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Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density

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631	Cation controlled rotation in anionic pillar[5]arenes and its application for fluorescence switch. <b>2023</b> , 14,	Ο
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628	Synthesis of functionalized aminopyrazole and pyrazolopyrimidine derivatives: Molecular modeling and docking as anticancer agents. <b>2023</b> , 16, 104645	Ο
627	HOAX: a hyperparameter optimisation algorithm explorer for neural networks.	O
626	Electronic Structures and NLO Properties of a Series of TMDs Lateral-CoreBhell Heterostructures Quantum Dots. <b>2023</b> , 6,	0
625	Spectral analysis (FT-IR, FT-Raman, UV and NMR), molecular docking, ADMET properties and computational studies: 2-Hydroxy-5-nitrobenzaldehyde. <b>2023</b> , 100, 100927	O
624	Pyridinecarboxaldehydes: Structures, Vibrational Assignments and Molecular Characteristics Using Experimental and Theoretical Methods. <b>2023</b> , 53,	0
623	The structure-based optimization of 3-substituted indolin-2-one derivatives as potent and isoform-selective c-Jun N-terminal kinase 3 (JNK3) inhibitors and biological evaluation. <b>2023</b> , 250, 115167	O
622	Mechanistic Insights into Substrate Positioning That Distinguish Non-heme Fe(II)/Exetoglutarate-Dependent Halogenases and Hydroxylases. <b>2023</b> , 13, 2489-2501	0
621	Supramolecular structure and isomeric transformations of N-t-butyl-N?-trifluoromethanesulfonacetamidine.	O
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619	A conceptual DFT and information-theoretic approach towards QSPR modeling in polychlorobiphenyls. <b>2023</b> , 61, 1143-1164	O
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614	Vibrational frequency Analysis, DFT and in Vitro Fungicidal Activity Studies of Biphenyl-4-Carboxylic Acid, 2,4-Difluorobiphenyl and 4-Acetylbiphenyl- A Comparative Study. 1-33	0
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611	The syntheses, photophysical properties and pH-sensitive studies of heterocyclic azo dyes bearing coumarinthiophenethiazole.	O

610	Revealing the steric effects of cobalt porphyrin on the selectivity of oxygen reduction reaction. <b>2023</b> , 663, 131091	О
609	Millimeter-wave spectrum of 2-propanimine. <b>2023</b> , 520, 4089-4102	О
608	Thermal site energy fluctuations in photosystem I: new insights from MD/QM/MM calculations. <b>2023</b> , 14, 3117-3131	O
607	In-silico approaches towards development of model irreversible HIV-1 protease inhibitors.	o
606	Synthesis and functionalization of electron-deficient perfluoroalkyl porphyrin building blocks for supermolecular systems. A-P	0
605	Employing Long-Range Inductive Effects to Modulate Metal-to-Ligand Charge Transfer Photoluminescence in Homoleptic Cu(I) Complexes. <b>2023</b> , 62, 3248-3259	0
604	Molecular dynamics simulation studies of 1,3-dimethyl imidazolium nitrate ionic liquid with water. <b>2023</b> , 158, 084505	0
603	Dinuclear Phenoxo-Bridged Nickel(II) and Copper(II) Complexes of Phenolate-Based Tripodal Ligand: Theoretical and Experimental Insights. 1-20	О
602	Impact of the local atomic structure on the thermal conductivity of amorphous Ge2Sb2Te5. <b>2023</b> , 158, 084504	O
601	Instigating the in vitro antidiabetic activity of new tridentate Schiff base ligand appended M(II) complexes: From synthesis, structural characterization, quantum computational calculations to molecular docking, and molecular dynamics simulation studies. <b>2023</b> , 37,	О
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596	Tuning transport properties of deformed carbon nanocages by electric field, electrode material, and type of coupling. <b>2023</b> , 28, 101383	0
595	Encapsulation of xenon by bridged resorcinarene cages with high 129Xe NMR chemical shift and efficient exchange dynamics. <b>2023</b> , 4, 101281	o
594	Structural Features Governing the Metabolic Stability of Tetraethyl-Substituted Nitroxides in Rat Liver Microsomes. <b>2023</b> , 12, 402	0
593	Model Chemistry Recommendations for Scaled Harmonic Frequency Calculations: A Benchmark Study. <b>2023</b> , 127, 1715-1735	O

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589	An Oxytocin Sensor Based on an Organic Field-Effect Transistor Functionalized with a Molecularly Imprinted Polymer. <b>2022</b> ,	O
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587	A Systematic Study on the Redox Potentials of Phenazine-Derivatives in Aqueous Media: A Combined Computational and Experimental Work. <b>2023</b> , 16,	O
586	Theoretical simulations on metal nanocluster systems. <b>2023</b> , 201-231	O
585	Computational Investigation of Substituent Effects on the Alcohol + Carbonyl Channel of Peroxy Radical Self- and Cross-Reactions. <b>2023</b> , 127, 1686-1696	O
584	Small, Electron-Donating Substituents Give CO2 Activation by Permethylpentalene Zirconium Amido Complexes the Upper Hand: A DFT Study of Distortion and Interaction. <b>2023</b> , 62, 3000-3006	0
583	On the self-consistency of DFT-1/2. <b>2023</b> , 158, 094103	O
582	Local Reactivity on Carbon Quantum Dots: The Influence of the Geometries and Chemical Doping for Chemical Sensor Applications. <b>2023</b> , 127, 3819-3829	0
581	Mechanism of Calcium Permeation in a Glutamate Receptor Ion Channel. <b>2023</b> , 63, 1293-1300	1
580	Switching of Redox Levels Leads to High Reductive Stability in Water-in-Salt Electrolytes.	O
579	Ph2Te2: An Accessible Main Group Organometallic Target for Spectral Characterization and Modeling. <b>2023</b> , 100, 1313-1319	O
578	Benchmarking two-photon absorption strengths of rhodopsin chromophore models with CC3 and CCSD methodologies: An assessment of popular density functional approximations. <b>2023</b> , 158, 094106	O
577	The effects of experimentally obtained electron correlation and polarization on electron densities and exchange-correlation potentials. <b>2023</b> , 158, 124103	O
576	A combined experimental and theoretical study of RuO2/TiO2 heterostructures as a photoelectrocatalyst for hydrogen evolution. <b>2023</b> , 52, 3472-3481	О
575	Computational Evidence of the Incipient Oxocarbenium Ion as a Hidden IntermediateDuring the Cyclization of Hydroxyenol Ether into Spiroketal Under Mild Acidic Condition.	O

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573	Computational Approaches in Some Important Organometallic Catalysis Reaction. 2023, 375-407	O
572	Doping of Graphene Nanostructure with Iron, Nickel and Zinc as Selective Detector for the Toxic Gas Removal: A Density Functional Theory Study. <b>2023</b> , 9, 20	0
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570	Electronic Structures and Spectroscopic Signatures of Noble-Gas-Doped Nanodiamonds.	0
569	Search for immunomodulatory compounds with antiproliferative activity against melanoma. <b>2023</b> , 160, 114374	O
568	Thermochemistry of uranium sulfide cations: guided ion beam and theoretical studies of reactions of U+ and US+ with CS2 and collision-induced dissociation of US+.	О
567	Structure, Vibrational Spectra, and Cryogenic MatrixPhotochemistry of 6-Bromopyridine-2-carbaldehyde: From the Single Molecule of the Compound to the Neat Crystalline Material. <b>2023</b> , 28, 1673	O
566	The Selection of the Best Derivatization Reagents for the Determination of Polyamines in Home-Made Wine Samples. <b>2023</b> , 16, 1474	0
565	A pH-Activatable Prodrug and Metal Prodrug Conjugate of Gossypol: Synthesis, Emergent Photophysical, Nanoscopic, Computational, and in-Vitro Cellular Studies.	O
564	Mechanistic Insight into Cu-Catalyzed CN Coupling of Hindered Aryl Iodides and Anilines Using a Pyrrol-ol Ligand Enables Development of Mild and Homogeneous Reaction Conditions. <b>2023</b> , 13, 2904-2915	0
563	Design, Synthesis, and Optical and Electrochemical Properties of DA Type Organic Dyes with Carbazole-Based Donor Units for Efficient Dye-Sensitized Solar Cells: Experimental and Theoretical Studies. <b>2023</b> , 52, 2525-2543	O
562	Intramolecular interactions (O-HD, C-HD, N-HD in isomers of neutral, cation, and anion dopamine molecules: A DFT study on the influence of solvents (water and ethanol). <b>2023</b> , 29,	0
561	Absorption of ethylene dichloride with imidazolium-based ionic liquids. <b>2023</b> , 376, 121449	O
560	Benzothiazole and benzoxazole promoted cleavage of Ru IC(aryl) bond in a four-membered ortho-metalated ruthenium(II) organometallics.	0
559	Conformational analysis of cyclohexyl hydroperoxide by rotational spectroscopy. <b>2023</b> , 392, 111758	О
558	Resonance Raman and Visible Micro-Spectroscopy for the In-Vivo and In-Vitro Characterization of Anthocyanin-Based Pigments in Blue and Violet Flowers: A Comparison with HPLC-ESI- MS Analysis of the Extracts. <b>2023</b> , 28, 1709	0
557	Resonance-Enhanced Multiphoton Ionization Studies of the Lower Electronically Excited States of Flavone. <b>2023</b> , 127, 1649-1655	О

