697-704	263
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1632	The electronic structure and charge transfer excited states of the endohedral trimetallic nitride C80 (I(h)) fullerenes-Zn-tetraphenyl porphyrin dyads. <b>2015</b> , 17, 5832-9	14
1631	Dynamics of N2 Dissociation upon Inner-Valence Ionization by Wavelength-Selected XUV Pulses. <b>2015</b> , 6, 419-25	37
1630	Multiple orbital effects and magnetic ordering in a neutral radical. 2015, 137, 1044-7	23
1629	Density functional calculations of molecular structures of arsenic-binding 田omain of metallothioneins-2. <b>2015</b> , 1058, 54-60	2
1628	The ab-initio density matrix renormalization group in practice. <b>2015</b> , 142, 034102	214
1627	Magnetic circular dichroism and computational study of mononuclear and dinuclear iron(IV) complexes. <b>2015</b> , 6, 2909-2921	22
1626	Pyrene-based dyad and triad leading to a reversible chemical and redox optical and magnetic switch. <b>2015</b> , 21, 5504-9	5
1625	On the gold-ligand covalency in linear [AuX2](-) complexes. <b>2015</b> , 44, 5535-46	20
1624	Synthesis, structure, theoretical studies and luminescent properties of a ternary erbium(III) complex with acetylacetone and bathophenanthroline ligands. <b>2015</b> , 162, 41-49	12
1623	Theories of phosphorescence in organo-transition metal complexes From relativistic effects to simple models and design principles for organic light-emitting diodes. <b>2015</b> , 295, 46-79	83
1622	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. <b>2015</b> , 11, 1525-39	389

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1621	The effect of spinBrbit coupling on selenadiazolo- and thiadiazolo- fused 1,10-phenanthrolines. <b>2015</b> , 117, 149-156	7
1620	Electronic structure calculations of ESR parameters of melanin units. <b>2015</b> , 17, 7264-74	26
1619	Reversing the relative 3MLCT-3MC order in Fe(ii) complexes using cyclometallating ligands: a computational study aiming at luminescent Fe(ii) complexes. <b>2015</b> , 44, 13498-503	40
1618	Suppressing of slow magnetic relaxation in tetracoordinate Co(II) field-induced single-molecule magnet in hybrid material with ferromagnetic barium ferrite. <b>2015</b> , 5, 10761	23
1617	Adsorption and dissociation of H2O on the Ga-rich GaAs(001)-(42) surface: DFT and DFT-D computations with a Ga7As8H11 cluster model. <b>2015</b> , 1064, 51-55	4
1616	Heterometallic Second-Row Transition Metal Chain Compounds in Two Charge States: Syntheses, Properties, and Electronic Structures of [Mo-Mo-Ru](6+/7+) Chains. <b>2015</b> , 54, 7660-5	18
1615	Reaction barrier heights for cycloreversion of heterocyclic rings: An Achilles Theel for DFT and standard ab initio procedures. <b>2015</b> , 458, 1-8	51
1614	Symmetric bent-shaped liquid crystal dimers showing transitions between optically uniaxial and biaxial smectic phases. <b>2015</b> , 42, 1013-1023	12
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746	Graph Theoretic Molecular Fragmentation for Multidimensional Potential Energy Surfaces Yield an Adaptive and General Transfer Machine Learning Protocol.	0
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731	Halogen Atom Participation in Guiding the Stereochemical Outcomes of Acetal Substitution Reactions.	
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726	Generation of fluoro(thio)carbenes from Me3SiCF2SAr. <b>2022</b> , 261-262, 110025	
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724	One-pot fabrication of petroleum pitch derived hierarchical porous carbon via a recyclable MgO-templating strategy for p-nitrophenol removal. <b>2022</b> , 10, 108458	O
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720	A neglected pathway for the accretion products formation in the atmosphere. <b>2022</b> , 848, 157494	
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713	Degradation of three typical hydroxamic acids collectors via UVA-B activated H2O2 and persulfate: Kinetics, transformation pathway, DFT calculation and toxicity evaluation. <b>2023</b> , 451, 138639	O
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710	Dinuclear Copper(I) Complexes Supported by Bis-Tridentate N-Donor-Ligands: Turning-On Tyrosinase Activity.	O
709	Bis(2-hydroxyethyl) 2-phenylsuccinate. <b>2022</b> , 2022, M1456	1
708	Structure and bonding of proximity-enforced main-group dimers stabilized by a rigid naphthyridine diimine ligand.	O
707	A-value revisited: ring flip energy of chair structures in halogenated cyclohexanes by quantum chemical methods.	0
706	Umpolung Reactivity of Imine Ester: Visible-Light Mediated Transfer Hydrogenation of ⊞ryl Imino Esters by Phenylsilane and Water.	О
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704	Magnetism of pseudohalide Ni(II) complexes containing 4-methylpyridine ligands. <b>2022</b> , 227, 116135	O

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702	Theoretical insight and molecular recognition of oxatub[4]arene-based organic macrocycle as a supramolecular host for antipsychotic drug risperidone. <b>2022</b> , 366, 120195	O
701	Application of chemometric method and computational analysis in the spectroscopic study of Azure A dimerization. <b>2022</b> , 366, 120316	0
700	Molecular dynamics simulation of CO2 hydrate growth in salt water. <b>2022</b> , 366, 120237	1
699	Effect of oligothiophene spacer length on photogenerated charge transfer from perylene diimide to boron-doped diamond electrodes. <b>2022</b> , 248, 111984	0
698	Different phosphoric triamide [HN]3-nP(O)[N]n (n´=´1, 2) skeletons lead to identical non-covalent interactions assemblies: X-ray crystallography investigation, Hirshfeld surface analysis and molecular docking study against SARS-CoV-2. <b>2022</b> , 543, 121190	O
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696	CALPHAD modeling of uranium nitride (UN) fabrication routes enabled by first-principles calculations. <b>2022</b> , 79, 102463	O
695	Design of organic materials with tailored optical properties: Predicting quantum-chemical polarizabilities and derived quantities. <b>2023</b> , 653-674	0
694	Zwitterion to normal formation of L-Alanine in water solvation as an ultrasonic impact from their Gibbs energy barrier: Experiment with different molarities and DFT simulation for few basis sets. <b>2023</b> , 127, 106847	О
693	Design and development of conjugated polymer-ferrite composite for selective recognition of NO2 vapors. <b>2023</b> , 1271, 134149	0
692	Radical-promoted room-temperature terminal alkyne activation on Au(111). <b>2023</b> , 727, 122180	Ο
691	Stereospecific redox-mediated clusterization reconstruction for constructing long-lived, color-tunable, and processable phosphorescence cellulose. <b>2023</b> , 451, 138923	0
690	Synthesis, photophysics, and theoretical calculations of styryl-based fluorophores harboring substituted benzothiazole acceptors. <b>2023</b> , 435, 114287	O
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688	Towards determining molecular structure with ESI-MS backed by computational methods: structures of subnanoclusters of Pd and Cu chlorides, ion dynamics in vacuum, and challenges to the methodology.	O
687	Genome mining reveals a new cyclopentane-forming sesterterpene synthase with unprecedented stereo-control.	О
686	A first principles examination of phosphorescence. <b>2022</b> , 12, 25440-25448	0

685	Exchange-driven slow relaxation of magnetization in Nill2LnIII2 (LnIII = Y, Gd, Tb and Dy) butterfly complexes: experimental and theoretical studies. <b>2022</b> , 51, 14721-14733	1
684	DFT insights into superelectrophilic activation of <b>E</b> unsaturated nitriles and ketones in superacids. <b>2022</b> , 20, 6799-6808	O
683	Energetics of carboxylic acidpyridine heterosynthon revisited: A computational study of intermolecular hydrogen bond domination on phenylacetic acidficotinamide cocrystals. <b>2022</b> , 20, 949-957	0
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680	Hybridized Ag-CuCrO2 Nanostructured Composites for Enhanced Gas Sensing. <b>2022</b> , 5, 12690-12698	O
679	Early Lanthanide(III) Ate Complexes Featuring LnBi Bonds (Ln = La, Ce): Synthesis, Structural Characterization, and Bonding Analysis. <b>2022</b> , 61, 14288-14296	1
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677	Discovery of Cyclic Diarylheptanoids as Inhibitors against Influenza A Virus from the Roots of Casuarina equisetifolia. <b>2022</b> , 85, 2142-2148	О
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671	Photocatalytic Carbon Dioxide Reduction and Density Functional Theory Investigation of 2,6-(Pyridin-2-yl)-1,3,5-triazine-2,4-diamine and Its Cobalt and Nickel Complexes. <b>2022</b> , 5, 11077-11090	О
670	2D-FFCASPA New Approach for 2D Structure Prediction Applied to Self-Assemblies of DNA Bases. 2200308	O
669	Solution-Phase Conformational/Vibrational Anharmonicity in Comonomer Incorporation Polyolefin Catalysis. <b>2022</b> , 126, 6858-6869	О
668	Piezo-Responsive Hydrogen-Bonded Frameworks Based on Vanillin-Barbiturate Conjugates. <b>2022</b> , 27, 5659	O

667	A Systemic Insight into Exohedral Actinides and Endohedral Borospherenes: An&Bm and An@Bn (An=U, Np, Pu; $m = 28, 32, 34, 36, 38, 40$ ; $n = 36, 38, 40$ ). <b>2022</b> , 27, 6047	1
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665	Multiconfiguration Pair-Density Functional Theory for Chromium(IV) Molecular Qubits. <b>2022</b> , 2, 2029-2037	1
664	Antimicrobial and antibiofilm activities and bovine serum albumin binding properties of benzimidazolium derivative NHC salts and their Ag(I)-NHC complexes.	O
663	Control over the Hydrophilicity in the Pores of Covalent Organic Framework Membranes for High-Flux Separation of Dyes from Water.	1
662	Enhancement of SO2 sensing performance of micro-ribbon graphene sensors using nitrogen doping and light exposure. <b>2022</b> , 155059	1
661	New Methods for Preparation of the Monofluorosubstituted Derivative of the closo-Borate Anion [2-B10H9F]2[Ilts Properties, and Analysis of Its Reactivity. <b>2022</b> , 67, 1583-1590	O
660	Monitoring the photochemistry of a formazan over 15 orders of magnitude in time. 10,	1
659	Rhenium Selenide Clusters Containing Alkynyl Ligands: Unexpected Reactivity of Bound Phenylacetylide.	O
658	Homoatomic cations: From [P 5 ] + to [P 9 ] +. <b>2022</b> , 8,	2
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649	Auto3D: Automatic Generation of the Low-Energy 3D Structures with ANI Neural Network Potentials.	2
648	2-D Molecular Alloy Ru <b>M</b> (M = Cu, Ag, and Au) Carbonyl Clusters: Synthesis, Molecular Structure, Catalysis, and Computational Studies. <b>2022</b> , 61, 14726-14741	1
647	Enhancement of Thermally Activated Delayed Fluorescence (TADF) in Multi-Resonant Emitters via Control of Chalcogen Atom Embedding. <b>2022</b> , 34, 8022-8030	2
646	Deciphering Photochemical Reaction Pathways of Aqueous Tetrachloroauric Acid by X-ray Transient Absorption Spectroscopy. <b>2022</b> , 13, 8921-8927	O
645	Stacking Is Favored over Hydrogen Bonding in Azaphenanthrene Dimers. <b>2022</b> , 13, 8939-8944	0
644	Computational Insights of Selective Intramolecular O-atom Transfer Mediated by Bioinspired Copper Complexes.	0
643	Applications of quinoxaline-bridged bis(benzimidazolium) salts as ligand sources for the palladium-catalyzed Suzuki and Heck cross-coupling reactions in an aqueous medium.	0
642	Spectroscopic and QM/MM studies of the Cu(I) binding site of the plant ethylene receptor ETR1. <b>2022</b> ,	O
641	Enantiomeric resolution of pidotimod and its isomers in pidotimod oral solutions by using HPLC QDa.	0
640	Experimental and Theoretical Kinetic Studies of the Ozonolysis of Selected Allyl Sulfides (H2C?CHCH2SR, R = CH3, CH3CH2): The Effect of Nascent OH Radicals. <b>2022</b> , 126, 6751-6761	2
639	Critical Role of Iodous Acid in Neutral Iodine Oxoacid Nucleation. <b>2022</b> , 56, 14166-14177	О
638	Designing a Four-Ring Tubular Boron Motif through Metal Doping. <b>2022</b> , 61, 14553-14559	Ο
637	Catalytic nitrene transfer by an FeIV imido complex generated by a comproportionation process.	1
636	Understanding the reaction mechanism of the CO2 and cyclohexene oxide copolymerization catalyzed by zinc(II) and magnesium(II) catalysts: a DFT approach. <b>2022</b> , 28,	Ο
635	Disentangling Electronic Spectra of Linear and Cyclic Hydrogenated Carbon Cluster Cations, C2n+1H+ (n = 310). <b>2022</b> , 126, 6678-6685	1
634	Surface Modification-Dominated Space-Charge Behaviors of LDPE Films: A Role of Charge Injection Barriers. <b>2022</b> , 15, 6095	0
633	Fluoride Additive as a Simple Tool to Qualitatively Improve Performance of Nickel-Catalyzed Asymmetric Michael Addition of Malonates to Nitroolefins. <b>2022</b> , 87, 12182-12195	0
632	Predicting Experimental Heats of Formation via Deep Learning with Limited Experimental Data. <b>2022</b> , 126, 6295-6300	O