556	Solvent-Mediated Tunable Regiodivergent C6- and N1-Alkylations of 2,3-Disubstituted Indoles with p-Quinone Methides. <b>2023</b> , 88, 3132-3147	О
555	GeTe2 Phase Change Material for Terahertz Devices with Reconfigurable Functionalities Using Optical Activation.	О
554	The d Orbital Multi Pattern Occupancy in a Partially Filled d Shell: The KFeF3 Perovskite as a Test Case. <b>2023</b> , 16, 1532	О
553	The Boekelheide Rearrangement of PyrimidineN-oxides as a Case Study of Closed or Open Shell Reactions - Experimental and Computational Evidence for the Participation of Radical Intermediates.	O
552	Revealing Structural and Physical Properties of Polylactide: What Simulation Can Do beyond the Experimental Methods. 1-39	О
551	Naphthalene Phthalimide Derivatives as Model Compounds for Electrochromic Materials. <b>2023</b> , 28, 1740	O
550	Extending density functional theory with near chemical accuracy beyond pure water. 2023, 14,	О
549	Influence of Changing the Remote Substituents on Charge Transfer Properties of Cyanide-Bridged Trinuclear Fe <b>R</b> uffe Complexes.	Ο
548	Melatonin Activation by Cytochrome P450 Isozymes: How Does CYP1A2 Compare to CYP1A1?. <b>2023</b> , 24, 3651	О
547	Heteropolymetallic [FeFe]-Hydrogenase Mimics: Synthesis and Electrochemical Properties. <b>2023</b> , 62, 3409-3419	O
546	Operando characterization of rhodium catalyst degradation in hydroformylation. 2023, 13, 1788-1801	1
545	Mechanistic insights into catalyst-dependent divergent cycloaddition reactions via discrimination between diazo compounds. <b>2023</b> , 10, 1606-1616	Ο
544	Mechanistic insights into the Cu(ii)/DBU-catalyzed incorporation of CO2 into homopropargylic amines. <b>2023</b> , 47, 5691-5700	Ο
543	BODIPY-Based Photothermal Agents with Excellent Phototoxic Indices for Cancer Treatment. <b>2023</b> , 145, 4534-4544	O
542	A Silver-Based Integrated System Showing Mutually Inclusive Super Protonic Conductivity and Photoswitching Behavior. <b>2023</b> , 62, 3485-3497	O
541	Position of Geminal Substitution of 中mino Acid Residues Modulates Their Ability to Form Isolated Non-Helical C 12 毗urn Mimics. <b>2023</b> , 8,	O
540	Cooperative CO2 adsorption mechanism in a perfluorinated CeIV-based metal organic framework. <b>2023</b> , 11, 5568-5583	0
539	Vibrational Spectroscopies, Global Reactivity, Molecular Docking, Thermodynamic Properties and Linear and Nonlinear Optical Parameters of Monohydrate Arsenate Salt of 4-Aminopyridine.	O

538	Solvent Bolute interactions, electronic properties, topological and biological explorations of 6-Bromo-7-methylimidazo[1,2-a]pyridine. <b>2023</b> , 376, 121437	0
537	Regeneration and Degradation in a Biomimetic Polyoxometalate Water Oxidation Catalyst. <b>2023</b> , 13, 3007-3019	0
536	Modeling Adsorption of CO2 in Rutile Metallic Oxide Surfaces: Implications in CO2 Catalysis. <b>2023</b> , 28, 1776	0
535	Synthesis and Optoelectronic Features of Rhodamine-Triazole Dyads as Metallochromic Probes for Copper-Selective Chemosensing. <b>2023</b> , 18,	О
534	Evaluation of the affinity of asphaltene molecular models A1 and A2 by the water/oil interfaces based on a novel concept of solubility parameter profiles obtained from MD simulations. <b>2023</b> , 376, 121430	0
533	The CO 2 Reduction Reaction Mechanism on Silicene Nanoflakes. A Theoretical Perspective. <b>2023</b> , 8,	0
532	Machine Learning-Guided Computational Screening of New Candidate Reactions with High Bioorthogonal Click Potential.	0
531	Reductive Oligomerization of Nitroaniline Catalyzed by Fe3O4 Spheres Decorated with Group 11 Metal Nanoparticles. <b>2023</b> , 8, 7459-7469	Ο
530	Cell Survival Enabled by Leakage of a Labile Metabolic Intermediate. <b>2023</b> , 40,	0
529	Thermal Methane Conversion to Formaldehyde Mediated by NiAlO3+ in the Gas Phase. <b>2023</b> , 127, 1636-1641	Ο
528	Competing Si2CH4H2 and SiCH2BiH4 Channels in the Bimolecular Reaction of Ground-State Atomic Carbon (C(3Pj)) with Disilane (Si2H6, X1A1g) under Single Collision Conditions. <b>2023</b> , 127, 1901-1908	0
527	Spectroscopic characterization, DFT modeling and antimicrobial studies of some novel nanoparticles mixed ligand complexes of NS bidentate ligand in presence of 2,2?-bipyridine. <b>2023</b> , 376, 121404	О
526	Origins of Regioselectivity in CuH-Catalyzed Hydrofunctionalization of Alkenes. 2023, 88, 2750-2757	О
525	Mechanistic insight into the ligand-controlled regioselective hydrocarboxylation of aryl olefins with palladium catalyst: A computational study. <b>2023</b> , 989, 122645	O
524	Adamantyl-Substituted Triplet Diradical: Synthesis, Structure, Redox and Magnetic Properties. <b>2022</b> , 507, 270-280	0
523	Insights into the mechanism of cumene catalytic oxidation using ionic liquid [Bmim]OH. 2023, 538, 113008	O
522	Binding profile of a mixed-ligand silver(I) complex with DNA and Topoisomerase I. 2023, 103, 107831	0
521	The effect of long-range interactions on the infrared and Raman spectra of aragonite (CaCO3, Pmcn) up to 25 GPa. <b>2023</b> , 13,	O

520	A comprehensive DFT study on organosilicon-derived fungicide flusilazole and its germanium analogue: A computational approach to Si/Ge bioisosterism. <b>2023</b> , 100, 100939	О
519	Better big or strained? Deformations of shape persistent arylene butadiynylene macrocycles. <b>2023</b> , 47, 6086-6094	О
518	Nanobiomineralization of Carbon Dioxide by Molecularly Engineered Metal⊞istidine Complex Nanozymes. <b>2023</b> , 35, 1610-1623	0
517	Synergistic Steric and Electronic Effects on the Photoredox Catalysis by a Multivariate Library of Titania Metal@rganic Frameworks. <b>2023</b> , 145, 4589-4600	O
516	A Dinitrophenol-Based Colorimetric Chemosensor for Sequential Cu2+ and S2IDetection. <b>2023</b> , 11, 143	0
515	Quantitative Raman Cross-Sections and Band Assignments for Fentanyl and Fentanyl Analogs. 000370282317	1605
514	Structure elucidation of an aspidofractinine-type monoterpene indole alkaloid from Melodinus reticulatus. <b>2022</b> ,	О
513	Understanding the Exchange Interaction between Paramagnetic Metal Ions and Radical Ligands: DFT and Ab Initio Study on Semiquinonato Cu(II) Complexes. <b>2023</b> , 24, 4001	O
512	Dual Photochemistry of Benzimidazole. <b>2023</b> , 88, 2884-2897	О
511	Slater transition methods for core-level electron binding energies. <b>2023</b> , 158, 094111	O
510	Rational Design to Activate Tetrafluoromethane by Two-Coordinate Borinium. 2023, 62, 3518-3524	О
510 509	Rational Design to Activate Tetrafluoromethane by Two-Coordinate Borinium. 2023, 62, 3518-3524  A Trinuclear High-Spin Iron(III) Complex with a Geometrically Frustrated Spin Ground State Featuring Negligible Magnetic Anisotropy and Antisymmetric Exchange. 2023, 62, 3420-3430	0
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509	A Trinuclear High-Spin Iron(III) Complex with a Geometrically Frustrated Spin Ground State Featuring Negligible Magnetic Anisotropy and Antisymmetric Exchange. <b>2023</b> , 62, 3420-3430  Synthesis of tetrahydrochromenes and dihydronaphthofurans via a cascade process of [3 + 3] and	0
509	A Trinuclear High-Spin Iron(III) Complex with a Geometrically Frustrated Spin Ground State Featuring Negligible Magnetic Anisotropy and Antisymmetric Exchange. <b>2023</b> , 62, 3420-3430  Synthesis of tetrahydrochromenes and dihydronaphthofurans via a cascade process of [3 + 3] and [3 + 2] annulation reactions: mechanistic insight for 6-endo-trig and 5-exo-trig cyclisation. <b>2023</b> , 13, 5796-580  Mechanism and Origin of CuH-Catalyzed Regio- and Enantioselective Hydrocarboxylation of	o 3 <sup>o</sup>
509 508 507	A Trinuclear High-Spin Iron(III) Complex with a Geometrically Frustrated Spin Ground State Featuring Negligible Magnetic Anisotropy and Antisymmetric Exchange. 2023, 62, 3420-3430  Synthesis of tetrahydrochromenes and dihydronaphthofurans via a cascade process of [3 + 3] and [3 + 2] annulation reactions: mechanistic insight for 6-endo-trig and 5-exo-trig cyclisation. 2023, 13, 5796-580  Mechanism and Origin of CuH-Catalyzed Regio- and Enantioselective Hydrocarboxylation of Allenes. 2023, 26,  Slow Magnetic Relaxation and Modulated Photoluminescent Emission of Coordination Polymer	o 3 <sup>o</sup> o
509 508 507 506	A Trinuclear High-Spin Iron(III) Complex with a Geometrically Frustrated Spin Ground State Featuring Negligible Magnetic Anisotropy and Antisymmetric Exchange. 2023, 62, 3420-3430  Synthesis of tetrahydrochromenes and dihydronaphthofurans via a cascade process of [3 + 3] and [3 + 2] annulation reactions: mechanistic insight for 6-endo-trig and 5-exo-trig cyclisation. 2023, 13, 5796-580  Mechanism and Origin of CuH-Catalyzed Regio- and Enantioselective Hydrocarboxylation of Allenes. 2023, 26,  Slow Magnetic Relaxation and Modulated Photoluminescent Emission of Coordination Polymer Based on 3-Amino-4-hydroxybenzoate Zn and Co Metal Ions. 2023, 28, 1846  Deciphering the ground state of a C3-symmetrical Blatter-type triradical by CW and pulse EPR	o 3° o o

502	Palbociclib (PD 0332991) Interaction with Kinases. Theoretical and Comparative Molecular Docking Study. <b>2023</b> , 20,	0
501	Environmentally benign synthesis of unsymmetrical ureas and their evaluation as potential HIV-1 protease inhibitors via a computational approach.	O
500	Single Crystal Investigations, Hirshfeld Surface Analysis, DFT Studies, Molecular Docking, Physico-Chemical Characterization, and Biological Activity of a Novel Non-Centrosymmetric Compound with a Copper Transition Metal Precursor. <b>2023</b> , 8, 7738-7748	0
499	TFE assisted mechanochemical synthesis of new pyrazolones from Meldrum acid carbothioamides-Experimental and theoretical studies. <b>2023</b> , 539, 113002	O
498	Endohedral group-14 clusters Au@X12 (X´=´Ge, Sn, Pb) and their anions: A first-principles study. <b>2023</b> , 376, 121477	0
497	Mg(i) $\mathbf{He}(\mathbf{II})$ and Mg(0) $\mathbf{Mg}(\mathbf{i})$ covalent bonding in the MgnFe(CO)4 $\mathbf{II}$ (n = 1, 2) anion complexes: an infrared photodissociation spectroscopic and theoretical study. <b>2023</b> , 25, 7697-7703	O
496	USc2C2 and USc2NC Clusters with ULT Triple Bond Character Stabilized Inside Fullerene Cages. <b>2023</b> , 145, 5645-5654	0
495	Centrosymmetric Nickel(II) Complexes Derived from Bis-(Dithiocarbamato)piperazine with 1,1?-Bis-(Diphenylphosphino)ferrocene and 1,2-Bis-(Diphenylphosphino)ethane as Ancillary Ligands: Syntheses, Crystal Structure and Computational Studies. <b>2023</b> , 13, 343	o
494	A Self-Powered, Rechargeable, and Wearable Hydrogel Patch for Wireless Gas Detection with Extraordinary Performance. 2300046	O
493	Thermal Atomic Layer Etching of CoO, ZnO, Fe2O3, and NiO by Chlorination and Ligand Addition Using SO2Cl2 and Tetramethylethylenediamine. <b>2023</b> , 35, 2058-2068	О
492	Design and implementation of humidity sensor based on carbon nitride modified with graphene quantum dots. <b>2023</b> , 13,	O
491	Can Copper(I) and Silver(I) be Hydrogen Bond Acceptors?.	o
490	Molecular structures, chemical descriptors and pancreatic lipase (1LPB) inhibition by natural products: A DFT investigation and molecular docking prediction.	O
489	First-Principles Study of the Structural, Mechanical and Thermodynamic Properties of Al11RE3 in Aluminum Alloys. <b>2023</b> , 13, 347	1
488	NHC-Stabilised Parent Tripentelyltrielanes.	0
487	Mechanistic Basis for a Connection between the Catalytic Step and Slow Opening Dynamics of Adenylate Kinase. <b>2023</b> , 63, 1556-1569	O
486	A Multifunctional Biomass Zinc Catalyst for Epoxy-Based Vitrimers and Composites. <b>2023</b> , 188, 111936	0
485	Structure and nuclear quadrupole coupling interaction in hydroxylamines: The rotational spectrum of N,N-diethyl(2H)hydroxylamine. <b>2023</b> , 392, 111759	O

484	Infrared spectra of isoquinolinium (iso-C9H7NH+) and isoquinolinyl radicals (iso-C9H7NH and 1-, 3-, 4-, 5-, 6-, 7- and 8-iso-HC9H7N) isolated in solid para-hydrogen.	O
483	Identifying Ordered OH/F Anions in Hydroxyfluorides by a Terahertz Spectroscopic Approach. <b>2023</b> , 127, 4367-4373	O
482	Synthesis, DFT investigations, antioxidant, antibacterial activity and SAR-study of novel thiophene-2-carboxamide derivatives. <b>2023</b> , 17,	0
481	Enabling Peculiar Photophysics and Mechanochromic Luminescence by Introducing Bromine in Push <b>B</b> ull Pyridine Derivatives. <b>2023</b> , 127, 4176-4187	O
480	Theoretical Investigation on 1-Ethyl-3-Methylimidazolium Fluoride: A Density Functional Theory Study. <b>2022</b> , 14, 1732-1740	0
479	Elastic and bright assembly-induced luminescent crystals of platinum(ii) complexes with near-unity emission quantum yield.	O
478	Conformational landscapes of artificial peptides predicted by various force fields: are we ready to simulate hamino acids?. <b>2023</b> , 25, 7466-7476	0
477	Synthesis, molecular modelling and biological evaluation of new 4-aminothiophene and thienopyrimidine compounds. <b>2023</b> , 17,	O
476	A Poly(carbazole-alt-triazole) with Thiabendazole Side Groups as an IDn-Off-OnIFluorescent Probe for Detection of Cu(II) Ion and Cysteine.	О
475	Combined quantum mechanics and molecular dynamics study on the calcite scale inhibition mechanism of carboxymethyl dextran. <b>2023</b> , 553, 116503	О
474	Allosteric regulation of 骨eaction stage I in tryptophan synthase upon the 且igand binding. <b>2023</b> , 158, 115101	О
473	Selective synthesis of oleyl alcohol via catalytic and non-catalytic liquid-phase methyl oleate reduction.	O
472	Insights into the deviation from piecewise linearity in transition metal complexes from supervised machine learning models. <b>2023</b> , 25, 8103-8116	О
471	Gas-phase molecular formation mechanisms of cyanamide (NH2CN) and its tautomer carbodiimide (HNCNH) under Sgr B2(N) astrophysical conditions. <b>2023</b> , 672, A49	O
470	Hierarchical Aggregation in a Complex Fluid-The Role of Isomeric Interconversion. <b>2023</b> , 127, 2052-2065	O
469	Monocyclopentadienyltitanium(III) Complexes with Hydridoborato Ligands.	O
468	Photophysical Behavior of Self-Organizing Derivatives of 10- and 12-Vertex p -Carboranes, and their Bicyclo[2.2.2]octane and Benzene Analogues.	0
467	Naphthalene Carboxylation in the Sulfate-Reducing Enrichment Culture N47 Is Proposed to Proceed via 1,3-Dipolar Cycloaddition to the Cofactor Prenylated Flavin Mononucleotide. <b>2023</b> , 89,	O