631	Excited-State Barrier Controls E - ₹ Photoisomerization in p-Hydroxycinnamate Biochromophores. <b>2022</b> , 13, 9028-9034	O
630	Radical Activation of NH and OH Bonds at Bismuth(II). <b>2022</b> , 144, 16535-16544	3
629	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**.	2
628	Alliacane-Type Secondary Metabolites from Submerged Cultures of the Basidiomycete Clitocybe nebularis.	O
627	Long-term corona behaviour and performance enhancing mechanism of SiC/epoxy nanocomposite in SF6 gas environment.	0
626	Cu(II)-Based Coordination Polymer as a Pristine Form Usable Electrocatalyst for Oxygen Reduction Reaction: Experimental Evaluation and Theoretical Insights into Biomimetic Mechanistic Aspects. <b>2022</b> , 61, 15699-15710	0
625	Binding polyprotic small molecules with second-sphere hydrogen bonds. 1-10	0
624	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**.	10
623	Direct Reduction of NO to N2O by a Mononuclear Nonheme Thiolate Ligated Iron(II) Complex via Formation of a Metastable {FeNO}7 Complex. <b>2022</b> , 61, 14909-14917	0
622	Experimental Spectroscopic, Quantum Chemical, Molecular Docking, and Molecular Dynamic Simulation Studies on Hydantoin (Monomer and Dimer). 1-27	O
621	Modeling pyranose ring pucker in carbohydrates using machine learning and semi-empirical quantum chemical methods.	0
620	A variational model for the hyperfine resolved spectrum of VO in its ground electronic state. <b>2022</b> , 157, 124305	O
619	Revisiting the pyrolysis of 1,5-diaryl-1,2,5-triazapentadienes: A computational reaction mechanism study. <b>2022</b> , 7,	О
618	Single-Molecule Magnetism in Linear Fe(I) Complexes with Aufbau and Non-Aufbau Ground States. <b>2022</b> , 61, 15335-15345	O
617	A simple approximate solution for the H3+\$\$ ${\rm H}_3^{+} \$ ion.	0
616	Theoretical investigation on the reaction kinetics of NO2 with CH3OH and HCHO under combustion conditions. <b>2022</b> ,	O
615	Intermolecular Interactions in G Protein-Coupled Receptor Allosteric Sites at the Membrane Interface from Molecular Dynamics Simulations and Quantum Chemical Calculations.	2
614	Conformer Weighting and Differently Sized Cluster Weighting for Nicotine and Its Phosphorus Derivatives.	O

613	Formation of 2D Self-Assembled Layers of Allyl Cyanide on Pd(111). 2022, 126, 16643-16655	0
612	Direct Cℍ/Cℍ Coupling of the Azoloannulated Pteridines with Electron Rich (Hetero)Aromatic Compounds. <b>2022</b> , 87, 13011-13022	Ο
611	Mechanical Activation of Forbidden Photoreactivity in Oxa-di-Emethane Rearrangement. <b>2022</b> , 87, 12586-12	5950
610	Base-Free Alkoxide Dysprosium(III) Complexes with an Unusual Tetraphenylborate Coordination: Study of the Slow Relaxation of the Magnetization.	O
609	Physics-based representations for machine learning properties of chemical reactions.	O
608	Modeling the non Arrhenius ignition behavior of 2-butanol: A detailed theoretical and experimental study. <b>2022</b> ,	O
607	Fabrication of the polyethersulfone/functionalized mesoporous carbon nanocomposite nanofiltration membrane for dyes and heavy metal ions removal: Experimental and quantum mechanical simulation method.	0
606	LIDA: The Leiden Ice Database for Astrochemistry.	O
605	Insights into Two Novel Orthopalladated Chromophores with Antimicrobial Activity against Escherichia coli. <b>2022</b> , 27, 6060	0
604	Structures, biomimetic synthesis, and anti-SARS-CoV-2 activity of two pairs of enantiomeric phenylpropanoid-conjugated protoberberine alkaloids from the rhizomes of Corydalis decumbens.	O
603	ZORA Gaussian basis sets for Fr, Ra, and Ac. <b>2022</b> , 28,	0
602	Computer Simulation of Electron Transfer between the Cytochrome Active Center and Reactive Oxygen and Nitrogen Species. <b>2022</b> , 48-53	O
601	Expanding the Knowledge of the Selective-Sensing Mechanism of Nitro Compounds by Luminescent Terbium Metal©rganic Frameworks through Multiconfigurational ab Initio Calculations. <b>2022</b> , 126, 7040-7050	Ο
600	Solving the riddle of the high-temperature chemistry of 1,3-dioxolane. <b>2022</b> ,	2
599	13C ENDOR Characterization of the Central Carbon within the Nitrogenase Catalytic Cofactor Indicates That the CFe6 Core Is a Stabilizing ⊞eart of Steel□	1
598	ASBase: The universal database for aggregate science.	1
597	Conformational energies of microsolvated Na + clusters with protic and aprotic solvents from GFN n -xTB methods. <b>2022</b> , 43, 1856-1863	1
596	How Computations Can Assist the Rational Design of Drugs for Photodynamic Therapy: Photosensitizing Activity Assessment of a Ru(II)-BODIPY Assembly. <b>2022</b> , 27, 5635	O

595	Protonation structure of the closed-cubane conformation of the O2-evolving complex in photosystem II.	О
594	Transient Absorption Spectroscopy of a Carbazole-Based Room-Temperature Phosphorescent Molecule: Real-Time Monitoring of Singlet Transitions. 9381-9389	O
593	Computational Analysis of the Behavior of BODIPY Decorated Monofunctional Platinum(II) Complexes in the Dark and under Light Irradiation.	О
592	Gold-Catalyzed Bidirectional Access to Planar Heptacyclic Benzobispyrido[1,2- a ]indoles and Benzobispyrrolo[1,2- a ]Quinolines for Materials Science.	O
591	Rapid calculation of internal conversion and intersystem crossing rate for organic materials discovery. <b>2022</b> , 157, 134106	0
590	Photocatalytic reduction of CO2 by highly efficient homogeneous FeII catalyst based on 2,6-bis(1段B驻riazolyl-methyl)pyridine. Comparison with analogues.	О
589	Contribution of Methanesulfonic Acid to the Formation of Molecular Clusters in the Marine Atmosphere.	1
588	Energy Transfer Mechanism and Quantitative Modeling of Rate from an Antenna to a Lanthanide lon.	1
587	A Solid/Liquid High-Energy-Density Storage Concept for Redox Flow Batteries and Its Demonstration in an H2-V System.	1
586	Competition between In-Plane vs Above-Plane Configurations of Water with Aromatic Molecules: Non-Covalent Interactions in 1,4-Naphthoquinone-(H2O)1B Complexes. 9510-9516	1
585	A Combined XPS and Computational Study of the Chemical Reduction of BMP-TFSI by Lithium**.	O
584	Development of a novel ReaxFF reactive potential for organochloride molecules.	O
583	The new Ca(Fe,Al)2O4 phase with calcium ferrite-type structure, a likely carrier of Al in the transition zone and lower mantle. <b>2022</b> , 111031	O
582	Charge-Transfer and Spin-Flip States: Thriving as Complements.	2
581	Theoretical Study for Evaluating and Discovering Organic Hydride Compounds as Potential Novel Methylation Reagents.	О
580	Mechanistic Analysis of Nanocellulose Formation Tuned by Deep Eutectic Solvents.	О
579	A hydroxylated tetracationic viologen based on dimethylaminoethanol as a negolyte for aqueous flow batteries.	О
578	Elucidating Conformation and Hydrogen-Bonding Motifs of Reactive Thiourea Intermediates. 12689-12700	O

577	Charge-Transfer and Spin-Flip States: Thriving as Complements.	O
576	Alumina-Based Bifunctional Catalyst for Efficient CO2 Fixation into Epoxides at Atmospheric Pressure.	2
575	The d-d transitions and ligand field parameters for Cr3+/Co2+ doped (Mg, Zn)Al2O4: Multi-reference Ab initio investigations. <b>2022</b> , 16, 100188	O
574	Structures of the (Imidazole)nH+ Ar (n=1,2,3) complexes determined from IR spectroscopy and quantum chemical calculations.	O
573	Stable High-Conductivity Ethylenedioxythiophene Polymers via Borane-Adduct Doping. 2208541	2
572	Comparative investigation of Cu(II) complexes with dithiocarbazate: Structural design, theoretical calculation, and in vitro antitumor activity. <b>2022</b> , 237, 112015	1
571	Benzimidazole-substituted bisanthracene: a highly efficient deep-blue triplet <b>t</b> riplet fusion OLED emitter at low dopant concentration. <b>2022</b> , 26, 101185	0
570	A conversion strategy to disaggregate asphaltenes via mild hydrotreatment: Theoretical and experimental investigation. <b>2022</b> , 264, 118106	O
569	The effect of halides and coordination mode of 4-amino-2,1,3-benzothiadiazole on the luminescence properties of its Zn complexes.	O
568	Single-precision CCSD and CCSD(T) Calculations with Density Fitting Approximations on Graphics Processing Units. <b>2022</b> , 80, 1401	O
567	Q-Band relaxation in chlorophyll: new insights from multireference quantum dynamics.	1
566	Local Structure of Molten Lithium Fluoride. I. Ab Initio and Molecular Dynamics Calculations of Three-Particle and Radial Functions. <b>2022</b> , 2022, 972-977	O
565	Ultrafast electron diffraction from transiently aligned asymmetric top molecules: Rotational dynamics and structure retrieval. <b>2022</b> , 9, 054303	O
564	On the Role of Noncovalent Ligand-Substrate Interactions in Au(I) Catalysis: An Experimental and Computational Study of Protodeauration. 13158-13163	O
563	Push-Pull Structures Based on 2-Aryl/thienyl Substituted Quinazolin-4(3H)-ones and 4-Cyanoquinazolines. <b>2022</b> , 27, 7156	1
562	The missing conformer: A comprehensive rotational spectroscopy study and astronomical search of two conformers of methyl cyanoacetate. 9,	1
561	The Source of Proton in the Noyorilkariya Catalytic Cycle. 13149-13157	О
560	High- and low-temperature ignition delay time study and modeling efforts on vinyl acetate. 2022,	O

559	Modeling of the Electrostatic Interaction and Catalytic Activity of [NiFe] Hydrogenases on a Planar Electrode. <b>2022</b> , 126, 8777-8790	O
558	Novel Chelating Agents for Zirconium-89-Positron Emission Tomography (PET) Imaging: Synthesis, DFT Calculation, Radiolabeling, and In Vitro and In Vivo Complex Stability. <b>2022</b> , 7, 37229-37236	1
557	<del>                                      </del>	O
556	Yellow-Emitting, Pseudo-Octahedral Zinc Complexes of Benzannulated N^N^O Pincer-Type Ligands.	1
555	Substituent Effects in Iron Porphyrin Catalysts for the Hydrogen Evolution Reaction.	1
554	Theoretical Investigation of Key Properties of the Pyrolysis of Methyl, Ethyl, and Dimethyl Dioxolane Isomers.	O
553	Constitutional isomerism of the linkages in donor covalent organic frameworks and its impact on photocatalysis. <b>2022</b> , 13,	4
552	Field-Induced Slow Magnetic Relaxation in Coll Cyclopropane-1,1-dicarboxylates. <b>2022</b> , 27, 6537	O
551	Synthesis, DFT Analyses, Antiproliferative Activity, and Molecular Docking Studies of Curcumin Analogues. <b>2022</b> , 11, 2835	0
550	Naphthalimide-phenothiazine dyads: effect of conformational flexibility and matching of the energy of the charge-transfer state and the localized triplet excited state on the thermally activated delayed fluorescence. 18, 1435-1453	O
549	Computational Study of Two Three-Dimensional Co(II)-Based Metal Drganic Frameworks as Quercetin Anticancer Drug Carriers.	0
548	Modelling of excited state potential energy surfaces with the BetheBalpeter equation formalism: The 4-(dimethylamino)benzonitrile twist.	3
547	Synthesis of Aluminum N,NElialkylcarbamates by Insertion of CO2 into Al® Bonds.	0
546	Correlation between Absorption and Substitution of Photochromic 1,2-Bis(thienyl)ethenes (BTEs) Using Modified Spectroscopic Hammett Equations.	O
545	Dehydrogenation Induced Formation of Chiral Core-Shell Arrays of Melamine on Ag(111). <b>2022</b> , 39, 116401	O
544	Porous Mn2+ Magnet with a Pttl Framework: Correlation between Water Vapor Adsorption/Desorption and Slow Magnetic Relaxation.	O
543	Interaction of Glutamic Acid/Protonated Glutamic Acid with Amide and Water Molecules: A Theoretical Study. <b>2022</b> , 126, 7750-7762	0
542	Electronic structure, cationic and excited states of nitrogen-containing spiroborates.	О

541	Atomistic structure search using local surrogate model.	0
540	Non-empirical double-hybrid density functionals as reliable tools for electronic structure calculations. <b>2022</b> , 4, 043001	1
539	Constructing Nonaqueous Rechargeable Zinc-Ion Batteries with Zinc Trifluoroacetate. <b>2022</b> , 5, 12437-12447	0
538	Reductive Elimination or CL bond Activation with Model Ni, Pd, Pt Complexes? A High-Accuracy Comparative Computational Analysis of Reactivity	O
537	Mechanistic Insights into Cobalt-Catalyzed Regioselective C4-Alkenylation of 3-Acetylindole: A Detailed Theoretical Study.	О
536	Cluster-in-Molecule Method Combined with the Domain-Based Local Pair Natural Orbital Approach for Electron Correlation Calculations of Periodic Systems.	O
535	Binding of piperine to mycobacterial RNA polymerase improves the efficacy of rifampicin activity against Mycobacterium leprae and nontuberculous mycobacteria. 1-11	O
534	Reliable Isotropic Electron-Paramagnetic-Resonance Hyperfine Coupling Constants from the Frozen-Density Embedding Quasi-Diabatization Approach.	O
533	Quintet Dinitrenes with Negative Zero-Field Splitting: Effect of Spin Drbit Coupling on the Sign of Magnetic Anisotropy. <b>2022</b> , 126, 7591-7597	0
532	Predicting Solvent Effects on SN2 Reaction Rates: Comparison of QM/MM, Implicit, and MM Explicit Solvent Models.	2
531	Classical vs. Non-Classical Cyclometalated Pt(II) Complexes. <b>2022</b> , 27, 7249	1
530	Transition-Metal-Stabilized Heavy Tetraphospholide Anions.	0
529	Distinguishing the Quantum Yield and Lifetime of Carbazole-Based Room-Temperature Phosphorescence Materials: QM/MM Study. 2200342	0
528	Mutactimycin AP, a New Mutactimycin Isolated from an Actinobacteria from the Atacama Desert. <b>2022</b> , 27, 7185	O
527	Tailored Charge Transfer Kinetics in Precursors for Organic Radical Batteries 🖪 Joint Synthetic-Theoretical Approach.	0
526	Slow Magnetic Relaxation in a Co(III)Io(II)Io(III) Mixed-Valence Complex with Negative Anisotropy. <b>2022</b> , 22, 6792-6800	O
525	Mechanisms of Reactions between HOI and HY (Y = Cl, Br, I) on a Water Nanodroplet Surface. <b>2022</b> , 126, 8028-8036	0
524	Enhancing NO Uptake in Metal-Organic Frameworks via Linker Functionalization. A Multi-Scale Theoretical Study. <b>2022</b> , 4, 1300-1311	1