466	Electronic, intermolecular, quantum computational investigations, molecular docking and simulation studies of the potent antiviral drug EIDD-2801. <b>2023</b> , 100, 100953	O
465	Molecular and electronic structures, bonding analysis, and UVI∕I is spectra predictions of quinolino[3,2-b]benzodiazepine and quinolino[3,2-b]benzoxazepine metal transition M(L)2Cl2 and M(L)Cl2 complexes.	O
464	Mechanism and Selectivity of Copper-Catalyzed Bromination of Distal C(sp3)⊞ Bonds.	0
463	A new freely-downloadable hands-on density-functional theory workbook using a freely-downloadable version of deMon2k. <b>2023</b> ,	Ο
462	Theoretically Revealing the Response of Intermolecular Vibration Energy Transfer and Decomposition Process of the DNTF System to Electric Fields Using Two-Dimensional Infrared Spectra. <b>2023</b> , 24, 4352	0
461	Application of DFT/TD-DFT Frameworks in the Drug Delivery Mechanism: Investigation of Chelated Bisphosphonate with Transition Metal Cations in Bone Treatment. <b>2023</b> , 5, 365-380	O
460	Polymeric Solar Cell with 19.69% Efficiency Based on Poly(o-phenylene diamine)/TiO2 Composites. <b>2023</b> , 15, 1111	0
459	Synthesis of a Novel Hydrazone of Thieno[2,3-d]pyrimidine Clubbed with Ninhydrin: X-ray Crystal Structure and Computational Investigations. <b>2023</b> , 13, 384	0
458	The Role of the Transient Atropisomerism and Chirality of Flurbiprofen Unveiled by Laser-Ablation Rotational Spectroscopy.	0
457	Hydroxycinnamic acid derivatives for UV-selective and visibly transparent dye-sensitized solar cells. <b>2023</b> , 13,	O
456	Synergistic mixture of Eupatorium adenophora spreng leaves extract and KI as a novel green inhibitor for steel corrosion in 5.0 M H3PO4. <b>2023</b> , 23, 5082-5104	0
455	Electrochemical Opening of Impermeable Nanochannels in Laminar Graphene Membranes for Ultrafast Nanofiltration. <b>2023</b> , 57, 3843-3852	O
454	Comparative Study of Molecular Docking, Structural, Electronic, and Fukui Function Studies on Favipiravir and its Newly Designed Derivatives (Potential Inhibitors) for COVID-19 Protease. <b>2023</b> , 407,	0
453	Remote-Group-Assisted Facile Oxidative Arylation of Furans and Pyrroles. <b>2023</b> , 13, 3520-3531	0
452	Fluorine-based Zn salan complexes. <b>2023</b> , 52, 4044-4057	0
451	Molecular modeling of mordant black dye for future applications as visible light harvesting materials with anchors: design and excited state dynamics. <b>2023</b> , 29,	O
450	Hirshfeld and AIM Analysis of the Methylone Hydrochloride Crystal Structure and Its Impact on the IR Spectrum Combined with DFT Study. <b>2023</b> , 13, 383	1
449	Histidine oxidation in lytic polysaccharide monooxygenase. <b>2023</b> , 28, 317-328	0

448	Quantum-Chemical Insight into Self-Organization of Complex Molecules from Acetylene and Anilines Catalyzed by Superbase KOH/DMSO: One-Pot Cascade Assembly of 1,3-Bis(arylamines). <b>2023</b> , 12,	O
447	In silico discovery of potent inhibitors against monkeypox\ major structural proteins. 1-16	O
446	Insights into the binding mechanism of ascorbic acid and violaxanthin with violaxanthin de-epoxidase (VDE) and chlorophycean violaxanthin de-epoxidase (CVDE) enzymes.	O
445	Revealing Internal Rotation and 14N Nuclear Quadrupole Coupling in the Atmospheric Pollutant 4-Methyl-2-nitrophenol: Interplay of Microwave Spectroscopy and Quantum Chemical Calculations. <b>2023</b> , 28, 2153	O
444	A quantum chemical study of the mechanism of thermal decomposition of N?-methoxy-N-methyldiazene N-oxide. <b>2022</b> , 71, 2595-2604	O
443	Design of N-11-Azaartemisinins Potentially Active against & amp;lt;i& amp;gt;Plasmodium falciparum& amp;lt;/i& amp;gt; by Combined Molecular Electrostatic Potential, Ligand-Receptor Interaction and Models Built with Supervised Machine Learning Methods. 2023, 14, 1-29	O
442	Crystal Structure, Photophysical Study, Hirshfeld Surface Analysis, and Nonlinear Optical Properties of a New Hydroxyphenylamino Meldrum Acid Derivative. <b>2023</b> , 28, 2181	О
441	On structural factors determining the nature of the fluorescent properties of OIHMs based on 8-hydroxyquinoline. <b>2023</b> , 25, 1993-2002	O
440	DFT and ONIOM Simulation of 1,3-Butadiene Polymerization Catalyzed by Neodymium-Based Ziegler Natta System. <b>2023</b> , 15, 1166	0
439	Hydroxymethylfurfural oxidation over unsupported Pd-Au alloy catalysts prepared by pulsed laser ablation: Synergistic and compositional effects. <b>2023</b> , 656, 119121	O
438	Dipole Cooperativity and Polarization Frustration Determine the Secondary Structure Distribution of Short Alanine Peptides in Water. <b>2023</b> , 127, 3126-3138	O
437	DFT CALCULATIONS IN MONOMERIC AND DIMERIC FORMS OF N-BENZYLMALEIMIDE (NBM) COMBINED WITH VIBRATIONAL SPECTROSCOPIC PARAMETERS.	O
436	The study on gas phase dehydrogenation reactions of transition metal cation and ethylene. <b>2023</b> , 121,	O
435	Catalytic activity of OH functionalized N-doped graphene in oxygen reduction reaction for fuel cell applications: a DFT study. <b>2023</b> , 129,	O
434	Electronic Effects of Substituents on the Reactivity of Silenes: A Computational Analysis.	O
433	Protonated Forms of Naringenin and Naringenin Chalcone: Proteiform Bioactive Species Elucidated by IRMPD Spectroscopy, IMS, CID-MS, and Computational Approaches. <b>2023</b> , 71, 4005-4015	O
432	Newly Synthesized Aminothiazole Based Disazo Dyes and Their Theoretical Calculations. 1-23	O
431	A DFT Investigation of the Reactivity of Guanidinium Salts in Tandem aza-Michael Addition/Intramolecular Cyclization. <b>2023</b> , 28, 2218	O

430	NIR Absorbing Aromatic E-Ethylene Bridged Hexaphyrins (2.1.1.2.1.1): Synthesis, Characterization, and Protonation Studies. <b>2023</b> , 25, 1491-1496	О
429	Colorful patterned polyacrylate films prepared using cholesteric liquid-crystalline mixtures with a smectic order. 1-10	O
428	The design and synthesis of green emissive iridium(iii) complexes guided by calculations of the vibrationally-resolved emission spectra. <b>2023</b> , 52, 4112-4121	O
427	Molecular Orbitals. 2023,	Ο
426	3D Hollow Porous Radio-Granular Hydrogels for SPECT Imaging-Guided Cancer Intravascular Brachytherapy. 2215110	О
425	The Contribution of Theoretical Prediction Studies to the Antioxidant Activity Assessment of the Bioactive Secoiridoids Encountered in Olive Tree Products and By-Products. <b>2023</b> , 28, 2267	O
424	Comparative Theoretical Study of Quinazolinone Derivatives in Different Solvents and Gas Phase. A Density Functional Theory (DFT) Calculations.	О
423	Ein Kooperatives Rhodium/Sekundles Phosphinoxid [Rh/P(O) n Bu 2 ]-Template zur Katalytischen Hydrodefluorierung von Perfluoroarenen.	O
422	Comparisons of bpy and phen Ligand Backbones in Cr-Mediated (Co-)Electrocatalytic CO2 Reduction.	O
421	Antioxidant Properties of Thymoquinone, Thymohydroquinone and Black Cumin (Nigella sativa L.) Seed Oil: Scavenging of Superoxide Radical Studied Using Cyclic Voltammetry, DFT and Single Crystal X-ray Diffraction. <b>2023</b> , 12, 607	O
420	Effect of Molybdenum Disulphide Thin Films on Enhancing the Performance of Polycrystalline Silicon Solar Cells. <b>2023</b> , 2023, 1-12	O
419	Exploring the Interaction Between the Newly Designed Antitumor Zn(II) Complex and CT-DNA/BSA: Spectroscopic Methods, DFT Computational Analysis, and Docking Simulation.	O
418	Density Functional Theory Guided Investigation of Ligand-Induced Neptunyl-Neptunyl Interactions.	О
417	A DFT study of Ni-catalyzed (3 + 3)-annulation between donorEcceptor cyclopropanes and diaziridines. <b>2023</b> , 10, 1948-1958	О
416	Synthesis of 4-Amino-N-[2 (diethylamino)Ethyl]Benzamide Tetraphenylborate Ion-Associate Complex: Characterization, Antibacterial and Computational Study. <b>2023</b> , 28, 2256	О
415	Phenothiazine-Based LSD1 Inhibitor Promotes T-Cell Killing Response of Gastric Cancer Cells. <b>2023</b> , 66, 3896-3916	O
414	Spin-crossing in heterogeneous ethane dehydrogenation by atomically dispersed Co/SiO2. <b>2023</b> , 3, 100534	О
413	Toward DMC Accuracy Across Chemical Space with Scalable EQML. 2023, 19, 1711-1721	O