523	Hygroscopicity and CCN potential of DMS-derived aerosol particles. 2022, 22, 13449-13466	0
522	Binuclear Nickel Complexes of a New Di(hydroxyphenyl)imidazolate. <b>2022</b> , 8, 132	O
521	Theoretical research on the relationships between aromatic ligands and spectroscopic properties of Pt(II) complexes.	0
520	Constructing Bull-Frequency pectra via Moment Constraints for Coupled Cluster Green Functions.	1
519	High-Spin S = 3/2 Ground-State Aminyl Triradicals: Toward High-Spin Oligo-Aza Nanographenes. <b>2022</b> , 144, 19576-19591	0
518	Self-Assembly of a Graphene Oxide Liquid Crystal for Water Treatment. <b>2022</b> , 14, 47549-47559	O
517	Thionation toward High-Contrast ACQ-DIE Probes by Reprogramming the Aqueous Segregation Behavior: Enlightenment from a Sulfur-Substituted G-Quadruplex Ligand.	1
516	Molecular Basis for the Difference in Singlet Oxygen Quantum Yield Between the First Genetically Encoded Photosensitizer, KillerRed, and its Monomeric Counterpart, SuperNova. <b>2022</b> , 7,	o
515	Piers Borane-Catalyzed Dimerization of Arylallenes via Transborylation: A Synthetic and Mechanistic Study. 13961-13968	0
514	Benchmark Thermochemistry of Polycyclic Aromatic Hydrocarbons.	o
513	Crystallographic Detection of the Spin State in FeIII Complexes. 2022, 22, 6429-6439	2
512	Theoretical Insight into B $\Omega$ Chemical Bonding in Closo-Borate [BnHn $\Omega$ CH3]2 $\Omega$ n = 6, 10, 12) and Monocarborane [ $\Omega$ nHnCH3] $\Omega$ n = 5, 9, 11) Anions. <b>2022</b> , 10, 186	o
511	Reversible Dioxygen Binding to Co(II) Complexes with Noninnocent Ligands. 2022, 61, 16664-16677	0
510	Functional and Mechanistic Study of a Lytic Polysaccharide Monooxygenase That Contributes to Xylan Degradation by Xylanase. <b>2022</b> , 10, 13955-13963	o
509	Ring-to-Chain Structural Relaxation of Elemental Sulfur upon Photoexcitation. 2362-2367	O
508	Synthesis, Biological Activity and Molecular Docking of Chimeric Peptides Targeting Opioid and NOP Receptors. <b>2022</b> , 23, 12700	0
507	The capture of carbonyl sulfide by N-methyldiethanolamine: A systematic density functional theory investigation.	0
506	Effect of the SilicaMagnetite Nanocomposite Coating Functionalization on the Doxorubicin Sorption/Desorption. <b>2022</b> , 14, 2271	1

505	Role of Exact Exchange in Difference Projected Double-Hybrid Density Functional Theory for Treatment of Local, Charge Transfer, and Rydberg Excitations. <b>2022</b> , 126, 8058-8069	0
504	Unexpected Strengthening of the H-Bond Complexes in a Polar Solvent Due to a More Efficient Solvation of the Complex Compared to Isolated Monomers. <b>2022</b> , 126, 7938-7943	1
503	Investigations of an Unexpected [2+2] Photocycloaddition in the Synthesis of ( PScabrolide A from Quantum Mechanics Calculations.	0
502	Mechanistic Insight into Phenol Dearomatization by Hypervalent Iodine: Direct Detection of a Phenoxenium Cation.	1
501	Together, Not Separately, OH and O3 Oxidize Hg(0) to Hg(II) in the Atmosphere.	2
500	Confinement of the Triplet States in EConjugated BODIPY Dimers Linked with Ethynylene or Butadiynylene Bridges: A Different View on the Effect of Symmetry.	О
499	Global Kinetics and Spectral Modeling of p-Methoxyphenyl Azide Photooxidation.	O
498	Geometries and electronic structures of Pn 🗈 Al (n´= 20월0) cages: A DFT study. <b>2022</b> , 1217, 113922	О
497	Reliable gas-phase tautomer equilibria of drug-like molecule scaffolds and the issue of continuum solvation.	2
496	Reactivities of silane coupling agents in the silica/rubber composites: Theoretical insights into the relationships between energy barriers and electronic characteristics.	О
495	The Effect of Methylation on the Triplet-State Dynamics of 2-Thiouracil: Time-Resolved Photoelectron Spectroscopy of 2-Thiothymine.	0
494	Intercalative binding of two new five-coordinated anticancer Pt(II) complexes to DNA: experimental and computational approaches. 1-11	o
493	Confinement of the Triplet States in Econjugated BODIPY Dimers Linked with Ethynylene or Butadiynylene Bridges: A Different View on the Effect of Symmetry.	0
492	The impact of the electric field of metal ions on the vibrations and internal hydrogen bond strength in alkali metal ion di- and triglycine complexes. <b>2022</b> , 157, 174301	o
491	Redox-active ligands as a challenge for electronic structure methods.	0
490	Revealing the Unexplored Mechanism of Photochemical Oxaziridine Conversion Process of 2H-imidazole 1-oxides. <b>2022</b> , 7,	О
489	Pyrrolidine-2,5-dione-derived ionic liquids promoted efficient transformation of flue gas CO2 into ⊞lkylidene cyclic carbonates at room temperature. <b>2022</b> , 65, 102227	O
488	Exploring 129Xe NMR parameters for structural investigation of biomolecules: relativistic, solvent, and thermal effects. <b>2022</b> , 28,	О

487	Impact of the electric field on isotropic and anisotropic spin Hamiltonian parameters.	О
486	New Aspects of the Synthesis of closo-Dodecaborate Nitrilium Derivatives [B12H11NCR][[R = n-C3H7, i-C3H7, 4-C6H4CH3, 1-C10H7): Experimental and Theoretical Studies. <b>2022</b> , 10, 196	1
485	Oxygen Evolution Reaction Electrocatalysis on Cobalt(oxy)hydroxide: Role of Fe Impurities.	2
484	Modelling the electric field in non-fullerene organic solar cells: The effect of 1-chloronaphthalene additive. <b>2022</b> , 247, 286-294	O
483	Identification of the active triple-phase boundary of a non-Pt catalyst layer in fuel cells. 2022, 8,	1
482	Picosecond Charge-Transfer-State Dynamics in Wide Band Gap PolymerNon-Fullerene Small-Molecule Blend Films Investigated via Transient Infrared Spectroscopy. 10418-10423	O
481	Study of interaction between different solvents and neurotransmitters dopamine, l-adrenaline, and l-noradrenaline using LED, QTAIM and AIMD. <b>2022</b> , 120708	2
480	Spin-vibronic interaction induced reverse intersystem crossing: A case study with TXO-TPA and TXO-PhCz molecules. <b>2022</b> , 157, 174101	1
479	Complex structures, formation thermodynamics and substitution reaction kinetics in the copper(II) Iglycylglycyl-l-tyrosine II/d-histidine systems. <b>2022</b> , 228, 116176	1
478	Separation of ethyl acetate-isopropanol using low transition temperature mixtures: Vapor-liquid equilibrium experiments and quantum chemical calculation. <b>2022</b> , 367, 120589	O
477	Syntheses, crystal structures, DFT calculation and solid-state spectroscopic properties of new zincate(II) complexes with N-(4-substituted phenyl)-N'-(4-nitrophenyl)-oxamate. <b>2022</b> , 15, 104349	O
476	Studies on the thermal degradation mechanism of polyethylene terephthalate and its 2-carboxy ethyl (phenyl) phosphinic acid copolymers. <b>2022</b> , 206, 110185	O
475	Synthesis and spectral studies of Ni(II) complexes involving functionalized dithiocarbamates and triphenylphosphine: X-ray crystal structure, thermal stability, Hirshfeld surface analysis, DFT and biological evaluation. <b>2023</b> , 545, 121271	0
474	Effects of nitrogen and oxygen on electrochemical reduction of CO2 in nitrogen-doped carbon black. <b>2023</b> , 202, 1-11	O
473	Femtosecond transient absorption spectroscopy on the thermally activated delayed fluorescence of bis[4-(9-H-carbazole)phenyl] sulfone. <b>2023</b> , 253, 119459	0
472	Exploring the separation mechanism of Gemini surfactant in scheelite froth flotation at low temperatures: Surface characterization, DFT calculations and kinetic simulations. <b>2023</b> , 305, 122358	O
471	Understanding the unceasing evolution of Co(II) based single-ion magnets. 2023, 475, 214871	3
470	Mechanism of photo-assisted atomic layer etching of chlorinated Si(111) surfaces: Insights from DFT/TDDFT calculations. <b>2023</b> , 153, 107169	O

469	Efficient ultralong and color-tunable room-temperature phosphorescence from polyacrylamide platform by introducing sulfanilic acid. <b>2023</b> , 453, 139753	0
468	Solvent interaction and dynamics of neurotransmitters -aspartic acid and -glutamic acid with water and ethanol. <b>2023</b> , 1273, 134347	1
467	Design, synthesis, characterization, antioxidant, antiproliferative activity and molecular docking studies of new transition metal complexes of 1,2,4-triazole as combretastatin A-4 analogues. <b>2023</b> , 1274, 134437	О
466	Rh-Pd/TiO2 as bilateral catalysts for reductive and oxidative degradation of fluorinated pharmaceutical contaminants. <b>2023</b> , 322, 122089	O
465	New insight to the catechol photochemistry: The role of different monomer and dimer configurations in radiationless decay of S1 electronic excited state.	1
464	Diterpenoids from Sigesbeckia glabrescens with anti-inflammatory and AChE inhibitory activities. <b>2023</b> , 205, 113503	O
463	Single-molecule Aflatoxin B1 Sensing via Pyrrole-based Molecular Quantum Dot. 2022,	1
462	Electronic Configuration Assignments for UO from Electric Dipole Moment Measurements. 10799-10804	O
461	Kinetics in DMS: Modeling Clustering and Declustering Reactions.	O
460	Cluster-Continuum Model as a Sanity Check of Sodium Ions@ibbs Free Energies of Transfer.	Ο
459	Calculation of Mass Spectra with the QCxMS Method for Negatively and Multiply Charged Molecules.	O
458	MBius-Strip Topology of Expanded Porphyrins: A Minireview on EPR, ENDOR and DFT MO Studies.	O
457	Pathway exploration in low-temperature oxidation of a new-generation bio-hybrid fuel 1,3-dioxane. <b>2022</b> ,	1
456	Quantum Computational, Spectroscopic, Hirshfeld Surface Analysis of 3-Picoline (Monomer and Dimer) by DFT/TD-DFT with Different Solvents, Molecular Docking, and Molecular Dynamic Studies. 1-25	O
455	Influence of Tartrate Ligand Coordination over Luminescence Properties of Chiral Lanthanide-Based Metal Drganic Frameworks. <b>2022</b> , 12, 3999	O
454	ESIPT-based benzazole-pyromellitic diimide derivatives. A thermal, electrochemical, and photochemical investigation. <b>2022</b> , 122050	O
453	Phthalocyanine-Carbon Nanotube Hybrid Materials: Mechanism of Sensor Response to Ammonia from Quantum-Chemical Point of View. <b>2022</b> , 10, 479	0
452	Amine-Reactive BODIPY Dye: Spectral Properties and Application for Protein Labeling. <b>2022</b> , 27, 7911	O

451	Mechanistic Insights into the Oxidative and Reductive Quenching Cycles of Transition Metal Photoredox Catalysts through Effective Oxidation State Analysis.	О
450	Libra: A modular software library for quantum nonadiabatic dynamics. <b>2022</b> , 100445	О
449	Biobased additives for asphalt applications produced from the hydrothermal liquefaction of sewage sludge. <b>2022</b> , 108974	0
448	Graph-Theoretic Molecular Fragmentation for Potential Surfaces Leads Naturally to a Tensor Network Form and Allows Accurate and Efficient Quantum Nuclear Dynamics.	O
447	An account of noncovalent interactions in homoleptic palladium(II) and platinum(II) complexes within the DFT framework: A correlation between geometries, energy components of symmetry-adapted perturbation theory and NCI descriptors. <b>2022</b> , 8, e11408	0
446	Carboxylic Acid Catalysis on the Imine Formation Versus Aza-Michael Reaction in Apolar Aprotic Solvent.	O
445	Thermal degradation and flame retardancy prediction of Fe, Al, and Cu-based metal-organic framework and polyethylene terephthalate nanocomposites using DFT calculation. <b>2022</b> , 125496	0
444	NMR chiral recognition of lipoic acid by cinchonidine CSA: A stereocenter beyond the organic function.	О
443	Synthesis, characterization, and quantum chemical study of cobalt(II) chelates with N-phenethyl-iminodiacetate(2-)-like ligands. Influence of p-(R)-phenethyl group on crystal pattern. 1-15	0
442	Synthesis of Apigenin and Quercetin-Like Compounds, Molecular Docking Simulation, and Investigation of Their Bioactivity on A549 Cell Lines. <b>2022</b> , 7,	O
441	Arene Variation of Highly Cytotoxic Tridentate Naphthoquinone-Based Ruthenium(II) Complexes and In-Depth In Vitro Studies. <b>2022</b> , 14, 2466	1
440	Tetranuclear Copper Complexes with Bulky Aminoalcohol Ligands as Catalysts for Oxidative Phenoxazinone Synthase-like Coupling of Aminophenol: A Combined Experimental and Theoretical Study. <b>2022</b> , 12, 1408	O
439	Alkaline earth metals (Be, Mg, Ca) doped hexamine complexant with enhanced electronic and nonlinear optical properties. <b>2022</b> , 28,	O
438	Erythrosin B as a New Photoswitchable Spin Label for Light-Induced Pulsed EPR Dipolar Spectroscopy. <b>2022</b> , 27, 7526	O
437	High-level quantum chemistry exploration of reduction by group-13 hydrides: insights into the rational design of bio-mimic CO2 reduction. <b>2022</b> , 4, 044001	О
436	Study of the dynamics of the interaction of glycine and GABA with water and ethanol using theoretical tools. <b>2022</b> , 368, 120721	1
435	Optical and computational analysis of red light emitting Eu(III) complexes for applications in luminescent devices. <b>2022</b> , 134, 113095	О
434	Point-defect engineering on phosphorene quantum dots for DNA bases adsorption and sensor performance. <b>2022</b> , 33, 104868	O

433	Transferable Potential Function for Flexible H2O Molecules Based on the Single-Center Multipole Expansion.	2
432	Investigation of the Structure of Atomically Dispersed NiNx Sites in Ni and N-Doped Carbon Electrocatalysts by 61Ni MBsbauer Spectroscopy and Simulations.	О
431	A simple quantum model for solving two-electron diatomics approximately.	О
430	Disproportionation and ligand lability in low oxidation state boryltin chemistry.	О
429	Caging of a Strongly Pairing Fluorescent Thymidine Analog with Soft Nucleophiles.	O
428	Energy transfer processes in 1,3- bis(pyridyl) iminoisoindoline based donor-acceptor system - Synthesis, photophysics, and TD-DFT study. <b>2022</b> , 110215	o
427	Molecular investigation of interplay mechanism between polydopamine and graphene oxide: The effect of oxidation degree on the adsorption behavior of polydopamine. <b>2022</b> , 155759	О
426	Z-scheme transfer pathway assisted photoelectrocatalyst Zn2SnO4/rGO/Ag/AgBr for organic pollutants treatment. <b>2023</b> , 657, 130552	O
425	Influence of the complete basis set approximation, tight weighted-core, and diffuse functions on the DLPNO-CCSD (T1) atomization energies of neutral H,C,O-compounds.	О
424	Biophysical investigation of the interaction between NSAID ibuprofen and cationic biodegradable Cm-E2O2-Cm gemini surfactants. <b>2023</b> , 370, 120972	1
423	Quantum chemistry insight into the interactions of 1,3-diisopropoxycalix[4]arenecrown-6 with alkali metal cations: Structure, selectivity, and solvation. <b>2023</b> , 370, 121054	О
422	Interaction studies of levofloxacin with human lysozyme in a ternary complex using multispectroscopic and computational analysis: A circular dichroism method for the quantitation of levofloxacin. <b>2023</b> , 370, 121023	О
421	A Bioinspired, One-Step Total Synthesis of Peshawaraquinone.	О
420	Complexation of sodium sulfamerazine with an ionic resorcin[4]arene: Thermodynamic and computational study. <b>2023</b> , 370, 120954	1
419	Spodium bonding to anticrown-Hg3 boosts phosphorescence of cyclometalated-PtII complexes.	0
418	Fluoroalkoxyaluminate-based ionic liquids as electrolytes for sodium-ion batteries. <b>2023</b> , 369, 120919	O
417	Electronic structures of zwitterionic and protonated forms of glycine betaine in water: Insights into solvent effects from ab initio simulations. <b>2023</b> , 369, 120871	0
416	In situ prepared all-fluorinated polymer electrolyte for energy-dense high-voltage lithium-metal batteries. <b>2023</b> , 55, 642-651	O

415	High methylation potential of mercury complexed with mixed thiolate ligands by Geobacter sulfurreducens PCA. <b>2023</b> , 342, 74-83	0
414	The formation mechanism of highly oxygenated organic molecules produced by toluene in the urban atmosphere. <b>2023</b> , 295, 119555	O
413	Molecular simulation investigations on interaction properties of the teriflunomidelhitosan complex in aqueous solution. <b>2023</b> , 174, 111171	1
412	Adsorption behavior of methylene blue on graphene and hexagonal boron nitride monolayers in aqueous solution: A first-principles treatment. <b>2023</b> , 174, 111151	o
411	Synthesis, crystal structure and theoretical studies of 1-sulfonyl-1,2,3-triazole derivatives. <b>2023</b> , 1276, 134806	0
410	Solvent effects on glyphosate deprotonation: DFT theoretical studies. 2023, 6, 100140	O
409	Nonadiabatic molecular dynamics study of a complete photoswitching cycle for a full-size diarylethene system. <b>2023</b> , 438, 114513	0
408	Comment on Multiple locations of boron atoms in the exohedral and endohedral C60 fullerene 2022, 106,	O
407	IIYCIReaction between Alkynes and Catechol-Thiol Derivatives Prompted by Metal Nanocatalysis: Mechanism Study by DFT Calculation.	O
406	Design of the Smallest Intramolecular Singlet Fission Chromophore with the Fastest Singlet Fission. <b>2022</b> , 13, 11076-11085	1
405	Density Functional Theory Study on the H2-Acceptorless Dehydrogenative Boration of Alkenes Catalyzed by a Zirconium Complex. <b>2022</b> , 87, 16632-16643	0
404	A reaction mechanism for plasma electrolysis of AgNO3 forming silver nanoclusters and nanoparticles. <b>2022</b> , 132, 203302	1
403	Mitigating Polysulfide Shuttles with Upcycled Alkali Metal Terephthalate Decorated Separators. <b>2022</b> , 8, 253	0
402	The vertical excitation energies and a lifetime of the two lowest singlet excited states of the conjugated polyenes from C2 to C22 : Ab initio, DFT, and semiclassical MNDO-MD simulations.	1
401	Manganese(III) Acetate-Based Radical Cyclization Reactions for Pyranocoumarin and Pyranoquinoline Compounds: Synthesis, DFT and Molecular Docking Studies. <b>2022</b> , 7,	0
400	Not All 3MC States Are the Same: The Role of 3MCcis States in the Photochemical N?N Ligand Release from [Ru(bpy)2(N?N)]2+ Complexes. <b>2022</b> , 61, 19907-19924	O
399	A computational study of Mg m H n nanoclusters with n : m f2:1 for efficient hydrogen storage.	0
398	Steric and Electronic Effects in N-Heterocyclic Carbene Gold(III) Complexes: An Experimental and Computational Study. <b>2022</b> , 27, 8289	0

397	Coupled Cluster Molecular Dynamics of Condensed Phase Systems Enabled by Machine Learning Potentials: Liquid Water Benchmark. <b>2022</b> , 129,	0
396	Toward Reliable and Insightful Entropy Calculations on Flexible Molecules. <b>2022</b> , 18, 7166-7178	O
395	Growing Spicy ONIOMs: Extending and generalizing concepts of ONIOM and many body expansions.	0
394	Silver(I) Complexes Based on Oxadiazole-Functionalized Aminophosphonate: Synthesis, Structural Study, and Biological Activities. <b>2022</b> , 27, 8131	О
393	Influence of H2SO4IIIH2O and (H2SO4)2 on the Hydrolysis of Formaldehyde: A Potential Source of Methanediol in the Troposphere. <b>2022</b> , 6, 2779-2789	1
392	Ambimodal Bispericyclic [6 + 4]/[4 + 6] Transition State Competes with Diradical Pathways in the Cycloheptatriene Dimerization: Dynamics and Experimental Characterization of Thermal Dimers. <b>2022</b> , 144, 22251-22261	О
391	Final Products of One-Electron Oxidation of Cyclic Dipeptides Containing Methionine Investigated by IRMPD Spectroscopy: Does the Free Radical Choose the Final Compound?. <b>2022</b> , 126, 10055-10068	О
390	Massive Assessment of the Binding Energies of Atmospheric Molecular Clusters. <b>2022</b> , 18, 7373-7383	O
389	Symmetry analysis of irregular objects.	О
388	Accurate Crystal Structures of C12H9CN, C12H8(CN)2, and C16H11CN Valence Isomers Using Nonspherical Atomic Scattering Factors. <b>2022</b> , 87, 16213-16229	О
387	Occurrence and stability of anionInteractions between phosphate and nucleobases in functional RNA molecules. <b>2022</b> , 50, 11455-11469	0
386	Hydroalumination of 1,8-DiethynylanthracenesAl-based Bis-Lewis-Acids and their Isomerization and Complexation Behavior. <b>2022</b> , 41, 3600-3611	О
385	Supramolecular Diversity, Theoretical Investigation and Antibacterial Activity of Cu, Co and Cd Complexes Based on the Tridentate N,N,O-Schiff Base Ligand Formed In Situ. <b>2022</b> , 27, 8233	О
384	Diboraanthracene-Doped Polymer Systems for Colour-Tuneable Room-Temperature Organic Afterglow.	1
383	Hydrolysis of SO3 in Small Clusters of Sulfuric Acid: Mechanistic and Kinetic Study. <b>2022</b> , 6, 3078-3089	О
382	Toward Large-Scale Restricted Active Space Calculations Inspired by the Schmidt Decomposition.	О
381	Enantiomeric Resolution of Pidotimod and Its Isomers in Pidotimod Oral Solutions Using Chiral RP-HPLC with Quadrupole Dalton Analyzer Detection.	О
380	Consistent Evaluation of Magnetic Exchange Couplings in Multicenter Compounds in KS-DFT: The Recomposition Method.	O

379	Structural Determination of the Hexacoordinated [Zn(L)2]2+ Complex Isomer Type Using Solution-State NMR, DFT Calculations and X-ray Crystallography. <b>2023</b> , 13, 16	O
378	Evaluation of experimental, computational, molecular docking and dynamic simulation of flucytosine. 1-20	О
377	Understanding the Stability of EConjugated Diradicaloid Organic Molecules.	O
376	Electron Density Analysis of MetalMetal Bonding in a Ni4 Cluster Featuring Ferromagnetic Exchange.	O
375	Triplets with a Twist: Ultrafast Intersystem Crossing in a Series of Electron Acceptor Materials Driven by Conformational Disorder.	О
374	Molecular Dynamics and Structural Studies of Zinc Chloroquine Complexes.	O
373	Biodegradation of 2,5-Dihydroxypyridine by 2,5-Dihydroxypyridine Dioxygenase and Its Mutants: Insights into OID Bond Activation and Flexible Reaction Mechanisms from QM/MM Simulations. <b>2022</b> , 61, 20501-20512	O
372	Boronated Cyanometallates.	O
371	Manganese(II) Bromide Compound with Diprotonated 1-Hydroxy-2-(pyridin-2-yl)-4,5,6,7-tetrahydrobenzimidazole: Dual Emission and the Effect of Proton Transfers. <b>2022</b> , 10, 245	2
370	Tetrafluorosubstituted Metal Phthalocyanines: Study of the Effect of the Position of Fluorine Substituents on the Chemiresistive Sensor Response to Ammonia. <b>2022</b> , 10, 515	1
369	Spin-defect qubits in two-dimensional transition metal dichalcogenides operating at telecom wavelengths. <b>2022</b> , 13,	1
368	Visible Light Accelerates Cr(III) Release and Oxidation in Cr <b>E</b> e Chromite Residues: An Overlooked Risk of Cr(VI) Reoccurrence. <b>2022</b> , 56, 17674-17683	O
367	Novel Orientation-Sensitive Spin Probes for Graphene Oxide Membranes Study. <b>2022</b> , 12, 1241	1
366	On the Mechanism of Soot Nucleation. IV. Molecular Growth of the Flattened E-Bridge. <b>2022</b> , 126, 9259-9267	O
365	Influence of the Side Chain Structure on the Electronic Structure and Self-Organization Properties of Low Band Gap Polymers. <b>2022</b> , 5, 15290-15301	O
364	Heterometallic Porphyrin Conjugated Polymer Thin Films A Gas-Phase Approach for the Engineering of New Fused Porphyrin Systems. 2202237	O
363	Electrochemical and Structural Study of the Buried Tryptophan in Azurin: Effects of Hydration and Polarity on the Redox Potential of W48.	О
362	Total Synthesis of Atrachinenins A and B. <b>2022</b> , 144, 22844-22849	О