412	Investigation of morphological, structural and electronic transformation of PVDF and ZnO/rGO/PVDF hybrid membranes. <b>2023</b> , 55,	0
411	A Cooperative Rhodium/Secondary Phosphine Oxide [Rh/P(O) n Bu 2 ] Template for Catalytic Hydrodefluorination of Perfluoroarenes.	Ο
410	Mechanism for the synthesis of medium-chain 1-alkenes from fatty acids catalyzed by binuclear iron UndA decarboxylase. <b>2023</b> , 420, 123-133	0
409	Dehydrogenation reaction of triethylamine by an electrophilic terminal phosphinidene complex. <b>2023</b> , 52, 3275-3278	O
408	Insights into the regioselectivity and diastereoselectivity of the Nazarov cyclization of 3-alkenyl-2-indolylmethanol with tryptophol. <b>2023</b> , 10, 1721-1730	0
407	Reactivity and Selectivity of the DielsAlder Reaction of Anthracene in [Pd6L4]12+ Supramolecular Cages: A Computational Study. <b>2023</b> , 62, 4330-4340	O
406	Light-induced infrared difference spectroscopy on three different forms of orange carotenoid protein: focus on carotenoid vibrations.	0
405	Extension of the TraPPE Force Field for Battery Electrolyte Solvents. <b>2023</b> , 127, 2224-2236	O
404	Synthesis and characterization of novel acrylamide derivatives and their use as corrosion inhibitors for carbon steel in hydrochloric acid solution. <b>2023</b> , 13,	0
403	Computation Study on Copper-Catalyzed Aerobic Intramolecular Aminooxygenative C?C Bond Cleavage to Imides: Different Roles of Mononuclear and Dinuclear Copper Complexes. <b>2023</b> , 13, 3815-3829	O
402	Spectroscopy, molecular structure, and electropolymerization of Ni(ii) and Cu(ii) complexes containing a thiophene-appending fluorinated Schiff base ligand. <b>2023</b> , 52, 4224-4236	0
401	Fabrication of a Cd(ii) metalorganic framework as a dual functional material: efficient iodine capture and selective adsorption of a cationic dye. <b>2023</b> , 25, 2280-2297	O
400	Brfisted Acids Promote Olefin Oxidations by Bioinspired Nonheme Colll(PhIO)(OH) Complexes: A Role for Low-Barrier Hydrogen Bonds. <b>2023</b> , 145, 5739-5749	1
399	Cobalt-catalyzed radical-mediated carbondarbon scission via a radical-type migratory insertion. <b>2023</b> , 14, 3352-3362	O
398	Mechanistic insights into H3B4NMeH2 dehydrogenation by Co-based complexes: a DFT perspective. <b>2023</b> , 47, 6661-6672	0
397	Improving Accuracy and Transferability of Machine Learning Chemical Activation Energies by Adding Electronic Structure Information. <b>2023</b> , 63, 1454-1461	O
396	Prediction of the structures and heats of formation of MO2, MO3, and M2O5 for M = V, Nb, Ta, Pa. <b>2023</b> , 25, 8355-8368	0
395	Isostructural coordination polymers of the tethering naphthalene anchored bis(2-methylpyridinecarboxamide) ligand: single crystal, XPS, EDS and theoretical studies. <b>2023</b> , 47, 5477-548	7 <sup>°</sup>

394	Triterpene Derivatives as Potential Inhibitors of the RBD Spike Protein from SARS-CoV-2: An In Silico Approach. <b>2023</b> , 28, 2333	О
393	A comparable DFT study on reaction of CHCllwith O3 and S2O. <b>2023</b> , 29,	O
392	Strongly constrained and appropriately normed density functional theory exchange-correlation functional applied to rare earth oxides. <b>2023</b> , 107,	О
391	Mechanistic Insights into Enantioselective C(sp 3) H Acylation to Construct Amino Ketones via Photoredox and Ni(II) Dual Catalysis: A DFT Study. <b>2023</b> , 18,	Ο
390	Theoretical insights into luminescence mechanism of Naphthyridine-based thermally activated delayed fluorescence emitter with aggregation-induced emission. <b>2023</b> , 817, 140407	0
389	Unveiling the theoretical aspects of superelectrophilic activation in an inverse demand Diels-Alder reaction. <b>2023</b> , 29,	O
388	Nonlinear optical response and characteristic Raman spectra of phagraphene quantum dots. <b>2023</b> , 98, 045109	0
387	Perchlorate-induced structural diversity in thiosemicarbazone copper(ii) complexes provides insights to understand the reactivity in acidic and basic media. <b>2023</b> , 25, 2213-2226	O
386	Synthesis of Ester-Containing Chroman-4-Ones via Cascade Radical Annulation of 2-(Allyloxy)Arylaldehydes with Oxalates under Metal Free Conditions. <b>2023</b> , 24, 5028	0
385	Influence of Transition Metal Electron Configuration on the Structure of Metal <b>E</b> DTA Complexes. <b>2023</b> , 127, 2258-2264	Ο
384	Performance of Density Functionals and Semiempirical 3c Methods for Small GoldII hiolate Clusters. <b>2023</b> , 127, 2242-2257	0
383	Dual emission of ESIPT-capable 2-(2-hydroxyphenyl)-4-(1H-pyrazol-1-yl)pyrimidines: interplay of fluorescence and phosphorescence. <b>2023</b> , 47, 6361-6377	O
382	Probing the n -d carbonylarbonyl interactions in the formaldehydel ifluoroacetone dimer by rotational spectroscopy. <b>2023</b> , 158, 124304	0
381	Solvation Effects on Polarizability of Aromatic Fluids. <b>2023</b> , 127, 2237-2249	O
380	Molecular Dynamic, Hirshfeld Surface, Computational Quantum and Spectroscopic analysis of 4-Hydroxy-1-Naphthaldehyde.	0
379	Mechanism and origins of ligand-controlled regioselectivity of copper-catalyzed borocarbonylation of imines with B2pin2 and alkyl iodides: a computational study. <b>2023</b> , 10, 2024-2032	O
378	Theoretical Aspects of Nanometal Oxides. <b>2023</b> , 47-56	O
377	Retrosynthesis from transforms to predictive sustainable chemistry and nanotechnology: a brief tutorial review.	O

376	Photoactivities of thiophene monomer/polymer transition in gelbased photoelectrochemical assembly: A theoretical/experimental approach. <b>2023</b> , 18, 100077	0
375	Experimental and computational studies of tautomerism pyridine carbonyl thiosemicarbazide derivatives.	O
374	Efficient Synthesis of 1H-Benzo[4,5]imidazo[1,2-c][1,3]oxazin-1-one Derivatives Using Ag2CO3/TFA-Catalyzed 6-endo-dig Cyclization: Reaction Scope and Mechanistic Study. <b>2023</b> , 28, 2403	0
373	Stabilisation and reactivity studies of donor-base ligand-supported gallium-phosphides with stronger binding energy: a theoretical approach. <b>2023</b> , 13, 7738-7751	O
372	Stereodivergent Construction of [5,5]-Oxaspirolactones of Phainanoids. <b>2023</b> , 88, 3987-3991	0
371	Oxidation Products from the Neolignan Licarin A by Biomimetic Reactions and Assessment of in vivo Acute Toxicity.	O
370	Terpenic Constituents of Essential Oils with Larvicidal Activity against Aedes Aegypti: A QSAR and Docking Molecular Study. <b>2023</b> , 28, 2454	0
369	Theoretical Study of Hydroxylation of ∃and ₱inene by a Cytochrome P450 Monooxygenase Model. <b>2023</b> , 24, 5150	O
368	DFT Study on Corrosion Inhibition by Tetrazole Derivatives: Investigation of the Substitution Effect. <b>2023</b> , 8, 9978-9994	0
367	DELTA50: A Highly Accurate Database of Experimental 1H and 13C NMR Chemical Shifts Applied to DFT Benchmarking. <b>2023</b> , 28, 2449	O
366	A dispersion-corrected DFT calculations on encapsulation of Favipiravir drug used as antiviral against COVID-19 into carbon-, boron-, and aluminum-nitride nanotubes for optimal drug delivery systems combined with molecular docking simulations.	0
365	Synthesis, Structure, Hirshfeld Surface Analysis, Non-Covalent Interaction, and In Silico Studies of 4-Hydroxy-1-[(4-Nitrophenyl)Sulfonyl]Pyrrolidine-2-Carboxyllic Acid.	O
364	Eremoxylarins DI, Antibacterial Eremophilane Sesquiterpenes Discovered from an Endolichenic Strain of Xylaria hypoxylon.	0
363	One-Component Artificial Gustatory System Based on Hydrogen-Bond Organic Framework for Discrimination of Versatile Analytes. 2300091	O
362	Cyclopentadiene: Explaining Its Deviation from the Correlation of pKa versus Number of Nitrogen Atoms of the Pyrrole to Pentazole Series and Its Closeness to the Correlation of pKa versus Number of Phosphorous Atoms of the Phosphole to Pentaphosphole Series. <b>2023</b> , 93, 116-119	0
361	Supramolecular Organization in Salts of Riluzole with Dihydroxybenzoic AcidsThe Key Role of the Mutual Arrangement of OH Groups. <b>2023</b> , 15, 878	O
360	A Multiple Proton Transfer Mechanism for the Charging Step of the Aminoacylation Reaction at the Active Site of Aspartyl tRNA Synthetase. <b>2023</b> , 63, 1819-1832	0
359	Evaluating performance of the approximate 3D-RISM-KH molecular solvation theory for solvation free energies in alkanes and alkane-water partition coefficients. <b>2023</b> , 378, 121597	O