361	Lanthanide and Actinide Ion Complexes Containing Organic Ligands Investigated by Surface-Enhanced Infrared Absorption Spectroscopy.	0
360	Mechanism study of the conductivity characteristics of cellulose electrical insulation influenced by moisture. <b>2022</b> , 132, 215104	O
359	Double Hybrid Density Functionals for the Electronic Excitation Energies of Linear Cyanines.	O
358	Role of CH2O moiety on laminar burning velocities of oxymethylene ethers (OMEn): A case study of dimethyl ether, OME1 and OME2. <b>2022</b> ,	O
357	The effect of various partial atomic charges on the bulk and liquid/vacuum interface properties of iodobenzene derivatives at their melting points. <b>2022</b> , 108400	О
356	Magneto-Structural Correlations in a Mixed Porphyrin(Cu2+)/Trityl Spin System: Magnitude, Sign and Distribution of the Exchange Coupling Constant.	O
355	Synthesis, characterization, computational studies and in vitro antiparasitic activity of novel flavanoidal-1,2,4,5-tetrazinane-6?-thione. 1-13	0
354	Solvent selection in membrane preparation from polyethylene terephthalate plastic waste: computational and experimental study. <b>2022</b> , 9, 125302	1
353	Diverse Cooperative Reactivity at a Square Planar Aluminium Complex and Catalytic Reduction of CO2.	O
352	A deep transfer learning-based protocol accelerates full quantum mechanics calculation of protein.	0
351	DFT, Hirshfeld Surface, Molecular Docking and Drug Likeness Studies of Medicinally Important Coumarin Molecule.	O
350	Pump-probe spectroscopy of chiral vibrational dynamics. <b>2022</b> , 8,	O
349	Zero-Field Splittings and Redox Potentials in an Isostructural Series of Dinuclear Fe II Ti IV , Fe III Ti IV , and Mn II Ti IV Complexes with a Face-Sharing Bridging Motive.	O
348	Quantification of the Steric Properties of 1,8-Naphthyridine-Based Ligands in Dinuclear Complexes.	O
347	Structurally Regulated Carbazole <b>P</b> yridine Derivatives Based on Space-Crowded Theory for Efficient Narrowband Ultraviolet Nondoped Organic Light-Emitting Diodes from the High-Lying Reverse Intersystem Crossing Process.	O
346	Insights into the role of the cobalt(III)-thiosemicarbazone complex as a potential inhibitor of the Chikungunya virus nsP4.	O
345	Efficient hydrogen storage capacity of La3B18: A DFT study. <b>2022</b> ,	О
344	Interexcited State Photophysics I: Benchmarking Density Functionals for Computing Nonadiabatic Couplings and Internal Conversion Rate Constants.	0

343	Quantum Chemical Prediction of the Acidities of Sulfonamide Inhibitors of Carbonic Anhydrase. <b>2022</b> , 126, 9207-9217	0
342	Constructing high-efficiency orange-red thermally activated delayed fluorescence emitters by three-dimension molecular engineering. <b>2022</b> , 13,	O
341	Hydrogen storage capacity of the niobium atom adsorbed on carbon and boron nitride planar nanoflakes. <b>2022</b> ,	0
340	URVA and Local Mode Analysis of an Iridium Pincer Complex Efficiently Catalyzing the Hydrogenation of Carbon Dioxide. <b>2022</b> , 10, 234	O
339	Selectivity Rule of Cryptands for Anions: Molecular Rigidity and Bonding Site.	0
338	Competing Routes in the Extraction of Lanthanide Nitrates by 1,10-Phenanthroline-2,9-diamides: An Impact of Structure of Complexes on the Extraction. <b>2022</b> , 23, 15538	1
337	Cross Second Virial Coefficients of the H2O⊞2S and H2OBO2 Systems from First Principles.	0
336	Oxygen versus Sulfur Coordination in Cobalt Superoxo Complexes: Spectroscopic Properties, O2 Binding, and H-Atom Abstraction Reactivity.	O
335	A multiconfigurational approach to the electronic structure of electro-generated species of the Re 2 (EP.h 2 PCH 2 PPh 2 )(S 2 CNEt 2 ) 4 complex.	О
334	On the intensity of light scattered by molecular liquidsComparison of experiment and quantum chemical calculations. <b>2022</b> , 157, 244501	O
333	Theoretical Investigation of Geometries and Bonding of Indium Hydrides in the In2Hx and In3Hy (x = $0$ 4,6; y = $0$ 5) Series. <b>2023</b> , 28, 183	0
332	Diboraanthracene-Doped Polymer Systems for Colour-Tuneable Room-Temperature Organic Afterglow.	O
331	Change in the Electronic Structure of the Cobalt(II) Ion in a One-Dimensional Polymer with Flexible Linkers Induced by a Structural Phase Transition. <b>2023</b> , 24, 215	O
330	Oligomerization of ethylene promoted by methylaluminoxane activated arylchalcogenyl-sulfonate nickel(II) complexes.	O
329	The dominant nature of Herzberg Teller terms in the photophysical description of naphthalene compared to anthracene and tetracene. <b>2022</b> , 12,	0
328	Modular Approach to Creating Functionalized Surface Arrays of Molecular Qubits. 2208998	1
327	Uncovering the Mechanism of Thermally Activated Delayed Fluorescence in Coplanar Emitters Using Potential Energy Surface Analysis. 310-317	O
326	Overall structure of Au12Ag60(S-c-C6H11)31Br9(Dppp)6: achieving stronger assembly of icosahedrons M13 units.	O

325	Thiosemicarbazonecopper/Halido Systems: Structure and DFT Analysis of the Magnetic Coupling. <b>2023</b> , 11, 31	0
324	Computational design of quinone electrolytes for redox flow batteries using high-throughput machine learning and theoretical calculations. 4,	О
323	Understanding the emergence of the boson peak in molecular glasses. 2023, 14,	O
322	Understanding the Role of Intramolecular Ion-Pair Interactions in Conformational Stability Using an Ab Initio Thermodynamic Cycle.	o
321	The oxidation dissolution of uranium oxides in carbonate-peroxide aqueous solution.	O
320	F2BMF (M = B and Al) Molecules: A Matrix Infrared Spectra and Theoretical Calculations Investigation. <b>2023</b> , 28, 554	o
319	Quantitative Descriptions of Dewar-Chatt-Duncanson Bonding Model: A Case Study of Zeise and Its Family Ions.	o
318	Branching mechanism of photoswitching in an Fe(II) polypyridyl complex explained by full singlet-triplet-quintet dynamics. <b>2023</b> , 6,	O
317	Antiviral Activity of Benzoheterocyclic Compounds from Soil-Derived Streptomyces ĵiujiangensis NBERC-24992. <b>2023</b> , 28, 878	0
316	Hydroxylated Coumarin-Based Thiosemicarbazones as Dual Antityrosinase and Antioxidant Agents. <b>2023</b> , 24, 1678	О
315	Spectroscopic snapshot for neutral water nonamer (H2O)9: Adding a H2O onto a hydrogen bond-unbroken edge of (H2O)8. <b>2023</b> , 158, 014301	O
314	Homochiral SCM Built of Tetrahedral and Pentagonal Bipyramidal Fe(II) Units Bridged by Chlorine.	О
313	Investigation of enhanced Am selectivity for Eu in solvent extraction using a BTPhen ligand substituted with halogen. <b>2023</b> , 13, 2476-2482	О
312	Denitrative hydroxylation of unactivated nitroarenes.	О
311	Study on endogenous inhibitors against PD-L1: cAMP as a potential candidate. <b>2023</b> , 123266	O
310	Investigating the Solvent Effects on Binding Affinity of PAHsExBox4+ Complexes: An Alchemical Approach. <b>2023</b> , 127, 249-260	О
309	Adsorption of water and organic solvents on the calcite [101[4] surface: implications for marble conservation treatments. <b>2023</b> , 156438	O
308	Charge-Induced Structure Variations of 1D-Iodine Inside Thin SWCNTs.	О

307	Benchmarking computational chemistry approaches on iminodiacetic acid. 2023, 100895	0
306	A novel paper-based microfluidic device and UV-visible spectroscopy coupled method for the field detection and analysis of seized marijuana samples.	O
305	Computational Studies on the Interaction of Organophosphorus Pesticides with Acetylcholinesterase and Butyrylcholinesterase: Quantum Chemical Cluster Model and HSAB Approaches. <b>2023</b> , 13, 153	О
304	Theoretical and Cyclic Voltammetric Analysis of Asparagine and Glutamine Electrocatalytic Activities for Dopamine Sensing Applications. <b>2023</b> , 13, 100	4
303	Photocatalytic Activity of the V2O5 Catalyst toward Selected Pharmaceuticals and Their Mixture: Influence of the Molecular Structure on the Efficiency of the Process. <b>2023</b> , 28, 655	О
302	SQMBox: Interfacing a semiempirical integral library to modular ab initio electronic structure enables new semiempirical methods .	O
301	Catalytic Oxidation of Benzoins by Hydrogen Peroxide on Nanosized HKUST-1: Influence of Substituents on the Reaction Rates and DFT Modeling of the Reaction Path. <b>2023</b> , 28, 747	1
300	Projection-Based Density Matrix Renormalization Group in Density Functional Theory Embedding. 716-722	O
299	The theoretical study of the oxidation reaction of hydroxyl radical for the removal of volatile organic aliphatic and aromatic aldehydes from the atmosphere.	O
298	Self-Catalyzed Hydroxyl-Yne Click Reaction: A Powerful Tool toward Red-Emitting Nontraditional Small Organic Luminogens.	O
297	Investigating the Unbinding of Muscarinic Antagonists from the Muscarinic 3 Receptor.	0
296	Theoretical Study of Charge Mobility in Crystal Porphine and a Computer Design of a Porphine-Based Semiconductive Discotic Liquid Mesophase. <b>2023</b> , 24, 736	O
295	The Boundary between Two Modes of Gas Evolution: Oscillatory (H2 and O2) and Conventional Redox (O2 Only), in the Hydrocarbon/H2O2/Cu(II)/CH3CN System. <b>2023</b> , 4, 74-102	O
294	Origin of Ferromagnetic Exchange Coupling in DonorAcceptor Biradical Analogues of Charge-Separated Excited States. <b>2023</b> , 62, 739-747	O
293	Screening out the Transition Metal Single Atom Supported on Onion-like Carbon (OLC) for the Hydrogen Evolution Reaction. <b>2023</b> , 62, 1001-1006	0
292	Probing the Pyrolysis of Ethyl Formate in the Dilute Gas Phase by Synchrotron Radiation and Theory.	O
291	Antioxidant Activities of Hydroxylated Naphthalenes: the Role of Aryloxyl Radicals.	О
290	Ab Initio Investigation of the Na3[Ln(ODA)3][2NaClO4[6H2O (Ln = CeNb; ODA = Oxydiacetate) Series.	O

289	Toward more accurate adiabatic connection approach for multireference wave functions.	О
288	Captodative Effect Facilitates the Excitation in Diboron Molecule (CAAC)2B2(SH)2.	О
287	Molecular insights into the functionalization of Au13 nanocluster with mercaptopurine anti-cancer drug. <b>2023</b> , 414547	O
286	Additive-Free Organic Radical Batteries Prepared through Electrochemical Polymerization of TEMPO-Decorated Terthiophene.	О
285	Microsolvation of phenol in water: structures, hydration free energy and enthalpy. 1-12	0
284	Processing Gray Selenium in Phosphonium-Based Ionic Liquids.	O
283	[4FeßS]-Mediated Proton-Coupled Electron Transfer Enables the Efficient Degradation of Chloroalkenes by Reductive Dehalogenases. 1173-1185	0
282	Pyrolysis of Trifluoroacetic Acid and Trifluoroacetic Anhydride Studied with Mass Spectrometry and Synchrotron Radiation: Decomposition and Free Radical Formation. <b>2023</b> , 8,	O
281	Anisotropically Fused Clusters Form a 2D Superatomic Sheet Exhibiting Polarized Light Emission.	O
280	Thermochemical study of the antioxidant activity of some hydroxycoumarins. 2023, 107006	O
279	Electron Attachment to Wobble Base Pairs. 2023, 127, 457-467	2
278	Incinerability of PFOA and HFPO-DA: Mechanisms, kinetics, and thermal stability ranking. <b>2023</b> , 457, 141235	O
277	The first supraicosahedral osmacarboranes and dynamic behavior of 13-vertex carborane. <b>2023</b> , 232, 116291	O
276	Understanding the photodynamics of 3-hydroxypyran-4-one using surface hopping simulations. <b>2023</b> , 438, 114538	O
275	Comprehensive study of substituent effects on structure and photochromic properties of 1,3-benzoxazine-4-one spiropyrans. <b>2023</b> , 1277, 134898	O
274	Insights into the HCl formation and volatilization mechanism from organochlorine in coal: A DFT study. <b>2023</b> , 338, 127271	O
273	Synthesis and Antiproliferative Activity against Cancer Cells of Indole-Aryl-Amide Derivatives. <b>2023</b> , 28, 265	0
272	The Effect of the Ancillary Ligand on Optical and Redox Properties of Cyclometalated Iridium(III) 2,5-Diphenyloxazole Complexes. <b>2022</b> , 48, 846-858	O

271	Planar Elongated B12 Structure in M3B12 Clusters (M = Cu-Au). 2023, 28, 236	O
270	A PYRIMIDINE-DERIVED DIPHOSPHINE P-MONOXIDE AND A Ag(I) COORDINATION POLYMER THEREOF: SYNTHESIS, STRUCTURE, AND LUMINESCENCE. <b>2022</b> , 63, 2020-2027	О
269	Synthesis of Novel 1,3,4-Oxadiazole-Derived Aminophosphonates/Aminophosphonic Acids and Evaluation of Their In Vitro Antiviral Activity against the Avian Coronavirus Infectious Bronchitis Virus. <b>2023</b> , 15, 114	Ο
268	Zn(II)-Catalyzed Selective N-Alkylation of Amines with Alcohols Using Redox Noninnocent Azo-Aromatic Ligand as Electron and Hydrogen Reservoir. <b>2023</b> , 88, 771-787	O
267	Catalytic isomerization of glucose to fructose over organic ligands: a DFT study. 2023, 29,	O
266	Application of Screen Printed Diamond Electrode, Coupled with Point-of-CarelPlatform, for Nanomolar Quantification of Phytonutrient Pterostilbene in Dietary Supplements: An Experimental Study Supported by Theory. 2023, 11, 15	O
265	Probing the Size Limit of Dispersion Energy Donors with a Bifluorenylidene Balance: Magic Cyclohexyl. <b>2023</b> , 88, 1024-1035	O
264	A Guide to In Silico Drug Design. <b>2023</b> , 15, 49	O
263	Synthesis and structural characterization of new spiropyran containing conjugated vinyl-3\(\text{H}\)ndolium moiety and its hydrolysis product. <b>2022</b> , 58, 712-720	0
262	Multifaceted View on the Mechanism of a Photochemical Deracemization Reaction. <b>2023</b> , 145, 2354-2363	O
261	A computational study of the gas-phase interstellar formose-like reactions. 2023, 2431, 012091	0
260	Highly Efficient Light-Driven CO 2 to CO Reduction by an Appropriately Decorated Iron Porphyrin Molecular Catalyst.	О
259	Conversion of Ketones into Blue-emitting Electron-deficient Benzofurans.	O
258	XPS and quantum chemical analysis of 4Me-BODIPY derivatives. <b>2023</b> , 25, 5211-5225	О
257	Uncovering Triradicaloid Structures in S 1 Benzene Photochemistry**.	0
256	Synthesis and biological activity of iron(II), iron(III), nickel(II), copper(II) and zinc(II) complexes of aliphatic hydroxamic acids. 1-30	O
255	Investigation of the Structures and Chemical Bonding of Mn2Ge6land Mn2Ge7lClusters via Anion Photoelectron Spectroscopy and Theoretical Calculations. <b>2023</b> , 62, 2033-2039	0
254	Exploring the Quantum Chemical Energy Landscape with GNN-Guided Artificial Force.	Ο

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253	A study of the thermodynamics and mechanisms of the atmospherically relevant reaction dimethyl sulphide (DMS) with atomic chlorine (Cl) in the absence and presence of water, using electronic structure methods. <b>2023</b> , 25, 4780-4793	O
252	Enhancing effect of choline chloride-based deep eutectic solvents with polyols on the aqueous solubility of curcuminshight from experiment and theoretical calculation. <b>2023</b> ,	O
251	Multi-Technique Experimental Benchmarking of the Local Magnetic Anisotropy of a Cobalt(II) Single-Ion Magnet.	О
250	CO2 Aggregation on Monoethanolamine: Observation from Rotational Spectroscopy.	O
249	Ab Initio Mo-lecular Dynam-ics Calculation on Electron Ion-ization Induced Fragmentations of C4F7N and C5F10O for Un-derstanding Their Decompo-sitions under Discharge Con-ditions.	O
248	Molecular interaction of di-ester bonded cationic Gemini surfactants with pepsin: in vitro and in silico perspectives. 1-16	O
247	Redox Potentials with COSMO-RS: Systematic Benchmarking with Different Databases.	O
246	Phosphine Reactivity and Its Implications for Pyrolysis Experiments and Astrochemistry. <b>2023</b> , 127, 1000-10	<b>12</b> o
245	Manifestation of Hydrogen Bonding and Exciton Delocalization on the Absorption and Two-Dimensional Electronic Spectra of Chlorosomes. <b>2023</b> , 127, 1097-1109	O
244	Linearly bridging N2 versus CO: Chemical bonding and spin-controlled reactivity	O
243	Exploring the Limits of Intramolecular London Dispersion Stabilization with Bulky Dispersion Energy Donors in Alkane Solution. <b>2023</b> , 145, 2093-2097	O
242	Promotion of adsorptive and catalytic properties of zeolitic Brfisted acid sites by proximal extra-framework Si(OH)x groups. <b>2023</b> , 6, 68-79	O
241	Inverse Sandwich Arene-Bridged Titanium Complexes Supported by a Bulky Tridentate [O, P, O] Ligand.	O
240	Tetranuclear Copper(I) and Silver(I) Pyrazolate Adducts with 1,1?-Dimethyl-2,2Ebibenzimidazole: Influence of Structure on Photophysics. <b>2023</b> , 28, 1189	1
239	CO2 Aggregation on Monoethanolamine: Observation from Rotational Spectroscopy.	O
238	Relativistic QTAIM. <b>2023</b> , 245-267	O
237	Practical guidance for easily interpreting the emission and physicochemical parameters of Eu3+ in solid-state hosts. <b>2023</b> ,	O
236	Molecular Dynamics with Chemical Accuracy-Alkane Adsorption in Acidic Zeolites. <b>2023</b> , 13, 2011-2024	O

235	In-situ construction of grass-like hybrid architecture responsible for extraordinary corrosion performance: experimental and theoretical approach.	O
234	Bis(pentafluorophenyl)borane-catalyzed E-selective isomerization of terminal alkenes to internal alkenes.	O
233	Theoretical Kinetic Studies on Thermal Decomposition of Glycerol Trinitrate and Trimethylolethane Trinitrate in the Gas and Liquid Phases. <b>2023</b> , 127, 1283-1292	О
232	Mechanism of Radical Initiation and Transfer in Class Id Ribonucleotide Reductase Based on Density Functional Theory.	O
231	Photophysical, photobiological, and biomolecule-binding properties of new tri-cationic meso-tri(2-thienyl)corroles with Pt(II) and Pd(II) polypyridyl derivatives. <b>2023</b> , 242, 112149	1
230	Improved surface flashover voltage of epoxy following polythiourea-assisted coating with high gas adsorption ability. <b>2023</b> , 618, 156546	О
229	An integrated ion trap for the photonion spectrometer at PETRA III. <b>2023</b> , 94, 023201	O
228	Cy3 Cyanine Dye with Strong Fluorescence Enhancement for AGRO100 and Its Derivative. <b>2023</b> , 127, 1811-1818	O
227	In Silico Design of Dihydroazulene/Vinylheptafulvene Photoswitches for Solar-Energy Storage Guided by an All-Around Performance Descriptor**.	О
226	Structure and Optical Properties of Polymeric Carbon Nitrides from Atomistic Simulations. <b>2023</b> , 35, 1547-1559	O
225	Ultrafast structural changes direct the first molecular events of vision. <b>2023</b> , 615, 939-944	O
224	Discovery of novel anti-cyanobacterial allelochemicals by multi-conformational QSAR approach. <b>2023</b> , 256, 106420	О
223	Molecular modification effects on the electrochromic and photochromic properties of diarylethene with intramolecular isomerization behavior. <b>2023</b> , 158, 114701	О
222	A study of the valence photoelectron spectrum of uracil and mixed water Dracil clusters. 2023, 158, 114301	О
221	Thermochemical and kinetics investigation of the CH2CN + CN system leading to NCCH2CN. <b>2023</b> , 815, 140371	О
220	Chemical Prepotassiation Realizes Scalable KC 8 Foil Anodes for Potassium-Ion Pouch Cells. 2300453	О
219	Nanomagnet-inspired design on molecularly imprinted nanofiber membrane: Mechanisms for improved transport selectivity of sufficient specific sites. <b>2023</b> , 672, 121467	О
218	Unveiling the thermodynamic and molecular mechanisms for the separation of diethoxymethane and ethanol azeotrope by deep eutectic solvents. <b>2023</b> , 376, 121451	О

217	Investigation of Dynamic Behavior of Confined Ionic Liquid [BMIM]+[TCM]In Silica Material SBA-15 Using NMR. <b>2023</b> , 24, 6739	О
216	Weak intra and intermolecular interactions via aliphatic hydrogen bonding in piperidinium based ionic Liquids: Experimental, topological and molecular dynamics studies. <b>2023</b> , 375, 121354	Ο
215	Zero-Field Splitting in Hexacoordinate Co(II) Complexes. <b>2023</b> , 9, 100	О
214	In-situ preparation of yeast-supported Fe0@Fe2O3 as peroxymonosulfate activator for enhanced degradation of tetracycline hydrochloride. <b>2023</b> , 324, 138340	Ο
213	Understanding of three different polyvinylpyrrolidone (PVP) based battery binders blends on graphene surfaces from first principles via DFT simulations. <b>2023</b> , 301, 127548	0
212	Structural evolution, electronic and magnetic properties investigation of V3Si[[n´=´14fl8]) clusters based on photoelectron spectroscopy and density functional theory calculations. <b>2023</b> , 820, 140423	Ο
211	A highly selective BnBffffluorescent sensor for detection of Fe3+ ion in protein and aqueous media: Synthesis, structural characterization, and computational studies. <b>2023</b> , 551, 121484	Ο
210	Reversible hydrogen storage on multiple Ti-doped B12C6N6 nanocage. <b>2023</b> , 62, 106910	Ο
209	Know your building blocks: Time-resolved EPR spectroscopy reveals NDI-T2 and not T-NDI-T to resemble the electronic structure of PNDIT2. <b>2023</b> , 117, 106790	Ο
208	1,4,9,9-tetramethyloctahydro-4,7-(epoxymethano)azulen-5(1H)-one, a natural product as a potential inhibitor of COVID-19: Extraction, crystal structure, and virtual screening approach. <b>2023</b> , 35, 102628	Ο
207	Theoretical approach to the one-step versus two-step spin transitions in Hofmann-like FeII SCO metal-organic frameworks. <b>2023</b> , 30, 101489	Ο
206	Synthesis, characterization and antimicrobial properties of silver complexes derived from 5,6-Dimethylbenzimidazol-2-ylidene. <b>2023</b> , 237, 116383	O
205	Theoretical insights into the spectroscopic properties of ferrocenyl hetaryl ketones. 2023, 296, 122635	0
204	Design and fabrication of nickel lanthanum telluride microfibers for redox additive electrolyte-based flexible solid-state hybrid supercapacitor. <b>2023</b> , 65, 107286	Ο
203	Modification of a commercial activated carbon with nitrogen and boron: Hydrogen storage application. <b>2023</b> , 64, 107193	Ο
202	Complexes of NiII, CoII, ZnII, and CuII with Promising Anti-Tuberculosis Drug: Solid-State Structures and DFT Calculations. <b>2023</b> , 11, 167	Ο
201	Combining Theoretical and Experimental Methods to Probe Confinement within Microporous Solid Acid Catalysts for Alcohol Dehydration. 5955-5968	0
200	Regioselective one-step alkoxy-aryloxycarbonylation of alkenes. <b>2023</b> , 421, 431-440	O

199	An advanced organic cathode for non-aqueous and aqueous calcium-based dual ion batteries. <b>2023</b> , 569, 232995	O
198	Studies towards investigation of Naphthoquinone-based scaffold with crystal structure as lead for SARS-CoV-19 management. <b>2023</b> , 1283, 135256	O
197	Simulation of uranyl-biomolecule interaction using a cationic dummy atom model. 2023, 822, 140479	0
196	Asymmetric counteranion-directed photoredox catalysis. <b>2023</b> , 379, 494-499	O
195	Liquid Dynamics Determine Transition Metal- N -Heterocyclic Carbene Complex Formation. <b>2023</b> , 29,	O
194	Photosensitizers Dispersed on Nanosized Triterpenoid Matrix with Deaggregation-Enhanced Singlet Oxygen Production. <b>2023</b> , 15, 4973-4983	O
193	In situ ligand restraints from quantum-mechanical methods. <b>2023</b> , 79, 100-110	O
192	Synthesis, Crystal, and Electronic Structure of (HpipeH2)2[Sb2I10](I2), with I2 Molecules Linking Sb2X10 Dimers into a Polymeric Anion: A Strategy for Optimizing a Hybrid Compound⊠ Band Gap. <b>2023</b> , 24, 2201	1
191	Analysis of non-covalent interactions in the acetone-chloroform system by MP2/CBS quantum chemical calculations.	O
190	Computational Study on Chemoselective Difunctionalization of Unactivated Alkenes with Radical-mediated Remote Functional Group Migration.	O
189	Photoisomerization of 1, 2-Di (4-pyridyl)ethylene According to NMR and UV Spectroscopy Data and Density Functional Modeling.	O
188	The reactions of 2-furfuryl alcohol with hydrogen atom: A theoretical calculation and kinetic modeling analysis. <b>2023</b> , 250, 112627	O
187	Halogen-Bonded Thiophene Derivatives Prepared by Solution and/or Mechanochemical Synthesis. Evidence of NIIIS Chalcogen Bonds in Homo- and Cocrystals. <b>2023</b> , 23, 2442-2454	O
186	Nitrocellulose-based propellants: elucidation of the mechanisms of the diphenylamine stabilizer employing density functional theory. 1-19	O
185	Intermolecular potential energy surfaces of NeH3+ and . <b>2023</b> , 1222, 114050	0
184	Pyrrolizidine alkaloids from Jacobaea vulgaris Gaertn and theoretical studies on intramolecular interactions. 1-6	O
183	Artificial Neural Network-Derived Unified Six-Dimensional Potential Energy Surface for Tetra Atomic Isomers of the Biogenic [H, C, N, O] System. <b>2023</b> , 19, 1186-1196	О
182	Design of Pyrrole-Based Gate-Controlled Molecular Junctions Optimized for Single-Molecule Aflatoxin B1 Detection. <b>2023</b> , 23, 1687	O

181	Evidence That Less Can Be More for Transferable Force Fields. 2023, 63, 1188-1195	0
180	Computational Study of Mechanisms and Tether Length Effects of Rh-Catalyzed [3+2] and [3+2+1] Reactions of Ene/Yne-Vinylcyclopropanes. <b>2023</b> , 18,	O
179	Hydration Structure of Diamondoids from Reactive Force Fields. 2023, 127, 3217-3227	О
178	Torsional Rotation in Ditopic Receptor Host and its Complex Formation with Resorcinol Guest: A Computational Study.	Ο
177	Dynamic molecular ordering in multiphasic nanoconfined ionic liquids detected with time-resolved diffusion NMR. <b>2023</b> , 4,	1
176	A catastrophe theory-based model for optimal control of chemical reactions by means of oriented electric fields. <b>2023</b> , 142,	O
175	Experimental and Theoretical Exploration of ESIPT in a Systematically Constructed Series of Benzimidazole Based Schiff Base Probes: Application as Chemosensors. <b>2023</b> , 29,	0
174	Structural Features Governing the Metabolic Stability of Tetraethyl-Substituted Nitroxides in Rat Liver Microsomes. <b>2023</b> , 12, 402	0
173	Outstanding improvement in removing the delocalization error by global natural orbital functional. <b>2023</b> , 158, 084110	1
172	Static and Dynamic Magnetic Properties of a Co(II)-Complex with N 2 O 2 Donor Set IA Theoretical and Experimental Study. <b>2023</b> , 26,	O
171	Evolution of Solute Water Interactions in the Benzaldehyde-(H2O)1 Clusters by Rotational Spectroscopy.	О
170	Two highly photoluminescent Eu3+ Ediketonates complexes with $\bar{\mu}$ -caprolactam as ancillary ligands: From synthesis to the first example as gunshot residue markers. <b>2023</b> , 137, 113527	O
169	Trihalide-included (I2, Br2 and IBrClDbambus[6]urils in halogenation and iodine-catalysed reactions. <b>2023</b> , 103, 81-87	О
168	Synthesis of Disubstituted Carboxonium Derivatives of Closo-Decaborate Anion [2,6-B10H8O2CC6H5][]Theoretical and Experimental Study. <b>2023</b> , 28, 1757	O
167	Heuristic-Based Alkaline Hydrolysis Mechanism of Nitrate Ester (Nitrocellulose Monomer) and Nitroamine (Hexogen) Compounds: Electrostatic Attraction Effect of the Nitro Group. <b>2023</b> , 127, 1609-1618	О
166	New Low-Dimensional OrganicIhorganic Lead Halide Hybrid Systems Directed by Imidazo[1,5-a]pyridinium-Based Cation or Imines: Synthesis, Structures, Non-Covalent Interactions and Optical Properties. <b>2023</b> , 13, 307	O
165	Regeneration and Degradation in a Biomimetic Polyoxometalate Water Oxidation Catalyst. <b>2023</b> , 13, 3007-3019	О
164	First X-ray Crystal Structure Characterization, Computational Studies, and Improved Synthetic Route to the Bioactive 5-Arylimino-1,3,4-thiadiazole Derivatives. <b>2023</b> , 24, 3759	0