358	Interaction of tacrine-coumarin derivatives with double stranded DNA: spectroscopic and molecular docking study.	0
357	Understanding the mechanism and origins of stereoconvergence in nickel-catalyzed hydroarylation of 1,3-dienes with aryl boronates. <b>2023</b> , 52, 4849-4855	Ο
356	Synthesis, Structure, and Non-Covalent Interactions of 5-Methyl-2,3-dihydrothiazolo[2,3-b]thiazolium Halides. <b>2023</b> , 93, 22-30	0
355	Theoretical Insights into the Selectivity of Hydrophilic Sulfonated and Phosphorylated Ligands to Am(III) and Eu(III) Ions. <b>2023</b> , 62, 4581-4589	Ο
354	A general highly efficient synthesis of biocompatible rhodamine dyes and probes for live-cell multicolor nanoscopy. <b>2023</b> , 14,	0
353	Reactions of Zinc Hydride with Silylenes: From Oxidative Addition to Ligand Exchange Reactions. <b>2023</b> , 42, 457-464	Ο
352	Graphene Embedded with Transition Metals for Capturing Carbon Dioxide: Gas Detection Study Using QM Methods. <b>2023</b> , 5, 403-417	0
351	Understanding the solvation structures of glyme-based electrolytes by machine learning molecular dynamics. <b>2023</b> , 100061	O
350	Photodehydration of Ethanol Mediated by CuCl2Ethanol Complex. 2023, 14, 2750-2757	0
349	Infrared spectra of gaseous peroxychloroformyl radical ClC(O)OO: A key intermediate in the conversion of CO to CO2 in the Venus atmosphere. <b>2023</b> , 393, 111771	Ο
348	Multicomponent wavefunction-in-DFT embedding for positronium molecules. 2023, 158, 134101	0
347	Hydrothiolation of alkynes with thioldatechol derivatives catalysed by CuNPs/TiO2: exploring the reaction mechanism by DFT calculations. <b>2023</b> , 13, 8025-8033	O
346	Synthesis of Sulfilimines Enabled by Copper-Catalyzed S-Arylation of Sulfenamides. 2023, 145, 6310-6318	0
345	Aluminabenzene-based Lewis superacids and weakly coordinating anions.	Ο
344	Determination of the molecular structure and spectroscopic properties of capsaicin. 2023, 208, 110879	0
343	Synthesis, molecular structure, FMO, spectroscopic, antimicrobial and in-silico investigation of (E)-1-(benzo[d][1,3]dioxol-5-yl)-3-(4-aryl)prop-2-en-1-one derivative: Experimental and computational study. <b>2023</b> , 5, 100887	Ο
342	Stereochemical Properties of Two Schiff-Base Transition Metal Complexes and Their Ligand by Using Multiple Chiroptical Spectroscopic Tools and DFT Calculations. <b>2023</b> , 28, 2571	0
341	Comparative study of the gas phase reaction of SiCl4, SiHCl3, SiH2Cl2, and SiH3Cl by thermodynamic analysis. <b>2023</b> , 62, 048002	Ο

340	Solvation Shell Structures of Ammonia in Reline and Ethaline Deep Eutectic Solvents. <b>2023</b> , 127, 2499-2510	0
339	ElCatalysis Made AsymmetricEnantiomerization Catalysis Mediated by the Chiral Esystem of a Perylene Bisimide Cyclophane.	O
338	Theoretical Study on the Gas-Phase and Aqueous Interface Reaction Mechanism of Criegee Intermediates with 2-Methylglyceric Acid and the Nucleation of Products. <b>2023</b> , 24, 5400	0
337	Stabilized Molecular Diphosphorus Pentoxide, P2O5L2 (L = N-Donor Base), in the Synthesis of Condensed Phosphate Drganic Molecule Conjugates. <b>2023</b> , 145, 6045-6050	O
336	Assessments of DFT-based energy decomposition analysis methods for intermolecular interactions. <b>2023</b> , 158, 124116	0
335	Identification of novel potential inhibitor of thymidylate kinase from Variola virus. 1-11	O
334	Synergistic Catalysis in Heterobimetallic Complexes for Homogeneous Carbon Dioxide Hydrogenation. <b>2023</b> , 28, 2574	0
333	Spectroscopic and Theoretical Analysis of the Interaction between Plasma Proteins and Phthalimide Analogs with Potential Medical Application. <b>2023</b> , 13, 760	O
332	Theoretical study on the kinetics of hydrogen cyanide and hydrogen isocyanide reactions with the methyl radical. <b>2023</b> , 25, 10121-10128	0
331	Controlling doping efficiency in organic semiconductors by tuning short-range overscreening. <b>2023</b> , 14,	O
330	Quantitative Solvation Energies from Gas-Phase Calculations: First-Principles Charge Transfer and Perturbation Approaches. <b>2023</b> , 127, 2546-2551	0
329	Target State Optimized Density Functional Theory for Electronic Excited and Diabatic States. <b>2023</b> , 19, 1777-1789	O
328	Impact of active sites on encapsulation of curcumin in Metal Organic Frameworks. 2023, 10, 035102	0
327	Influence of the Thiophene Ring on the Molecular Order of Structurally Simple EConjugated Smectogens: 13 C NMR Study.	O
326	Cobalt-catalysed nucleophilic fluorination in organic carbonates. <b>2023</b> , 52, 4585-4594	0
325	Theoretical Research Methods Involved in This Book. <b>2023</b> , 19-43	O
324	Characterizing the Impact of Mg-Doped Li Metal Anode and Excess Electrons on High Concentration Electrolyte Interfacial Stability: A Theoretical Study. <b>2023</b> , 6, 3291-3300	0
323	Reciprocity of C?O?IInteractions with the dominant anionIbn fullerene (C60)Ibmine-based organocatalysts: a mechanistic elucidation for addition vs. decarboxylation reaction. <b>2023</b> , 25, 10647-10660	O

322	Emerging Metabolic Profiles of Sulfonamide Antibiotics by Cytochromes P450: A Computational Experimental Synergy Study on Emerging Pollutants. <b>2023</b> , 57, 5368-5379	O
321	Correlated energy from radial densityBnergy relations. 2023, 10,	1
320	A $\{Cu2I3$ Thain hybrid with two-step phase transition, switchable dielectrics, thermochromism and piezochromism.	Ο
319	Classification of doubly excited molecular electronic states. <b>2023</b> , 14, 4012-4026	O
318	Syntheses, Structures, and Electronic Properties of Mono- and Bimetallic Thiolato Complexes Containing Unusual Coordination Modes of Thiolato Ligands.	0
317	Oxidative cyclopalladation triggers the hydroalkylation of alkynes. <b>2023</b> , 108339	O
316	Development of Dipeptide NEcetyllldysteine Loaded Nanostructured Carriers Based on Inorganic Layered Hydroxides. <b>2023</b> , 15, 955	0
315	Brfisted acidflatalyzed asymmetric dearomatization for synthesis of chiral fused polycyclic enone and indoline scaffolds. <b>2023</b> , 9,	0
314	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	0
313	Unveiling the Mechanistic Singularities of Caspases: A Computational Analysis of the Reaction Mechanism in Human Caspase-1. <b>2023</b> , 13, 4348-4361	O
312	Room-Temperature Cu-Catalyzed Amination of Aryl Bromides Enabled by DFT-Guided Ligand Design. <b>2023</b> , 145, 6966-6975	0
311	Molecular Basis of RNA-Driven ATP Hydrolysis in DExH-Box Helicases. <b>2023</b> , 145, 6691-6701	O
310	Influence of Rare-Earth Ion Radius on Metal <b>M</b> etal Charge Transfer in Trinuclear Mixed-Valent Complexes. <b>2023</b> , 62, 4799-4813	0
309	Theoretical Spectroscopy Aided Validation of the Hydration Structure of Trimethylamine N-Oxide (TMAO). <b>2023</b> , 127, 2774-2783	O
308	Mechanistic aspect for the atom transfer radical polymerization of itaconimide monomers with methyl methacrylate: a computational study. <b>2023</b> ,	0
307	Computational Exploration of Cu(II)-en Chelate Catalyzed Hydrolysis of O-isopropyl methylphosphonofluoridate.	0
306	Experimental-Theoretical Approach for the Chemical Detection of Glyphosate and Its Potential Interferents Using a Copper Complex Fluorescent Probe. <b>2023</b> , 11, 194	0
305	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	0