163	Designing an Apparently Orbital-Symmetry-Forbidden [3s,5s]-Sigmatropic Shift through Transition-State Complexation and Stereoelectronic Effects. <b>2023</b> , 62,	O
162	Designing an Apparently Orbital-Symmetry-Forbidden [3s,5s]-Sigmatropic Shift through Transition-State Complexation and Stereoelectronic Effects. <b>2023</b> , 135,	O
161	Supramolecular Recognition of Cytidine Phosphate in Nucleotides and RNA Sequences. 2023, 3, 964-977	О
160	Interactions of Sodium Salicylate with Ecyclodextrin and an Anionic Resorcin[4]arene: Mutual Diffusion Coefficients and Computational Study. <b>2023</b> , 24, 3921	O
159	Dibenzyl-(1S*,2S*)-2,3-dihydro-1H-indene-1,2-dicarboxylate. <b>2023</b> , 2023, M1586	O
158	Insensitive High-Energy Density Materials Based on Azazole-Rich Rings: 1,2,4-Triazole N-Oxide Derivatives Containing Isomerized Nitro and Amino Groups. <b>2023</b> , 24, 3918	O
157	Slow Magnetic Relaxation and Modulated Photoluminescent Emission of Coordination Polymer Based on 3-Amino-4-hydroxybenzoate Zn and Co Metal Ions. <b>2023</b> , 28, 1846	O
156	Efficient removal of trace uranium from nuclear effluents using irradiation-functionalized fibrous adsorbents with very high salt tolerance. <b>2023</b> , 461, 141978	O
155	Electronic structure, cationic, and excited states of nitrogen-containing spiroborates. 2023, 29,	O
154	Dinitrogen Complexes of Cobalt(I) Supported by Rare-Earth Metal-Based Metalloligands. 2023, 62, 3836-38	<b>46</b> o
153	Metallodrugs against Breast Cancer: Combining the Tamoxifen Vector with Platinum(II) and Palladium(II) Complexes. <b>2023</b> , 15, 682	O
152	Computational and optoelectronic quantification of semi-conducting, warm ruby red color emanating Eu3+ complexes with hetro-cyclic ligands.	O
151	Solvent- and additive-free liquid-phase acceptorless dehydrogenation of benzyl alcohol to benzaldehyde catalyzed by carbon-encapsulating Cu nanoparticles: a combined experimental and theoretical study. <b>2023</b> , 136, 953-962	0
150	Pyridine-Based Small-Molecule Fluorescent Probes as Optical Sensors for Benzene and Gasoline Adulteration. <b>2023</b> , 3, 109-126	O
149	A Promising 1,3,5-Triazine-Based Anion Exchanger for Perrhenate Binding: Crystal Structures of Its Chloride, Nitrate and Perrhenate Salts. <b>2023</b> , 28, 1941	O
148	3-Aryl-5-aminobiphenyl Substituted [1,2,4]triazolo[4,3-c]quinazolines: Synthesis and Photophysical Properties. <b>2023</b> , 28, 1937	O
147	NHC-Stabilised Parent Tripentelyltrielanes.	О

145	Highly Efficient Purely Organic Phosphorescence Light-Emitting Diodes Employing a Donor Acceptor Skeleton with a Phenoxaselenine Donor. 2207003	O
144	Boradigermaallyl: (4+3) Cycloaddition-Initiated Boron Insertion into Benzene. <b>2023</b> , 135,	O
143	Unprecedented endo-oxidative cyclometallation and $[4'+3]$ cycloaddition of diene-vinylcyclopropanes. <b>2023</b> ,	0
142	Melamine Barbiturate as a Light-Induced Nanostructured Supramolecular Material for a Bioinspired Oxygen and Organic Radical Trap and Stabilization. <b>2023</b> , 8, 8276-8284	O
141	Atmospheric Sulfuric AcidMulti-Base New Particle Formation Revealed through Quantum Chemistry Enhanced by Machine Learning. <b>2023</b> , 127, 2091-2103	O
140	Strain-Release-Controlled [4 + 2 + 1] Reaction of Cyclopropyl-Capped Diene-ynes/Diene-enes and Carbon Monoxide Catalyzed by Rhodium. <b>2023</b> , 145, 5496-5505	O
139	Molecular Dynamics Simulation of CO2 Hydrate Growth in NaCl Aqueous Solution. 2023, 1-7	O
138	How Doping Affects the Activity of the Aluminum Oxide Support.	O
137	Synthesis of ONO-Ligated Tetrylenes Based on 2,6-bis(2-Hydroxyphenyl)pyridines: Influence of Ligand Sterics on the Structure of the Products. <b>2023</b> , 26,	O
136	Toward Atomistic Understanding of Materials with the ConversionAlloying Mechanism in Li-Ion Batteries. <b>2023</b> , 35, 2835-2845	О
135	The Role of Ligands in Oxidative Addition Chemistry of Low-Valent Main Group Derivatives: Not Only Stabilization but Also Activation.	O
134	Isolation, Structure Elucidation, and First Total Synthesis of Quinomycins K and L, Two New Octadepsipeptides from the Maowei Sea Mangrove-Derived Streptomyces sp. B475. <b>2023</b> , 21, 143	O
133	Quantum Computational, Spectroscopic (FT-IR, FT-Raman, NMR, and UV\(\mathbb{I}\)is) Hirshfeld Surface and Molecular Docking-Dynamics Studies on 5-Hydroxymethyluracil (Monomer and Trimer). <b>2023</b> , 28, 2116	0
132	AQME: Automated quantum mechanical environments for researchers and educators.	1
131	Modelling Complex Bimolecular Reactions in a Condensed Phase: The Case of Phosphodiester Hydrolysis. <b>2023</b> , 28, 2152	O
130	DFT and ONIOM Simulation of 1,3-Butadiene Polymerization Catalyzed by Neodymium-Based ZieglerNatta System. <b>2023</b> , 15, 1166	O
129	Citrated cellulose nanocrystals from post-consumer cotton textiles. 2023, 11, 6854-6868	0
128	Ancillary Ligand Coordination Directed Modes of Aggregation in Mixed-Valence Tetranuclear Cobalt Complexes: Synthesis, Structure, Field-Induced SIM Behavior, and Theoretical Insights. <b>2023</b> , 2169-2181	O

127	Surface Reaction of Methyl Mercaptan (CH3SH) with Hydrogen Atoms on Amorphous Solid Water. <b>2023</b> , 944, 219	O
126	Clusteromics V: Organic Enhanced Atmospheric Cluster Formation. <b>2023</b> , 8, 9621-9629	О
125	Formation of 3-Oxa- and 3-Thiacyclohexyne from Ring Expansion of Heterocyclic Alkylidene Carbenes: A Mechanistic Study. <b>2023</b> , 25, 1364-1369	О
124	Characterization of the Fe(III)-Tiron System in Solution through an Integrated Approach Combining NMR Relaxometric, Thermodynamic, Kinetic, and Computational Data. <b>2023</b> , 62, 4272-4283	О
123	A novel strategy for producing low-sugar pomegranate jam with better anthocyanin stability: Combination of high-pressure processing and low methoxyl & midated pectin. <b>2023</b> , 179, 114625	О
122	Testing the Limits of Imbalanced CPET Reactivity: Mechanistic Crossover in H-Atom Abstraction by Co(III) Dxo Complexes. <b>2023</b> , 145, 5664-5673	O
121	Multiscale theoretical tools for in silico macromolecular chemistry and engineering. 2023, 17-69	О
120	Electron heat transport in low-rank lignite: combining experimental and computational methods.	O
119	Mononuclear mononitrosyl iron complex with 8-mercaptoquinoline. Synthesis, structure and properties. <b>2023</b> , 1284, 135285	0
118	Interaction Modification of Transition Metal Dichalcogenide Layers by Halogenation. 2023, 127, 5134-5144	O
117	Engineering Flexible Metal-Phenolic Networks with Guest Responsiveness via Intermolecular Interactions. <b>2023</b> , 135,	0
116	Green Synthesis of Na abietate Obtained from the Salification of Pinus elliottii Resin with Promising Antimicrobial Action. <b>2023</b> , 12, 514	О
115	Copper and Nickel Complexes of OxamatePhenol Containing Ligands: A Structural Dichotomy in Oxidized Species.	О
114	Engineering Flexible Metal-Phenolic Networks with Guest Responsiveness via Intermolecular Interactions. <b>2023</b> , 62,	О
113	Aromaticity in P8 allotropes and (CH)8 analogues: significance of their 40 valence electrons?. <b>2023</b> , 25, 9364-9372	O
112	Influence of chirality on the aggregation of a new A-ED-EA small molecule with a benzodithiophene core: Spectroscopic and morphological investigations. <b>2023</b> , 138, 113619	1
111	Cold Oxidative Demetalation of Aryl Organometallics: A Novel Route to Demetalate Ullmann Intermediates without Heating. <b>2023</b> , 8,	0
110	Bis(perfluoroaryl)chalcolanes ArF2Ch (Ch = S, Se, Te) as ÆHole Donors for Supramolecular Applications Based on Noncovalent Bonding. <b>2023</b> , 23, 2593-2601	O

109	Electron Attachment to DNA: The Protective Role of Amino Acids. 2023, 127, 2215-2227	1
108	Electrochemistry of Uranyl Peroxide Solutions during Electrospray Ionization. <b>2023</b> , 62, 4456-4466	O
107	Free-Radical Propagation Rate Coefficients of Diethyl Itaconate and Di-n-Propyl Itaconate Obtained via PLPBEC. <b>2023</b> , 15, 1345	0
106	Stability of a Silica-Supported Second Generation Hoveyda-Grubbs Catalyst Under Atmospheric Conditions: Experimental and Computational Studies.	O
105	Relativistic Effects on Rate and Product Formation in the Gas-Phase Methane Chemistry of Late Atomic Transition Metal Cations.	O
104	New Hybrid Compound Candidate as Photothermal Agent Based on DPP Derivatives and Toluidine Blue: A Theoretical Perspective.	O
103	Reactions of Zinc Hydride with Silylenes: From Oxidative Addition to Ligand Exchange Reactions. <b>2023</b> , 42, 457-464	0
102	Is DFT Accurate Enough to Calculate Regioselectivity? The Case of 1,3-Dipolar Cycloaddition of Azide to Alkynes and Alkenes.	O
101	Benchtop 19F Nuclear Magnetic Resonance (NMR) Spectroscopy Provides Mechanistic Insight into the Biginelli Condensation toward the Chemical Synthesis of Novel Trifluorinated Dihydro- and Tetrahydropyrimidinones as Antiproliferative Agents. <b>2023</b> , 8, 10545-10554	Ο
100	Multicomponent wavefunction-in-DFT embedding for positronium molecules. <b>2023</b> , 158, 134101	O
99	Assessing the Role of the KohnBham Density in the Calculation of the Low-Lying BetheBalpeter Excitation Energies. <b>2023</b> , 127, 2618-2627	О
98	Synergistic Catalysis in Heterobimetallic Complexes for Homogeneous Carbon Dioxide Hydrogenation. <b>2023</b> , 28, 2574	O
97	Sulfur X-ray Absorption and Emission Spectroscopy of Organic Sulfones.	O
96	Oxidation State Tuning of Room Temperature Phosphorescence and Delayed Fluorescence in Phenothiazine and Phenothiazine-5,5-dioxide Dimers.	O
95	Quantitative Solvation Energies from Gas-Phase Calculations: First-Principles Charge Transfer and Perturbation Approaches. <b>2023</b> , 127, 2546-2551	О
94	Extended-sampling QM/MM simulation of biochemical reactions involving PN bonds. <b>2023</b> , 25, 9824-9836	O
93	Synthesis and Properties of a Through-Space Interacting Diradicaloid.	О
92	Exploring the Accuracy Limits of PNO-Based Local Coupled-Cluster Calculations for Transition-Metal Complexes. <b>2023</b> , 19, 2039-2047	Ο