304	Molecular Structure, Spectral Analysis, Molecular Docking and Physicochemical Studies of 3-Bromo-2-hydroxypyridine Monomer and Dimer as Bromodomain Inhibitors. <b>2023</b> , 28, 2669	0
303	Theoretical Kinetic Isotope Effects in Establishing the Precise Biodegradation Mechanisms of Organic Pollutants. <b>2023</b> , 57, 4915-4929	O
302	The Origin of Anion[Autocatalysis.	O
301	Electrophilicity and nucleophilicity scales at different DFT computational levels.	O
300	ReDD-COFFEE: a ready-to-use database of covalent organic framework structures and accurate force fields to enable high-throughput screenings. <b>2023</b> , 11, 7468-7487	O
299	Pd/Xu-Phos-catalyzed asymmetric elimination of fully substituted enol triflates into axially chiral trisubstituted allenes. <b>2023</b> , 9,	0
298	Molecular Structure, Electronic Properties, Reactivity (ELF, LOL, and Fukui), and NCI-RDG Studies of the Binary Mixture of Water and Essential Oil of Phlomis bruguieri. <b>2023</b> , 28, 2684	0
297	Insights into selectivity of some oxygen containing gases by the CHClhnion from molecular simulation. <b>2023</b> , 49, 758-768	O
296	Determination of tilt angle and its behavior in chiral smectic phases by exploring molecular conformations using complementary methods. <b>2023</b> , 107,	O
295	Unraveling Binding Mechanism and Stability of Urease Inhibitors: A QM/MM MD Study. <b>2023</b> , 28, 2697	O
294	Introduction of Methyl Group in Substituted Isoselenazolones: Catalytic and Mechanistic Study. <b>2023</b> , 88, 4273-4285	O
293	Mechanistic Investigation into the Regio-Controllable Hydroallylations of Alkynes with Allylborons under Pd-Based Synergetic Catalyses. <b>2023</b> , 88, 4536-4545	O
292	Coexistence of Three Different Spin States in a Cyanido-Bridged Trinuclear Iron(III) Complex with an Unusual Fe III to Ligand Charge Transfer.	O
291	Origin and Quantitative Description of the NESSIAS Effect at Si Nanostructures. 2200065	O
<b>2</b> 90	Investigation of the dual role of acyl phloroglucinols as a new hope for antibacterial and anti-SARS-CoV-2 agents employing integrated in vitro and multi-phase in silico approaches. 1-18	O
289	Quantum Chemical Characteristics of Additives That Enable the Use of Propylene Carbonate-Based Electrolytes. <b>2023</b> , 2023, 1-14	0
288	Stereochemistry of the Reactions between Palladacycle Complexes and Primary Alkyl Iodides. <b>2023</b> , 42, 606-614	0
287	Gas phase synthesis of the C40 nano bowl C40H10. <b>2023</b> , 14,	O

286	Spontaneous and Simultaneous Oxidation and Reduction of o-Quinones in Water Microdroplets. <b>2023</b> , 127, 2805-2809	0
285	Substituent-Guided Cluster Nuclearity for Tetranuclear Iron(III) Compounds with Flat {Fe4(B-O)2} Butterfly Core. <b>2023</b> , 24, 5808	Ο
284	Chemistry in Fungal Bioluminescence: Theoretical Studies on Biosynthesis of Luciferin from Caffeic Acid and Regeneration of Caffeic Acid from Oxidized Luciferin. <b>2023</b> , 9, 369	0
283	Cooperativity and intermolecular hydrogen bonding in donor-acceptor complexes of phenol and polyhydroxybenzenes.	Ο
282	Interactions of N-Mannich Bases of Pyrrolo[3,4-c]pyrrole with Artificial Models of Cell Membranes and Plasma Proteins, Evaluation of Anti-Inflammatory and Antioxidant Activity. <b>2023</b> , 13, 349	Ο
281	Solvent effect on adsorption of benzylidene oxindole to C 20 nanocage: A DFT approach.	Ο
280	Reducing Exact Two-Component Theory for NMR Couplings to a One-Component Approach: Efficiency and Accuracy. <b>2023</b> , 19, 2010-2028	Ο
279	Structure Performance Correlation of N-Heterocyclic Oligomer Leveler for Acid Copper Plating of Advanced Interconnects. <b>2023</b> , 28, 2783	Ο
278	Ultrafast T1 generation in pyrene-4,5-dione and pyrene-4,5,9,10-tetrone. <b>2023</b> , 441, 114695	Ο
277	Electronic Born Dppenheimer approximation in nuclear-electronic orbital dynamics. 2023, 158, 114118	Ο
276	A new voltammetric approach for the determination of the growth retardant paclobutrazol in the presence of difenoconazole in pesticide preparations. <b>2023</b> , 935, 117360	Ο
275	Selective Oxidation of Sulfuric Acid to Peroxydisulfuric Acid on a Tungsten Trioxide Anode. <b>2023</b> , 8,	Ο
274	A DFT Study of Ruthenium fcc Nano-Dots: Size-Dependent Induced Magnetic Moments. 2023, 13, 1118	О
273	Exploring the potential as molecular quantum-dot cellular automata of a mixed-valence Ru2 complex deposited on a Au(111) surface. <b>2023</b> , 10, 2484-2492	Ο
272	Looking for chiral recognition in photoinduced bimolecular electron transfer using ultrafast spectroscopy.	Ο
271	Crystal Structure, DFT Investigation, Molecular Docking, Antioxidant and Thrombolytic Investigation of Thioxo Pyrimidine-5-Carboxylate. 1-14	О
270	Quantum mechanical studies of p-azoxyanisole and identification of its electro-optic activity. <b>2023</b> , 25, 9576-9585	О
269	High-performance low temperature curable copolyimides via multidimensional modulation in alkaline environment and electronic effects of monomers. <b>2023</b> , 4, 1731-1739	О

268	Thiocarbohydrazone and Chalcone-Derived 3,4-Dihydropyrimidinethione as Lipid Peroxidation and Soybean Lipoxygenase Inhibitors. <b>2023</b> , 8, 11966-11977	0
267	A DFT study of structural-stability, Mulliken charges, MEP, FMO, and NLO properties of trans alkenyl substituted chalcones conformers: theoretical study.	O
266	How the Conformational Movement of the Substrate Drives the Regioselective CN Bond Formation in P450 TleB: Insights from Molecular Dynamics Simulations and Quantum Mechanical/Molecular Mechanical Calculations. <b>2023</b> , 145, 7252-7267	0
265	Glassy and liquid Sb2S3: insight into the structure and dynamics of a promising functional material. <b>2023</b> , 11, 4654-4673	О
264	DFT Treatment of Some Cantharidine Isomers and Some Radicals from Them. 77-91	0
263	Molecular Docking, DFT, and Antibacterial Activity Study of a Newly Synthesized Mixed Ligand Complex of Co(II), 1,10-Phenanthroline, Adenine and Acetamide.	O
262	UVIVis, FTIR and DFT Studies of the Fluoroquinolone [Pyrido Pyrolo Quinoxaline (PPQ)] Tethered to Gold Nanoparticles as a Novel Anticancer.	О
261	New Insights into the Nature of Ti(II) and Ti(III) Active Sites in the Heterogeneous ZieglerNatta Catalyst. <b>2023</b> , 127, 5720-5730	O
260	Nucleolar Essential Protein 1 (Nep1): Elucidation of Enzymatic Catalysis Mechanism by Combined Molecular Dynamics Simulation and Quantum Chemical Calculations.	0
259	Bimodal structural tuning of pyrrole-2-carboxamide-based transmembrane ion transport systems.	О
258	Hirshfeld Atom Refinement of Metal Drganic Complexes: Treatment of Hydrogen Atoms Bonded to Transition Metals. <b>2023</b> , 127, 3020-3035	0
257	Diplomeroterpenoid G: An unusual meroterpenoid from Mimosa pudica Linn. (Mimosaceae). <b>2023</b> , 120, 154451	O
256	Molecular recognition of tripeptides containing tryptophan by cucurbit[8]uril: A computational study. <b>2023</b> , 16, 104819	0
255	A simple strategy to simultaneously improve the lifetime and activity of classical iridium complex for photocatalytic water-splitting.	O
254	Ab Initio Dynamics of Graphene and Graphyne Electrodes in Vacuum and in the Presence of Electrolytes. <b>2023</b> , 127, 6515-6523	O
253	Understanding the fundamentals of TiO2 surfacesPart II. Reactivity and surface chemistry of TiO2 single crystals. <b>2022</b> , 38, 846-906	0
252	Synthesis, biological evaluation and theoretical studies of (E)-1-(4-sulfamoyl-phenylethyl)-3-arylidene-5-aryl-1H-pyrrol-2(3H)-ones as human carbonic anhydrase inhibitors. <b>2023</b> , 38,	0
251	Exciton states in ultrathin crystalline films of 3,4,9,10-perylene tetracarboxyl dianhydride and their optical properties. <b>2023</b> ,	O