91	Methanol Synthesis on Copper-Doped F Centers. 2023, 127, 5321-5333	O
90	Modeling the Effect of Disorder in the Two-Dimensional Electronic Spectroscopy of Poly-3-hexyltiophene in an Organic Photovoltaic Blend: A Combined Quantum/Classical Approach. <b>2023</b> , 127, 6793-6801	O
89	Excited-State Intramolecular Proton Transfer in Salicylidene-Hydroxy Carboxylate Derivatives: Direct Detection of the Triplet Excited State of the cis-Keto Tautomer. <b>2023</b> , 127, 2765-2778	О
88	Unraveling Binding Mechanism and Stability of Urease Inhibitors: A QM/MM MD Study. <b>2023</b> , 28, 2697	O
87	Dense and Acidic Organelle-Targeted Visualization in Living Cells: Application of Viscosity-Responsive Fluorescence Utilizing Restricted Access to Minimum Energy Conical Intersection. <b>2023</b> , 95, 5196-5204	О
86	How the coordination modes change the performance of Rh-PPh3 for complexes catalyst allyl alcohol hydroformylation: A theoretical study. <b>2023</b> , 177, 106647	O
85	Gas phase synthesis of the C40 nano bowl C40H10. <b>2023</b> , 14,	O
84	Do Models beyond Hybrid Density Functionals Increase the Agreement with Experiment for Predicted NMR Chemical Shifts or Electric Field Gradient Tensors in Organic Solids?. <b>2023</b> , 127, 2846-2858	O
83	Coating of SPIONs with a Cysteine-Decorated Copolyester: A Possible Novel Nanoplatform for Enzymatic Release. <b>2023</b> , 15, 1000	1
82	Control of Molecular Packing in Crystal and Electron Communication of Two Ferrocenyl Moieties across Chiral Isomannide or Isosorbide Bridge. <b>2023</b> , 13, 520	O
81	Acceptor substitution engineering of BODIPY-based organic photosensitizers with aggregation-induced emission for organelle localization and photodynamic anticancer therapy. <b>2023</b> , 228, 111838	О
80	Ultrafast Photoelimination of Nitrogen from Upper Excited States of Diazoalkanes and the Fate of Carbenes Formed in the Reaction. <b>2023</b> , 88, 4286-4300	Ο
79	SchNetPack 2.0: A neural network toolbox for atomistic machine learning. 2023, 158, 144801	O
78	First-principles study of square chalcogen bond interactions and its adsorption behavior on silver surface. <b>2023</b> , 25, 10836-10844	O
77	Hirshfeld Atom Refinement of Metal©rganic Complexes: Treatment of Hydrogen Atoms Bonded to Transition Metals. <b>2023</b> , 127, 3020-3035	0
76	Path separation of dissipation-corrected targeted molecular dynamics simulations of protein I gand unbinding. <b>2023</b> , 158, 124106	O
75	Interactive Organic Reaction Trajectory Animation iPhone Application (iORA) and Web Site (webORA). <b>2023</b> , 100, 1659-1663	О
74	Influence of Oxygen Atoms and Ring Strain on the Low-Temperature Oxidation Pathways of 1,3-Dioxolane. <b>2023</b> , 127, 2992-2999	Ο

73	Multiple resonance induced thermally activated delayed fluorescence: effect of chemical modification. <b>2023</b> , 5, 014010	О
72	Structural, Spectroscopic, and Bonding Analyses of La(III)/Ce(III)-Tetrel Ate-Complexes. 2023, 62, 5660-5668	О
71	A novel phthalocyanine based discotic liquid crystal for efficient corrosion inhibition of mild steel. 1-9	0
70	New Guaiane-Type Sesquiterpenoids Biscogniauxiaols A <b>©</b> with Anti-Fungal and Anti-Inflammatory Activities from the Endophytic Fungus Biscogniauxia Petrensis. <b>2023</b> , 9, 393	О
69	Theoretical studies on spiro[acridine-fluorene]-based emitters with efficient thermally activated delayed fluorescence. <b>2023</b> , 1284, 135431	0
68	Structure of the green heme isolated from allylbenzene-modified chloroperoxidase: A novel heme architecture implicating the mechanisms of CPO inactivation and epoxidation. <b>2023</b> , 21, 2365-2372	O
67	Exploring Spin-Phonon Coupling in Magnetic 2D Metal-Organic Frameworks. <b>2023</b> , 13, 1172	0
66	Magnetic frustration and fractionalization in oligo(indenoindenes). 2023, 107,	О
65	Origin of the Distinctive Electronic Structure of Co- and Fe-Porphyrin-Nitrene and Its Effect on Their Nitrene Transfer Reactivity. <b>2023</b> , 62, 5810-5821	0
64	Screening Efficient Tandem Organic Solar Cells with Machine Learning and Genetic Algorithms. <b>2023</b> , 127, 6179-6191	О
63	Roles of the Zinc Ion and Water Molecule in the Active Site of the Copper-Zinc SOD Catalyst. 2023, 55-59	O
62	Polyhedral Dicobaltadithiaboranes and Dicobaltdiselenaboranes as Examples of Bimetallic Nido Structures without Bridging Hydrogens. <b>2023</b> , 28, 2988	О
61	A density functional theory insight into the extraction mechanism of lithium recovery from alkaline brine by Ediketones.	О
60	Photooxidation Chemistry of Hydrofluoroolefins: Assessing the Impact of Substituents on the Greenhouse Gas Replacements. <b>2023</b> , 7, 876-884	O
59	Toward a Combined Molecular Dynamics and Quantum Mechanical Approach to Understanding Solvent Effects on Chemical Processes in the Pharmaceutical Industry: The Case of a Lewis Acid-Mediated SNAr Reaction. <b>2023</b> , 27, 742-754	0
58	Quantum Chemical Study of the Pressure-dependent Phosphorescence of [Cr(ddpd)2]3+ in the Solid State.	O
57	Electroluminescence of Tetradentate Pt(II) Complexes: O^N^N^O versus C^N^N^O Coordination. <b>2023</b> , 62, 5772-5779	0
56	Theoretical design of a new hydrogen storage based on the decorated phosphorene nanosheet by alkali metals. <b>2023</b> , 178, 111354	O

55	Revisiting the Spectrum of Co(CN)63[IThe Role of Correlation, Solvation, and Vibronic and Spin Drbit Couplings. <b>2023</b> , 127, 3200-3209	O
54	The physicochemical properties of the CeF3 IFLiNaK molten mixture: an in silico study. <b>2023</b> , 49, 845-854	Ο
53	Solvation Dynamics of Oxadiazoles as Potential Candidate for Drug Preparation. 2023, 35, 991-998	О
52	A General Picture of Cucurbit[8]uril Host <b>ū</b> uest Binding: Recalibrating Bonded Interactions. <b>2023</b> , 28, 3124	O
51	Spectroscopic and Magnetic Studies of Co(II) Scorpionate Complexes: Is There a Halide Effect on Magnetic Anisotropy?. <b>2023</b> , 62, 5984-6002	O
50	Acceleration of Stepwise Carbon-Polygold Bonding Cleavage in Hypercoordinated Carbon-Centered Gold(I) Clusters. <b>2023</b> , 62, 6147-6154	O
49	Investigating the Thermodynamics and Kinetics of Catechin Pyrolysis for Environmentally Friendly Binders. <b>2023</b> , 8, 12693-12701	O
48	How Metal Nuclearity Impacts Electrocatalytic H2 Production in Thiocarbohydrazone-Based Complexes. <b>2023</b> , 11, 149	O
47	Multiscale Theoretical Study of Sulfur Dioxide (SO2) Adsorption in Metal®rganic Frameworks. <b>2023</b> , 28, 3122	0
46	C-P/C=O bonds assisted desolvation effect in ultra-micropores carbon for boosting Zn-ion storage capability. <b>2023</b> , 58, 332-343	O
45	Ring-opening reactions of phosphoramidate heterocycles. <b>2023</b> , 137, 133390	O
44	Liquid-assisted mechanochemical synthesis, crystallographic, theoretical and molecular docking study on HIV instasome of novel copper complexes: (µ-acetato)-bis(2,2?-bipyridine)-copper and bromidotetrakis(2-methyl-1H-imidazole)-copper bromide.	O
43	Additivity of Diene Substituent Gibbs Free Energy Contributions for DielsAlder Reactions between Me2C?CMe2 and Substituted Cyclopentadienes. <b>2023</b> , 8, 14160-14170	0
42	Anomalous deep-red luminescence of perylene black analogues with strong IIInteractions. <b>2023</b> , 14,	O
41	Multiconfigurational Calculations and Photodynamics Describe Norbornadiene Photochemistry.	0
40	Luminescent Zirconocene Complexes with Pendant Phosphine Chalcogenide Donor Groups.	O
39	Calculation of Excited State Internal Conversion Rate Constant Using the One-Effective Mode Marcus-Jortner-Levich Theory.	0
38	Separation of phenolic compounds from water by using monoterpenoid and fatty acid based hydrophobic deep eutectic solvents. <b>2023</b> , 381, 121806	O

37	High-Valent Iridium Complexes Containing a Tripodal Bis-Cyclometalated C^N^C Ligand.	O
36	Two Shared Icosahedral Metallacarboranes through Iron: A Joint Experimental and Theoretical Refinement of M\( \begin{align*} \text{Results and Shauer Spectrum in [Fe(1,2-C2B9H11)2]Cs. \textbf{2023}, 8, 13993-14004 \end{align*}	О
35	Terahertz (6-18 THz) spectroscopic characterization of benzoic acid class liquid crystals using Fourier Transform Infrared technique. 1-7	0
34	Molecular Engineering to Tune Functionality: The Case of Cl-Substituted [Fe(terpy)2]2+.	О
33	Structure determination and magnetic studies of triazole chelated Co(II) coordination polymers.	O
32	MOF-derived Co/Fe@NPC-500 with large amounts of low-valent metals as an electro-Fenton cathode for efficient degradation of ceftazidime. <b>2023</b> , 333, 122755	О
31	Iron(II) Complexes with Porphyrin and Tetrabenzoporphyrin: CASSCF/MCQDPT2 Study of the Electronic Structures and UVI∕vis Spectra by sTD-DFT. <b>2023</b> , 24, 7070	О
30	A conserved hymenopteran-specific family of cytochrome P450s protects bee pollinators from toxic nectar alkaloids. <b>2023</b> , 9,	O
29	Dynamical Simulations of Carotenoid Photoexcited States Using Density Matrix Renormalization Group Techniques.	0
28	Peroxo-Diiron(III/III) as the Reactive Intermediate for N-Hydroxylation Reactions in the Multidomain Metalloenzyme SznF: Evidence from Molecular Dynamics and Quantum Mechanical/Molecular Mechanical Calculations. 5808-5818	О
27	Spectroscopical and Molecular Studies of Four Manganese(I) PhotoCORMs with Bioinspired Ligands Containing Non-Coordinated Phenol Groups. <b>2023</b> , 28, 3439	0
26	Rhenium(V) Tris(pyrazolyl)borate Complexes as Ligands in Square Planar Palladium and Platinum Complexes. <b>2023</b> , 49, 33-40	О
25	Cobalt and Iron Phthalocyanine Derivatives: Effect of Substituents on the Structure of Thin Films and Their Sensor Response to Nitric Oxide. <b>2023</b> , 13, 484	0
24	On the Dynamic Behavior of Pacman Phosphanes-A Case of Cooperativity and Redox Isomerism.	O
23	Tristhiolato Pseudopeptides Bind Arsenic(III) in an AsS3 Coordination Environment Imitating Metalloid Binding Sites in Proteins.	0
22	Structural and Dynamic Characterization of Lilbnic Liquid Electrolyte Solutions for Application in Li-Ion Batteries: A Molecular Dynamics Approach. <b>2023</b> , 9, 234	O
21	Structural Features of 4-VP-HEMA-SiO2 Hybrid Membranes and Their Proton Conductivity. <b>2023</b> , 5, 92-97	0
20	Kinetic, Thermodynamic, and Dynamic Control in Normal vs. Cross [2 + 2] Cycloadditions of Ene-Keteniminium Ions: Computational Understanding, Prediction, and Experimental Verification.	O

19	Adsorption Capacity of Silica SBA-15 and Titanosilicate ETS-10 toward Indium Ions. 2023, 16, 3201	0
18	Environmental theoretical calculation for non-periodic systems. 2023,	O
17	Halogen bonding: a designer strategy for graphyne-like two-dimensional architectures. 2023, 142,	О
16	Regiodivergent Nucleophilic Fluorination under Hydrogen Bonding Catalysis: A Computational and Experimental Study.	O
15	Understanding the Origins of Site Selectivity in Hydrogen Atom Transfer Reactions from Carbohydrates to the Quinuclidinium Radical Cation: A Computational Study.	0
14	Flexible Molecular Electrochromic Devices Run by Low-Cost Commercial Cells.	O
13	Exploring the Interaction of Pyridine-Based Chalcones with Trinuclear Silver(I) Pyrazolate Complex. <b>2023</b> , 11, 175	О
12	Transient and general synthesis of high-density and ultrasmall nanoparticles on two-dimensional porous carbon via coordinated carbothermal shock. <b>2023</b> , 14,	O
11	Enhancement of Atmospheric Nucleation Precursors on Iodic Acid-Induced Nucleation: Predictive Model and Mechanism.	0
10	Covalent Adduct Formation as a Strategy for Efficient CO2 Fixation in Crotonyl-CoA Carboxylases/Reductases. 6230-6241	O
9	The gas-phase pyrolysis of cyclopropylamine. A computational study on the kinetics and reaction mechanism. <b>2023</b> , 253, 112774	0
8	Understanding Antioxidant Abilities of Dihydroxybenzenes: Local and Global Electron Transfer Properties. <b>2023</b> , 11, 88	O
7	Ozonation of Gabapentin in Water-Investigating Reaction Kinetics and Transformation Mechanisms of a Primary Amine Using Isotopically Labeled Ozone.	О
6	Static and Dynamical Quantum Studies of CX3-AlX2 and CSiX3-BX2 (X = F, Cl, Br) Complexes with Hydrocyanic Acid: Unusual Behavior of Strong Ehole at Triel Center. <b>2023</b> , 24, 7881	O
5	Combined Structural and Computational Study of the mRubyFT Fluorescent Timer Locked in Its Blue Form. <b>2023</b> , 24, 7906	0
4	Including vibrational effects in magnetic circular dichroism spectrum calculations in the framework of excited state dynamics. <b>2023</b> , 158,	O
3	A Chain of Vertex-Sharing (Colli2Coll2)n Squares with Single-Ion Magnet Behavior. 2023, 9, 130	О
2	Performance of Functionals and Basis Sets in Calculating Redox Potentials of Nitrile Alkenes and Aromatic Molecules using Density Functional Theory. <b>2023</b> , 8,	О

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