250	Heteronuclear Trimetallic MFe 2 and M 2 Fe (M=V, Nb, and Ta) Clusters for Dinitrogen Activation.	O
249	Direct Dynamics Trajectories Demonstrate Dynamic Matching and Nonstatistical Radical Pair Intermediates during Fe-Oxo-Mediated CH Functionalization Reactions. <b>2023</b> , 145, 7628-7637	O
248	Electric-field induced entropic effects in liquid water.	O
247	Polymorph Screening of the Antitumor Drug Ripretinib-Selective Preference of Dimer Synthons. <b>2023</b> , 23, 2470-2484	O
246	Effect of Boron Species on Carbon Surface on Oxidative Dehydrogenation of Propane. 2023,	O
245	Helical allophycocyanin nanotubes absorb far-red light in a thermophilic cyanobacterium. <b>2023</b> , 9,	O
244	A DFT study on structural evolution, electronic property and spectral analysis of yttrium-doped germanium clusters. <b>2023</b> , 121,	O
243	Diffusion Monte Carlo calculations on the low-lying states of LaX (X´=´Ge, As, Te).	O
242	Modulation of metal species as control point for Ni-catalyzed stereodivergent semihydrogenation of alkynes with water. <b>2023</b> , 14,	0
241	Manganese-based flow battery based on the MnCl2 electrolyte for energy storage. <b>2023</b> , 465, 142602	O
240	Influence of water on the conformations and interactions within two choline chloride-based deep eutectic solvents: a density functional theory investigation.	O
239	Molecular Screening of Different Linker-Based Organic Dyes for Optoelectronic Applications: Quantum Chemical Study.	O
238	Complexation behaviour of piceatannol ligand with Ti(IV) and Zr(IV) metal ions: a combined DFT and deep learning investigation.	O
237	Triplet Separation after the Fastest Intramolecular Singlet Fission in the Smallest Chromophore. <b>2023</b> , 19, 2092-2101	O
236	Gas-phase formation of Grignard-type organolanthanide (III) ions RLnCl 3 🛭 The influences of lanthanide center and hydrocarbyl group. <b>2023</b> , 37,	O
235	Noncollinear and Spin-Flip TDDFT in Multicollinear Approach.	O
234	Propane Oxidative Dehydrogenation on Nanosized Boron Carbide: Effect of Boron Content and Its Oxidation Implicated by DFT Calculations. <b>2023</b> , 127, 6280-6293	O
233	Integrating Molecular Simulations with Machine Learning Guides in the Design and Synthesis of [BMIM][BF4]/MOF Composites for CO2/N2 Separation. <b>2023</b> , 15, 17421-17431	O

232	Substituent and redox effects on the second-order NLO response of Ru(ii) complexes with polypyridine ligands: a theoretical study. <b>2023</b> , 47, 7326-7334	О
231	How Does Pseudo-Jahn-Teller Effect Induce the Photoprotective Potential of Curcumin?. <b>2023</b> , 28, 2946	Ο
230	Diserinol Isophthalamide: A Novel Reagent for Complexation with Biomolecular Anions in Electrospray Ionization Mass Spectrometry. <b>2023</b> , 34, 745-753	0
229	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	О
228	The Quantum Chemical Cluster Approach in Biocatalysis. <b>2023</b> , 56, 938-947	0
227	Improved Elastic Image Pair Method for Finding Transition States.	О
226	Theoretical studies on the mechanism of molybdenum-catalysed deoxydehydration of diols.	0
225	Histamine Recognition by Carbon Dots from Plastic Waste and Development of Cellular Imaging: Experimental and Theoretical Studies.	O
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36	The gas-phase pyrolysis of cyclopropylamine. A computational study on the kinetics and reaction mechanism. <b>2023</b> , 253, 112774	О
35	Role of simulated in vitro gastrointestinal digestion on biotransformation and bioactivity of astragalosides from Radix Astragali. <b>2023</b> , 115414	Ο

34	A molecular electron density theory study of mechanism and selectivity of the intramolecular [3+2] cycloaddition reaction of a nitronelinylphosphonate adduct.	0
33	Vibrational circular dichroism spectra of natural products by means of the nuclear velocity perturbation theory. <b>2023</b> , 122769	O
32	Molecular mechanism for the activation of the potent hepatotoxin acetylhydrazine: Identification of the initial N-centered radical and the secondary C-centered radical intermediates. <b>2023</b> ,	0
31	The geometry of calix[3]pyrrole and the formation of the calix[3]pyrrole Flbomplex in solution. <b>2023</b> , 142,	O
30	Toward combined photobiological photochemical formation of kerosene-type biofuels: which small 1,3-diene photodimerizes most efficiently?.	0
29	Indotricarbocyanine dyes relevant for photodynamic therapy and their radicals: Substituent effects studied by optical and electrochemical methods. <b>2023</b> , 216, 111344	O
28	Selective synthesis of two-dimensional semiconductive coordination polymers with silverBulfur network. <b>2023</b> , 25, 2990-2994	0
27	An organic (4-nitrophenyl) methionine single crystal: growth, optical properties and quantum chemical investigations for NLO device fabrication.	O
26	Experimental and Theoretical Investigation of Inclusion Complexes of Ecyclodextrin with Fingolimod. <b>2023</b> , 97, 469-476	0
25	Multi-scale modeling of natural organic matterfleavy metal cations interactions: Aggregation and stabilization mechanisms. <b>2023</b> , 238, 120007	O
24	Intramolecular Hiyama Coupling: Synthesis of 1,8,13-Trisubstituted Chiral Triptycenes with Three Different Substituents by Intramolecular Substituent Transfer.	0
23	A druggable copper-signalling pathway that drives inflammation. <b>2023</b> , 617, 386-394	О
22	Arylazo under Extreme Conditions: [2 + 2] Cycloaddition and Azo Metathesis. <b>2023</b> , 127, 8482-8492	О
21	Pyrene-Based Polyimide Covalent Organic Framework with Temperature-Dependent Fluorescence.	О
20	A semilocal machine-learning correction to density functional approximations. 2023, 158,	O
19	Ultralong excimer phosphorescence by the self-assembly and confinement of terpyridine derivatives in polymeric matrices.	О
18	Computational Study of the Fe(II) and Eketoglutarate-Dependent Aryloxyalkanoate Dioxygenase (AAD-1) in the Degradation of the Herbicide 2,4-Dichlorophenoxyacetic Acid. <b>2023</b> , 63, 2759-2768	О
17	Including vibrational effects in magnetic circular dichroism spectrum calculations in the framework of excited state dynamics. <b>2023</b> , 158,	O

16	Comparative (magneto)optical, redox, and photophysical properties of phosphorous octacarbazole-and tetra-tert-butyltetrabenzotriazacorroles. <b>2023</b> , 216, 111361	O
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14	Ab Initio Molecular Dynamics: A Guide to Applications. <b>2023</b> ,	0
13	Mono-nuclear ruthenium catalyst for hydrogen evolution. 2023,	O
12	Computational studies on optoelectronic and nonlinear optical properties of para-substituted nitrobenzofurazan compound. <b>2023</b> , 35, 106133	0
11	Blends of nitrophenylmaleimide isomers with carboxymethylcellulose for the preparation of supramolecular polymers. <b>2023</b> , 9, e16108	O
10	Adsorption of CO, NO and SO on Fe2-10 clusters: A computational investigation on the metal catalysed activation of atmospheric pollutants. <b>2023</b> , 1225, 114160	0
9	Advances in understanding the phosphate binding to soil constituents: A Computational Chemistry perspective. <b>2023</b> , 887, 163692	O
8	Designing a promising sensor for SF6 decomposed gases by using platinum doped-aluminum nitride nanotubes. <b>2023</b> , 153, 110743	0
7	Nonlinear Optical Materials: Predicting the First-Order Molecular Hyperpolarizability of Organic Molecular Structures. <b>2023</b> , 10, 545	O
6	Insights into the carbonization mechanism of PAN-derived carbon precursor fibers and establishment of a kinetics-driven accelerated reaction template for atomistic simulation.	0
5	Mechanistic Insights of Copper Catalyzed Trifluoromethyl Aziridine Opening: Regioselective and Stereospecific Aryl Grignard Addition.	O
4	Synthesis, physico-chemical characterization and theoretical exploration of some 2,4,5-triaryl imidazole derivatives.	0
3	Asymmetric catalysis by l-prolinamide based small molecules: synthesis, characterization and first principle studies on their enantioselectivity. <b>2023</b> , 545, 113185	O
2	Black Gold-Based AntennaReactor To Activate Non-Plasmonic Nickel: Photocatalytic Hydrodechlorination and Hydrogenation Reactions. 7395-7406	0
1	High-temperature reactivity of vanadium oxide clusters in methane activation: Vibrational degrees of freedom matter. <b>2023</b> , 158,	O